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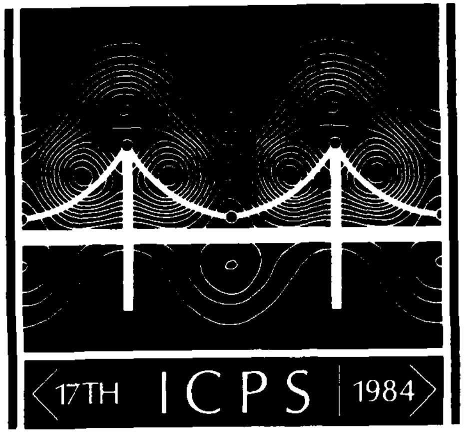

San Francisco, California, USA
August 6-10, 1984

ABSTRACTS

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17th International Conference on the Physics of Semiconductors

ABSTRACTS

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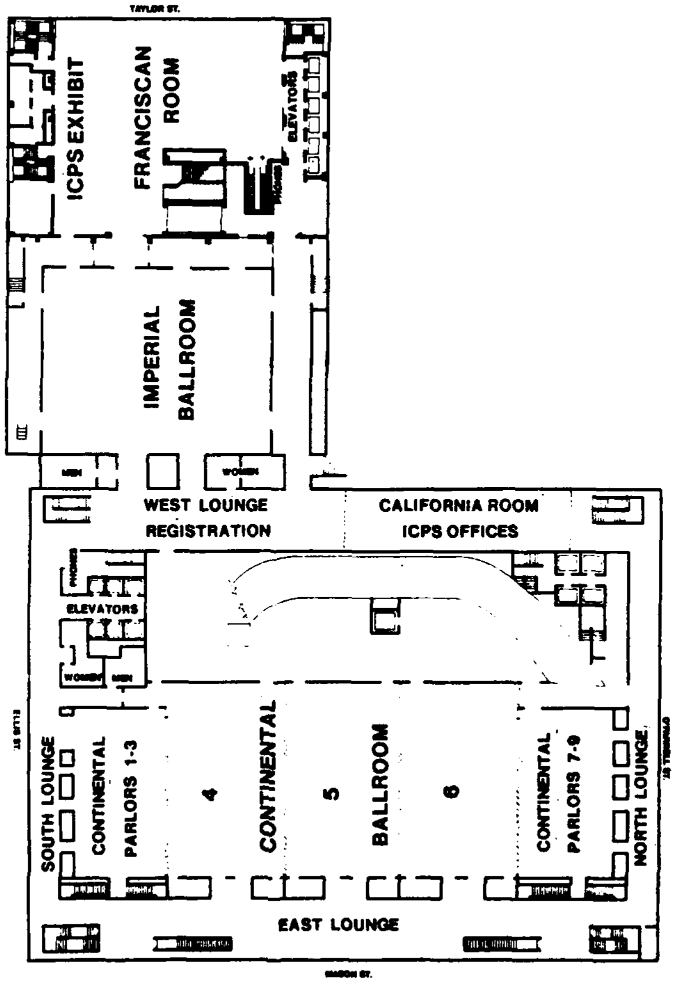

MORNING

7:30 8:00 8:45 9:00 9:40 10:40 12:20

MONDAY	REGISTRATION	OPENING	PLENARY ESAKI	break	A	Surface Structure (Rowe)	Lunch
Aug. 6					B	Metal-Insulator Transition	
					C	Quantum Wells (Gornik)	
					D	Two Dimensional Materials	
TUESDAY	POSTER SETUP	A	Symposium on (Cho, Matsushita)	break	A	Materials and Devices (Bhargava, Capasso)	Lunch
Aug. 7		B	Surface (Bringars)		B	Electronic Structure (Grazhulis)	
		C	Transport in		C	2D Systems (Sakaki)	
		D	Excitons and		D	Polarons (Cohen)	
WEDNESDAY			PLENARY GRIMMEISS BINNIG	break	A	Symposium on Characterization (Shank, Petroff)	
Aug. 8					B	Phase Transitions (Newman)	
					C	Quantum Wells	
					D	Transport	
THURSDAY		A	Interface (Williams)	break	A	Electronic Properties (Rossi)	Lunch
Aug. 9		B	Electronic		B	States	
		C	Multiple (Voos)		C	Quantum Wells	
		D	Deep Level		D	Impurities (Kaminska)	
FRIDAY			PLENARY TSUI LAUGHLIN	break	A	Adsorption on Surface	Lunch
Aug. 10					B	Electronic States (Yin)	
					C	Quantum Hall Effect	
					D	Deep Level Impurities (Estle)	
					E	Narrow Gap Semiconductors	

8:00 9:00 9:40 10:20 10:40 12:20

AFTERNOON

		14:00	15:40		16:00	17:20	18:00
MONDAY	A	Surface (Uhrberg, Olmstead)	break	A	Reconstruction (Tromp)	ICPS RECEPTION at the EXPLORATORIUM	
	B	Amorphous (Street)		B	Semiconductors		
	C	Two Dimensional (Queisser)		C	Electron Systems		
	D	One Dimensional Systems (Orenstein)		D	Resonance Raman Scattering		
TUESDAY	A	Amorphous Superlattices	break	A	POSTERS		
	B	Interface Structure (Sebenne)		B			
	C	Heterostructures (McGill)		C			
	D	Electron-Hole Liquid		D			

WEDNESDAY EXCURSION

THURSDAY	A	Phonons (Nizzoli)	break	A	Phonons	BANQUET
	B	Amorphous Semiconductors (Ley)		B	Amorphous Semiconductors	
	C	Multiple Quantum Wells		C	Multiple Quantum Wells (Masumoto)	
	D	Impurities and (Car)		D	Defects	
FRIDAY	A	Semiconductor Structure (Phillips, Mikkelson)	break		CLOSING	
	B	Optical Properties				
	C	Laser Annealing				
	D	Recombination and Spins (Alvarado)				
	E	Magnetic Semiconductors (Ramdas)				
		14:00	15:40 16:20		16:40	17:20

Monday, August 6th

Morning 8:45 am Continental Ballroom

MoA Opening Session

Chair: R.Z. Bachrach

8:45 Welcome: M.L. Cohen, ICPS Chairman
R. Hofstader, IUPAP National Chairman

Reflections: Sir Neville Mott
Announcements: P.Y. Yu

MoA Plenary Session

Chair: M.L. Cohen

9:40 L. Esaki (Yorktown Heights)
MoA-1 Semiconductor Superlattices and Quantum Wells
Plenary 1

10:20 Intermission

Monday, August 6th

Morning 10:40 am Imperial Ballroom

MoA-A Surface Structure

Chair: W.E. Spicer

10:40 MoA-A1 Invited	J. E. Rowe (Gainesville) Surface EXAFS Studies of Semiconductor *Surface Structure*	2
11:20 MoA-A2	S. Y. Tong, G. Xu (Milwaukee) The Geometric Structure of the GaAs(111) and (110) Surfaces	3
11:40 MoA-A3	L. Smit, J. F. van der Veen (Amsterdam) Atomic Geometry and Dynamics of the InAs(110) Surface	4
12:00 MoA-A4	J. Ihm (Murray Hill), D. H. Lee, J. D. Joannopoulos, J. J. Xiong(Cambridge MA) Structural Phase Diagrams for the Surface of a Solid: A Total Energy/Renormalization-Group Approach	5

17th International Conference on the Physics of Semiconductors

Monday, August 6th

Morning 10:40 am Continental Ballroom 4

MoA-B Metal - Insulator Transition

Chair: G.A. Thomas

10:40 W. N. Shafaraman, T. G. Castner (Rochester)
MoA-B1 Low Temperature Magnetoresistance Measurements on Arsenic-Doped Silicon Near the Metal-Insulator Transition 6

11:00 M. A. Paalanen, G. A. Thomas, A. Ruckenstein (Murray Hill)
MoA-B2 Evidence of Strong Spin Correlations in Si:P 7

11:20 T. Suski, E. Litwin-Staszewska, W. Szymanska (Warsaw)
MoA-B3 Influence of Disorder on Semiconductor-Metal Transition in InSb 8

11:40 S. Shin, S. Suga, M. Taniguchi, M. Seki, H. Kanzaki (Tokyo), Y. Ueda, K. Kosuge, S. Kachi (Kyoto)
MoA-B4 Electron Correlation Energies and Metal-Insulator Transition of VO_2 9

12:00 F. Meloni, M. Serra (Cagliari)
MoA-B5 Valence-Conduction Charge Transfer in the Semiconductor-Metal Transition : Si 10

Monday, August 6th

Morning 10:40 am Continental Ballroom 5

MoA-C Quantum Wells

Chair: G. Chiarotti

10:40 MoA-C1	J. P. Eisenstein, H. L. Stormer, V. Narayanamurti, A. C. Gossard (Murray Hill) High-Precision de Haas-van Alphen Measurements on a Two-Dimensional Electron Gas	11
11:00 MoA-C2 Invited	E.Gornik (Innsbruck, Murray Hill), R. Lassnig (Innsbruck), H. L. Stormer, A. C. Gossard, W. Wiegmann (Murray Hill), M. v. Ortenberg (Grenoble) Specific Heat Measurements on 2D-Electrons in GaAs/GaAlAs Multilayer Structures	12
11:40 MoA-C3	E. J. Pakulis, F. F. Fang, M. Heiblum (Yorktown Heights) New Microwave Induced Resonances in the Conductance of a GaAs/Ga$_{1-x}$Al$_x$As Heterojunction	13
12:00 MoA-C4	S.J. Allen, Jr., F. DeRosa , G.J. Dolan, C.W. Tu (Murray Hill) Collective Resonances in the Laterally Confined 2D Electron Gas	14

Monday, August 6th

Morning 10:40 am Continental Ballroom 6

MoA-D Two-Dimensional Materials

Chair: T. Geballe

10:40 MoA-D1	A. Koma, K. Sunouchi, T. Miyajima (Ibaraki) Electronic Structure of a Monolayer NbSe$_2$ Film Grown Heteroepitaxially on the Cleaved Face of 2H-MoS$_2$	15
11:00 MoA-D2	M. Naito, S. Tanaka (Tokyo) NQR and NMR Study of ^{181}Ta in the Commensurate CDW State of 1T-TaS$_2$ and 1T-TaSe$_2$- on the Semiconductor Nature of 1T-TaS$_2$	16
11:20 MoA-D3	S. A. Solin, B. R. York (Lansing), H. R. Resing (Washington) Graphite Intercalated with K and NH$_3$ - A Metal-Ammonia Solution in 2 Dimensions	17
11:40 MoA-D4	R. S. Markiewicz, C. Zahopoulos (Boston, Cambridge MA) Magnetic Breakdown in Graphite Intercalation Compounds	18
12:00 MoA-D5	T. Takahashi, Y. Hayasi, H. Tokailin, H. Asahina, A. Morita, T. Sagawa (Sendai), I. Shirotani (Muroran) Electronic Structure of Black Phosphorus Studied by Angle-Resolved Photoemission and Polarized Soft X-Ray Emission and Absorption	19

Monday, August 6th

Afternoon 14:00 pm Imperial Ballroom

MoP-A Surface Reconstruction

Chair: J. Chadi

14:00	R. Uhrberg (Linkoping)	
MoP-A1	Angle Resolved Photoemission Studies of Reconstructed	
Invited	Silicon Surfaces	20
14:40	K. C. Pandey (Yorktown Heights)	
MoP-A2	Reconstruction of the Si(100)-2x1 Surface	21
15:00	M. A. Olmstead, N. M. Amer (Berkeley)	
MoP-A3	Polarization Dependence of Ge and Si(111)2x1 Surface State	
Invited	Optical Absorption: A Test of Surface Reconstruction	
	Models	22
15:40	Intermission	
16:00	R. M. Tromp (Yorktown Heights)	
MoP-A4	Ion Scattering Studies of the Structure of Silicon Surfaces	
Invited		23
16:40	C. B. Duke, A. Paton (Webster), B.W. Holland (Coventry)	
MoP-A5	The Atomic Geometry of Si(100)-(2x1) Revisited	24
17:00	J. E. Northrup (Palo Alto)	
MoP-A6	Theory of the Al-Si(111) - $\sqrt{3}$x$\sqrt{3}$ Surface	25
18:30	Conference Reception	

Monday, August 6th

Afternoon 14:00 pm Continental Ballroom 4

MoP-B Amorphous Semiconductor

Chair: H. Fritzsche

14:00 MoP-B1 Invited	R. A. Street (Palo Alto) Doping Effects in Hydrogenated a-Si	26
14:40 MoP-B2	H. A. Stoddart, D. Pfost (Providence), M. Pollak (Riverside), J. Tauc (Providence) Study of Dispersive Relaxations in Amorphous Si_xGe_{1-x}:H by Photoinduced Absorption	27
15:00 MoP-B3	F. Boulitrop (Orsay), J. Dijon (Grenoble), D. J. Dunstan (Guilford), A. Herve (Grenoble) ESR Study of Metastable Carriers in Hydrogenated Amorphous Silicon	28
15:20 MoP-B4	N.M. Johnson, D. K. Biegelsen (Palo Alto) Gap-State Distribution in a-Si:H Measured by Photocapacitance Spectroscopy	29
15:40	Intermission	
16:00 MoP-B5	J. R. Eggert (Cambridge MA) Carrier Loss in Dispersive Transport	30
16:20 MoP-B6	E. V. Anda, S. S. Makler (Niteroi) Real Space Renormalization Formalism for a-Si:H	31
16:40 MoP-B7	B. Hoheisel, J. Stuke (Marburg), M. Stutzmann (Palo Alto), W. Beyer (Julich) Electron Spin Resonance of Amorphous III-V-Compounds	32
17:00 MoP-B8	A. F. J. Levi (Murray Hill), M. C. Payne (Cambridge) Phonon Structure of Amorphous Germanium by Inelastic Electron Tunneling Spectroscopy	33
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MoP-C Two-Dimensional Electron Systems

Chair: G. Landwehr

14:00 MoP-C1 Invited	H. Queisser (Stuttgart) Persistent Photoconductivity in Semiconductors	34
14:40 MoP-C2	G. Timp, A. B. Fowler, A. Hartstein (Yorktown Heights) The Temperature and Electric Field Dependence of the HoppingConductivity in a 2-D Impurity Band	35
15:00 MoP-C3	U. Kunze, G. Lautz, E. Behnen (Braunschweig) Tunneling Studies of Uniaxially Stressed (001) Si Inversion Layers	36
15:20 MoP-C4	R. J. Nicholas, T. H. H. Vuong, M. A. Brummell (Oxford), J. C. Portal (Grenoble), M. Razeghi (Orsay) Temperature and Magnetic Field Dependent Thermoelectric Power in GaInAs-InP Heterojunctions	37
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16:00 MoP-C5	T. P. Smith III (Providence), M. Heiblum (Yorktown Heights), P. J. Stiles (Providence) Capacitively Coupled Measurements of the Magnetoconductivity Tensor in Heterostructures	38
16:20 MoP-C6	Z. Schlesinger (Yorktown Heights), S. J. Allen (Murray Hill), J. C. M. Hwang (Murray Hill), H. Le (Cambridge MA) Cyclotron Resonance in the Fractionally Quantized 2D Electron Gas	39
16:40 MoP-C7	N. Miura, Y. Iwasa, S. Tarucha, H. Okamoto (Tokyo) Magneto-Optics of Two-Dimensional Excitons in GaAs-AlAs Heterostructures in High Magnetic Fields	40
17:00 MoP-C8	A. Zrenner, H. Reisinger, F. Koch (Garching), K. Ploog (Stuttgart) Subband Structure and Magnetotransport for Electron Layers in $\delta(z)$-Doped, MBE-Grown GaAs	41
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MoP-D One Dimensional Systems

Chair: K. Seeger

14:00 MoP-D1 Invited	J. Orenstein (Murray Hill) 1D Semiconductors-polyacetelyene	42
14:40 MoP-D2	H. Kahlert, G. Leising, O. Leitner, R. Uitz, F. Stelzer (Graz) Transport and Optical Properties of Fully Oriented Non-Fibrous Crystalline $(CH)_x$	43
15:00 MoP-D3	Y. Iye (Murray Hill), L. E. McNeil, G. Dresselhaus, P. M. Berglund (Cambridge MA) The Electronic Phase Transition in Graphite Under Strong Magnetic Field	44
15:20 MoP-D4	T. Rasing (Berkeley) Electronic Bandstructure of an Incommensurate Crystal	45
15:40	Intermission	

MoP-D Resonance Raman Scattering

Chair: M.V. Klein

16:00 MoP-D5	Z. Vardeny, O. Brafman, E. Ehrenfreund (Haifa) Resonant Raman Scattering from Amplitude Modes in Polyacetylene	46
16:20 MoP-D6	N. Mestres, F. Cerdeira, M. Cardona (Stuttgart) Light Scattering by Plasmons in Heavily Doped n-Type Ge and Si	47
16:40 MoP-D7	P. B. Allen (Stuttgart, Stony Brook) Theoretical Calculation of Resonant Two-Phonon Raman Scattering in Si and Ge	48
17:00 MoP-D8	S. Katayama (Niigata), T. Ando (Tokyo) Electronic Excitations and Resonant Light Scattering Spectra in Doped $GaAs/Al_xGa_{1-x}As$ Superlattices	49
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Tuesday, August 7th

Morning 9:00 am Continental Ballroom 4

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Chair: C. Hilsum

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9:40 TuA-A2 Invited	Y. Matsushita (Kawasaki) Silicon: On the Behaviour of Microdefects and their Applications	51
10:20	Intermission	
10:40 TuA-A3 Invited	R. Bhargava (Briarcliff Manor) II-VI Semiconductor Materials and Devices: Recent Progress	52
11:20 TuA-A4 Invited	F. Capasso (Murray Hill) Bandgap Engineering via Superlattice and Graded-Gap Materials: New Phenomena and their Device Applications	53
12:00 TuA-A5	P. P. Ruden (Raleigh), G. H. Dohler (Palo Alto) Low-Power Non-Linear Optical Phenomena in n-i-p-i Doping Superlattices	54

Tuesday, August 7th

Morning 9:00 am Continental Ballroom 5

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Chair: Y. Petroff

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9:40 TuA-B2	H. H. Farrell (Murray Hill), J. Q. Broughton (Stonybrook), J. C. Bean (Murray Hill) Electronic States on Si(100) and Si/Ge (100) Alloy Surfaces	56
10:00 TuA-B3	F. J. Himpsel, T. Fauster, D. Straub (Yorktown Heights) Inverse Photoemission at Semiconductor Surfaces	57
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10:40 TuA-B4 Invited	V. A. Grazhulis (Moscow) Atomic Structures and Electronic Properties of Ge(111) Cleaved Surfaces at Low Temperatures	58
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11:40 TuA-B6	M. Y. Chou, S. G. Louie, M. L. Cohen (Berkeley) Theoretical Study of Stacking Faults in Silicon	60
12:00 TuA-B7	F. Flores, C. Tejedor (Madrid), E. Louis (Alicante) Electron-Phonon and Correlation Effects at Silicon Surfaces	61

Tuesday, August 7th

Morning 9:00 am Continental Ballroom 6

TuA-C Transport in Two-Dimensional Electron Systems

Chair: P. Stiles

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9:20 TuA-C2	T. Ando, Y. Murayama (Tokyo) Self-Consistent Screening in a Heterojunction in Strong Magnetic Fields	63
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10:00 TuA-C4	A. Kastalsky, S. Luryi (Murray Hill) Hot Electron Injection in Double-Layered Heterostructures	65
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10:40 TuA-C5 Invited	H. Sakaki (Tokyo) *Transport in Two-Dimensional* Electron System in GaAs/AlGaAs Heterostructures	66
11:20 TuA-C6	T. W. Nee (China Lake) Surface-Irregularity-Enhanced Dissipation in Semiconductor Two-Dimensional Electron Gas Devices	67
11:40 TuA-C7	S. Kawaji, K. Kuboki, J. Wakabayashi, J. Yoshino, H. Sakaki (Tokyo) Inelastic Scattering and Spin-Orbit Scattering in 2D Systems of GaAs/AlGaAs Heterostructures	68
12:00 TuA-C8	T. W. Hickmott, P. M. Solomon, F. F. Fang (Yorktown Heights), R. Fischer, H. Morkoc (Urbana) Magnetotunneling and Magnetic Freezeout in n-GaAs-Undoped $Al_xGa_{1-x}As$-n^+ GaAs Capacitors	69

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9:00 am Continental Parlor 7-9

TuA-D Excitons and Polarons

Chair: F. C. Brown

Tuesday, August 7th

Afternoon 14:00 pm   Continental Ballroom 4

TuP-A   Amorphous Superlattices and Junctions

Chair: H. Kamimura

14:00 TuP-A1	G. H. Dohler (Palo Alto) Amorphous Doping Superlattices	78
14:20 TuP-A2	M. Hundhausen, J. Wagner, L. Ley (Stuttgart) Amorphous Silicon Based Doping Superlattices	79
14:40 TuP-A3	P. D. Persans, C. R. Wronski, B. Abeles, T. Tiedje, G. D. Cody (Annandale) Electronic Properties of Amorphous Si:H/Ge:H Semiconductor Superlattices	80
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Chair: B. Pistoulet

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Chair: T. Masumi

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Chair: C. Benoit a la Guillaume

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TuP-PB	**Phonons**	Imperial Ballroom
TuP-PC	**Surfaces and Interfaces**	Imperial Ballroom
TuP-PD	**Transport**	Imperial Ballroom
TuP-PE	**Heterostructures**	Imperial Ballroom
TuP-PF	**Optical Properties**	Imperial Ballroom
TuP-PG	**Excitons and Polarons**	Continental Parlor 1-3
TuP-PH	**Magnetic Properties**	Continental Parlor 1-3
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TuP-PC Surfaces and Interfaces (continued)

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TuP-PE Heterostructures (continued)

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TuP-PF Optical Properties

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TuP-PG Excitons and Polarons

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TuP-PJ Impurities (continued)

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Morning 9:00 am Continental Ballroom

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Chair: H. Kawamura

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Chair: G. Martinez

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Chair: F. Koch

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WeA-C1 W. Wiegmann (Murray Hill)
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11:40 L. L. Chang, E. E. Mendez, W. I. Wang, L. Esaki
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Chair: R. A. Stradling

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ThA-A Interface: Electronic Properties

Chair: L. Brillson

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ThA-B Electronic States: Surface

Chair: S. Louie

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ThA-B Electronic States: Bulk

Chair: F. Bassani

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ThA-C Multiple Quantum Wells

Chair: Y. Uemura

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ThA-D Deep Level Impurities

Chair: M. Schluter

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ThP-A Phonons

Chair: Y. Toyozawa

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17:00 ThP-B8	H. Tokumoto, K. Kajimura, S. Yamasaki, K. Tanaka (Ibaraki) Evidence for Existence of Two-Level Tunneling States in a-Si	276
17:20 ThP-B9	Y. J. Chabal, C. K. N. Patel, J. B. Harbison (Murray Hill) Infrared Absorption in α-Si:H: First Observation of Gaseous Molecular H_2 and Si-H Overtone	277
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Afternoon 14:00 pm Continental Ballroom 5

ThP-C Multiple Quantum Wells

Chair: J. Worlock

14:00 ThP-C1	R. Sooryakumar, D. S. Chemla, A. Pinczuk (Holmdel), A. Gossard, W. Wiegmann (Murray Hill), L. J. Sham (LaJolla) Band Mixing in GaAs -(AlGa)As Heterostructures	278
14:20 ThP-C2	J. F. Ryan, R. A. Taylor, A. J. Turberfield, A. Maciel (Oxford) J. M. Worlock (Holmdel), A. C. Gossard, W. Wiegmann (Murray Hill) Hot Electron Relaxation and Trapping in Modulation-Doped GaAs-AlGaAs Multi-Quantum Well Heterostructures	279
14:40 ThP-C3	M. C. Smith, A. Petrou, C. H. Perry (Boston), J. M. Worlock (Holmdel), R. L. Aggarwal (Cambridge MA), A. C. Gossard, W. Wiegmann (Murray Hill) Photoluminescence Studies of Landau Transitions in GaAs/AlGaAs Multiple Quantum Wells	280
15:00 ThP-C4	J. Shah, A. Pinczuk (Holmdel), H. L. Stormer, A. C. Gossard, W. Wiegmann (Murray Hill) Hole Heating and Hole-Phonon Interaction in Modulation Doped 2D Hole System	281
15:20 ThP-C5	Y. Aoyagi, Y. Segawa, T. Miyoshi, S. Namba (Saitama) Picosecond Carrier Dynamics in GaAs/$Ga_{1-x}Al_xAs$ Single and Multi Quantum Well Structure	282
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16:00 ThP-C6 Invited	Y. Masumoto, S. Shionoya, H. Okamoto (Tokyo) Slow Energy Relaxation of Excitons in GaAs-AlAs Multi-Quantum-Well Structures	283
16:40 ThP-C7	R. W. J. Hollering, H. J. A. Bluyssen, P. Wyder (Nijmegen), M. Leys, J. Wolter (Eindhoven) Electron Hole Relaxation and Recombination in GaAs/GaAlAs Quantum-Well Structures from Picosecond Photoluminescence	284
17:00 ThP-C8	R. Hoger, E. O. Gobel, J. Kuhl, K. Ploog (Stuttgart) Investigation of Carrier Dynamics in AlGaAs/GaAs Quantum Well Structures by Picosecond Luminescence Spectroscopy	285
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Afternoon 14:00 pm   Continental Ballroom 6

ThP-D Impurities and Defects

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14:20 ThP-D2	G. A. Baraff, M. Schluter (Murray Hill) Migration of Interstitials in Silicon	287
14:40 ThP-D3 Invited	R. Car (Yorktown Heights) Atomic Diffusion in Silicon	288
15:20 ThP-D4	M. Kobayashi, T. Hattori, Y. Akahama, S. Endo, S. Narita (Osaka) Reasonant Polaron Effect in Non-Polar Semiconductor Black Phosphorus	289
15:40	Intermission	
16:00 ThP-D5	E. E. Haller, R. E. McMurray Jr., N M. Haegel, L. M. Falicov (Berkeley) Positively Charged Acceptors with $(1s)^3$ and $(1s)^4$ Configurations	290
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16:40 ThP-D7	M. Baj, S. Huant, L. C. Brunel (Grenoble), Z. Wasilewski (Warsaw, St. Andrews), R. Stradling (St. Andrews) Magnetooptical Study of Shallow Donors in InSb Under High Pressures	292
17:00 ThP-D8	S. R. Hetzler, T. C. McGill (Pasadena), A. T. Hunter (Malibu) S-Like Excited States of the 78-meV Acceptor in GaAs	293
17:20 ThP-D9	L. T. Canham, G. Davies, E. C. Lightowlers (London) A Novel Near-Infrared Vibronic Series in Irradiated Silicon	294
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Morning 9:00 am Continental Ballroom

FrA Plenary Session

Chair: K. von Klitzing

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Plenary		295
9:40	R. B. Laughlin (Livermore)	
FrA-P2	Theory of Anomalous Quantum Effect	296
Plenary		
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Morning 10:40 am Continental Ballroom 4

FrA-A Adsorption on Surfaces

Chair: R. Ludeke

10:40 FrA-A1	M. K. Kelly, G. Margaritondo (Madison), M. N. Piancastelli (Roma), J. Anderson, D. J. Frenkel, G. J. Lapeyre (Bozeman) Surface Vibrational Studies of Chemisorption on Silicon	297
11:00 FrA-A2	H. Tochihara, M. Kubota (Tokyo), M. Miyao (Hamamatsu), Y. Murata (Tokyo) Surface Electronic Structure Change by Cs Adsorption on Si(111)2x1	298
11:20 FrA-A3	J. R. Myron, G. J. Lapeyre (Bozeman) GaAs(110) +Sb p(1x1): An Adatom Case Study of Adsorption on Compound Semiconductor Surfaces	299
11:40 FrA-A4	J.-G. Che, K. Zhang, X. Xie (Shanghai) Chemisorption of Ag, Cu and Au on Si(111) and Ge(111) Surfaces	300
12:00 FrA-A5	H. Richter, L. J. Brillson (Webster) Laser Induced Chemical Reactions at the Al-III -V Semiconductor Interface	301

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FrA-B Electronic States : Theory

Chair: J. Chelikowsky

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11:20 FrA-B3	N. E. Christensen, G. B. Bachelet (Stuttgart) 1s Core Shifts and the Gap of Tetrahedral Semiconductors	304
11:40 FrA-B4 Invited	M. T. Yin (Murray Hill) Theory of the Ground State Properties of Crystalline Semiconductors	305

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Morning 10:40 am Continental Ballroom 6

FrA-C Quantized Hall Effect

Chair: S. Kawaji

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Morning 10:40 am Continental Parlor 1-3

FrA-D Deep Level Impurities

Chair: C. Concalves da Silva

10:40 FrA-D1 Invited	T. L. Estle (Houston) Muonium Impurity Centers in Semiconductors	312
11:20 FrA-D2	H. P. Gislason, B. Monemar, M. E. Pistol, (Linkoping) P. J. Dean, D. C. Herbert, (Great Malvern), B. C. Cavenett, A. Kana ah (Hull) Electronic and Vibrational Structure of Isoelectronic Cu-Li Centres in GaP	313
11:40 FrA-D3	B. K. Meyer, T. Hangleiter, J. M. Spaeth (Paderborn), G. Strauch, T. Zell, A. Winnacker (Heidelberg), R. H. Bartram (Storrs) Optical and ODMR Investigation of Antisite Defects in GaP	314
12:00 FrA-D4	R. S. Berg, P. Y. Yu (Berkeley) Raman Study of Neutron Irradiated GaAs	315

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Morning 10:40 am Continental Parlor 7-9

FrA-E Narrow Gap Semiconductors

Chair: M. Grynberg

10:40 FrA-E1	W. Szuszkiewicz, A. M. Witowski (Warsaw) The First Observation of Temperature Dependence of Free Carrier Absorption by Photon-Ionized Impurity-Plasmon Processes in Semiconductors	316
11:00 FrA-E2	D. G. Seiler, C. L. Littler, R. J. Justice (Denton), P. W. Milonni (Fayetteville) Nonlinear Oscillations, Bifurcation and Chaos in n-InSb	317
11:20 FrA-E3	S. W. McKnight, M. K. El-Rayess (Boston) High-Pressure Far-Infrared Studies of PbTe and Indium-Doped $Pb_{1-x}Sn_xTe$	318
11:40 FrA-E4	T. Ichiguchi, H. D. Drew (College Park) Magneto-Optical Studies of In Doped $Pb_{1-x}Sn_xTe$	319
12:00 FrA-E5	P. M. Amirtharaj, K. K. Tiong, P. Parayanthal, F. H. Pollak (Brooklyn), J. K. Furdyna (West Lafayette) Raman Scattering in the Narrow Gap Alloy $Hg_{1-x}Cd_xTe$	320

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Chair: A. Baldereschi

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Invited
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Solids in Limbo: Structure and Properties of Non Crystalline Semiconductors 321

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D. E. Aspnes (Murray Hill), C. E. Bouldin, E.A. Stern (Seattle)
Structural and Microstructural Determinations of Crystalline and Amorphous Fractions of Microcrystalline Ge: A Comparison 322

15:00
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Invited
J. C. Mikkelsen, Jr. and J. B. Boyce (Palo Alto)
Atomic-Scale Structure of Zincblende Alloys 323

15:40
FrP-A4
P. Boguslawski (Trieste, Warsaw), A. Baldereschi (Trieste, Lausanne)
Bond Lengths and Average Lattice Constant of $Ga_xIn_{1-x}As$: A Microscopic Theory 324

16:00
FrP-A5
K. Murase, T. Fukunaga (Toyanaka)
Stability and Formation of the Clusters with Tetrahedral Units in Germanium-Tin-Selenium Glasses 325

16:20 Intermission

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FrP-B Optical Properties

Chair: K. P. Jain

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14:40 FrP-B3	G. Contreras, A. K. Sood, M. Cardona (Stuttgart) *Light Scattering Due to Intervalley Electron Density* Fluctuations in n-Si	328
15:00 FrP-B4	R. B. James (Livermore), D. L. Smith (Pasadena) Theory of Spectral Hole Burning in p-Type Germanium by *a Frequency-Domain Technique*	329
15:20 FrP-B5	A. Borghesi, G. Guizzetti, L. Nosenzo, E. Reguzzoni, A. Stella (Pavia), F. Levy (Lausanne) Optical Investigation of Phase Transitions and "Anomalies" in $Ti_{1-x}Hf_xSe_2$ Crystals	330
15:40 FrP-B6	H. Presting, H. Voght (Stuttgart) Observation of Anomalous Faust-Henry Coefficients in the Hyper-Raman Scattering from II-VI Semiconductors	331
16:00 FrP-B7	L. K. Vodopyanov, S. P. Kozyrev, Y. A. Aleshchenko (Moscow), R. Triboulet (Meudon) Optical Observation of Clusters in Distribution of Cd and Hg Ions in Cation Sublattice of $Cd_{1-x}Hg_xTe$	332
16:20	Intermission	

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Afternoon 14:00 pm Continental Ballroom 6

FrP-C Laser Annealing

Chair: D. Biegelsen

14:00 FrP-C1	M. O. Thompson (Ithaca), J. M. Poate (Murray Hill), P. S. Peercy (Albuquerque), J. W. Mayer (Ithaca) Melting Temperature and Dynamics During Pulsed Laser Irradiation of Amorphous Silicon	333
14:20 FrP-C2	M. Combescot, J. Bok, C. Benoit a la Guillaume (Paris) Symmetry Breaking Mechanism at the Melting Threshold of Laser Irradiated Silicon	334
14:40 FrP-C3	K. Murakami, H. Itoh, K. Takita, K. Masuda (Ibaraki), T. Nishino (Osaka) Supersaturated Substitutional-Nitrogen Impurities in Nanosecond-Pulsed Laser Annealed Silicon	335
15:00 FrP-C4	D. H. Lowndes, G. E. Jellison, Jr., R. F. Wood (Oak Ridge), R. Carpenter (Tempe) Time-Resolved Studies of Ultrarapid Solidification of Highly Undercooled Molten Silicon Formed by Pulsed Laser Irradiation	336
15.20 FrP-C5	P. M. Fauchet, A. E. Siegman (Stanford) Ultrafast Spectroscopy of Very Dense and Hot Electron-Hole Plasmas in Crystalline and Amorphized Semiconductors	337
15:40 FrP-C6	W. Marine, J. Marfaing, F. Salvan, B. Mutaftschiev (Marseille) Free Carrier Density Dependence of the Melting Temperature of Amorphous Germanium	338
16:00 FrP-C7	L. Tapfer, H. C. Alt (Stuttgart) X-Ray Diffraction Study of Self-Implanted Silicon	339
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FrP-D Recombination and Spin-Dependent Properties

Chair: M. Balkanski

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14:20 FrP-D2	D. V. Lang, M. C. Chen (Murray Hill) Determination of the Electronic Structure of Si Dangling Bonds at the Si/SiO_2 Interface	341
14:40 FrP-D3	C. N. Ironside, R. A. Taylor, J. F. Ryan (Oxford) Stimulated Recombination and the Dynamic Mott Transition in GaTe	342
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16:00 FrP-D6	H.-J. Drouhin, C. Hermann (Palaiseau), M. Eminyan (Palaiseau, Paris), G. Lampel (Palaiseau) Photoelectron Energy Distribution and Spin Polarization Measurements from GaAs with Negative Affinity	345
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FrP-E Magnetic Semiconductors

Chair: D.R. Penn

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15:00 FrP-E3	R. Planel, J. Cernogora, J. Gaj, C. Benoit a la Guillaume (Paris) Magnetic Polaron Effects on Bound Excitons	348
15:20 FrP-E4	J. Mycielski, A. Witowski, A. Wittlin, M. Grynberg (Warsaw) Hopping Magnetoabsorption *in Semimagnetic* Semiconductor n-$Cd_{1-x}Mn_xSe$	349
15:40 FrP-E5	R. L. Aggarwal, S. N. Jasperson, Y. Shapira, S. Foner (Cambridge MA), T. Skakibara, T. Goto, N. Miura (Tokyo), K. Dwight, A. Wold (Providence) Determination of the Antiferromagnetic Exchange Coupling Constant Between the Mn^{++} Ion Pairs with $S = 5/2$ in $Cd_{0.95}Mn_{0.05}Se$	350
16:00 FrP-E6	J. A. Gaj, L. S. Dang (St. Martin d' Heres) Optical Pumping in $Cd_{1-x}Mn_xTe$	351
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Afternoon 16:40 pm Continental Ballroom

FrP Closing Ceremony

Chair: R. Z. Bachrach

16:40	Epiloque:	R. Z. Bachrach L. J. Sham M. L. Cohen

SEMICONDUCTOR SUPERLATTICES AND QUANTUM WELLS*

L. Esaki
IBM Thomas J. Watson Research Center
Yorktown Heights, NY 10598

During the last fifteen years, since the first proposal for a semiconductor superlattice by Esaki and Tsu, remarkable developments of an interdisciplinary nature have been witnessed on this subject. Indeed, in recent years, increased attention has been given to the engineering of artificial structures such as superlattices, quantum wells and heterojunctions. Obviously, the intriguing physics, particularly regarding the electron gas system of the reduced dimensionality involved in such structures, has provided fuel for this advance. Modern thin-film growth techniques have facilitated heterostructures having designed potential profiles and impurity distributions with a dimensional control close to interatomic spacing and with virtually defect-free interfaces. Such "engineered" structures which possess predetermined two-dimensional or quasi-two-dimensional quantum states, exhibit extraordinary transport and optical properties: Some of them, such as ultrahigh carrier mobilities, semimetallic coexistence of electrons and holes, etc., may not even exist in any "natural" crystal. The electron system with the quasi-one-dimensionality may be achievable on the surface inversion layer of a semiconductor superlattice. Thus, this new degree of freedom offered in semiconductor research has inspired many ingenious experiments, resulting in observations of not only predicted effects but also totally unknown phenomena such as fractional quantization which often require novel interpretations.

This talk, following a brief overview on the evolution of superlattices and quantum wells, is focussed on highlights of our group's studies in the four hetero-systems: InAs/GaSb, InAs/AlSb, GaSb/AlSb and GaAs/AlAs.

1) InAs/GaSb quantum wells: The quantum wells for both electrons and holes are made of a thin InAs layer from 70Å to 200Å sandwiched between GaSb layers. This unique structure is an outgrowth of our previously-studied semimetallic superlattices. Because of "interpenetration" between the GaSb valence band and the InAs conduction band at the junction, a conductive dipole layer with electron mobilities as high as 2×10^5 cm^2/V-sec is produced by electron transfer from GaSb to InAs leaving holes behind. Magnetotransport in such a layer at low temperatures down to 0.005K exhibited, in addition to the quantized Hall effect, anomalous structures which arise from the magnetic field-enhanced and temperature-activated interaction between two-dimensional electrons and holes coexisting across the interface.

2) InAs/AlSb quantum wells and superlattices: Transport measurements suggest that the bandedge relationship of InAs/AlSb heterostructures is similar to that of their InAs/GaSb counterparts.

3) GaSb/AlSb superlattices: Since a lattice mismatch of 0.65% in this hetero-system requires considerable elastic deformations of each layer, if no misfit dislocations are created during the MBE growth, the effect of strains (4 ~ 8 kbar) on the superlattice subbands is anticipated to be observable. In optical absorption, the reversal of the heavy- and light-hole exciton positions as well as the shift of absorption edges were observed, which are attributed to this strain effect. The data are interpreted according to a simple effective-mass theory.

4) GaAs/AlAs heterojunctions: Magnetotransport measurements, at 0.51K and up to 28T, were performed for a dilute two-dimensional electron gas with 6×10^{10} cm^{-2} in a GaAs/GaAlAs heterojunction. The existence of a fractional Hall quantization for a filling factor of 1/3 was confirmed. The magnetoresistance showed a substantial deviation from linearity above 18T and exhibited no additional features for filling factors below 1/5 down to 1/11. The results suggest that a transition from a quantum liquid to a crystalline state may take place.

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* Supported in part by the U.S. Army Research Office

17th International Conference on the Physics of Semiconductors

Surface Structure MoA-A1 Invited

SURFACE STRUCTURE OF SEMICONDUCTORS FROM EXTENDED X-RAY ABSORPTION FINE STRUCTURE.*

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University of Florida
Gainesville, Florida 32611

The application of extended x-ray absorption fine structure (EXAFS) to the local structure of semiconductor overlayers is reviewed. Since EXAFS is an impurity-based structural probe, only foreign atoms not present in the semiconductors substrate can be studied. However, both ordered and disordered substrates and overlayers have been studied. We concentrate in the review on some of the basic structural problems and issues that can be addressed by EXAFS and attempt to summarize the physics of the measurement and its limitations. Three different methods for determining the near-neighbor bond length from EXAFS are compared. Typical examples of overlayers are chlorine on Si(111), Ge(111) and Si(100) as well as on amorphous Si and Ge, tellurium on Si(111) and Ge(111). Interface reactions are observed for tellurium on Ge(111) and nickel on Si(111). Future directions of these studies are briefly discussed.

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*Collaborators are P.H. Citrin and F. Comin, AT&T Bell Laboratories, Murray Hill, N.J. 07974.

THE GEOMETRIC STRUCTURE OF THE GaAs(111) AND (110) SURFACES

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Because of the many technological applications and the scientific importance of semiconductor surfaces, their geometric structure has been diligently studied for over three decades. Semiconductor surface structures are scientifically challenging because a bulk-terminated surface is usually unstable; the surface atoms rearrange to occupy equilibrium sites other than bulk-terminated sites. We call this surface reconstruction. Monopolar (e.g. Si, Ge) and heteropolar (e.g. GaAs, ZnSe) semiconductor surfaces exhibit a wide variety of reconstructed structures. On Si surfaces, for example, there are the (2x1) structures of (100) and (111) faces, and (7x7) structure of the (111) face. For III-V compound semiconductors, there are the (1x1) structure of the (110) face, (2x2) structures of (111) and ($\bar{1}\bar{1}\bar{1}$) faces, and a series of structures (e.g. c(4x4), c(2x8), p(1x6), p(4x6), etc.) on the (100) face.

In this talk, we present results which, for the first time, confirm that a common driving mechanism is responsible for the reconstructed structures of the (110) and (111) faces of GaAs. This reconstruction mechanism explains why the stable structure on the (110) face has a (1x1) periodicity, while that on the (111) face has a (2x2) periodicity. Moreover, we have determined the surface atomic positions of both the (111) and (110) faces. Results of this work suggest that similar processes could occur on the (110) and (111) faces of other III-V compound semiconductors.

This work is supported in part by NSF Grant No. DMR-81-01203.

ATOMIC GEOMETRY AND DYNAMICS OF THE InAS(110) SURFACE

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The structure of the relaxed InAs(110) surface has been determined using mass-resolved Rutherford backscattering of He^+ ions. The relaxation embodies a rotation of the bond between the In and As atom out of the surface plane. Until recently it was commonly accepted that all cleavage faces of III-V compounds show such a bond rotation, with the rotation angle ω lying in the range $25^\circ < \omega < 31^\circ$ 1). However, recent evaluations based on LEED and ion channeling spectroscopy also appear to be consistent with a significantly smaller rotation angle ($\omega \approx 7^\circ$). The purpose of the present study is to determine accurately ω and the directions in which the surface atoms are displaced. Contrary to LEED, the technique of ion channeling and blocking used here is highly sensitive to displacements of atoms parallel to the surface plane, permitting a clear distinction between a bond-length-conserving relaxation model and a model that involves normal displacements only. It is concluded that the relaxation is purely bond-length-conserving and involves a rotation of the In-As surface bond by an angle of $\omega = 31^\circ$ out of the surface plane. The r.m.s. thermal vibration amplitude of the surface atoms is found to be enhanced with respect to the bulk amplitude by a factor 1.5.

1) A. Kahn, J. Vac. Sci. Technol. A1, 684 (1983) and references cited therein.

MoA-A4

STRUCTURAL PHASE DIAGRAMS FOR THE SURFACE OF A SOLID: A TOTAL ENERGY/RENORMALIZATION-GROUP APPROACH

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and
D. H. Lee, J. D. Joannopoulos, and J. J. Xiong
Massachusetts Institute of Technology
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Total energy calculations based on microscopic electronic structure are combined with position-space renormalization-group calculations to predict the structural phase transitions of the Si(100) surface as a function of temperature. It is found that two distinct families of reconstructed geometries can exist on the surface, with independent phase transitions occurring within each. Two critical temperatures representing order-disorder transitions are calculated.

LOW TEMPERATURE MAGNETORESISTANCE MEASUREMENTS ON ARSENIC-DOPED SILICON NEAR THE METAL-INSULATOR TRANSITION

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University of Rochester, Rochester, NY 14627

Magnetoresistance measurements have been made on uncompensated Si:As samples in the donor concentration range 6.6×10^{18}/cc to 9.5×10^{18}/cc. The measurements were made using the 4-terminal approach (welded Au-wire contacts) on bar-shaped samples approximately 5 mm long, in the temperature range $0.050 \text{ K} < T < 4.2 \text{ K}$, and in magnetic fields up to 23 T. The zero-field temperature dependence of G_{DC} exhibits Mott variable range hopping behavior, $\sigma_{DC} \propto \exp[-(T_0/T)^m]$ where $m \approx 1/4$ and T_0 scales rapidly to zero as $N_D \to N_C$. The N_C estimated from scaling of T_0 with N_D is in reasonable agreement with the value $N_C = 8.5 \times 10^{18}$/cc obtained by Newman and Holcomb[1] from measurements of σ_{DC} for $N_D > N_C$. The magnetoresistance results show $\ell n\,\rho(H)/\rho(0) \propto H^2 f(N_D,T)$ above a field $H \approx 3$T for the dilute samples and $H \approx 7$T for a metallic sample. The H^2 dependence of $\ell n\,\rho(H)/\rho(0)$ is the expected low field behavior for $\gamma < 1$ ($\gamma^2 = \varepsilon_h a^{*3} H^2/m^* c^2$). The density dependence of $\ell n\,\rho(H)/\rho(0)$ in the H^2 regime is of order N_D^{-p} with $p \approx 5$ in the range $7.5 \times 10^{18}/\text{cc} < N_D < 9.5 \times 10^{18}$/cc, a dependence much faster than the percolation prediction[2] of N_D^{-1}. The temperature dependence in this regime is of order T^{-m} with m density dependent and decreasing from $m = 1.0$ for the most dilute sample to $m \approx 0.2$ for a sample with $N_D = 9.4 \times 10^{18}$. The H^2 range of $\ell n\,\rho(H)/\rho(0)$ can be qualitatively explained by a modified variable range hopping approach taking account of the diamagnetic interaction term. These results also place a limit on the magnitude of the localization length barely on the insulating side of the metal-insulator transition.

[1] P. Newman and D. Holcomb, Phys. Rev. B 28, 638 (1983).
[2] B. I.Shklovskii, Sov. Phys. Semicond. 6, 1053 (1973).

Dilution refrigerator results were obtained in collaboration with J. Brooks, M. Naughton, and K. Martin of Boston University.
We are also grateful for the hospitality we received at the Francis Bitter National Magnet Laboratory.
This work was supported in part by NSF Grant # DMR-8306106.

Metal-Insulator Transition **MoA-B2**

EVIDENCE OF STRONG SPIN CORRELATIONS IN Si:P

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We observe an enhancement of the spin-lattice relaxation rate by a factor of 25 in metallic Si:P. We find this effect in NMR experiments at a frequcney of 7.48 MHz, T=10 mK, and a donor density near 3.8x10**18 cm**-3. For T up to 300 mK, the rate follows an anomalous form: proportional to T**1/2. Within the Korringa formulation, these results can be parameterized as an increase in the spin susceptibility by a factor of 5, strengthening previous evidence based on enhancements of 50% [1]. Both our observations appear to indicate spin correlations resulting from many body Coulomb interactions. We also observe a linear dependence of the relaxation rate on magnetic field, and argue that our results indicate a slowing down of the spin diffusion relative to the charge diffusion.

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Metal-Insulator Transition **MoA-B3**

INFLUENCE OF DISORDER ON SEMICONDUCTOR-METAL TRANSITION IN InSb

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The results of low temperature ($T \simeq 4$ K) electric transport and magnetotransport in the region of semiconductor-metal transition in n-type InSb are presented. It is well known that two processes contribute to this transition, i.e. the Anderson localization due to disorder present in the semiconductor and the effects of electron-electron interactions (correlation effects). Separation of these contributions has become one of the main interest of the carrier localization problem in three dimensions.
The change of electron concentration through its critical value, n_{cr}, (Mott condition) is usually achieved by changes in compensation rate. We adopt an alternative method of the high pressure freeze-out of carriers on the metastable donor states which enables us to obtain extremaly low carrier concentrations ($n \simeq 1_{10}12$ cm^{-3}). The first method introduces a significant disorder to the matrix of InSb whereas the second one does not change the content of acceptors. Moreover it causes a decrease in the number of ionized donors acting as scattering centers. Comparison of the results obtained in different samples of InSb with electron concentrations (between $5_{10}14$ cm^{-3} and $2_{10}12$ cm^{-3}) modified by the above mentioned methods shows that for the samples prepared by the high pressure method: ^{i}the low temperature conductivity, σ, is higher (by two orders of magnitude for $n \simeq 2_{10}13$ cm^{-3}) and instead of a collapse it exhibits almost linear dependence of $\ln\sigma$ versus $\ln n$ down to $n = 2_{10}12$ cm^{-3}, ^{ii}Hall coefficient does not exhibit a maximum as temperature is lowered. Additionally the magnitude of the negative magnetoresistance is influenced by the high pressure freeze-out of carriers. We believe that the obtained results demonstrate the effect of disorder on the low temperature electric conductivity processes in the region of semiconductor-metal transition of InSb crystal.

ELECTRON CORRELATION ENERGIES AND METAL-INSULATOR TRANSITION OF VO_2

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We report the changes of band structures and correlation energies of VO_2 on the metal to insulator(M-I) phase transition at $T_c=340^\circ K$, elucidated for the first time by the synchrotron radiation spectroscopy. Reflectance spectra were measured on single crystals in the region between $h\nu=2$ and 60 eV. On the M-I transition, the structures due to the excitation from the O 2p valence bands to the π^* conduction bands have shown a remarkable energy shift of 0.5 eV to the higher energy region, in contrast to the negligible shift of the excitation to the (s,p) conduction bands. The structures ascribed to the excitation to the $d_{\parallel}$ conduction band have shown an anomalous energy shift of 1.2~1.6 eV on the M-I transition.

Meanwhile, the ultraviolet photoemission spectra(UPS) have demonstrated a clear Fermi edge in the metal phase. On the contrary, the UPS in the insulator phase have shown the $d_{\parallel}$ valence band with a width of 1.5 eV. The energy difference between the top of the $d_{\parallel}$ valence band and the Fermi level is evaluated as 0.2 eV. Almost no change is observed, however, for the O 2p valence bands.

These experimental results are consistently understood by considering the electron correlation energies between $d_{\parallel}$-$d_{\parallel}$ and $d_{\parallel}$-π^* electrons , in addition to the changes of band structures on the M-I transition. If one excites an extra $d_{\parallel}$ electron from the O 2p valence bands, the excited $d_{\parallel}$ electron is subjected to a strong Coulomb interaction(comparable to the band width) with the $d_{\parallel}$ electron of the bonding orbitals, in the insulator phase. The degeneracy of this transition with that to the π^* conduction bands in the metal phase is explained by the screening effect of this intra-atomic $d_{\parallel}$-$d_{\parallel}$ correlation energy by the π^* electrons partly populated at the Fermi level. The π^*-$d_{\parallel}$ interaction is also evaluated as 0.2~0.4 eV, in consistence with other experimental results.

VALENCE-CONDUCTION CHARGE TRANSFER IN THE SEMICONDUCTOR-METAL TRANSITION : Si

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Recent experiments (1) evidenciate some anomalies during the pressure-induced metal transitions in group IV and III-V semiconductors. In particular the intensity I of the (222) forbidden X-ray reflection in Silicon and in InSb, measured as a function of high hidrostatic pressure, decreases sharply before the semiconductor-metal phase transition. Focusing the importance of the order-parameter I(222) in the definition of the transition from the covalent bonding to the metallic one (2), we here propose a possible solution of the phenomenon.

In the local density self-consistent approach we have verified the constance of the (222) Fourier component of the valence charge density by extending the volume variation in order to reproduce the experiment. As recently commented (3) the bonding charge does not change very much in the region of the phase variation. In the limit of the same diamond structure we find, however, that the (222) component is very rapidly lowered in the semimetal transition. The valence electron is sharply transferred in the conduction band at X explaining in this way the observed decrease. At the same time we suggest that the observed anomalies before the phase transition, may be accounted for as due to localized crystallizations in the bulk originated by the pressure. A simple H_2-like model is also discussed to explain the charge density constance in the (110) plane.

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HIGH-PRECISION deHAAS-van ALPHEN MEASUREMENTS ON A TWO-DIMENSIONAL ELECTRON GAS

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The transport properties of a 2-dimensional (2-D) electron system have been investigated extensively for more than a decade.[1] Much of the work has involved electrical transport in high magnetic fields (B) in 2-D Si MOSFET's and modulation doped (MD) GaAs/AlGaAs heterostructures. In contrast, static properties, e.g. heat capacity and magnetic susceptibility, have not received as much attention.

In this paper we report new, high-precision static magnetization measurements on the two-dimensional electron gas in MD GaAs/AlGaAs heterostructures in fields up to 10T. Using a newly developed torsional magnetometer technique we have made qualitative improvements on our earlier[2] SQUID magnetometer results. The torsional technique is ideally suited for detecting the small anisotropic moment of the 2-D electrons in the presence of other, far larger, isotropic background moments. Due to the 2-D nature of the electron gas in the heterojunction a magnetic field applied at a slight angle to the normal of the 2-D plane produces a torque on the sample directly proportional to the induced magnetic moment (μ). The sample is mounted on a thin wire which twists due to the torque and this twist is measured by capacitive techniques. A minimum value of about 10^{-12} J/T for μ has been detected at a field of 10T.

This value is approximately 100 times more sensitive than the SQUID technique and the sensitivity to anisotropic moments allows a nearly complete rejection of isotropic background moments. Beautiful deHaas-van Alphen oscillations have been observed in MD GaAs/AlGaAs heterostructures with clear signals seen in as few as 13 superlattice layers. A detailed comparison with a variety of theoretical models for the electronic density of states will be presented.

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Quantum Wells **MoA-C2** **Invited**

SPECIFIC HEAT AND SCREENING OF 2D ELECTRONS IN GaAs

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Measurements of the specific heat of 2-dimensional (2D) electrons are of great interest since they reveal directly the density of states. In GaAs the specific heat of 2D electrons becomes comparable to the lattice specific heat at liquid Helium temperatures for pure multilayer structures.

We have investigated two multilayer samples consisting of 172 and 94 double layers of 200 Å GaAs and 200 Å GaAlAs having mobilities of 30.000 cm^2/Vs and 100.000 cm^2/Vs at 4.2 K respectively. The samples are thermally isolated with 5 μm thick superconducting wires.

Two methods are applied to determine the specific heat:

In the first method the sample temperature is measured as a function of a fast magnetic field sweep. Oscillations proportional to the derivative of the specific heat in respect to magnetic field are observed.

In the second method the specific heat is directly measured using 2 carbon films, one for heating and one for detecting the temperature change. The investigated temperature range is 4,2 K to 2 K in fields up to 10 T. Oscillations of the sample temperature up to 20 mK are observed revealing a broadened density of states with no significant overlap between the levels for fields above 6 T.

In addition the temperature dependent screening of the electron-polar optical phonon interaction was investigated for 2-dimensional electrons in GaAs.

The analysis of the splitting between different Landau level transitions reveals the influence of the nonparabolicity of the bandstructure and the so called polaron effect on the effective mass.

We have investigated Landau level transitions in high mobility GaAs/GaAlAs heterostructures ($\mu \sim 5 \times 10^5 cm^2/Vs$) as a function of electron heating in cyclotron resonance experiments. Electric fields up to 300 V/cm were applied. Clear evidence for an electron heating dependent polaron effect is found.

NEW MICROWAVE INDUCED RESONANCES IN THE CONDUCTANCE OF A GaAs/$Ga_{1-x}Al_xAs$ HETEROJUNCTION

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We have observed microwave induced resonances in the conductance of a modulation doped GaAs/$Ga_{1-x}Al_xAs$ heterojunction placed in a uniform magnetic field and cooled to 1.7K. In addition to the narrow spin resonance and the broad oscillations due to microwave heating reported by Stein et al[1], we observed a new series of resonances when $\hbar\omega_c >> \hbar\omega_m >$ spin splitting, where $\hbar\omega_c$ and $\hbar\omega_m$ are the cyclotron energy and the microwave energy respectively. This series consists of two resonances per Landau level and is observed already at microwave powers one to two orders of magnitude lower than the minimum required to see the microwave heating signal. We believe these new resonances to result from *non-resonant* spin transitions within each Landau level. It is the Landau level structure itself which converts these *non-resonant* spin transitions into *resonant* changes in conductance.

The experimental procedure consisted of mounting the sample in a microwave cavity (f=23 GHz), placing it into the bore of a superconducting magnet, and cooling it to 1.7K. Two terminal measurements of the conductance in the plane of the 2DEG as a function of magnetic field were made prior to irradiation with microwaves. The familiar Shubnikov de Haas (SdH) oscillations were obtained. Changes in this conductance due to 500 Hz amplitude modulated microwave irradiation were measured using phase-sensitive detection. The microwave related signal was studied as a function of the microwave power incident on the cavity over the range 10^{-5} to 10^{-1} watts. At or below about 10^{-4} watts, the microwave heating signal, which has the same periodicity as the SdH oscillations but is 180° out of phase, was no longer observed. The remaining "low power" spectrum has two peaks per Landau level - a small peak as the Fermi level enters the Landau level, and a larger peak as the Fermi level leaves the Landau level.

A model based on non-resonant electric-dipole-induced spin flips within each Landau level is in excellent agreement with the data. This model provides us with a sensitive experimental probe of the Landau level density of states, which we find to be distinctly non-gaussian and in qualitative agreement with theoretical predictions.

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COLLECTIVE RESONANCES IN THE LATERALLY CONFINED 2D ELECTRON GAS

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Transport of high mobility electrons confined in a submicron semiconductor structure is controlled by the interaction of the carriers with the boundaries. To experimentally probe the effects of such confinement we have fabricated structures consisting of a 2D electron gas at the interface of a selectively doped (Ga,Al) As and GaAs heterostructures patterned as arrays of narrow (< 1 micron) wires. These wires are uniformly distributed as a grating or two dimensional grid. The bulk, two dimensional mean free path is substantially larger than the width of the wires.

The collective resonances are observed by measuring the far infrared magneto transport. At low magnetic fields with the electric vector polarized perpendicular to the grating a single resonance is observed that moves to higher frequency in strong magnetic fields. With the electric vector polarized parallel to the wires no resonance is observed until the cylcotron frequency is comparable to the to the resonance observed in the perpendicular polarization. The two dimensional grid exhibits more complex behavior.

The electron density in these narrow wires is a basic parameter controlling the collective behavior and can be independently determined from Shubnikov-de Haas oscillations in the d.c. magneto transport. The predictions of a model calculation for the collective behavior at this measured density differs from that observed. This indicates that the 2D electrons are not responding in a classical manner in these small structures. Contributions to the response due to boundary scattering or quantum mechanical confinement are considered.

ELECTRONIC STRUCTURE OF A MONOLAYER $NbSe_2$ FILM GROWN HETEROEPITAXIALLY ON THE CLEAVED FACE OF $2H$-MoS_2

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Low-energy electron energy loss spectroscopy (LEELS) is a powerful technique espeially to investigate the electronic structure of an ultrathin film, since its information depth can be made as short as 0.3 nm. We have made full use of this technique to investigate the electronic structure of monolayer $NbSe_2$ film epitaxially grown on a cleaved face of 2H-MoS_2.

Usually there appear dangling bonds on the clean surfaces of semiconductors, and this makes it difficult to grow good heteroepitaxial film having atomic order thickness except in such very few case as GaAs and AlAs, in which beautiful lattice matching is realized. Both $NbSe_2$ and MoS_2, however, have layered crytal structures, which are formed from unit layers consisting of transition metal atoms sandwitched by chalcogen atoms. The atoms in a layer are bound by strong covalent bonds, whereas the layers are weakly bound to each other by van der Walls forces. The crystal can be easily cleaved along the layers, and there appear no dangling bonds on their cleaved faces. The epitaxial growth proceeds through van der Waals forces in those layered materials. Thus we have succeeded in growing an ultrathin metallic NbSe film heterepitaxially on the cleaved face of semiconducting MoS_2, in spite of the large differnece between the lattice constants of those materials.

$NbSe_2$ film was grown on clean cleaved face of natural molybdenite by molecular beam epitaxy. The reflection high energy electron diffraction and Auger electron spectroscopy showed that good $NbSe_2$ film was grown epitaxially. The thickness of the film was 0.6 nm which is about that of a unit layer. The LEELS spectra of the prepared $NbSe_2$ film were measured in situ, and it was found that the spectrum was almost the same as that of single-crystalline $NbSe_2$, which agrees well with the optical reflection spectrum yielding bulk electronic structure of 2H-$NbSe_2$. Thus it is concluded that the electronic structure of monolayer $NbSe_2$ is very close to that of bulk $NbSe_2$, indicating that the electronic structures of layered materials are determined predominantly by intralayer interactions.

Two-Dimensional Materials **MoA-D2**

NQR AND NMR STUDY OF ^{181}Ta IN THE COMMENSURATE CDW STATE OF 1T-TaS$_2$ AND 1T-TaSe$_2$ -- ON THE SEMICONDUCTIVE NATURE OF 1T-TaS$_2$

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1T-TaS$_2$ and 1T-TaSe$_2$ have attracted much attention as two-dimensional metals showing striking CDW effects. Below 180K in 1T-TaS$_2$ and 475K in 1T-TaSe$_2$, the $\sqrt{13}\times\sqrt{13}$ commensurate structure appears. The structural unit in this phase is considered to be a star-shaped cluster of 13 Ta atoms, consisting of three inequivalent Ta sites with population ratios 1:6:6. Until recently, it has been believed that 1T-TaS$_2$ would be isostructural to 1T-TaSe$_2$ in the commensurate phase. But the electrical transport properties at low temperatures are quite different between the two compounds. 1T-TaS$_2$ is semiconducting, while 1T-TaSe$_2$ is metallic. At the moment this difference between the two, especially the semiconductive nature of 1T-TaS$_2$, is a matter of controversy and several pictures, such as the Mott or Anderson localization model, are proposed. However, none of them are satisfactory. We report here pulsed NQR and NMR studies on the ^{181}Ta nuclei in 1T-TaS$_2$ and 1T-TaSe$_2$ at 4.2K in order to understand the semiconductive nature of 1T-TaS$_2$ from a microscopic standpoint. The observed spectra show that in the commensurate phase there exist $6\sim7$ inequivalent Ta sites in 1T-TaSe$_2$ and $12\sim15$ sites in 1T-TaS$_2$, contrary to the expectation from the simple cluster model. This inconsistency can be removed if the effect of the three-dimensional ordering of clusters is taken into account. In 1T-TaSe$_2$ it is suggested from X-ray and electron diffraction that clusters are periodically stacked with a stacking wave vector $\vec{c}_0+2\vec{a}_0$. For this simple stacking case, the cluster consists of seven inequivalent Ta sites with population ratios 1:2:2:2:2:2:2. Our experimental results are consistent with this simple stacking model. On the other hand, in 1T-TaS$_2$, such simple stacking is not realized. Then we propose the "bicluster" model that a unit cell in the commensurate phase of 1T-TaS$_2$ contains two star-shaped clusters on the two successive layeres. According to this model, the unit cell includes even number (26) of electrons, so the semiconductive behavior of 1T-TaS$_2$ at low temperatures can be explained without relying upon the Mott localization. Furthermore the line shapes of the NQR and NMR spectra of 1T-TaS$_2$ are broad as compared with 1T-TaSe$_2$. This fact may indicate that the stacking order of the CDW is of short-range character in 1T-TaS$_2$. The incomplete stacking order may be a possible cause of the low-temperature Anderson localization.

GRAPHITE INTERCALATED WITH K AND NH_3 - A METAL-AMMONIA SOLUTION IN 2 DIMENSIONS

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The ternary graphite intercalation compound $K(NH_3)_xC_{24}$, $0 \leq x \leq 4.38$ can be prepared by exposing stage 2 KC_{24} to NH_3 vapor. We will show that this compound represents a 2-D analog of the famous 3-D metal-ammonia systems which are the foci of numerous investigations of the metal-insulator transition.[1,2] For instance, from high resolution x-ray diffraction studies we know that the NH_3 enters the carbon layer interspace in monolayer form. Thus, one would expect K in the two-dimensional metal-NH_3 system to be dynamically 4-fold planar coordinated to NH_3 in contrast to the 6-fold octahedral coordination of the 3-D system. The saturation value of $x = 4.38$ is consistent with a 4-fold coordination plus ≈10% of spacer NH_3 molecules. Indeed, angle-dependent proton NMR studies of $K(NH_3)_{4.38}C_{24}$ indicate that two NH_3 species are present, one of which is 10% of the other. Our NMR studies, coupled with color 3D-real time space filling computer graphics modeling of the K-NH_3-graphite system indicate that the NH_3 molecules are spinning rapidly about their 3-fold axes which are simultaneously reorienting about the graphite c-axis. Moreover, the NH_3 molecules' c_3 axes are tilted towards their K neighbors in response to the binding of the nitrogen lone pair to the K^+ ion. But unlike the case for 3-D metal-ammonia solutions, the alignment of the NH_3 c_3 axis along the line of centers between the NH_3 molecule and the K^+ ion is sterically precluded by the carbon planes. We have also studied the effect of NH_3 insertion on the charge exchange and charge distribution in the interlayer space by monitoring the (00ℓ) x-ray diffraction patterns of $K(NH_3)_xC_{24}$ as a function of NH_3 vapor pressure (i.e. of x) and by carefully measuring intercalation isotherms. Calculations of the x dependence of the x-ray structure factor which include the effect of electron charge transfer back into the K-NH_3 layer from the carbon layers are in good agreement with experiment. The electrons in the K-NH_3 layer are solvated by the NH_3 molecules in analogy with the 3D-metal-ammonia solutions. This solvation (charge localization) contributes significantly (30%) to the c-axis expansion of the carbon layers which has been quantitatively accounted for with a model for the staging free energy in ternary graphite intercalation compounds.

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17th International Conference on the Physics of Semiconductors

Two-Dimensional Materials **MoA-D4**

MAGNETIC BREAKDOWN IN GRAPHITE INTERCALATION COMPOUNDS

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The presence of large, in-plane superlattices in acceptor graphite intercalation compounds (GIC) can lead to extensive restructuring of the Fermi surfaces. We present the first direct evidence of these extra Fermi surfaces, showing that they can be broken down in a large magnetic field to reveal the simpler, graphitic-derived Fermi surfaces. Similar results are found in GIC with H_2SO_4, HNO_3, and Br_2. The superlattice sizes determined from deHaas-van Alphen orbit areas are in good agreement with direct x-ray diffraction studies of the same samples. While the lattices are only weakly stage-dependent, the breakdown field is found to increase as the stage decreases, suggesting a three-dimensional enhancement of the superlattice cohesive energy.

A detailed analysis of the experimental data shows the presence of significant magnetic interaction (Schoenberg effect).

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Two-Dimensional Materials **MoA-D5**

ELECTRONIC STRUCRURE OF BLACK PHOPHORUS STUDIED BY ANGLE-RESOLVED PHOTOEMISSION AND POLARIZED SOFT X-RAY EMISSION AND ABSORPTION

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Orthorhombic black phosphorus (black P) is the most stable form of phosphorus and is a narrow gap (about 0.3 eV) layered semiconductor. After our recent success in growing a relatively large single crystal of black P, the physical properties are now being extensively studied by various experimental techniques as well as the possibilities of intercallation with alkali metals and alloying with arsenic. In this paper, we present the comprehensive study of the electronic structure of black P using the highly-angle-resolved ultraviolet photoelectron spectroscopy (ARUPS) and the polarized soft x-ray emission and absorption spectroscopy (PSXEAS). The experimental band structure determined by the ARUPS study has been compared with the self-consist pseudopotential calculations. Some special points and bands with almost no dispersion along the interlayer direction have been successfully assigned in the experimentally determined band structure. The PSXEAS study has clearly identified the respective contribution of each atomic orbital ($3p_z$ etc.) to the valence and conduction band structures.

ANGLE RESOLVED PHOTOEMISSION STUDIES OF RECONSTRUCTED SILICON SURFACES

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Recent angle resolved photoemission studies have been concentrated on the dangling-bond band dispersion on the cleaved Si(111)2x1 surface. For good single domain 2x1 surfaces different experimental groups agree on a highly dispersive dangling-bond band along $\bar{\Gamma}$-$\bar{J}$ in the surface Brillouin zone. Reconstruction models giving flat or nearly flat dangling-bond bands, such as the buckling-model, are ruled out by the experiments, which instead support the π-bonded chain model.

In addition to the dangling-bond structure, spectra from Si(111)2x1 exhibit another dominating structure reported by Rowe[1] et al. in the first angle resolved measurements on the 2x1 surface. Due to its sensitivity to contamination and threefold azimuthal emission pattern this structure has hitherto been interpreted as a back-bond surface state in the literature.

From polarization dependent measurements[2] we identify this structure as instead due to direct transitions from the uppermost valence band. Direct transitions from the second highest valence band are also identified. The experimental $E_i(\bar{k}_{//})$ dispersions for these transitions are in good agreement with calculated dispersions for direct transitions to a free-electron final band in the photon energy range 10.2 - 21.2 eV investigated. These direct transition structures are also observed in the spectra from Si(111)7x7 and Si(111) $\sqrt{3}$x $\sqrt{3}$:Al.

The Si(111)7x7 surface exhibits three surface states at $\sim$-0.2, $\sim$-0.8 and $\sim$-1.8 eV. The $\sim$-1.8 eV surface state is found to have a $\sim$ 0.3 eV downwards dispersion along $\bar{\Gamma}$-$\bar{M}$ and $\bar{\Gamma}$-$\bar{K}$ in the 1x1 SBz. The polarization dependence of emission suggests that all three surface states on 7x7 are dangling-bond derived. A relative difference in the contamination sensitivity to oxygen and chlorine has been found for the two upper surface states.

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RECONSTRUCTION OF THE Si(100)-2x1 SURFACE

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Our self-consistent pseudopotential calculations of total energy and surface energy bands show that the accepted buckled dimer model for the Si(100)-2x1 surface implies a very soft and metallic surface. We show that both of these features are inconsistent with existing data. We present an alternative model for the reconstruction of this surface which has geometrical features of buckling - as suggested by experiments. However, the physical mechanism for reconstruction in our model is quite different from buckling. In contrast to buckling, which is based on ionic bonding, our model is based on the reduction of the number of broken bonds present at the surface and a π-bonding between the broken bonds. We show that our model is energetically favored over buckled dimer models and is consistent with data. New experiments to test the validity of the model are suggested.

The Si(100)-2x1 is one of the most thoroughly studied of Si surfaces. A variety of experiments - LEED, ion-scattering, photoemission - have all been interpreted by others as supporting the buckled dimer model. Theoretical calculations by others have also supported the buckled dimer model.

Our self-consistent pseudopotential calculations for buckled dimer models where the degree of buckling is varied show that the total energy of this surface, relative to the unbuckled surface, is remarkably insensitive to buckling up to relatively large buckling of about 12 degrees. This implies a wide distribution of buckling (-10 to 10 degrees) of the dimers on the surface. Such a distribution seems inconsistent with LEED and ion scattering data. In addition, we find that the surface stays metallic - contrary to photoemission data and earlier theoretical calculations. Only for unacceptably large buckling (about 20 degrees) the surface becomes semiconducting. However, we find that for buckling larger than about 15 degrees total energy increases very sharply with buckling. Thus our calculations suggest that the buckled dimer model is not a valid model.

We propose a new reconstruction model for this surface that is based on elimination of broken bonds present at the surface and a π-bonding between them. We show how this model accounts for the existing data. We also show that this model is energetically favored over the buckled dimer model.

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Surface Reconstruction **MoP-A3** Invited

POLARIZATION DEPENDENCE OF Ge AND Si (111)2×1 SURFACE STATE OPTICAL ABSORPTION: A TEST OF SURFACE RECONSTRUCTION MODELS.

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The nature of the reconstruction geometry of cleaved Ge and Si (111)2×1 surfaces is an open question, with several models having been proposed to explain the various experimental results. An important prediction of these models, which we have tested, is the polarization dependence of the dangling bond absorption.[1] This polarization dependence arises from symmetry considerations, and is not critically dependent on calculations requiring accurate atomic positions, such as those required to simulate photoemission or LEED data. The π-bonded chain model predicts strong absorption for light polarized parallel to the chains (along $[\bar{1}10]$) and no absorption perpendicular to these chains, as they are well separated in space, leading to a $\cos^2\vartheta$ dependence. The π-bonded molecule model leads to a maximal absorption along the molecular axis, or at a small angle to $[11\bar{2}]$. The buckling and anti-ferromagnetic insulator models lead to a maximal absorption perpendicular to the rows of atoms with either position or spins up or down (along $[11\bar{2}]$), with the absorption reduced by 1/3 along $[\bar{1}10]$. The polarization-dependent absorption measurements reported here for Si and Ge (111)2×1 support the π-bonded chain model for both surfaces, in agreement with total energy calculations for both surfaces which find the π-bonded chain to be the minimum energy structure for both Si[2] and Ge[3] (111)2×1 surfaces. The results are inconsistent with other models proposed for these surfaces. For Si, other experimental results also appear to support the chain model, including photoemission and ion backscattering measurements. Less experimental evidence exists for Ge(111)2×1, with two recent photoemission measurements in contradiction. Measurements by Nicholls *et al.*,[4] indicate a dispersion similar to that predicted by the chain model, while measurements by Solal *et al.*,[5] from Ge(111)2×1 surfaces are not consistent with the chain model. Thus, the structure of Ge(111)2×1 is the subject of some controversy, with the results reported here strongly supporting a similarity between the reconstructions on cleaved silicon and germanium.

Using photothermal displacement spectroscopy, we have measured the polarization-dependent absorption by surface states on Si(111)2×1 and Ge(111)2×1 surfaces.[6] Photothermal displacement spectroscopy is based on the optical detection of the thermal expansion of a sample as it is heated by the absorption of light. Being a direct absorption measurement which can discriminate the surface state absorption from the weak bulk impurity absorption background, it is not necessary to obtain a difference spectrum as it is in reflectivity, photovoltage and photoconductivity experiments. For Si(111)2×1, the ∼2% dangling bond absorption is peaked at ∼0.46 eV; for Ge(111)2×1, the absorption is also ∼2%, but has a maximum at ∼0.50 eV. For both Si and Ge we have found the absorption in a single domain region to be highly peaked for light polarized parallel to the $[\bar{1}10]$ direction on the surface, or perpendicular to the reconstruction direction as determined by LEED. The absorption follows a $\cos^2\vartheta$ dependence as the polarization is rotated, with no detectable surface absorption of light polarized parallel to $[11\bar{2}]$, the dependence predicted by the π-bonded chain model.

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ION SCATTERING STUDIES OF THE STRUCTURE OF SEMICONDUCTOR SURFACES AND INTERFACES

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Medium energy ion scattering (50-200keV H^+, He^+), combined with the effects of channeling and blocking, is a technique very sensitive to the structure of the (near) surface region of a solid. The technique has been used to study the structure of clean Si, Ge, GaSb and InAs surfaces, and the interaction of very thin metal films (≤ 20 Å) with Si surfaces. Surface geometries have been determined with high accuracy on the clean surfaces. For the thin metal films intermixing with substrate atoms, morphology of the film, surface segregation and epitaxial growth have been studied in detail. In this talk the analytic capabilities of the technique will be explained and illustrated with recent experimental results.

THE ATOMIC GEOMETRY OF Si(100)-(2x1) REVISITED

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A new atomic geometry for the (2x1) structure on Si(100) is proposed on the basis of dynamical calculations of the elastic low-energy electron diffraction (ELEED) intensities. A systematic X-ray R-factor comparison of calculations for hundreds of trial structures with published ELEED intensity data reveals the existence of an asymmetric dimer structure which is fully compatible with ion-scattering measurements.[1,2] This structure provides a description of the measured ELEED intensities which is improved relative to that afforded by structures proposed on the basis of prior ELEED intensity analyses[3] which are, however, not compatible with the ion-scattering results.[2] Moreover this structure is similar to but not identical with those predicted by several energy-minimization calculations.[4,5] Consequently, our analysis resolves an apparent incompatibility between ELEED and ion-scattering results as well as reveals the qualitative correctness of modern total-energy minimization methods for semiconductor surface-structure determinations.

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Surface Reconstruction **MoP-A6**

Theory of the Al -Si(111) -$\sqrt{3}$x$\sqrt{3}$ Surface

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The deposition of 1/3 monolayer of Al onto the Si(111) surface produces a $\sqrt{3}$x$\sqrt{3}$ reconstruction. Based on periodicity and coverage considerations, Lander and Morrison [1] proposed that the surface structure consisted of Al adatoms resting in the threefold hollow sites. However, no conclusive determination of the structure of this phase has been given.

We have carried out total energy minimization calculations for this surface using the pseudopotential method and the local density approximation. We find that in addition to the Lander-Morrison model, adsorption of Al in the threefold site above the second layer Si atoms is a possible candidate for the structure. The preference for one site over the other is strongly influenced by substrate relaxation. The structural properties for both sites will be presented.

More importantly, we have determined the energy and dispersion of the adatom induced surface states for these geometries. Experimentally [2] , it has been found that the dispersion of these surface states is characteristic of a 1x1 Brillioun zone rather than the $\sqrt{3}$x$\sqrt{3}$ zone. In fact, these surface states appear to exist only near the outer regions of the 1x1 zone. This fact is provocative because surface states with these characteristics also occur on many of the clean Si(111) and Ge(111) surfaces [3]. The explanation of this effect will be given for the Al-Si(111)-$\sqrt{3}$x$\sqrt{3}$ surface. The same theory may be used to explain the photoemission intensity patterns [3] for the Si(111)-(7x7) surface in terms of Si adatom models.

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Amorphous Semiconductor **MoP-B1** **Invited**

DOPING EFFECTS IN HYDROGENATED AMORPHOUS SILICON

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Early models of bonding in amorphous semiconductors (Mott's 8–N rule) concluded that substitutional doping is impossible. Its observation in hydrogenated amorphous silicon was therefore surprising. Recent experiments will be described which show that the doping process involves much more than the addition of shallow donors and acceptors, and results in profound changes in the structure of the material, and in its transport and optical properties. In particular, excess dangling bonds are introduced whose density increases as the square root of the impurity concentration. The doping efficiency is low and also varies with the impurity density. In contrast, compensated amorphous silicon has a low dangling bond density, but instead contains gap states of a different origin. From these measurements it is deduced that the position of the Fermi energy exerts a controlling influence on the doping process. Starting from a modification of the 8–N rule we have developed a unifying description of the dopant and defect states based on the location of the Fermi energy. Doping occurs through an interplay of 3– and 4–fold coordinated dopants and charged dangling bonds. The model quantitatively accounts for the increase in dangling bond density and also provides insight into the difference between doping of an amorphous and crystalline semiconductor.

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Amorphous Semiconductor MoP-B2

STUDY OF DISPERSIVE RELAXATIONS IN AMORPHOUS Si_xGe_{1-x}:H BY PHOTOINDUCED ABSORPTION

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The decays of the photoinduced absorption (PA) band in a-Si:H follow the power law $t^{-\alpha}$ indicating that the underlying recombination process is dispersive. We studied the dependence of the dispersion parameter α on temperature, hydrogen content, doping with P or B, concentration of Ge in the alloy, and bias illumination. The temperature dependence of α can in general be represented by two straight lines of different slope. The high temperature branch has the larger slope and extrapolates to $\alpha=0$ at $T=0$. This behavior is attributed to multiple trapping in an exponential band tail. The low temperature branch extrapolates to a non-zero value α_o at $T=0$. Both α_o and the slope depend on sample composition and other parameters Various theoretical models for non-radiative recombination by tunnelling are explored and compared with the experimental data in order to determine a realistic model for recombination at low temperatures.

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Amorphous Semiconductor **MoP-B3**

ESR STUDY OF METASTABLE CARRIERS IN HYDROGENATED AMORPHOUS SILICON

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Evidence of metastable carriers at low temperature in a-Si:H has been given by Electron Spin Resonance (ESR)[1], photoconductivity[2] and thermostimulated currents[3]. ESR has been extensively used to study gap states in a-Si:H. In undoped material, ESR detects a single signal at g=2.0055 attributed to dangling bonds[4], while at low temperature light induced ESR (LESR) selects two resonances at g=2.004 and g=2.012 thought to be due to carriers trapped respectively in conduction and valence band tail states[5]. This LESR signal has a very broad lifetime distribution which extends up to hours and there remains several $10^{16}cm^{-3}$ metastable photoexcited carriers in the material which disappear after annealing at room temperature. We have used an original ESR technique which consists in studying the evolution with the temperature of isochronal anneals, of an ESR signal measured at a given temperature. This technique yields information on the detrapping and retrapping of carriers in the states monitored by ESR. We have observed that electrons in the conduction band tail were annealed first from temperature as low as 50K, while holes in the valence band tail start vanishing for annealling above 100K. For annealing above 170K when almost no LESR signal at g=2.004 and g=2.012 remains, a quenching of the 2.0055 ESR is observed and disappears for annealings above 230K. From these results trapping depths of 150, 300 and 500 meV are estimated for carriers in conduction and valence band tails and dangling bonds respectively. These results and their implications on trapping and retrapping mechanisms of carriers will be discussed.

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Amorphous Semiconductor **MoP-B4**

GAP-STATE DISTRIBUTION IN a-Si:H MEASURED BY PHOTOCAPACITANCE SPECTROSCOPY*

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In amorphous silicon it is generally found that electronic defect levels are continuously distributed in energy in the semiconductor band gap and of sufficient density to dominate the transport properties of the material. Both features introduce unique difficulties in the measurement of the gap-state distribution, as compared to deep-level characterization in crystalline semiconductors. The gap-state distribution in hydrogenated amorphous silicon (a-Si:H) has previously been measured by deep-level spectroscopies based on thermal emission of trapped electrons.[1] In the present study, photocapacitance spectroscopic techniques have been implemented to measure the distribution and optical cross-section of the gap states, based on photoemission of trapped charge, in both Schottky-barrier and p-n junction diodes. The measurement involves cooling a diode to low temperature in order to freeze out thermal emission from deep levels while retaining band-tail mediated charge transport and sufficient electrical conductivity in the neutral region of the device for monitoring the low-frequency capacitance. After voltage biasing the diode to populate deep levels with electrons (in n-type material), a reverse bias establishes a layer depleted of free carriers. Illumination with sub-band gap light of energy $h\nu$ photoemits electrons from a thermal-emission depth to $h\nu$ below the mobility edge, and a positive space charge builds up in the depletion layer as these electrons are swept away. This deep-level photodepopulation dominates in Schottky barriers for $h\nu$ less than the threshold for internal photoemission and in p-n junctions up to the energy for minority-carrier photoemission. The light-induced transient response is time resolved in two detection modes. First, under constant-capacitance conditions, the applied voltage is servoed to maintain a fixed depletion width, thereby yielding directly the change in space charge, ΔQ_t. The total density of gap states is computed from the steady-state values of $\Delta Q_t(h\nu)$, and the initial-slope method,[2] reformulated here for a continuous deep-level distribution, yields the optical cross-section. The results identify a broad peak centered ~0.8 eV below the mobility edge. Secondly, from analogous measurements of ESR-detected photodepopulation, the energy distribution of doubly occupied Si dangling orbitals (designated D^-) has been obtained.[3] The distribution $D^-(h\nu)$ is identical, within experimental accuracy, in position and density with the electronic states deduced from the photocapacitance.

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CARRIER LOSS IN DISPERSIVE TRANSPORT

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In a variety of amorphous semiconductors carrier transport is seen to be dispersive, where the average mobility of injected carriers is a decreasing function of time over the large experimentally accessible time range. This dispersion is due to the nonequilibrium repopulation of carriers in a thermally wide distribution of localized states near the mobility edge. The time varying mobility of dispersive transport complicates the dynamics of carrier loss due to deep trapping or monomolecular recombination, and calls into question the simple deduction of $\mu\tau$ products from charge collection experiments. Here we show that the Hecht analysis of carrier loss is, in fact, valid in the presence of dispersive transport in an arbitrary shallow state distribution. A simple method is presented by which the form of the current transient in a photoconductivity or time-of-flight experiment can be calculated for the case of carrier loss from the case of no or less carrier loss. An approximate solution is given for transport in an exponential band tail.

REAL SPACE RENORMALIZATION FORMALISM FOR a-Si:H

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The electronic properties are studied for a-Si:H described by a tight binding Hamiltonian defined on a Bethe lattice. Each Si atom is represented by four sp^3 orbitals and the nearest neighbour interactions by six transfer matrix elements V_1 to V_6(1). The hydrogen is included saturating the four dangling bonds produced by a Si vacancy characterized by different matrix elements.

To calculate the local densities (LDS) of states the Dyson equations for the Green function are solved using a real space renormalization technique(2) which permits the study of the effect of a finite concentration of hydrogen taking into account compositional fluctuation at all orders.

The gap increases with H concentration. Interacting monohydrates(3) do not explain the three characteristic peaks seen in photoemission. Due to its simplicity this method can be easily extended in order to study ring statistics, the effects of other components in a a-Si:H etc.

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ELECTRON SPIN RESONANCE OF AMORPHOUS III-V-COMPOUNDS

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In this paper the first ESR-spectra of amorphous GaAs, GaP and InP are presented. For material obtained by rf-sputtering in Argon with varying admixture of hydrogen the dependence of the line parameters on hydrogen content and annealing has been studied. For hydrogen free samples resonances with a positive g-shift (g=2.01-2.07) and a linewidth ΔH_{pp}=300-650 G are obtained (line 1). With increasing hydrogen content C_H a second line reveals with a negative g-shift (g=1.93-1.98) and a smaller linewidth ΔH_{pp}=140-230 G; at high C_H this narrower line 2 predominates. For a-GaAs the transition from line 1 to line 2 with increasing C_H is connected with a shift of the Fermi level E_F from a position about 0.4 eV above E_v, the valence band mobility edge, nearer to midgap. Annealing of samples with high C_H-values and the resulting hydrogen evolution leads to the reverse process: a transition from line 2 to line 1 takes place and E_F moves back nearer to E_v. From variation of preparation conditions it can be concluded that the broad line 1 is due to defect states created by a surplus of chalcogen atoms, the narrower line 2, however, by a surplus of Ga or In. Since the multiplicity of the resonances characteristic for As- or P-antisites in crystalline material is not observed, line 1 is assigned to As or P dangling bonds, with a density of states distribution about in the midst between midgap and E_v. The narrower line 2, on the other hand, is attributed to Ga or In dangling bonds with a density of states distribution centered near midgap.

PHONON STRUCTURE OF AMORPHOUS GERMANIUM BY INELASTIC ELECTRON TUNNELING SPECTROSCOPY

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Knowledge of the vibrational density of states g(w) is a prerequisite for an adequate understanding of the properties of amorphous materials. Infrared, Raman and neutron spectroscopies give results for g(w) which differ through the details of the energy dependencies of the relevant matrix elements. In this paper we show that inelastic electron tunneling spectroscopy provides an alternative technique with which to investigate the structural and vibrational properties of the minute amounts of material which make up tunnel junction barriers.

Accurate measurements of inelastic electron tunneling through barriers of amorphous germanium are reported. The matrix element coupling vibrational states in the barrier to the tunneling electrons has been calculated using a bond model for the vibrational modes. This model includes nearest neighbor correlations and assumes that the disorder in the material is sufficient for the scattering of the electrons from different bonds to be uncorrelated. The calculated matrix element allows the determination of g(w) from the experimental measurements. The results show a broadened spectrum characteristic of highly disordered amorphous germanium. We conclude that the very thin films of amorphous germanium that form the barriers in the tunneling experiments contain a broader distribution of bond angle variations than the thicker films used in optical and neutron experiements.

It should be noted that the calculation for amorphous germanium may be directly applied to amorphous silicon.

This work established inelastic tunneling spectroscopy as a valuable technique for the study of the amorphous state. The method is of particular interest in view of the importance of thin films in semiconductor technology.

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PERSISTENT PHOTOCONDUCTIVITY

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Photoconductivity persists for long time periods beyond an illumination in many semiconductor materials at low temperatures,[1] whenever any of various physical mechanisms preclude recombination of the photo-generated carriers. Restoration of the original conductance requires thermal activation by raising the sample temperature. Persistent photoconductivity may be utilized to adjust the density of a two-dimensional electron gas,[2] to measure cumulative photon dose,[3] or to profile distributions of deep traps.[4] Reduction of device speeds, parasitic field effects, and complication of transport dynamics are some of the detrimental consequences of persistent photoconductivity.

Junctions, barriers, dopant and compositional fluctuations, clusters of radiation damage defects, and surfaces cause potential gradients, which have been demonstrated to lead to persistence through carrier pair separation in real space. An effective-medium theory is used to describe transport in such inhomogeneous samples. Quantitative interpretations of the build-up of the persisting enhanced conductivity have been achieved for well-defined configurations of Si and GaAs.[3] The densities of the carriers are usually enhanced within the potential minima, mobilities are generally increased by screening of the ionized impurities, and the geometries of conducting pathways may be severely altered by changes of adjacent space charge configurations.[3]

Many observations of persistence, especially in ternary alloy compound semiconductors, are interpreted by microscopic potentials.[5] Recombination is suppressed at defect level configurations having extremely large lattice relaxations after changes of the charge state, thus presenting a potential barrier against recapture of the liberated carrier. An alternative interpretation considers carrier separation in momentum space, when photons excite electrons from defect states associated with subsidiary conduction band minima.[6]

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THE TEMPERATURE AND ELECTRIC FIELD DEPENDENCE OF THE HOPPING CONDUCTIVITY IN A 2-D IMPURITY BAND

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Thermally assisted tunnelling (hopping) between localized states determines the low temperature conductivity of Na^+-induced impurity bands in silicon MOSFETs[1]. Two distinct regimes in the hopping transport can be discriminated. The observed temperature dependence of the conductivity in the range $1.30 < T < 4.2$ K is consistent with the formula for variable range hopping, $\ln(\sigma./\sigma_0) = -(T_0/T)^n$ where $n = 1/3$, σ_0 is a constant, and T_0 is a characteristic temperature depending on the reciprocal of the density of states. At higher temperatures $8 < T < 30$K, the conductivity is activated, and the activation energy is related to the width of the impurity band. Non-ohmic conduction has been observed in the hopping conductivity in the field range below 400V/cm for temperatures below 8K. In the variable range hopping regime the current is approximately exponentially dependent on the field in the range $20 < F < 200$ V/cm. For fields greater than 200V/cm the current is only weakly temperature dependent. In this paper we present the results of an extensive investigation of the dependence of the 2-D hopping conductivity on the electric field and temperature. A detailed comparison is given to a modification of Mott's theory for hopping conductivity in three dimensions as made Pollack and Reiss[2] which includes the effect of the field on the current for a two dimensional system.

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MoP-C3

TUNNELING STUDIES OF UNIAXIALLY STRESSED (001) Si INVERSION LAYERS

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Metal/SiO_2/p-Si tunnel junctions are prepared in a geometry similar to a field-effect transistor. Narrow slabs containing the junctions are bent upwards and downwards resulting in an uniaxial tension or compression in the surface layers[1]. The electron inversion layer of the MOS junction is created by a gate metal of a work function lower than the Si electron affinity. In this quasi two-dimensional space-charge layer the motion of the electrons perpendicular to the interface is quantized resulting in a sequence of surface subbands. Due to the small thickness of the thermally grown gate oxide tunneling occurs between subband and metal states. At low temperatures the tunneling characteristics dI/dV vs V and d^2I/dV^2 vs V show structures due to the cutoff of the density of states at the bottoms of the subbands. The corresponding biases reflect their energies relative to the semiconductor Fermi-level. Since on (001) Si the probability for tunneling into electron states of the lower ladder of twofold degenerate subbands E_n is considerably lower than of the higher fourfold degenerate subbands E_n' the corresponding structures can easily be distinguished[2]. When a compressive (or tensile) stress is applied in the [110] - direction we observe a shift of the primed ladder to lower (higher) energies relative to the unprimed ladder. Stress experiments in the [100]-direction give the expected splitting of the E_n' levels each into two levels. From the magnitude of the change in energy as a function of the applied stress we derive directly the shear deformation potential constant. The result is in accordance with values previously obtained from measurements in the volume[2].

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MoP-C4

TEMPERATURE AND MAGNETIC FIELD DEPENDENT THERMOELECTRIC POWER IN GaInAs-InP HETEROJUNCTIONS

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Measurements have been made of the thermo-electric power of the two dimensional electron gas in GaInAs-InP heterojunctions, as a function of temperature and magnetic field. At low temperatures (2K - 20K), the diagonal component of thermopower, α_{xx}, shows strong oscillations which are in phase with the Shubnikov-deHaas oscillations in the resistivity. The absolute magnitude of the thermopower is lower than the theoretically predicted value of $k \ln 2/(N + \frac{1}{2})e$ (1,2), and falls with increasing temperature, in contrast to theoretical predictions(3).

At higher temperatures the thermopower shows a very rapid increase as a function of temperature, in zero magnetic field. A power law behaviour is observed, with $\alpha \sim T^x$, with the power x lying in the range 3 - 5. The onset of this increase is sample dependent, and lies in the range 25K - 50K. The explanation of this rapid increase is the importance of phonon drag, which occurs due to the transfer of momentum from the thermal flow of phonons to the electron gas. Consideration of the elastic and inelastic phonon scattering rates, leads to the conclusion that the phonons with wavevector comparable with the size of the Fermi sphere, are under the rather unusual conditions necessary for the existence of Poiseuille flow. Simple arguements show that this causes a phonon-drag thermopower proportional to T^4.

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CAPACITIVELY COUPLED MEASUREMENTS OF THE MAGNETOCONDUCTIVITY TENSOR IN HETEROSTRUCTURES

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Using large area capacitors in place of ohmic contacts we have studied the Hall voltage and magnetoresistance of high mobility (10^5-10^6 cm^2/V-s) GaAs-$Ga_{1-x}Al_xAs$ heterostructures. Measurements were made at frequencies between 10 and 10^7 Hz and at temperatures between 1.0 and 4.2K.

We find that the vanishing capacitance of a two dimensional electron gas between Landau levels replaces the flats in the Hall voltage with minima. This structure is highly frequency dependent and this dependence may be due to changes in other properties of the two dimensional electron system along with the capacitance. In addition, this technique improves Landau level resolution. For example, we were able to observe spin splitting at 0.2 Tesla where the Landau level index was 30. When only the lowest Landau levels are filled we observe additional structure but the lack of flats in the Hall voltage make precise determination of fractional values difficult. Again, the shape and amplitude of this structure was highly frequency dependent.

Finally, we have observed that the weak field magnetoresistance of a two dimensional electron system is frequency dependent and deviates from the parabolic DC behavior reported previously[1].

Further work is planned at magnetic fields up to 29 Tesla and temperatures down to 0.5K to further identify the structure due to the fractional quantum Hall effect.

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Two-Dimensional
Electron Systems

MoP-C6

CYCLOTRON RESONANCE IN THE FRACTIONALLY QUANTIZED 2D ELECTRON GAS

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In a charge density wave or Wigner crystalline state of a 2D electron gas an upward shift of the cyclotron frequency, associated with pinning to a lattice bound potential, is expected [1]. Thus motivated we have attempted to probe the enigmatic fractionally quantized state[2] by concurrently measuring cyclotron resonance and magnetotransport of a highly mobile 2D electron gas in GaAs/(GaAl)As at $T \gtrsim 0.,4K$, $B \lesssim 200kG$ and Landau level filling $\nu \gtrsim 0.2$. The occurence of the fractionally quantized behavior in our sample is verified by the observation of a deep activated minimum in the conductance at $\nu = 1/3$ as well as weaker minima at 2/5, 3/5, 2/3 and 4/3. The cyclotron resonance was measured used fixed frequency radiation $(239\ cm)^{-1}$ from a CO_2 pumped gas laser, yielding a resonance field, H_C and width of roughly 190kG and 0.8kG respectively. The filling factor at resonance is varied using a transparent backside gate with which the 2D electron density can be adjusted between 1 and $2\times 10^{11}\ cm^{-2}$ (without leakage).

As the filling factor (density) is reduced from $\nu = 0.4$ to 0.2, H_C shifts upward by ~ 4kG at both $T \simeq 0.4K$ and 4K. This shift is roughly linear in ν and does not appear to be associated with the 1/3 state, which is seen only at the former temperature. We are thus left with a rather large depression of the cyclotron frequency with decreasing density which cannot be accounted for by band non-parabolicity (wrong sign). The possibility that this depression is associated with an enhancement of the LO phonon-2D electron coupling at low densities will be examined.

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17th International Conference on the Physics of Semiconductors

Two-Dimensional Electron Systems

MoP-C7

MAGNETO-OPTICS OF TWO-DIMENSIONAL EXCITONS IN GaAs-AlAs HETEROSTRUCTURES IN HIGH MAGNETIC FIELDS

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Magneto-absorption spectra of excitons were investigated in GaAs-AlAs superlattices in pulsed high magnetic fields up to 40 T. The GaAs-AlAs superlattices were grown with various quantum well widths L_z and barrier layer thicknesses L_d by molecular beam epitaxy. The magneto-optical spectra were measured at the top of the magnetic field pulse by using an optical multichannel analyser. In zero field, two well-defined absorption peaks were observed corresponding to the excitons associated with the heavy and the light hole bands. These peaks were observed even at room temperature owing to the large binding energies of the two-dimensional excitons. In high magnetic fields, the two exciton peaks showed a diamagnetic shift, the amount of which was much larger for the heavy hole exciton than for the light hole exciton due to the anisotropic nature of the Kohn-Luttinger Hamiltonian for an exciton. The energy shift caused by the magnetic field decreased for the heavy hole exciton with decreasing L_z because of the enhancement of the two-dimensional character. By extrapolating the photon energies of the many observed excited state peaks to zero field, the energy gap and thus the exciton binding energy E_B was obtained as a function of L_z. The L_z v.s. E_B curve appears to be the most accurate one among previously reported data, and it showed clearly the change of the character of the excitons from three-dimensional to two-dimensional with decreasing L_z. The linewidth of the absorption peaks was also investigated as a function of L_z and L_d.

17th International Conference on the Physics of Semiconductors
Two-Dimensional Electron Systems
MoP-C8

SUBBAND STRUCTURE AND MAGNETOTRANSPORT FOR ELECTRON LAYERS IN $\delta(z)$-DOPED, MBE-GROWN GaAs

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Samples have been grown in which a single layer of Si dopant atoms with areal densities $N_D = 1 - 6 \times 10^{12}$ cm^{-2} is incorporated into the lightly n-type GaAs crystal during growth. It appears that these dopant atoms remain as a sharply defined, δ-function layer embedded in the material and acting as a V-shaped potential well for a number of electrons $N_s \sim N_D$.

We have studied the conductivity and magnetoconductivity to identify the carrier density and mobility in the δ-layer. For densities N_D up to 6×10^{12} cm^{-2} the number of electrons grows linearly with dopant density. Samples with even greater N_D are currently being prepared. The carrier density N_s can be increased through illumination by an approximately constant ΔN_s. The low-temperature mobility for the carriers in the subbands of the δ-doped layer is $\sim$ 2800 cm^2/Vsec. This value rises for the higher lying subbands. Using Shubnikov-de Haas oscillations and cyclotron resonance we have examined the individual subband contributions to the electrical transport in the 2-D layer.

A calculation of the subband structure for a typical $N_s = 4 \times 10^{12}$ cm^{-2} shows 4 partially occupied bands, for which the $n = 0$ to $n = 1$ separation is $\sim$ 60 meV. We are engaged in measurements of the subband energies using an infrared grating spectrometer.

The δ-doped layer represents a novel example of a 2-D system, closely related to the grain boundary layer in Ge. The N_s densities in the layer are several times higher than those achieved at the modulation-doped interfaces.

One-Dimensional Systems **MoP-D1** **Invited**

PHOTOEXCITATIONS OF A 1D-SEMICONDUCTOR

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The polymer *trans*-polyacetylene, $(CH)_x$ is a particularly simple realization of a quasi-1D system with one electron per site. The combined effects of the Peierls instability and electron-electron repulsion give rise to a semiconducting material with a gap of $\sim$1.5 eV. Recently there has been a great deal of speculation concerning the nature of single-particle and electron-hole (e-h) pair excitations across this "Peierls-Hubbard" gap. Specifically, it has been proposed that a photogenerated e-h pair in $(CH)_x$ will create a pair of mobile defects. These defects are thought to be domain walls which separate the two degenerate ground state structures of $(CH)_x$. If they exist, such domain walls (or solitons) would constitute a type of carrier new to solid state physics. Experimentally we have looked for solitons using the techniques of photoinduced absorption and EPR. We create e-h pairs in $(CH)_x$ by excitation with above-gap photons and single e's (or h's) by photoionization of impurity levels. The new, metastable gap states which appear upon photoexcitation are detected by transient absorption and EPR spectroscopy. In this talk we compare the results of these experiments with theoretical predictions for soliton and polaron states in $(CH)_x$. Our results indicate that current framework for understanding excitations in $(CH)_x$ must be modified to include the dominant effects of electron-electron interaction.

TRANSPORT AND OPTICAL PROPERTIES OF FULLY ORIENTED NON-FIBROUS CRYSTALLINE $(CH)_x$

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All previous experimental investigations on transport and optical properties of polyacetylene,$(CH)_x$, were performed on fibrous samples, where the individual fibers were randomly oriented in space or poorly aligned by stretching the already prepared material. We succeeded in synthesizing almost perfectly oriented $(CH)_x$ by converting films of a prepolymer produced from bis-(trifluoromethyl)-tricyclo-deka-triene under applied stress to $(CH)_x$. X-ray and HEED-patterns obtained from these films allow to determine the direction of the carbon chains and to deduce high-quality structural data. We report on the optical transmission of these films for polarized light from the near UV to 400 cm^{-1}. Particularly dramatic polarization effects are observed in the vicinity of the optical gap of the undoped material and for the characteristic IR-active modes. Of peculiar interest is the polarization behavior of the IR-modes which develop upon doping with O_2, I_2, and AsF_5. In addition, our samples permit to obtain what we believe to be the first intrinsic data on the anisotropy of the conductivity of $(CH)_x$ not obscured by fibrous-morphology problems. Montgomery-type measurements on the undoped trans-$(CH)_x$ samples indicate a ratio of $\sigma_{\parallel}/\sigma_{\perp} = 40$. From the temperature dependence of the conductivity of the undoped material, if interpreted as an intrinsic semiconductor, a transport gap of 1.0 eV is deduced. These transport experiments are supplemented by measurements of the Hall effect and the conductivity as a function of temperature. The existing models for the transport in $(CH)_x$ are critically examined in view of these new data on non-fibrous crystalline material.

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One-Dimensional Systems **MoP-D3**

THE ELECTRONIC PHASE TRANSITION IN GRAPHITE UNDER STRONG MAGNETIC FIELD

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The magnetic field induced electronic phase transition [1] in graphite has been studied by galvanomagnetic measurements in fields of up to 280 kG and at temperatures down to 110 mK. The magnetic field dependence of the transition temperature can be expressed as $Tc(B)=T^*\exp(-B^*/B)$, where the values of the parameters T^* and B^* are approximately 100 K and 1000 kG, respectively. This functional form is consistent with Yoshioka and Fukuyama's model [2] of a charge density wave instability originating from the one-dimensional character of the Landau subbands in the extreme quantum limit, although the precise nature of the ordered phase is yet to be elucidated, because of a subtle competition between various kinds of possible instabilities inherent to this system.

The conductivity shows a sharp decrease at the transition, reflecting the development of a gap at the Fermi level. The detailed behavior of the conductivity shows considerable diversity among the samples investigated. Nevertheless, two distinctive types of behavior have been recognized. The differences between the two types of behavior are characterized by a small difference in the transition temperature at a given field and a difference in sharpness of the transition as observed by the change in conductivity. These differences are found to be correlated with the ionized impurity concentration which has been deduced from the high field Hall measurements. Some aspects of the differences in behavior of the conductivity in the ordered phase can be understood by taking account of the pair breaking effect of the impurities.

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ELECTRONIC BANDSTRUCTURE OF AN INCOMMENSURATE CRYSTAL

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The lattice translational symmetry of crystalline matter leads to the well known concepts of the Brillouin zones, Bloch electrons, phonons, and the like. In a crystal where the lattice is periodically distorted with a period that is incommensurate with the underlying lattice, this translational symmetry is broken. Nonetheless, an incommensurate crystal is perfectly ordered and as such it provides an intermediate case between periodic and amorphous materials.

In this paper we show how the superspace approach, introduced to describe the microscopic symmetries of incommensurate crystals,[1] provides a natural framework to understand their electronic bandstructure as well. The recovery of lattice translational symmetry leads again to a Bloch formalism (though now in a higher dimensional space) which can be used to solve a simple tightbinding model. The resulting predictions of new energy levels and their dependence on the modulation parameters are confirmed by optical absorption spectra in the bandgap region of the modulated crystal Rb_2ZnBr_4.

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MoP-D5

RESONANT RAMAN SCATTERING FROM AMPLITUDE MODES IN POLYACETYLENE

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The three resonantly enhanced Raman Vibrations in trans and cis isomer of polyacetylene are described in terms of amplitude modes associated with the 1D gap. The observed frequencies are determined by the dressed phonon propagator in the dimerized lattice; it contains an effective e-p coupling constant λ and the bare phonon frequencies in the undimerized lattice. This description differs considerably from previous models for the phonons in polyacetylene and can explain known as well as new experiments.

In the trans isomer the excitation energy dependence of the Raman line profiles can be accounted for by a distribution of the Peierls gap. A narrow distribution of λ and a resonant Raman cross-section with a 1-D type singularity at the gap, describe the observed spectra in detail[1]. The isotope shifts observed in the Raman frequencies of $(CD)_x$ compared to $(CH)_x$ can be properly explained only when the isotope shift in their bare frequencies are considered[2].

The phonon frequencies follow the Variations of the 1D gap with temperature and high pressure. When the temperature is lowered both the phonon frequencies and the 1D gap decrease. This can be explained by the decrease of λ at low temperature due to lattice contraction. All Raman line intensities decrease sharply at high pressure due to a reduction in the 1D singularity as a result of an increase in the 3D effects.

In cis polyacetylene the energy gap is determined also by an extrinsic non spontaneous mechanism. Using a modified relation between λ and the excitation energy in resonance, we found that the extrinsic part of the gap is about 10% of the full gap.

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LIGHT SCATTERING BY PLASMONS IN HEAVILY DOPED n-TYPE Ge AND Si

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The observation of light scattering by plasmons in n-Ge has been recently reported.[1] In the present paper we discuss the scattering mechanism. Two mechanisms are possible: The "charge density fluctuations mechanism" which involves carriers in extrema of the resonant gap and the Fröhlich forbidden quadrupole mechanism in which the carrier valleys need not be related to the resonant gap. It is shown that the observed scattering by plasmons resonates strongly at the E_1-$E_1+\Delta_1$ gaps in the manner expected for the Fröhlich quadrupole mechanism, a fact which suggests that this mechanism is dominant. This conjecture is confirmed by observations of plasmon scattering in n-Si resonant at the E_1 gap (3.4 eV). Such scattering cannot be due to the "charge density fluctuations mechanism" since the carriers do not occupy extrema involved in the E_1 gap. The absolute scattering intensities and the observed line shapes are compared with theoretical predictions based on the Lindhard-Mermin dielectric function generalized to a multivalley semiconductor. Effects of spatial dispersion and Landau damping are seen. Scattering by two plasmons has also been observed.

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THEORETICAL CALCULATION OF RESONANT TWO-PHONON RAMAN SCATTERING IN Si AND Ge

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Resonant two-phonon Raman scattering involves a virtual electron-hole pair (resonant with the laser photon) which subsequently emits two phonons in branches $\underset{\sim}{Q}_j$, $-\underset{\sim}{Q}_j$ and ultimately recombines emitting the Raman photon. Thus the resonant Raman spectrum contains a wealth of information on the coupling between electrons at the band edges and phonons of all branches and wavevectors. Precisely the same kind of information is needed for two other problems: The thermal self-energy shift of the band gap with temperature, and the renormalization of phonon energies by electron-hole pairs or doping. The first microscopic calculation is reported of all three components (Γ_1, Γ_{12}, $\Gamma_{25'}$) of the second-order Raman spectrum of Si and Ge, for incident photons resonant with the lowest direct gap. The integrated second-order intensities, divided by the integrated ($\Gamma_{25'}$) first-order intensity, are calculated to be (.08, .003, .005) and (.02 , .002, .006) for Si and Ge in (Γ_1, Γ_{12}, $\Gamma_{25'}$) channels at T = 0. The results agree reasonably well with available data, and lend support to a recent calculation of the temperature shift of the band gaps.[1]

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17th International Conference on the Physics of Semiconductors

One-Dimensional Systems MoP-D8

ELECTRONIC EXCITATIONS AND RESONANT LIGHT SCATTERING SPECTRA IN DOPED GaAs/$Al_xGa_{1-x}As$ SUPERLATTICES

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The present work theoretically explores the spectra of the resonant inelastic light scattering in modulation doped GaAs/$Al_xGa_{1-x}As$ superlattices. The dynamical susceptibility is introduced to describe the resonance-enhanced scattering spectra for both charge-density and spin-density excitations. It is calculated by taking into account the Coulomb interaction between carriers, the exchange-correlation effect, and the interaction with LO phonons, based on the subband structure calculated self-consistently.[1]

Explicit numerical calculations have been performed for polarized and depolarized backscattering spectra with photon energies near the E_0 and $E_0+\Delta_0$ optical gaps of GaAs. The computed lineshape, peak positions and relative intensities for the two-dimensional plasmon and the intersubband charge-density and spin-density excitations, is in excellent agreement with experimental results so far obtaind.[2] It is further demonstrated that the local field effect resulting from interlayer couplings gives rise to a strong anisotropy in the dispersion relatin for the two-dimensional plasmon and intersubband charge-density modes. The interlayer coupling is not so important for spin--density excitations. This anisotropy effect can be observed by a careful measurement of the scatteringle-angle dependence of the spectra.

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Symposium on Semiconductor Materials and Devices **TuA-A1** **Invited**

RECENT DEVELOPMENTS IN III-V COMPOUND SEMICONDUCTOR MATERIALS AND DEVICES

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The demand for smaller and faster electronic and optical devices has motivated many new advances in III-V semiconductor materials preparation techniques. Liquid phase epitaxy (LPE) has been used mostly for optical devices and chemical vapor deposition (CVD) has been used for microwave devices. Molecular beam epitaxy (MBE) and metalorganic chemical vapor deposition (MOCVD) are relatively new and have contributed to most of the recent new novel structures and devices.

The halide CVD process can produce the highest-purity GaAs while the hydride CVD offers flexibility in the growth of binary, ternary, and quaternary III-V materials. A recent advance in CVD is the introduction of a "double-barrel" reactor,[1] which permits the growth of two different compounds without interrupting the growth for purging the reactor. Interruption of growth between epitaxial layers would introduce interfacial defects.

MOCVD has the capability of growing quaternary III-V[2] as well as aluminum containing III-V compounds[3] which are less suitable for growth by the halide or hydride CVD process.

MBE is a very versatile crystal growth technique. Because of the ease of preparing various doping and compositional profiles with this technique, many novel structures and devices were first demonstrated with MBE. Exciting discoveries such as the quantized Hall effect and fractional quantum numbers were reported.[4,5] Graded band-gap superlattices resulting in artificial variation of the impact ionization ratios of electrons and holes have been demonstrated.[6] This kind of "band-gap engineering" opened a whole new window in the search for design freedom in new generation devices.

Heterostructure epitaxy has been largely limited to lattice matched systems. Recently, the strained layer superlattice (SLS) has permitted the growth of mismatched materials without misfit defects by MBE[7] and MOCVD.[8] Independently variable bandgap and lattice constants in $GaAs_xP_{1-x}$ SLS were demonstrated. $In_xGa_{1-x}As/GaAs$ field-effect transistors[9] and double heterostructure lasers[10] have all been prepared from SLSs. The unique properties of SLS's provide a new area of applications with the freedom to achieve heteroepitaxy.

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17th International Conference on the Physics of Semiconductors
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Invited

FRONTIEERS OF SILICON SINGLE CRYSTALS AND DEVICES
- ON THE BEHAVIOR OF MICRODEFECTS AND THEIR APPRICATIONS -

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A current revolution of LSI (Large Scale Integration) technology has been demanding highly controlled silicon crystals. Silicon wafers used for LSI devices are generally cut from a crystal grown by Czochralski method (CZ) using a quartz crucible. Most of residual impurities in the CZ Si crystal are oxygen and carbon, which are introduced during crystal growth as much as 10^{18} and 10^{16} atoms/cm^3, respectively.

Since oxygen is supersaturated in the wafer, many microdefects, such as oxide precipitates, dislocations and stacking faults, are induced by heat treatments, which are actually necessary for a LSI manufacturing process. When the microdefects are induced in the interior of the wafer, many beneficial effects for the device can be brought, because the microdefects act as gettering centers for harmful impurities and killer sites of excess minority carriers. For example, it is possible to suppress the pn junction leakage, dark current generation for charge coupled devices and soft error probability for memory devices. Microdefects induced in a device active region, on the other hand, are detrimental for LSI devices. Therefore, it is very important to control the microdefect distribution in the whole wafer in order to get a LSI with high reliability.

The microdefects originated from supersaturated oxygen and oxide precipitates are formed by a heterogeneous nucleation mechanism. It has been confirmed that nuclei of oxygen precipitates are formed at cites correlated with carbon atoms or point defects by thermal history during crystal growth. Moreover, the microdefect distribution in the wafer can be controlled by a selection of heat treatment sequence, that is high temperature or low temperature sequence, during LSI manufacturing process. Designing Si wafers throughout the crystal growth to the device process, therefore, is becoming a key technology in the LSI manufacturing process.

II-VI SEMICONDUCTOR MATERIALS AND DEVICES - RECENT PROGRESS

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The II-VI semiconductors offer a wide range of band gap energies from $\leq$ 0.02 eV to $\geq$ 4.0 eV. To date, because of limited electrical properties of the material, useful devices from II-VI's have been made only in the spectral regions where Si and III-V devices cannot provide the required band gap energy. Two major applications where II-VI's have been successfully used are infrared imaging (3000-10,000 nm) and visible light sources (400-650 nm).

A resurgence in II-VI materials research in the last five years has occurred due to: (i) the need to improve current II-VI devices and (ii) the hope that when the semiconductor technology developed for Si and GaAs is applied to II-VI materials, better and novel devices will result. In the '60's, the inability to control the electrical and optical properties of II-VI's was usually attributed to intrinsic point defects. However, the studies made recently in ZnSe, ZnTe and HgCdTe reveal a stronger role of the extrinsic impurities rather than that of the intrinsic defects. Determining the nature and identification of shallow acceptors and donors in the above materials was only possible in recent years due to improved growth of 'pure' II-VI materials. These growth techniques are liquid phase epitaxy, organometallic CVD, and molecular beam epitaxy. For example, in ZnSe grown by LPE, hydrogenic acceptors (e.g., Li, Na, N, and P) and deep acceptors, like Cu, Ag, and Au, have been identified optically. Shallow donors due to B, Al, Cl, F, and alkali interstitials have also been identified. The recent use of such measurement techniques as high-resolution excitation spectroscopy, electron microscopy, optically detected magnetic resonance, and EXAFS has been successful in revealing the chemical identification as well as symmetry of defects. Similar detailed studies have been completed in ZnTe and CdTe. Another result of recent studies is the conclusion that interaction of fast diffusing impurities with native defects and precipitates frequently dictates the optical and electrical properties of the material.

These recent advances in the material preparation and characterization methods have resulted in better devices, such as high-intensity CRT's, electron-beam-pumped visible lasers, thin-film electroluminescent panels, and photoconductive/photovoltaic HgCdTe detectors.

NEW TRANSPORT PHENOMENA AND HETEROJUNCTION DEVICES BY BAND-GAP ENGINEERING

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Appropriate combinations of heterojunctions, superlattice structures and graded-gap materials allow one to modify continuously and in a nearly arbitrary fashion the energy band-diagram of a semiconductor structure (band-gap engineering[1]). This permits to modify to an unprecedented degree the transport properties and to taylor them to a given device application.

Many novel phenomena and devices have emerged from band-gap engineering. These include:

a. Enhancement of electron impact ionization in superlattices and graded gap materials. New low noise avalanche detectors.

b. Staircase potentials. Solid-state photomultipliers and repeated velocity overshoot devices.

c. New electrical polarization phenomenon in sawtooth superlattices. Displacement current photodetectors.

d. Parabolic band-gap grading. Elimination of the emitter-collector offset voltage in wide gap emitter bipolar transistors.

e. High speed graded base phototransistors and high gain graded base transistors.

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LOW-POWER NON-LINEAR OPTICAL PHENOMENA IN n-i-p-i DOPING SUPERLATTICES

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Semiconductors with n-i-p-i doping superlattices form an interesting new class of synthetic materials. The tunability of their electronic structure and of the related properties has recently been demonstrated in samples using GaAs as host material[1,2]. In the present paper we discuss the consequences of two of these unique features for non-linear optical behavior. Absorption studies have demonstrated, that in the whole range of photon energies larger than the effective band gap of the n-i-p-i structure and less than that of the host material, the absorption coefficient changes strongly if the (tunable) band gap is varied[3]. The extremely long electron-hole recombination lifetimes, achievable in n-i-p-i crystals[2] allow for large densities of photo excited carriers and, associated with it, for large changes of the effective band gap, even at very low light intensities. Consequentely, the light-induced change of the absorption coefficient as a function of light intensity at some given photon frequency can be quite dramatic. This non-linearity extends over a wide range of photon frequencies and differs in its nature from previously reported non-linearities in bulk semiconductors[4] or multiple quantum well structures [5], where either band-filling or exciton screening led to an intensity dependence of the dielectric function. Apart from the possibility of low-power self-induced transparency, the changes of the refrective index, which result from the variation of the absorption coefficient, are particularly appealing. We illustrate this by the results of our calculations of the non-linear optical behavior of GaAs, InAs and PbTe doping superlattices in Fabry-Perot interfrometers. It is found that large changes in the optical path length, in fact, can be achieved at modest power level, leading to optical bi- or multi-stability. Possible device applications are outlined.

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17th International Conference on the Physics of Semiconductors
Surface Electronic Structure TuA-B1 Invited

THE ELECTRONIC STRUCTURE OF POLAR GaAs SURFACES

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Of the four lowest index faces of GaAs, only one, the (110) surface, is non-polar, the (100), (111) and $(\bar{1}\bar{1}\bar{1})$ faces all being polar. A considerable amount of work, both experimental and theoretical, has been done on the (110) cleavage surface, and its surface properties seem to be fairly well understood. The three polar surfaces which will be discussed here, however, have only been examined in detail relatively recently.

Atomically smooth surfaces of the polar faces can be obtained with molecular beam epitaxy techniques and, in the case of GaAs(111), also with sputtering and annealing. As a direct consequence of the polar nature of these faces, the surface could, in principle, be a complete layer of Ga, a complete layer of As, or a partially filled layer of either species. Which of these alternatives occurs in a particular case would depend on the way in which the epitxial growth was terminated. Several stable structures have been found and are identified by their reconstruction. For GaAs(100) these are: c(4x4), c(2x8), c(8x2), (1x6) and (4x6). Both GaAs(111) and GaAs$(\bar{1}\bar{1}\bar{1})$ reconstruct with a (2x2) periodicity, with GaAs$(\bar{1}\bar{1}\bar{1})$ having, in addition, a $(\sqrt{19}x\sqrt{19})R23.4$ reconstruction.

Having available such a variety of reconstructions and thus of atomic arrangements in one compound, makes an examination of the electronic properties of these surfaces very interesting. A summary will be given of the experimentally known facts about the (100), (111) and $(\bar{1}\bar{1}\bar{1})$ surfaces of GaAs. In particular, angle-resolved photoemission measurements have been carried out on all three surfaces and the surface state dispersions which have been obtained will be compared. The photoemission experiment probes several atomic layers and influence of the surface reconstruction on the bulk-like states near the surface will also be discussed.

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ELECTRONIC STATES ON Si(100) AND Si/Ge(100) ALLOY SURFACES

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High Resolution Electron Energy Loss Spectroscopy (HREELS) has been used to investigate the unoccupied surface states on both Si(100) and Si/Ge alloy (100) surfaces. These surfaces reconstruct to form surface dimers across the total range of concentration. The unoccupied "anti-bonding" states associated with these dimers are found to have a minimum near the Γ point at about 0.3eV above the valence band maximum. The observation of this mimima at the Γ point, rather than at the edge of the Broullion zone, is significant in that it shows that the reconstruction of the surface actually involves larger unit cells than the simple (2x1) structure generally observed with LEED. Present evidence indicates that the Fermi level is pinned at the clean surface by the "anti-bonding" states associated with the surface dimers. Additional transitions are observed that are attributable to the occupied dimer states.

INVERSE PHOTOEMISSION AT SEMICONDUCTOR SURFACES

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Inverse photoemission is used as a probe for unoccupied electronic states. We have made the first observation of unoccupied surface states on silicon and have studied their dependence on crystallographic orientation. Critical points of the conduction bands of bulk silicon have been determined, e.g., L_1 at 2.2 eV above the valence band maximum.

For various silicide surfaces (e.g., Pd_2Si grown on Si(111)) we have studied the density of antibonding metal/silicon states which was not accessible to other techniques.

New high-resolution data from cleaved GaP(110) surfaces show a surface state located near the conduction band minimum. Various critical points can be derived within 6 eV above the conduction band minimum.

Surface Electronic Structure **TuA-B4** **Invited**

ATOMIC STRUCTURES AND ELECTRONIC PROPERTIES OF Ge(111) CLEAVED SURFACES AT LOW TEMPERATURES

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The Ge(111) cleaved surfaces have been investigated at about 10^{-10} Torr in the range 10–300 K. It is found by the LEED that the atomic structure of the cleaved surface depends essentially on the cleavage temperature, T_{cl}. At $T_{cl} \lesssim 40$ K one may observe a Ge(111) – 1x1 pattern, at $T_{cl} \gtrsim 60$ K a Ge(111) – – 2x1 LEED pattern is always observed. The temperature changes of the sample (after it has been cleaved) in the range 10–300 K does not effect the surface structure.

The conductivity measurements for Ge(111) – 1x1 and Ge(111) – – 2x1 surfaces are carried out too. Strong correlation between the values of the conductivity and the atomic structure is observed.

The results obtained by different authors on the atomic structure and the Ge(111) "surface" condusctivity are discussed. It is shown that a Ge(111) – 2x1 surface possesses high "surface" conductivity due to a spontaneous p-channel occuring at the cleaved surface. It is pointed out that these p-channels demonstrate some characteristic features of 2D systems.

Some possible models for Ge(111) – 2x1 and Ge(111) – 1x1 surfaces are briefly discussed.

ON THE TEMPERATURE COEFFICIENT OF THE IONIZATION ENERGY IN III-V COMPOUND SEMICONDUCTORS

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The work function $\Phi = E_{vac} - E_F$ of clean (110) surfaces cleaved from p- and n-type InP single crystals was measured in the range from room temperature up to 360 ^{o}C by using the Kelvin technique. At room temperature the work function varies by less than 50 meV on p- but by up to 250 meV on n-type samples. However, the largest differences of the work functions almost equal the band-gap energy minus the sum of the distances between the Fermi level to the nearest band edge in the bulk, i.e. $\Phi_p - \Phi_n = E_g - (E_F - E_{vb})_p - (E_{cb} - E_F)_n$. Thus, at such spots the bands are flat up to the surface for both n- and p-type samples. With increasing temperature the work function of n-type InP increases to almost the same extend as the band gap shrinks while for the samples used the Fermi level remains close to the conduction-band bottom in the temperature range investigated. Thus, the ionization energy $I = E_{vac}-E_{vs}$ is almost independent of temperature while the electron affinity $\chi = E_{vac}-E_{cs}$ varies with temperature as the band gap. The same result has been obtained with cleaved surfaces on p-GaAs. The small temperature coefficient of the ionization energy is quantitatively explained by considering the contributions of the Debye-Waller effect, the hydrostatic shift, the electron self-energy, and the V_{000} form-factor to the temperature coefficient of the valence-band top. These results are in good agreement with the temperature coefficient of the valence-band top as evaluated from measured energy shifts of transitions from core-levels into conduction-band states [1,2] and variations of the band-gap energy as a function of temperature [1,3]. In contrast to earlier conclusions [4], these results show that - at least for the semiconductors considered here - the bottom of the conduction band is much more sensitive to changes in temperature than the valence-band top.

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Surface Electronic Structure **TuA-B6**

THEORETICAL STUDY OF STACKING FAULTS IN SILICON

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The _ab initio_ pseudopotential method within the local density functional formalism is applied to study the stacking faults along the <111> direction in silicon. The total energies of the perfect crystal and of the crystal with stacking faults are compared. For the first time, a first principle calculation is used to obtain the stacking fault energy. This energy is extremely small since there is no bond-breaking mechanism involved. A supercell method is used to maintain the periodicity of the crystal. The one-particle equation is solved self-consistently using a plane wave basis set with the exchange-correlation functional approximated by the Ceperly-Alder formula. The calculated stacking fault energy is in reasonable agreement with the observed values.[1,2] The relaxation of the atoms near the faults is studied by using the Hellmann-Feynman theorem to calculate the forces. A recent charge collection scanning electron microscopy experiment on an extrinsic stacking fault in n-type silicon has suggested the existence of defect states with energies about 0.1 eV below the conduction band minimum.[3] Photoluminescence spectra of plastically deformed silicon suggested a stacking fault state near 0.15 eV above the valence band maximum.[4] The possible existence of these defect states in the gap region is examined and their energies are evaluated.

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ELECTRON-PHONON AND CORRELATION EFFECTS AT SILICON SURFACES

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We have analyzed the effects that both electron-phonon and electron-electron interactions create at Si surfaces for metal-like dangling bonds surface states. The system is described by a Hamiltonian which includes an intrasite Coulomb interaction U between electrons and a term giving the coupling of electrons to localized phonons with constant frequency. The Hamiltonian is solved by introducing in two successive steps the electronic part and the electron-phonon interaction. In both cases we use an adequate self-energy built up by means of an interpolation procedure between the two known limits of coupling much smaller/higher than the band width [1].

For very low temperatures we get:
(i) A very narrow Kondo-like peak (7 meV) at the Fermi level E_F.
(ii) Two rather broad peaks ($\sim$ 0.25 eV) at 0.75 eV above and below E_F.
(iii) Two features 0.2 eV above and below E_F which are clearly phonon satellites.

All these features are in satisfactory agreement with recent photoemission and energy loss experimental information [2]. That agreement is reinforced by the behaviour of this spectrum with increasing temperature. So for room temperature our results show that:
(i) The narrow peak at E_F disappears.
(ii) The peaks at 0.75 eV from E_F are further broadened by the temperature.
(iii) Phonon satellites are significantly broadened.

Our conclusion is that electron-phonon coupling becomes very important for the narrow peaks produced by electron-electron interaction, so that both effects are complementary and very important to understand the electronic structure of semiconductor surfaces.

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17th International Conference on the Physics of Semiconductors

Transport in Two-Dimensional Electron Systems **TuA-C1**

LOW-TEMPERATURE MAGNETOTRANSPORT IN InAs-GaSb QUANTUM WELLS*

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We report measurements of the magnetoresistance ρ_{xx} and Hall resistance ρ_{xy} in GaSb-InAs-GaSb heterostructures at magnetic fields up to 28T and temperatures as low as 0.005K. In addition to the quantized Hall effect, samples with high mobilities exhibited extraordinary structures which, because of their anomalous temperature dependence, cannot be accounted for in the framework of fractional quantization present in a one-carrier system (electrons or holes). These new features are attributed to the uniqueness of the InAs-GaSb system, where two-dimensional electrons and holes coexist.

The heterostructures consisted of a thin InAs layer sandwiched between two thick layers of GaSb, grown by molecular beam epitaxy on insulating substrates. Because the top of the valence band of InAs lies lower in energy than the bottom of the valence band of GaSb, electrons transfer naturally to the former from the latter where holes are generated. As this process is intrinsic, without the need of external doping, high mobilities are achievable, and the amount of charge transferred can be controlled by varying the InAs thickness L. For this work, L ranged from 70 to 200Å, corresponding to carrier concentrations between 4×10^{11} and $9\times10^{11}cm^{-2}$. The highest mobility at 4.2K was $2.1\times10^{5}cm^{2}/Vs$.

Samples with $L < 100Å$, for which the mobility was moderately low ($\leq 7\times10^{4}cm^{2}/Vs$) showed well-defined plateaus at values $h/\nu e^{2}$, with $\nu = 1,2,3$...corresponding to the number of filled magnetic levels, accompanied by wide regions of vanishing resistance with peaks between them. On the other hand, high mobility samples ($L \geq 150Å$) exhibited additional structures in ρ_{xx} whose magnetic field position and amplitude were temperature dependent. These structures gave rise to additional features in ρ_{xy}, sometimes even well-defined plateaus for non-integers values of $\nu > 1$.

The magnetic field dependence was particularly strong for the peaks occurring at high fields, where a down-shift of over 2T in the temperature range 2-0.56K was observed. With decreasing temperature the amplitude of these extra peaks decreased much faster than the regular ones, attributed to electrons, and finally disappeared completely for temperatures below 0.02K. The origin of these extraordinary structures appears to be exotic electron dynamics arising from the magnetic field-enhanced and temperature-activated interaction with the coexisting two-dimensional holes in GaSb.

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Transport in Two-Dimensional Electron Systems

TuA-C2

SELF-CONSISTENT SCREENING IN A HETEROJUNCTION IN STRONG MAGNETIC FIELDS

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In the two-dimensional system in strong magnetic fields, the screening of scattering potentials and the level broadening of Landau levels are mutuallly correlated and must be determined in a self-consistent way.[1] In this paper various transport quantities are determined theoretically in GaAs/$Al_xGa_{1-x}As$ heterojunctions in strong magnetic fields. Explicit numerical caluculatios are performed for scattering from remote donor ions in the $Al_xGa_{1-x}As$ layer.

The peak values of the diagonal conductivity, σ_{xx}, are shown to be almost independent of the Landau-level index in contrast to the case of Si inversion layers. This reflects the long-range nature of the scatterers and agrees with experimental results.[2] The broadening of the cyclotron resonance exhibits a strong oscillatory behavior as a function of the electron concentration[3] although its amplitude is much smaller than that of the level width itself. It is demonstrated that the level width is a strong function of the spacer thichness d_s and exhibits a drastic decrease when d_s is increased. This effect occurs around $d_s \sim 100$Å for the lowest Landau level and at somewhat larger d_s for higher Landau levels. This shows that in strong magnetic fields impurity potentials are dominated by mutual Coulomb interactions in heterojunctions having very high qualities.

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17th International Conference on the Physics of Semiconductors
Transport in Two-Dimensional Electron Systems TuA-C3

QUANTUM HOT ELECTRON EFFECTS IN LOW DIMENSIONAL STRUCTURES

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For electrons in the lowest sub-band of a quantum well the energy-relaxation rate remains constant with energy (deformation potential scattering in 2D) or reduces with energy (all other cases). As a result runaway effects are predicted at electric fields above a critical magnitude, and runaway will be contained only by scattering into other sub-bands, whether belonging to the same conduction valley or not. Corresponding jumps in the current are predicted.

Because of the abrupt optical-phonon emission threshold in a given sub-band, there is a tendency for a negative differential resistance (n.d.r.) to occur. Whether it does so or not appears to be dependent upon the intensity of electron-electron scattering. Too little of the latter allows the hot electrons to stream, without exhibiting n.d.r., too much effectively softens the emission threshold and destroys the n.d.r. It is possible to describe the situation by a simple model which applies in the field regime below runaway. At best, only a weak n.d.r. is predicted.

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HOT ELECTRON INJECTION IN DOUBLE-LAYERED HETEROSTRUCTURES

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We have studied the new effect of real-space electron transfer between two conducting layers in semiconductor heterostructures. The charge injection occurs due to heating of electrons in one of the layers separated from the other layer by a potential barrier and contacted separately. The hot-electron layer was realized as a high mobility two-dimensional channel at a modulation doped $GaAs/Al_{0.3}Ga_{0.7}As$ interface. The second conducting layer (heavily doped n^+ GaAs substrate) was isolated from the channel by an undoped graded $Al_xGa_{1-x}As$ barrier of thickness ~1500 Å.

The effect of hot electron injection was studied at 300, 77 and 4.2K at different electric (E) and magnetic (B) fields. From the measured magnitude of the injection current we were able to determine the electron temperature in the channel which was found to be proportional to the square of the heating field E and to decrease markedly with B. The real space transfer occurs at the rate of several kA/cm^2 and gives rise to a pronounced negative differential conductivity in the channel. The dependence of the electron heating on the substrate voltage is strong and nonmonotonic, giving rise to a dramatic negative differential resistance in the substrate circuit. At low temperatures (77, 4.2K) and in a certain range of applied voltages we observed an anomalous behaviour of the injection current corresponding to an absolute negative conduction in the substrate circuit. This effect is attributed to the development of a thermoelectric force of hot electrons.

The hot-electron injection physics discussed in this work underlies the operation of new devices proposed [1] and realized experimentally: a gate controlled microwave generator [2,3] and a charge injection transistor [4].

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17th International Conference on the Physics of Semiconductors

Transport in Two-Dimensional Electron Systems **TuA-C5** **Invited**

Transport in Two-Dimensional Electron System in the GaAs/AlGaAs Heterostructures

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One of the key features of GaAs/AlGaAs heterostructures is the capability of preparing the quantum potential $V(z)$ of nearly arbitrary profiles, by which the wavefunction of electron $\varphi(z)$ can be artificially controlled (Wave-function Engineering). By varying the thickness Lz of quantum wells from 50 A to 500 A, we have generated a variety of electronic states, spanning from the tightly-bound limit of two-dimensional electron gas to the bulk limit via the sophisticated case of multi-subband conductions. We describe our work to evidence such a transition of electronic states by investigating the anisotropy of Shubnikov de Haas effect. We discuss also the interaction of electrons with a periodic (superlattice) potential. By adjusting the doping level of a superlattice, we vary the wavenumber $\langle kz \rangle$ of electrons normal to the layer, and demonstrate the onset of Bragg reflection (or the minigap formation) as soon as $\langle kz \rangle$ reaches the minizone edge.

Despite the very attractive feature of achieving extremely high-electron mobility μ, selectively-doped N-AlGaAs/GaAs single heterojunction has an intrinsic limitation in that the maximum electron concentration that can be stored is rather low. This is very detrimental especially for FET applications. We have shown that such a difficulty can be solved by using double heterostructures DH, if the quality of notorious "inverted heterojunction" can be improved. Recently, we have succeeded in growing very high quality DH strctures having a very-high mobility ($\sim 2 \times 10^5$ cm^2/Vs) and a high carrier concentration (1.3×10^{12} cm^{-2}) at the same time. We discuss properties of such DH structures, including FET performances, electronic structures and wavefunctions, and a novel mean to assess relative qualities of two heterointerfaces.

Transport in Two-Dimensional Electron Systems **TuA-C6**

SURFACE-IRREGULARITY-ENHANCED DISSIPATION IN SEMICONDUCTOR TWO-DIMENSIONAL ELECTRON GAS DEVICES

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In a metal-insulator-semiconductor field effect transistor (MISFET), selectively-doped heterostructure transistor (SDHT), or modulation-doped superlattice transistor, the carrier transport due to interfacial irregularities — surface roughness and/or impurities — is an important and interesting problem. Extensive theoretic efforts have been made to calculate the scattering rate on the charge carriers — electrons or holes — by the surface roughness.[1-3] However, the possible additional forces due to the surface modes of the electromagnetic fields induced by these interfacial irregularities have never been investigated. In a recent investigation,[4,5] the effects on the optical infrared intersubband absorptions were calculated to explain the new experimental phenomena in MIS inversion or accumulation layer systems. In this paper, the enhanced power absorption of the two-dimensional electron gas due to these induced surface electromagnetic fields in a MISFET, SDHT, or modulation-doped superlattice transistor system is calculated and analyzed. Using simple models similar to that in Refs. 4 and 5, effective susceptibilities for intra- and intersubband transitions at different electronic population distributions — single and multiple subband occupations — are calculated to show the qualitative and quantitative characteristics.

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INELASTIC SCATTERING AND SPIN-ORBIT SCATTERING IN 2D SYSTEMS OF GaAs/AlGaAs HETEROSTRUCTURES

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Two-dimensional (2D) system in GaAs/AlGaAs heterojunction interfaces is the best material to test theoretical results in quantum corrections to the conductivity and the magnetoresistance due to localiztion and interaction effect. We report results of analysis of anomalous magnetoresistance in 2D systems of GaAs/AlGaAs interfaces measured in magnetic fields B up to 0.02T applied normal to the interface and at temperatures T between 40 mK and 6.5K. Our samples are modulation doped heterostructures grown by molecular beam epitaxy. Electron concentration and mobility are $1.8\times10^{11}/cm^2$ and 18000 $cm^2/V\cdot s$ in samples #1 and $4.4\times10^{11}/cm^2$ and 68000 $cm^2/V\cdot s$ in sample #2, respectively.
At $T > 1K$, magnetoresistance is negative. As reported[1], the negative magnetoresistance cannot be reproducted by Hikami, Larkin and Nagaoka's theory [2] except at low field region ($B<0.002T$). However, a theory developed by Kawabata[3] can be fitted to experimental data by adjusting only inealstic scattering time τ_ε in the whole region of B used. This fact shows that the interaction constant (g_2-2g_4) is very small as shown recently by Isawa and Fukuyama's theory[4].
The inelastic scattering time extracted from experiments by Kawabata's theory is about 1.5 times that by Hikami et al's theory. The exponenet in $\tau_\varepsilon \propto T^{-p}$ depends on sample and T. In the sample #1, p is 1.3 between 1K and 3.5K, and 2 at $T > 3.5K$. In the sample #2, p is about 2 at $T > 0.6K$ and less than 0.5 at $T < 0.6K$. Magnitude of τ_ε in the temperature region with $p \approx 2$ is about 0.3 times that predicted by Fukuyama and Abrahams's theory[5] for pure 2D metal limit. The exponenet $p = 1.3$ is explained by FA theory[5] for dirty limit and by Altshuler, Aronov and Khmelnitzky's theory[6]. In the magninude, FA's result gives smaller values and AAK's result gives larger values than experimental values.
In the sample #2 at $T < 1K$, we observed small positive magnetoresistance in a very low field region of B lower than 0.0003T. When we assume spin-orbit scattering, the magnetoresistance in low field region ($B<0.002T$) is well reproduce by Maekawa and Fukuyama's theory[7]. we obtain best results for the spin-orbit scattering time $\tau(so,z) \approx 1\times10^{-10}s$ which is nearly independent of T and $\tau(so,z)/\tau(so,x,y) \approx 0.1$. Here we obtain $\tau_\varepsilon = 1\times10^{-10}T^{-2}s$ at $T > 0.6K$ and $\tau_\varepsilon \approx 4\times10^{-10}T^{-0.25}s$ at $T < 0.6K$.

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Transport in Two-Dimensional Electron Systems TuA-C8

MAGNETOTUNNELING AND MAGNETIC FREEZEOUT IN n^-GaAs–UNDOPED $Al_xGa_{1-x}As$–n^+GaAs CAPACITORS

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We have recently shown that undoped $Al_xGa_{1-x}As$ is a nearly ideal dielectric in n^-GaAs–undoped $Al_xGa_{1-x}As$–n^+GaAs capacitors.(1) Capacitance-voltage (C–V) characteristics are closely fit by the theory of ideal semiconductor–insulator–semiconductor structures. For low voltages and for temperatures between 100 K and 300 K, I–V characteristics are determined by thermionic emission over the barrier at the $Al_xGa_{1-x}As$–GaAs interface. At low temperatures and higher voltages, tunneling is the dominant conduction mechanism; resonant Fowler–Nordheim tunneling is observed at 4.2 K in samples with $Al_xGa_{1-x}As$ thicknesses of 30–35 nm.(1) We find that direct tunneling occurs in samples with $Al_xGa_{1-x}As$ thickness of ~20 nm.

We have observed a remarkable periodic structure in the current–voltage curves of n^-GaAs–undoped $Al_xGa_{1-x}As$–n^+GaAs capacitors at 1.6 K in the presence of high magnetic fields. Current flow in the capacitor is due to direct electron tunneling from n^+GaAs through $Al_xGa_{1-x}As$ into n^-GaAs. The periodic structure is seen only for magnetic fields high enough ($B>4$ T) that magnetic freezeout of carriers in the n^-GaAs occurs. C–V curves are shown to provide a useful method to measure magnetic freezeout in GaAs. Contrary to the usual observations of magnetoconduction or magnetophonon effects in semiconductors, neither the voltage spacing nor the phase of the observed oscillations depends on the magnitude of the magnetic field. The voltage periodicity is 0.036 V, independent of orientation of magnetic field. Sixteen periods are observed for magnetic field perpendicular to the sample; twenty eight periods are observed for magnetic field parallel to the sample. The mechanism appears to involve sequential LO phonon emission events by ballistic electrons. This is the first example of sequential single-phonon emission observed in electron transport.

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Excitons and Polarons **TuA-D1**

CORE-EXCITONS IN Si_xGe_{1-x} ALLOYS

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We have examined the Si $L_{2,3}$ absorption edge as a function of changing chemical environment in a series of Si_xGe_{1-x} alloys as well as the compound SiC. Of primary interest is the shape of the absorption edge as a function of photon energy, and the comparison of the Si $L_{2,3}$ edge in the alloy with the well-known Si $L_{2,3}$ edge in pure Si.[1] Also of interest is the "chemical shift" of the threshold energy, which was measured to be a 99.7 eV for pure Si, 100.3 eV for the $Si_{.1}Ge_{.9}$, and 101.7 eV for SiC.

We find there to be a strong "enhancement" or increase in the absorption coefficient at threshold, for the Si_xGe_{1-x} alloy samples with compositions x near 0.2. Si_xGe_{1-x} alloys exhibit a crossover in the conduction-band minimum of from L, in Ge, to near X, in pure Si. The observed absorption enhancement occurs at compositions x near this crossover point. We have observed the enhancement in a number of samples, using both transmission and electron-yield techniques.

We hypothesize that the edge enhancement is due to transitions to localized excitonic states that have dropped into the band gap near the L-X crossover point, x ~ 0.2. Our experimental results are consistent with a transition from shallow, effective-mass-like excitons[2] (for low Si concentrations), to deep, localized core excitons for compositions near the L-X crossing[3], and back to shallow excitons (for higher Si concentrations).

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EVIDENCE FOR DISORDER-ENHANCED CORE EXCITONS IN AMORPHOUS SEMICONDUCTORS

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We investigated by photoemission techniques the Si2p absorption edges for core-to-conduction band transitions in crystalline Si (c-Si) and amorphous Si and Si-C alloys (a-Si, a-Si:H and a-$Si_{0.5}C_{0.5}$:H). In particular, we measured for all these materials the "photoemission gap" defined as the difference between the position in energy of the Si2p edge given by partial-yield spectroscopy and the Si2p binding energy with respect to the top of the valence band deduced from photoemission energy distribution curves. For each material we found a "photoemission gap" much smaller than the corresponding measured optical gap. In particular, the "photoemission gaps" were 1.0 eV for c-Si, 0.6 eV for a-Si, 0.8 eV for a-Si:H and 0.35 eV for a-$Si_{0.5}C_{0.5}$:H, while the corresponding optical gaps were 1.12 eV, 1.26 eV, 1.75 eV and 2.2 eV. The discrepancy between "photoemission gaps" and optical gaps cannot be explained in terms of one-electron transitions to localized states inside the gap. Furthermore, its magnitude appears directly related to the degree of disorder of the material. For c-Si the discrepancy is close to the core-excitonic binding energies reported by several authors. The large discrepancies found for the amorphous samples can be explained by a disorder-induced enhancement of the core-exciton binding energy, which in turn is due to a reduction of the screening effects affecting the optical excitation process. In fact, due to the disorder-induced localization of the states at the bottom of the conduction band, the excited electron has most of its charge very close to the hole it leaves behind. We shall discuss the important consequences of the above observations on the general problem of core excitons in semiconductors.

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Al 2p CORE EXCITON IN AlSb

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We have investigated using synchrotron radiation angle-integrated photoemission and high-resolution photoyield from polycrystalline and cleaved AlSb (110). At the Sb 4d threshold we observe only structures due to the conduction band density of states and no pronounced excitonic effects. In contrast the Al 2p threshold exhibits a sharp and intense doublet separated by 0.39 eV. These peaks are found to be insensitive to contamination and are therefore likely due to bulk excitons connected with the lowest conduction band in AlSb. The intensity ratio of the two components is 1:1 and deviates thus considerably from the statistical ratio 2:1 expected in the limit of j-j coupling. We attribute this deviation to a strong exchange interaction between core hole and excited electron. From the measured intensity ratio we obtain an exchange energy of 0.133 eV. The same mechanism reduces the separation of the two exciton components from the spin-orbit splitting of the Al 2p core level (0.41 eV [1]) by 6% to 0.39 eV as measured. The systematics of this effect in Al, Si, and P is discussed.

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PHYSICAL PROPERTIES OF Sm_3S_4: A NEW EXCITONIC STATE

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Sm_3S_4 is a semiconductor which crystallizes in the Th_3P_4 structure. The compound can be considered as being composed of SmS and Sm_2S_3 with divalent and trivalent Sm ions in the ratio one to two. Both ions occupy crystallographically equivalent lattice sites. The compound is thus similar to Fe_3O_4 or Eu_3S_4, where a thermally stimulated hopping process of electrons occurs between ions of different valency. For these compounds a so called charge ordering is expected at a critical temperature, associated with a lattice distortion. For Fe_3O_4 this is the Verwey transition at 119 K and in Eu_3S_4 the transition is at 186 K . In Sm_3S_4 no such transition has been observed so far .

We have investigated the solid solution system Sm_2S_3 - $Sm_{3-x}\square_xS_4$-Sm_3S_4 (where $\square$ denotes a vacancy in the Sm sublattice) which crystallizes in the same structure. The lattice constant exhibits a sudden increase from 8.516 Å to 8.545 Å near stoichiometric Sm_3S_4 . On single crystals of stoichiometric Sm_3S_4 we looked for structural changes down to 4 K and found none (Weissenberg camera). With a capacitance method capable of measuring length changes of 10^{-10} cm we investigated the thermal expansion down to 4 K and observed no anomaly. We thus conclude that there is neither a first nor a second order crystallographic transition related to charge ordering in Sm_3S_4.

The electronic structure of Sm_3S_4 is well known from optical measurements. The Sm^{2+} $4f^6$ ($^7F_0$) state is a few tenth of eV below the 5d conduction band and the Sm^{3+} $4f^5$ ($^6H_{5/2}$) state is about 6 eV below the conduction band. The Raman spectrum at 10 K is dominated by phonons below 300 cm^{-1} and electronic transitions within the ^7F_J multiplet above 294 cm^{-1}. In function of sample stoichiometry the above measurements show only minor variations.

The magnetic susceptibility is a sum of Sm^{2+} and Sm^{3+} contributions, the latter being subject to crystal field splitting, a Γ_7 doublet being lowest in energy. As function of composition the susceptibility changes by about 30% near stoichiometric samples in the sense that samples with a small lattice constant (8.516 Å) have a significant smaller Sm^{2+} and a larger Sm^{3+} contribution.

We propose that the lattice at the stoichiometric composition is instable against a contraction where a gain in lattice energy is compensated with an electronic excitation $4f^6 \rightarrow 4f^5 5d$ in an excitonic orbit for about 30% of the Sm^{2+} ions. This has to be demanded because the materials remain semiconductors, the radius of the $4f^5 5d$ configuration is mainly the one of the Sm^{3+} ion and the susceptibility of the $4f^5 5d$ state corresponds to a $^7K_4$ state. In contrast to usual excitons the 5d electron and the $4f^5$ "hole" state have parallel spins.

TuA-D5

K-DEPENDENT SPLITTING OF THE UPPER EXCITON POLARITON OF CuCl IN HIGH MAGNETIC FIELDS

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Nonlinear optics is a powerful tool to study the polariton structure of dipole allowed excitons. Contrary to linear absorption spectroscopy, where only the frequency ω of the absorbed photons is varied, one has in nonlinear optical spectroscopy the possibility to choose ω and the wave-number K of the driving photon field independently of each other. Sharp resonances are detected whenever the photons are coupled by nonlinear interaction to match the $\omega(K)$ dispersion of the polaritons in the crystal. By two-photon absorption (TPA) and sum frequency generation (SFG) we are able to resolve sharp resonances on the upper polariton and the longitudinal exciton branches of CuCl. Applying a magnetic field, the two-fold polariton is split and the longitudinal exciton interacts with the paraexciton. With proper orientation of the crystal and polarizations of the two light beams one can selectively excite the magnetic components ($M = \pm 1$) of the upper polariton. The Zeeman splitting of the upper polariton branch (B-field up to 9 T) shows a drastic K-dependence. Within the $\omega(K)$ tuning range of our experiments the splitting changes by about 50 %. The K-dependent splitting can be explained quantitatively by taking into account the field induced mixing of the Z_3 and $Z_{1,2}$ excitons. The analysis of the data yields reliable g-values which have to be compared to one-photon data. In addition the experimental results give information on the p-d mixing in the upper valence band.

TuA-D6

NONLINEAR SPATIAL DISPERSION OF EXCITONIC POLARITON IN CuCl

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Two-photon absorption for the direct generation of excitonic molecules (EM) in CuCl is known to induce the non-linear change in the excitonic polariton dispersion [1, 2]. By analogy with the spatial dispersion of exciton, that of EM is also expected to affect on the non-linear change. Under the existence of the pump polaritons having energy ω_1 and wavevector k_1, there appear, in addition to the "ordinary polariton branch *a*", two kinds of new spatial dispersion branches for the probe polariton having ω_2 and k_2: "self-induced branch *b*" where $\omega_2(k_2)=\omega_m/2+\hbar k_2^2/M_m$ and "induced branch *c*" where $\omega_2(k_2)=(\omega_m-\omega_1)+\hbar k_2^2/2M_m$ (ω_m and M_m are the Γ- point energy and the translational mass of the EM). Therefore, one can expect several kinds of two-photon resonant Raman scattering (TRRS) processes for the intense one-beam excitation with energy ω, being larger than $\omega_m/2$, where $\omega_m=3.18600$ eV. Three typical processes have been experimentally observed in CuCl. (1)Combination of 2*a* polaritons: the ordinary TRRS, M_T^R and M_L^R, with recoil of the transverse and longitudinal excitons, respectively. Here, the energy shift is twice as much as that of the incident light, δ. (2)Combination of *a*+*b*: the shift of the TRRS is about $+\delta$. New Raman lines, L_T and L_L, have been observed for $\omega>\omega_m/2$, separated from the M_T^R and M_L^R, respectively. The energy positions and intensities depend strongly on the pump power, indicating the non-linear character of this process. (3)Combination of 2*b* or *a*+*c*: the shift is about -2δ. This process is particular because it is always resonant with the EM state. Therefore, the secondary emission may have the character of luminescence. The recently observed hot luminescence bands, X_T and X_L, are thought to be caused by this process.

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INTRINSIC LINESHAPE OF EXCITON-POLARITON PHOTOLUMINESCENCE PEAK IN GaAs

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The origin of the pronounced dip at the free exciton energy (or in another view, the doublet structure) observed in the photoluminescence spectra of GaAs and some other compound semiconductors has been a matter of speculation for some time.[1-4] Originally it was proposed that the "doublet" was a consequence of the energy offset of the "bottleneck" emission of the upper and lower exciton-polariton branches[1,2] and later[3,4] that the dip was due to a resonant enhancement of exciton-polariton scattering at the exciton energy (the effect of this narrow "reabsorption" region is to convert a single narrow intrinsic peak into a broader doublet). We have observed a single narrow photoluminescence peak at the exciton energy in nominally undoped GaAs which is contrary to the prediction of the "bottleneck" model and consistent with the reabsorption model assuming few scattering centers. We report here on the lineshapes of exciton-polariton photoluminescence peaks in nominally undoped GaAs samples grown by molecular beam epitaxy which contain unusually small amounts of donor impurities as determined by low temperature photoluminescent spectra of samples excited by greater-than-bandgap laser radiation[5]. In our "best" samples we observed a single, narrow peak at the exciton energy with a full width at half maximum (0.4 meV) which is less than the splitting ($\approx$ 0.7 - 0.9 meV) observed in "good samples") grown by VPE. In these samples the donor luminescence (free-to-bound transitions and exciton-bound-to-donor peaks) was unobservable. There was excellent agreement between this peak's position and the energies of the transverse and longitudinal excitons measured in the same sample using resonant Brillouin scattering.[6] Comparing results from a number of our samples, a clear relationship is evident between the narrowness of the exciton halfwidth (and the magnitude of the doublet peaks' splitting which is directly related to the magnitude of the dip) and the intensities of the donor luminescence and some other impurity related peaks. As the intensities increase, the splitting increases. The lineshape of the exciton-polariton emission peak is fit with a model incorporating enhanced scattering in a narrow energy range near the exciton energy due to the reduction of the mode's group velocity which is a consequence of spatial dispersion.[6] Assuming no scattering centers, a narrow emission peak is predicted, as was observed in our "best" samples. We believe this represents the first observation of the intrinsic lineshape of the exciton-polariton photoluminescence emission in GaAs.

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EXCITON DYNAMICS IN WEAKLY DISORDERED SEMICONDUCTORS

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Time-resolved exciton luminescence experiments in mixed $Al_xGa_{1-x}As$ and CdS_xSe_{1-x} semiconductors are reviewed. Excitons in these disordered systems are subjected to random potential fluctuations. Depending on the exciton energy it can either be localized at such a fluctuation or scatter by it, while still be in an extended state. Using selective, pulse laser excitation (pulse width $\ll$ exciton lifetime) at low temperatures, non-exponential exciton decay curves are observed in both indirect-gap $Al_xGa_{1-x}As$ and CdS_xSe_{1-x}. In the latter case, fluorescence line narrowing is also observed. The data can be interpreted in terms of excitons localized by random potential fluctuations. In $Al_xGa_{1-x}As$ the non-exponential decay is due to inter-valley scattering while in CdS_xSe_{1-x} it is due to tunneling between localized states. Entended exciton states are also observed: In $Al_xGa_{1-x}As$ they have the same luminescence spectrum at the localized excitons. In CdS_xSe_{1-x} they lie higher than the localized excitons,but a sharp exciton mobility edge cannot be identified.

17th International Conference on the Physics of Semiconductors

Amorphous Superlattices
and Junctions

TuP-A1

AMORPHOUS DOPING SUPERLATTICES

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Recent experimental studies on crystalline n-i-p-i doping superlattices with GaAs as host material have fully confirmed our previous predictions about the anusual electronic properties of this new class of artificial semiconductors[1,2]. In contrast to compositional superlattices, where the most striking features rely on the formation of 2-dimensional quantum wells, the exotic properties of n-i-p-i doping superlattices include many features for which this is not the case. Therefore, such peculiarities can persist, even if the host of the superstructure is a (strongly disordered!) amorphous solid. These properties include an effective band gap, which can be "tuned" over a wide range by optical excitation, for instance[1], and extremely enhanced electron-hole recombination lifetimes[2]. After the successful investigation of crystalline doping superlattices, for which quantitative agreement between predicted and observed behavior was obtained because of well established data characterizing the host materials, the study of amorphous doping superlattices seems particularly appealing, since new information on the properties of the amorphous bulk material can be expected. As a first example we demonstrate how the gap density of states of the bulk host material can be obtained from a study of amorphous doping superlattices. Secondly we show, that interesting information about the energy relaxation mechanisms of photo-excited carriers can be obtained from steady-state and time-resolved luminescence and photoconductivity measurements. Amorphous silicon appears as a most suitable host for this new kind of doping superlattices.

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Amorphous Superlattices
and Junctions

TuP-A2

AMORPHOUS SILICON BASED DOPING SUPERLATTICES

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Doping superlattices consisting of up to 240 alternating layers of n-type, p-type, and intrinsic amorphous hydrogenated silicon (a-Si:H) were prepared in a computer controlled RF discharge deposition system. Various types of superlattices (nipi, nini, pipi, npnp) have been synthesized with layer thicknesses between 20 and 2000 Å. The gas exchange between layers was optimized using optical emission spectroscopy of the plasma to yield the sharpest transitions possible. Concentration profiles of dopant atoms and hydrogen were obtained using SIMS and depth resolved nuclear reaction techniques. We measure small ($\sim$20%) asymmetries in hydrogen content which appear to be related to the growth direction.

We have determined the width of the depletion layer in the doped regions of nini structures from the drop in dark conductivity as a function of n-layer thickness.

The optical absorption edge shifts by as much as 30 meV towards lower energy in nipi and npnp superlattices.

Carrier separation due to the strong built-in fields lowers the photoluminescence intensity of nipi's as a function of i-layer thickness down to less than 1% of its value in unstructured a-Si:H.

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Amorphous Superlattices and Junctions **TuP-A3**

Electronic Properties of Amorphous Si:H/Ge:H Semiconductor Superlattices

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We have synthesized semiconductor superlattices consisting of alternate layers of hydrogenated amorphous Si and Ge by periodically changing reactive gas in a low-pressure plasma-assisted CVD reactor. The layer pair repeat spacing was varied from 8 A to 100 A. X-ray and TEM measurements indicate uniform and parallel layers. A series of (a-Ge:H)/(a-Si:H) films with sub-layer thicknesses 4 A $< L_{Si} <$ 50 A and 4 A $< L_{Ge} <$ 50 A and $L_{Si}/L_{Ge} = 0.5$, 1 and 2 have been studied, as well as alloy films. When layers are thick (L_{Si}, $L_{Ge} >$ (40,40)) optical properties can be described by classical effective medium theory with the optical constants of each constituent considered separately. In-plane resistivity of thick layers is controlled by a-Ge:H layers whereas transverse resistivity is probably dominated by electron tunneling through a-Si:H layers. Transport in all samples is n-type as determined by thermoelectric power measurements. Photoluminescence and photoconductivity measurements indicate that a-Ge:H in layers is of higher electronic quality than bulk a-Ge:H prepared in the same manner. As layers are made thinner (L_{Si}, $L_{Ge} <$ (30,30)) quantum superlattice effects must be taken into account to interpret the increase in optical gap from 1.05 eV to 1.5 eV, the increase of in-plane resistivity and its activation energy and the disappearance of anisotropy in electronic transport. Metal Schottky junction height also increases as L_{Ge} is decreased showing that the electron mobility edge shifts upward as well as the optical gap. Electronic properties are consistent with a Kronig-Penney periodic potential model in which most of the band-edge discontinuity of a-Ge:H/a-Si:H junctions is in the conduction band. We will discuss the effect of disorder on quantum superlattice effects.

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Amorphous Superlattices and Junctions **TuP-A4**

OPTICAL AND ELECTRICAL PROPERTIES OF AMORPHOUS SEMICONDUCTOR SUPERLATTICES*

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Compositionally modulated amorphous n-p-n-p . . . . superlattices of doped hydrogenated amorphous silicon (a-Si:H) have been prepared in a closed two-chamber plasma reactor. We shall report on the effects of internal fields, space charge doping, and for thin sublayers the effect of two-dimensional confinement on the transport and optical properties. The properties of the multilayer films are compared with those of unlayered films prepared in each of the chambers simultaneously. Instead of a red-shift of the photoluminescence peak observed in doped and compensated a-Si:H, the n-p-n-p . . . . superlattices show a blue shift. As a result of the strong internal fields, the absorption edge is decreased. Compared to unlayered films the decay of the photoconductivity extends to longer times. The compositionally modulated amorphous superlattices show interesting changes in their properties after strong light exposure. For instance the in-layer dark conductance is decreased after exposure at 300K but is increased after exposure at 78K. These changes, of which some are related to the Staebler-Wronski effect in a-Si:H, can be reversed by annealing. Our results will be compared with the theoretical predictions of optical tuning and the effects of space charge modulation in compositionally modulated superlattices.

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TuP-A5

SCHOTTKY BARRIER FORMATION AT METAL-HYDROGENATED AMORPHOUS SILICON INTERFACES

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The formation of the Schottky barrier between Pt, Pd, Cr, and Au and undoped hydrogenated amorphous silicon (a-Si:H_x) has been investigated. The barrier was formed by evaporated metal on a-Si:H_x, produced by homogeneous chemical vapor deposition (HOMOCVD). Barrier height measurements were performed using forward current-voltage (J-V), capacitance-voltage (C-V), and photovoltaic techniques (V_{oc} - T) in the range from 295 to 500°K and the results were compared with photoresponse (I_{ph} - $h(\nu-\nu_o)^2$) measurements. Within the experimental accuracy, values of the intrinsic barrier heights (flat bands) (ϕ_{BF}) deduced from the different measurement techniques were found to be in good agreement. The barrier heights were found to depend on the metal deposited, and to decrease with increasing temperature with a coefficient nearly equal to the change in the energy band gap of a-Si:H_x. This suggests that the Fermi level at the metal-a-Si:H_x interface is pinned in relation to the valence band edge. The densities of interface states deduced from the variation of ϕ_{BF} with the metal work function were found to be $\sim 10^{13}$ $eV^{-1}cm^{-2}$, resulting in the pinning of the Fermi level to values ~0.7 eV above the valence band edge. These results are compared with the proposed theoretical models describing Schottky barrier formation and show for the first time the striking similarities in the behavior of the intrinsic Schottky barrier height on amorphous and single-crystal Si.

INITIAL STEPS OF METAL-SILICON INTERFACE FORMATION

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In the present talk, data obtained[*] through surface physics methods on the first steps of ultra high vacuum metal deposition on clean Si(111) surfaces are presented and discussed : structural, compositional and electronic properties are deduced as a function of metal coverage below, at and above the 1 monolayer range, from low energy electron diffraction, Auger electron spectroscopy and photoemission yield spectroscopy. The latest is well suited to the problem since it gives the values of the work function and ionization energy, and hence the surface barrier height of the semiconductor, together with the effective density of filled surface states in the gap and the highest part of the valence band.

Taking examples among the d-metals of the first column (Cu,Ag, Au), the simple trivalent metals (Al,Ga,In) and Sn as compared to Ge, the influence of several parameters on the atomic arrangement and the corresponding electronic properties are underlined. These parameters are either related to the nature of the metal — atom size, bond strength, valency, d-electrons — or to the Si substrate initial states — 2 x 1 or 7 x 7 reconstruction — or to the Si substrate temperature during or after metallisation. It is shown that most often a conflicting situation arises between opposite tendencies, which makes any prediction usually hazardous.

It demonstrates that the local atomic arrangement at the last atom of the true silicon crystal is of primary importance for the Schottky barrier,and that its determination, which cannot be considered as achieved in any system, command the understanding of the electronic properties.

[*] In collaboration with D. Bolmont, P. Chen, V. Mercier, F. Proix and A. Taleb-Ibrahimi.

THIN FILM KINETICS AND REACTIONS AT METAL-SILICON INTERFACES

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The solid state reactions at metal-silicon interfaces strongly affect the electronic properties of the structure. While the chemical nature of the constituents may determine the phase formation. the kinetic properties can influence the process. In this study Raman scattering and Rutherford backscattering (RBS) are used to determine the initial phase formation from metals deposited on silicon and then annealed to initiate the reaction. The metals that form the focus of the study are Ni, Pd. and Pt while results of other transition metals are also presented. Both crystalline and amorphous silicon substrates are used to explore the effects of initial disorder. The sensitivity of the Raman scattering experiment is increased by the use of the interference enhanced Raman scattering (IERS) configuration while channeling and glancing exit angle procedures are used to obtain similar enhancement of the RBS. Both techniques achieve a sensitivity of ~10A. The Raman scattering experiments determine the structure at the interface and are sensitve to crystalline or disordered nature, and the RBS determines the composition of the reacted region. Metal deposition and *in situ* measurements are performed on atomically clean and chemically etched silicon surfaces. The results indicate that low temperature annealing can yield both crystalline or disordered phases. These results are discussed in the context of a random diffusion process. A model is presented which includes both strain and chemical energy to account for the various processes which are experimentally observed. Within the context of the model, conditions which could lead to epitaxial silicide growth are discussed.

Pb/Ge(111) : FORMATION OF THE INTERFACE UNDER THERMODYNAMIC EQUILIBRIUM

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The lead-germanium system appears as a very promising one for the study of the formation of the metal-semiconductor interface and the evolution of the atomic and electronic structures as it is a typical example of a non-reactive interface growing from room temperature in a layer plus islands mode /1-4/. Until now it has been studied by several techniques in the course of adsorption or desorption kinetics experiments, in conditions very far from the thermodynamic equilibrium. The physical properties investigated in this way thus concerned eventually only metastable , but out-of-equilibrium, surface phases. Recent progress in the understanding of two-dimensional (2D) matter (e.g. physisorbed systems at low temperatures) comes for a large part from experiments performed under equilibrium between the gas phase and the adsorbate : one measures the adsorption isotherms and the presence of several steps and/or substeps reveal the first order transitions that correspond to the different surface phases.

For a metal/semiconductor system one can install such an equilibrium by using a molecular beam directly impinging on the substrate /5/ ; we have thus reexamined the Pb/Ge(111) system in conditions which are equivalent to a substrate exposed to an isotropic gas pressure. A lead beam impinges at a controlled rate Φ on the heated germanium crystal, cleaved in situ under UHV, and maintained at fixed temperature T. When the desorbing flux is equal to the incident one a stationnary equilibrium coverage $\Theta(\Phi,T)$ is reached : it is accurately determined by AES. Adsorption isotherms are then plotted by varying Φ and T. From the isotherms we derive the cohesive enthalpies of the different surface phases which we compare with our previous estimations deduced from desorption kinetic experiments. This gives some hint for structural models and the metal-semiconductor interaction.

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HIGH RESOLUTION ELECTRON ENERGY LOSS SPECTRA FROM SURFACES AND INTERFACES OF SEMICONDUCTOR OXIDES

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We report the observation of Fuchs-Kliewer surface phonons on various faces of SnO_2 and SiO_2 single crystals by high resolution electron energy loss spectroscopy (HREELS). These materials are characterized by anisotropic dielectric properties, and the resolution of our experimental spectra calls for a revision of the HREELS theory. We provide a new scheme based on the dielectric approach which incorporate anisotropy effects. The theory is equally applicable in the visible and UV range of energy losses associated with the excitation of interband transitions and surface plasmons. This scheme allows to distinguish between losses obtained at non-equivalent surfaces of a single crystal, or for different electron azimuthal directions on non-basal faces. The full quantum mechanical Poisson spectrum of multiple phonon peaks is obtained from the first order Born spectrum constructed from available dielectric tensors. This theory provides a remarkably accurate representation of the HREELS spectrum in the case of the uniaxial crystals presently measured. Such an agreement makes it possible to describe the dielectric tensor independently of any IR optical measurements and we present a detailed comparison between such independent data. In most observed excitation events a slight decrease of phonon lifetime is observed in the HREELS spectra when compared to the values deduced from infrared reflectivity. The theory has been extended to describe the surface and interface phonon spectrum of thin supported oxide films. Recent HREELS measurements on various oxide layer thicknesses of the Si/SiO_2 interface will be reported at the conference.

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POLARON CYCLOTRON RESONANCE AT AN INTERFACE

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Electron - LO phonon interaction can perturb significantly the cyclotron resonance frequency of electrons in bulk polar semiconductors, especially when the cyclotron frequency, ω_c, approaches ω_{LO}, the long wavelength LO phonon frequency. Analogous perturbations are expected to be even stronger for two dimensional electrons. This paper studies a model in which electrons, bound by a triangular potential to a surface, interact with bulk LO phonons and a magnetic field perpendicular to the surface. The dimensionless electron - LO phonon interaction constant, α, is assumed small and correlations due to electron - electron repulsion are neglected. The correction to the cyclotron energy is found to depend not only upon ω_c/ω_{LO} and α, but also upon the strength of the binding potential, the filling factor, ν, and the density of electrons with the same spin orientation as that of the optically excited electron. For electrons in the lowest subband the correction seems insensitive to the shape of the confining potential, provided that potentials are compared which produce the same energy difference between the ground and first excited subband states. Numerical results for the GaAs/(GaAℓ)As interface are presented for $\nu < 1$ and ω_c above and below ω_{LO} and compared to results for a two-dimensional model calculation. The two-dimensional model predicts corrections which are considerably larger than those found for realistic confining potentials.

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ONE-DIMENSIONAL LOCALISATION BEYOND FIRST ORDER IN NARROW SILICON MOSFET'S

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We report the observation of large conductivity corrections at temperatures below 1 Kelvin in Silicon MOSFETs of width ≈ 1μm (1), and show that these effects result from One-Dimensional electron localisation.
These measurements provide a powerful test of finite-temperature Scaling methods (2) and direct 1-D calculations (3). Both theories suggest that, in the low-temperature regime where the inelastic diffusion length is no longer smaller than the localisation length of the electron wavefunctions, the conductivity should depend linearly on the inelastic scattering rate. We experimentally confirm this prediction, and find that the dominant inelastic scattering mechanism is electron-electron. In addition, magnetoconductance measurements indicate the presence of localisation-enhanced electron-electron interaction effects.

We also discuss, in relation to recent theory (4), the effects of strong electric fields when conductivity is in this regime; and we present 2-terminal quantum Hall measurements made on these devices(5).

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EFFECTS OF SUBMICRON CONFINEMENT ON SHALLOW DONORS IN GaAs-$Ga_{1-x}Al_xAs$ MULTIQUANTUM WELL STRUCTURES

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The electronic states of shallow impurities in semiconductors are greatly affected by confinement on the scale of the effective Bohr radius, a_B. Such confinement can be achieved in GaAs quantum wells (a_B=104A^o) in GaAs-$Ga_{1-x}Al_xAs$ heterostructures grown by molecular beam epitaxy (MBE). Experimental studies of such systems have been limited to photoluminescence and, very recently, Raman scattering[1]. We report the first experimental observation of intraimpurity absorption spectra of shallow donors in GaAs in GaAs-$Ga_{1-x}Al_xAs$ multiquantum well (MQW) structures.

MBE-grown Samples having nominal Si donor densities between $1x10^{15}cm^{-3}$ and $1x10^{17}cm^{-3}$ and GaAs quantum well widths between 80A^o and 1000A^o have been investigated. Doping "spikes" of 50-60A^o nominal width were placed at the well centers and in some cases at the edges of the wells in order to determine the effects of impurity position within the wells. MQW structures of 20 repetitions have been investigated. The far infrared experiments were carried at liquid helium temperature in magnetic fields normal to the sample surface up to 9.3T. Results are compared with measurements on a Si doped "bulk" sample. For the 150A^o quantum well samples with impurities at the well center, the 1s-2p transition is observed at zero field at energies aproximately 2meV above that of the bulk sample. This line splits into two lines (1s-2p(+) and 1s-2p(-)) with increasing magnetic field as expected for the Faraday geometry of the experiments. A plot of the 1s-2p(+) transition energy vs. magnetic field for the quantum well samples crosses that of the bulk sample at approximately 2T, and remains at lower energies at all higher magnetic fields. These results will be compared with recent calculations that include the effects of an arbitrary magnetic field[2].

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17th International Conference on the Physics of Semiconductors

Heterostructure TuP-C4 Invited

SUPERLATTICES:NEW SEMICONDUCTOR MATERIALS

by

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Recent developments in fabrication techniques have made it possible to consider the fabrication of new, man-made materials which have structures not found in nature. These new materials can be constructed in such a way as to have properties that are ideally suited to specific applications. To illustrate this approach to new semiconductor materials, examples, such as HgTe-CdTe superlattices and various III-V superlattices, will be discussed. For the HgTe-CdTe superlattice, the band gap of the superlattice is controlled by varying the thicknesses of the layers even when the ratio of Hg to Cd is fixed. In contrast for the $Hg_{(1-x)}Cd_xTe$, the bandgap is changed by varying the relative concentration of Hg and Cd. In the case of the alloy, the effective mass is coupled strongly with the band gap. However, in the superlattice, the effective mass normal to the layers and the bandgap are decoupled. Hence, it is possible to have a material with a small band gap and a rather large mass which will lead to small tunneling currents in p-n junctions. The near band edge values of ϵ_2 for the electric field polarized parallel to the layers is comparable to that for the alloys. Further, the optical properties can be tailored by varying the thicknesses of the layers while at the same time fixing the band gap. Experimental verification of the results will be discussed. The major areas where there are unsolved problems will also be indicated.

DISSIPATION PROCESSES IN SEMICONDUCTORS DURING IRRADIATION WITH FEMTOSECOND PULSES.

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We study the exact dissipation processes in very dense electron hole plasma created by a femtosecond pulse in silicon and germanium, by measuring the total energy reflected from this pump pulse. The femtosecond laser is a very unique tool to study the conversion of photons into electronic excitations (the first step toward the fusion of the material), since all other charactetic times - e-h recombination, plasma expansion, electron-phonons interaction, lattice heating and atomic motion - are longer. During the pulse only effects coming from the created e-h plasma are observed through the plasma contribution to the dielectric constant. We calculate the reflected power taking into account the change is space and time, of that dielectric constant during the pulse by solving the highly non linear field propagation equation.

Experimentally, we are able to pass the minimum of reflectivity associated with the plasma resonance of the pump pulse at 0.62 μ and 0.31 μ, which indicates that e-h densities higher than 10^{22}cm^{-3} are reached. We find that the plasma resonance is very broad which means that the carrier relaxation time τ is extremelly short, a value as low as $\tau = 3.10^{-16}$s is necessary to fit the experimental data. Such a value, which cannot be attributed to e-phonons interaction, is associated to a new dissipation process, electron hole collisions, which can exist and dominate only in highly excited semiconductors.

A STUDY OF THE DYNAMICS OF THE ELECTRON-HOLE-LIQUID FREE-EXCITON SYSTEM IN Ge USING NO-PHONON LUMINESCENCE

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We present a new method of studying the dynamics of the electron-hole-liquid (EHL) free-exciton (FE) system in Ge which makes new information accessible to experiment. The technique involves using EHL no-phonon luminescence that is mediated by a defect (e.g. an impurity) onto which electron-hole-drops (EHD) are bound. A crystal that contains a uniform and low concentration of these defects is required ($\sim 10^{12}$ cm^{-3} or less). For such concentrations each EHD will be bound on at most one defect. The EHL no-phonon luminescence from an EHD bound on such a defect will emanate only from a small region in the droplet because the defect is very effectively screened by the electron-hole plasma. Thus the intensity of the EHL no-phonon luminescence will be independent of droplet size. This means that in a suitable crystal the EHL no-phonon luminescence intensity will be proportional to the number of EHD's.

As a demonstration of the power of this technique we show EHD cloud decay for a phosphorous doped crystal experiencing pulsed photoexcitation. We have demonstrated that EHD bind to phosphorous by measuring the hysteresis of the luminescence with steady state excitation power. We have made detailed time and position dependent measurements of both phonon assisted luminescence and defect mediated luminescence. These measurements enable us to determine the dynamics of cloud including both drop size and density during the decay. Temperature and excitation power dependences are planned for the future.

In conclusion, a powerful new probe of the EHL-FE system is available making previously difficult to measure parameters, such as the Richardson boil off constant for the EHL, accessible to measurement.

HIGH SPEED ELECTRON-HOLE PLASMA TRANSPORT IN SILICON

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We have investigated the spatial expansion of equilibrium ("electron-hole liquid EHL") and non-equilibrium ("electron-hole plasma EHP") ambipolar plasmas in Si at temperatures $<$ 50K using two new optical methods:

1) Optical time of flight technique - Using surface doping e.g. by ion implantation with In (E_{max} = 750keV, penetration depth 0.3 µm) we have introduced characteristic centers for bound exciton recombination in one side of high purity Si-crystals. In these structures carrier pairs are generated by ≅200 ps pulses from a mode locked frequency doubled NdYAG laser in the undoped surface of the sample and travel through the unexcited bulk (40µm-200µm) finally reaching the back-surface where they partially give rise to a characteristic bound exciton luminescence. Using time delayed spectra, we study the ambipolar transport
i) below the critical point for EHL-formation. We find, that the EHL-transport occurs along preferential axes ("phonon focussing") and obtain EHL-velocities up to $5\cdot 10^5$cm/s, i.e. close to the velocity of sound.
ii) above the critical point we observe a supersonic EHP propagation.

2) The EHP expansion is studied in detail using the Mott-Transition between EHP and free excitons (FE). We have monitored the onset and decay of the EHP and FE emission after strong surface excitation as described above. We observe an immediate rise of the EHP signal with the excitation, whereas the FE emission increases in proportion to the decay of the EHP intensity. The data clearly shows i) carriers are created in the EHP-state and ii) FE are formed only in those spatial regions in which the plasma density has fallen below the Mott density n_{Mott}. Using a simple model we can extract from the number of excited carrier pairs, $n_{Mott}(T)$ and the measured time dependence of the emissions average values for the plasma expansion velocity as a function of the excitation intensity and the temperature. Consistent with the results of the first method we obtain EHP velocities in the 10^6cm/s range.

TURBULENCE IN ELECTRON-HOLE PLASMA IN GE

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Spontaneous current oscillations in an electron-hole (e-h) plasma in Ge in an electric field E and a parallel magnetic field B are known to be the result of an unstable helical density wave [1]. We have discovered that when this instability is strongly excited by an increasing electric field, there is a transition to turbulence similar to that observed in fluids [2], and characterized by a rich dynamical structure. We produce an e-h plasma by double injection or laser pumping in rods of n-type Ge of size $\sim 1\times1\times10$ mm^3, with N(donor) $\sim 10^{12}$ cm^{-3}, $B \sim 1$-15 kG, $E \sim 1$-50 V/cm, $T \sim 77$K, and plasma density $\rho \sim 10^{13}$ cm^{-3}. The resulting spontaneous oscillations have a frequency $f \sim 10^4$-10^5 Hz.

For $B = 4$ kG, we find a sequence of threshold values of E at which the period of the spontaneous oscillations doubles, $f \to f/2 \to f/4, \ldots$, leading to a noisy state characterized by broadband noise. This noise is shown to be of chaotic nature [3], i.e. due to nonlinear plasma dynamics, not thermal fluctuations. For several different values of B we observe a quasiperiodic route to chaos -- as E is increased the onset of a quasiperiodic state (simultaneous oscillations at two incommensurate frequencies) is followed by a transition to turbulence. This turbulent state is described by motion on a strange attractor, a fractal surface in phase space. We measure the fractal dimension, finding it to vary between roughly 2 and 3 with the degree of excitation. Multiple probe contacts on the crystal surface enable the measurement of spatial variations in the plasma density $\rho(\vec{r},t)$, and hence data describing the spatio-temporal behavior of the chaotic states are obtained.

Although the possibility that plasmas could exhibit chaotic behavior has been discussed theoretically [4], no clear evidence for it in gas or solid state plasmas has been previously reported. We interpret the data by a rate equation model which includes nonlinear coupling between stable and unstable plasma density waves.

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DENSITY-TEMPERATURE RELATION OF QUASI-EQUILIBRIUM e-h PLASMA IN GaAs

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The properties of the electron-hole plasma (EHP) in high purity GaAs layers* are studied under conditions of carrier confinement. Raman spectroscopy of collective plasmon-LO phonon modes (PLP) and single particle excitations (SPE) as a function of temperature, excitation intensity and excess energy of the photocreated carriers are applied to determine the EHP-properties. The plasma density n_{EHP} and the effective carrier temperature T_{eff} are obtained from the energies of the collective modes and a lineshape analysis of the single particle spectra, respectively. The main results are summarized as follows:

1) at a constant power density the quasi-stationary plasma density initially increases with temperature up to a maximum value n^*; a further increase in temperature reduces the plasma density.
2) the maximum density n^* increases for increasing excitation level, whereas the corresponding temperature T^* is nearly independent of the excitation intensity and is approximately 170 K.
These investigations establish that the observed decrease of n_{EHP} above T^* is controlled by a strong temperature and density dependent carrier loss process. In conjunction with simultaneously measured luminescence spectra we believe that primarily the nonradiative decay process produces this density reduction in the high temperature range (T_{eff} > 170 K), whereas below the radiative component mainly governs the density-temperature relation. The data are interpreted in terms of an equilibrium balance equation including all possible recombination processes. This model is able to explain the sensitive dependence of the carrier density on the excitation level as well as the observed relationship between carrier density and temperature. The unexpected decrease of n_{EHP} above T^* is found to be controlled by the onset of the strongly temperature dependent phononless Auger recombination.

*The samples are grown by MBE and have been generously given to us by K. Ploog.

TuP-PA1

SELF - CONSISTENT SOLUTION FOR ELECTRONS IN a-Si.

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We have reported(1) a theory to deal with electronic problems in amorphous systems in a real space frame work. The Hartre-Fock self consistent formalism has been used to find the thermodynamically averaged green's function in a Bethe lattice.

In this work, we report some calculations, based on the mentioned theory, done in a lattice of coordination 4 and sp^3 orbitals.

This formalism gives good results for pure amorphous silicon and provides with an excellent saturator for finite cluster calculations.

The important case of hydrogenated a-Si can be treated with this theory by applying the cluster Bethe lattice method, but with the advantage that there are no adjustable parameters in the theory.

PSEUDOPOTENTIAL AND K.P CALCULATIONS OF OVERLAP INTEGRALS FOR AUGER PROCESSES IN DIRECT GAP SEMICONDUCTORS

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A realistic calculation of the Auger recombination rate in a semiconductor requires detailed information on the semiconductor bandstructure and the electronic states. Accurate E-k curves are required to determine the possible Auger transitions and simple approximations to the bandstructure can lead to large errors in rate calculations. The electronic wavefunctions are required to calculate the overlap integrals of the periodic parts of the Bloch functions that appear in the Auger transition matrix element. In Auger theory it has been conventional to make estimates of the overlap integrals by using effective mass sum rules and making assumptions about the dominant terms in the sums. In this paper we report both pseudopotential and k.p calculations which demonstrate that the sum rule approach is totally inadequate.

We have carried out direct calculations of the overlap integrals using both the pseudopotential bandstructure of Chelikowsky and Cohen and also a full zone k.p method. Theoretical estimates of the errors involved in using pseudowavefunctions for the overlap integrals suggest that the pseudopotential results are reasonably reliable even when the $|\text{overlap integral}|^2 \sim 10^{-4}$. This is confirmed by the good agreement between the pseudopotential and k.p methods.

We present data for overlap integrals relevant to the CCCH process in several direct gap semiconductors and give estimates of the integrals for alloys such as GaInAsP and CdHgTe. For antiparallel wavevectors the conduction band - heavy hole band overlap integral shows a very strong dependence on wavevector direction and a peak value an order of magnitude less than estimated from simpler indirect methods. For non-parallel wavevectors the overlap integral is rather larger and still varies substantially with wavevector direction. The directional dependences of both the overlap integrals and the threshold energy are significant complications in the calculation of Auger rates.

CORRELATION IN TIGHT-BINDING THEORY

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In tight-binding theory electron correlations enter through an intra-atomic Hubbard U . This U gives shifts in the atomic levels in compounds which may be calculated self-consistently and can produce a Mott transition in some systems. A systematic table of values for nontransition elements has been obtained using approximate elementary predictions, adjusted to accord with experimental differences between electron affinities and first and second ionization potentials. For most properties an effective U* enters which is reduced by a Madelung potential from the neighboring atoms. For tetrahedral semiconductors the two are found to very nearly cancel, so that reasonable tight-binding energy bands are obtained using free-atom term values. However, the increace in the expected energy gap over the value obtained in self-consistent-field (or density-functional) theory depends upon U rather than U* . The shift is found to be given approximately by U/ε where ε is the dielectric constant. The shift is larger for polar semiconductors because of the smaller ε and larger for lighter semiconductors both because of the smaller ε and the larger U . The cohesion, on the other hand depends upon U* so that reasonable values are obtained using free-atom term values. The corresponding analysis of ionic solids gives a similar cancellation, explaining why tight-binding theory remains appropriate there and why the tight-binding calculation of cohesion is essentially equivalent to the Born electrostatic theory. A condition for the Mott transition is derived-using unrestricted Hartree-Fock theory, based upon U* and universal tight-binding interatomic matrix elements. This criterion confirms the earlier finding(1) that an ideal silicon (111) surface would be antiferromagnetic.

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ISOMER SHIFT AND THE LOCAL CHEMICAL BOND IN SEMICONDUCTORS

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When studying the behaviour of various impurities in semiconductors in particular with implanted materials, it is very helpful to know the local chemical bond in more detail since it accounts for the site and the physical properties of the impurity. However, it is very often difficult in this connection to introduce simple reliable parameters which could be measured by the experiment. For example, the concept of the effective ionic charge in semiconducting compounds, which at first sight seems to be quite meaningful, turns out to be rather unreliable although our knowledge of the electron charge distribution in these materials is reasonably good. And yet, some experiments reflect the fact that certain electronic charge can be assigned to individual ions; unfortunately, since different experiments include various interactions, different values of the effective ionic charges have been obtained and, surprisingly, even different signs have been found.

In this paper an attempt is made to use Mössbauer Isomer Shift (IS) measurements to cast some new light on this problem. It is well known that the IS reveals the electronic configuration of the Mössbauer atom (ion), however, in general not in a straightforward way, so that either complementary experiments or theoretical calculations are needed to determine the real electronic configuration of the atom (ion) in terms of the occupancy numbers of the valence shells. One can thus anticipate that if the calculated occupancy numbers are compatible with the IS measurements, then the corresponding effective charge defines a certain electronic charge associated with the atom (ion) in question.

The situation is, however, more involved since different methods, though giving practically the same band structure, yield different electron distributions depending on the approximations made. Some aspects of this problem concerning group IV and $A^{III}B^{V}$ semiconductors are discussed in detail.

THERMOPOWER IN SILICON INVERSION LAYERS

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We have investigated the thermopower of electrons in silicon inversion layers for electron concentrations from 10^{11} cm^{-2} to 10^{12} cm^{-2} in the temperature range 1.7K-7K. We find that the transition from activated to metallic conductivity is accompanied by a change in the temperature dependence of the thermopower.

In the metallic regime the thermopower agrees with the theoretical expression $S = const.(kT/E_F)$ calculated for charged impurity scattering. One feature of this system we emphasize is that E_F is measured from the mobility edge E_c. We note that in the temperature range studied inelastic scattering is sufficiently strong to cut off the weak localisation arising from quantum interference. At low values of E_F there are departures from this behaviour because of non-degeneracy, while at high electron concentrations, surface roughness is seen to cause a deviation from the above formula.

In the localised regime the thermopower increases with decreasing temperature, characteristic of an excitation process. These features will be discussed in detail and a comparison will be made between the behaviour of thermopower and conductivity across the metal-insulator transition.

THE VALENCE BAND PARAMETERS OF CADMIUM ANTIMONIDE

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The first cyclotron resonance measurements of the holes in cadmium antimonide are presented. The cyclotron effective masses values for the magnetic field B parallel to the a, b, c axes of the orthorombic crystal was obtained with excitation wavelength radiations ranging form 119 µm to 699 µm using either D.C. or pulsed magnetic field up to 35 T.

Thermal excitation of the free holes is clearly evident on the absorption spectra at temperatures above 10 K and a single cyclotron line exists above 30 K. At 4 K, only impurity absorption lines are exhibited. Thoses lines was recently interpreted as cyclotron resonance ones giving thus erroneous values |1|.

In the temperature range where the thermal energy is lower than the cyclotron energy, the line corresponds to a transition between the two first Landau levels. Its magnetic field position could be followed unambigously as a function of the excitation energy taking seven values between 1.8 and 10.4 meV. At low excitation energy (1.8 meV) the following values of the cyclotron masses for B parallel to the axes a, b and c are measured :

$$m_a^* = 0.287 \pm .005, \qquad m_b^* = 0.180 \pm .005, \qquad m_c^* = 0.410 \pm .005$$

At higher energy values we found a substantial decrease for all the masses reaching the order of 10 %. The values come in agreement with the Shubnikov-de-Haas measurements of the masses in the same energy range of the holes. The present results strongly disagree with initially published cyclotron resonance ones for an unidentified type of sampe |2|.

The valence band model proposed by Yamada |3| includes eight parameters. A new method developed for the Landau energy levels calculation permits an overall fit of the parameters to our experimental data. For this new set of parameters the double humped structure given by Yamada is largely supressed. It should be mentionned however that the decrease of the effective cyclotron mass m_a^* remains unexplained.

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TEMPERATURE DEPENDENCE OF THE OPTICAL CONSTANTS OF Ge, α-Sn, and InSb: ELECTRONIC INTERBAND TRANSITIONS

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In spite of the vast information existing for the intrinsic dielectric constants of semiconductors at room temperature, data at other temperatures are scarce. The development of spectroscopic ellipsometry provides an efficient way of obtaining such data. Here we present dielectric function spectra from 100 to 850 K for Ge and InSb and from 100 to 343 K for α-Sn. Numerical second derivative spectra are fitted to theoretical line shapes and the parameters of the E_1, $E_1+\Delta_1$, E_0' and E_2 critical points (energy, Lorentzian broadening and exciton phase shift) vs. temperature are obtained. This is the first systematic investigation of the temperature dependence of the broadening and phase shift in semiconductors. The results are compared with recent full band structure calculations of Debye-Waller and self-energy terms in the temperature dependence of the electronic states. While both of these terms contribute to the shifts only the self-energy terms contribute to the broadenings.

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TuP-PA8

Excitons Spectroscopy in $Cd_xZn_{1-x}Te$ Alloys: Homogeneous and Inhomogeneous Broadening.

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The low temperature photoluminescence (PL) of $Cd_xZn_{1-x}Te$ alloys is investigated over the entire composition range $0 \leq x \leq 1$. A particular interest is devoted to the study of free and neutral impurity bound excitons, and their interaction with the alloy disorder state. The enhancement of the lower polariton band observed in PL spectra is discussed in the framework of polariton[1] and alloy disorder theories. The polariton absorption spectra measured from excitation spectra are discussed using a new theory of spatially extended quasiparticles [2, 3]. The spectra of neutral impurity bound excitons are studied. Besides the measurement of transition energies between the donor atomic states by selectively excited photoluminescence, attention is focused on the alloy induced spectral line broadening. A theoretical approach based on the Hopfield-Linch[4] exciton binding model in wich accounts for both impurity local environment effect [5, 6] and inhomogeneous broadening [7] is described. In the present case the latter broadening mechanism is shown to be dominant.

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INDUCED SUPERCONDUCTING STATE IN SEMICONDUCTORS AND SEMIMETALS*

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Along with the well-known mechanism of intervalley scattering (M. L. Cohen, 1964) leading to the appearance of superconducting state in semiconductors, there exist a possibility of induced superconductivity in semiconductors (SC) or semimetals (SM). Induced superconductivity is possible in proximity systems (S-SC or S-SM).

It turns out that the critical temperature of such systems strongly depends upon various parameters of SC, e.g., the electron concentration n. The behavior of a system in external field (penetration depth) also appears to depend strongly on these quantities.

Josephson contacts of the types S_1-I-SC-S_2, S_1-I-SM-S_2, etc., are examples of applications of such induced superconductivity, because we deal with Josephson current between S_1 and SC (or SM). The dependences of T_c and I_m upon n appear to be opposite (I_m is the maximum dc Josephson current): an increase of n results in a decrease of T_c and an increase of I_m.

A special case is presented by induced superconducting in a thin SC or SM size-quantizing film. A non-monotonic thickness dependence of T_c, I_m, the penetration depth, etc., appears in this case.

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ON THE FERMI SURFACE OF $Pb_{1-x}Sn_xTe$ AND SnTe IN THE RHOMBOHEDRAL PHASE

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The alloy system $Pb_{1-x}Sn_xTe$ exhibits structural phase transitions from the cubic to the rhombohedral structure and a band inversion transition leading to zero band gap at 0 K for $x = 0.35$. Shubnikov-de Haas studies in both phases and with normal and inverted band ordering in samples with $x = 0.32$ and 0.37 have been carried out and comparison of the observed frequencies with the band structure calculations of Dimmock (1), for the cubic phase, and of Bangert (2), for the rhombohedral phase, give excellent agreement. The parameters thus derived have been applied to the whole $Pb_{1-x}Sn_xTe$ system and their validity is confirmed by the agreement obtained with the Sn composition and the carrier concentration dependence of the anisotropy factor in the cubic phase. The complex nature of the Fermi surface in the rhombohedral phase is found to agree with the predicted splitting of the cubic phase ellipsoid into 'apple-like' composite surfaces and clear evidence is obtained of the presence of structural domains. Furthermore, the puzzle of the multiple parallel frequency branches observed in low carrier concentration SnTe by Savage et al in 1972 (3) has been resolved in terms of the structural phase transition taken in conjunction with the band parameters derived from our work and excellent agreement is achieved.

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INTERPRETATION OF THE FERMI-SURFACE WARPING IN NARROW GAP SEMICONDUCTORS USING A SIMPLE TIGHT-BINDING MODEL

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We have performed measurements of the Shubnikov-de Haas period on degenerate n-type $CdSnAs_2$ samples with carrier densities about 4.10^{18} cm^{-3}. This period exhibits an anisotropy of about 6% in the (1,1,0) plane and shows a warping of the Fermi-surface close to 1,5% in the (0,0,1) plane. We constructed a simple nearest-neighbour tight-binding model for chalcopyrites by extending the work of W.A. Harrison[1] on diamond-type and zinc-blended compounds. This model contains no fitting parameters but nevertheless it reproduces the anisotropy in the (1,1,0) plane to within 1% of the experimental values and provides a fair description of the warping in the (0,0,1)-direction. This remains true when the model is used to describe the zincblende compounds. From this work follows an interpretation for the warping and anisotropy which is entirely different from the usual interpretation based on the $\bar{k}.\bar{p}$ model: to describe both warping and anisotropy the translational symmetry, the configuration of the atoms in the unit cell and the lattice parameters have to be used explicitly. These characteristics of the material are eliminated formally in the usual $\bar{k}.\bar{p}$ description which uses only the pointgroup symmetry explicitly and therefore cannot describe warping despite the use of a set of fitting parameters.

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ENERGY BAND GAP IN QUASI-PARTICLE LOCAL DENSITY THEORY

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We present a general first principle approach to calculation of quasi-particle excitation in insulating crystal which is tested and found to work for both silicon and diamond. The method includes the energy dependence of the self-energy evaluated in the "GW approximation" of Hedin which is applied in the quasi-particle local density approximation (QPLDA) of Sham and Kohn. The essential ingredient is the model of a homogeneous insulating electron gas, built on the idea of Penn and of Levine and Louie. It is shown that this QPLDA self-energy for an insulator (a) is topologically distinct from its metallic counterpart due to discontinuous behavior either as the gap vanishes at fixed particle number or for changes in particle number which move the chemical potential out of the gap, and (b) always leads to an increase over the ground state gap. Connections to related non-analyticities in the ground state exchange-correlation potential are discussed.

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Phonons **TuP-PB1**

FIRST PRINCIPLES STUDY OF THE DYNAMICAL BEHAVIOR OF AlAs

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The lattice dynamical properties of AlAs are investigated using the ab initio pseudopotential theory within the local density functional formalism. The potentials used here are able to produce the lattice constant and bulk modulus in good agreement with experiment. With the use of only atomic input, i.e., the atomic number and mass, we calculate phonon frequencies and mode Gruneisen parameters at Γ and X in the Brillouin zone. The phonon frequencies are accurately estimated to within 2-7% compared to experiment. For the TO and TA modes at X, the eigenvectors are determined. In addition, we have computed the dynamical effective charges using supercell geometries.[1] The longitudinal effective charge is obtained from the electrostatic terms of the potential. The calculated longitudinal effective charge is underestimated: $e_L^* = 0.20$ (experiment, 0.25).

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CATIONS IN OFF-CENTER SITES IN Cu-HALIDES AND AgI - A QUANTITATIVE APPROACH

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Cu-halides and AgI exhibit a great number of anomalies in their low temperature phases as observed in Raman and i.r. spectra, inelastic neutron scattering, Bragg X-ray and neutron scattering. A dynamical model in which the cation may occupy four equivalent off-center sites or its ideal position in the lattice explained qualitatively all the irregular features in the pure [1,2] and mixed crystals [3], as well as their dependence on temperature, hydrostatic pressure and concentration.

We present here for the first time calculations which allow for the existence of a cation potential having two minima. We derive the frequencies of the $\vec{k} = 0$ phonons involving both "central" and "off-center" cations and the corresponding values of Δ, the energy difference between the minima. The relative population of the two potential wells depends exponentially on Δ/kT. It was measured using the ratio of the intensities of the corresponding Raman lines ($Cu_xAg_{1-x}I$, CuCl) or that of their oscillator strengths, obtained from phonon polariton measurements (CuCl, $CuCl_{1-x}Br_x$).

The potential includes the Madelung term and the following short range interactions: the van der Waals (vdW) attraction with a position dependent polarizability and the Born-Mayer-Verwey (BMV) repulsion. The parameters of the model are the ionic radii and the vdW and BMV interaction constants. They were used to fit the temperature (2K-300K) and pressure [4] (up to 35 kbar) dependence of Δ together with the Raman frequencies in CuCl.

The additional minimum of the potential was found to be at a distance of about 0.5 A from the ideal site along the (111) direction, towards the faces of the tetrahedron. Its position is temperature and pressure dependent. We discuss the model and its parameters referring also to EXAFS results.

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Phonons **TuP-PB3**

VERY STRONG LATTICE COUPLING IN DIAMOND AT PHOTON ENERGIES UP TO 1.5 eV ABOVE THE BANDGAP

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Due to the negative effective electron affinity [1] of the hydrogenated diamond (111) 1 x 1 surface, total photoelectric yield is closely related to the optical absorption coefficient. We report the observation of an oscillatory photoelectric yield from diamond as a function of incident photon energy over the range $5.5 \leq h\nu \leq 7$eV. The oscillations are spaced by approximatedly the optical phonon energy ($\simeq$160 meV). This structure is strongly dependent on temperature; the peak to valley ratio increasing strongly as the termperature is decreased from 300°K to 200°K. Structures with essentially identical peak and valley positions have been reported [2] in photoluminescence at 77°K. Because of the $h\nu$ range over which the photoelectric yield oscillations occur, and the small dependence of the strength of the oscillations on photon energy (the first five oscillations are of roughly the same strength), this result can not be explained by conventional indirect band edge optical adsorption. A very crude explanation will be given in terms of the Franck-Condon effect. However, it is recognized that this presents great difficulties in its departure from the one electron approximation for optical absorption up to 1.5 eV above the band gap. Thus, the main objective of this paper is to bring attention to important phenomena not previously recognized in order to stimulate appropriate theoretical and experimental work.

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MAGNETOPHONON RESONANCE RECOMBINATION OF HEATED ELECTRON AND HOLE DEU TO TWO TA-PHONON EMISSION IN LPE-HgTe

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This paper reports a new magnetophonon effect of electron-hole recombination accompanied by two TA-phonon emission in HgTe. The observation was succeeded for the first time by using a thin layer of high quality LPE-grown crystal on CdTe. It has become possible to measure the resistance in heated electron condition without using pulse technique because of the usage of thin layer immersed in liquid helium and this DC measurement has made it possible to detect a small oscillation signal induced by the application of magnetic field.

Second derivatives of longitudinal magnetoresistance under heated electron condition were investigated for several different samples with different crystallographic orientation. Oscillation with 3-5 peaks were observed in 2$\sim$9T under the electric field of order 1 V/cm. It is found that these peaks are different from the higher order peaks of the magnetophonon oscillation deu to LO-phonon reported earlier by Russian groups.1)

Analysis of the peak position strongly suggests that the oscillation is due to magnetophonon resonance recombination of heated electron and hole accompanied by two TA-phonon emission. According to this interpretation, near zone edge TA-phonon energy at low temperatures has been obtained for the first time. The result indicats that the TA-phonon density of states has two peaks at 2.6 meV and 3.1 meV, respectively. These very small phonon energy may explain the anomalies of HgTe found in many properties at low temperatures such as heat capacity and reflectivity spectra. Quantitative result of the present experiment supports the resonance two phonon absorption model proposed by Witowski and Grynberg2) in their interpretation of absorption below TO-phonon energy.

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TuP-PB5

PHONON SPECTRA OF MIXED CRYSTAL $Cd_xHg_{1-x}Te$ AND $Cd_xMn_{1-x}Te$

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Phonon vibration behaviour of the mixed crystals $Cd_xHg_{1-x}Te$ and $Cd_xMn_{1-x}Te$ has been investigated with absorption and reflection spectra in wavenumber region of 10 to 400 cm^{-1} and temperature region of 4.2 to 300K. A low frequency absorption band has been found in far infrared absorption spectra for the first time for both mixed crystal materials with different composition. The fine structures have also been observed in reflection spectra for both CdTe-like band and HgTe-like band of $Cd_xHg_{1-x}Te$. The low frequency absorption band has been attributed to TA phonon band modes by an estimation of phonon densities of states for the mixed crystal and induced by the disorder and "impurity" effects. The fine structures of the reflection band have been discussed with a poly-oscillator model and associated with the clustering effects and the coupling modes between LO phonon and plasmon.

Phonons **TuP-PB6**

URBACH TAIL AND PHASE TRANSITION OF FERROELECTRIC SEMICONDUCTOR SBSBR

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Antimony sulfo-bromide(SbSBr) is a ferroelectric semiconductor like antimony sulfoiodide (SbSI) with strong photoconductivity at room temperature. In perovskite ferroelectrics, SbSI and SbSBr, the band-gap energy cannot be determined precisely owing to the exponential character of the absorption edge, which is called Urbach tail. This tail is considered to originate in the strong electron-phonon interaction. In this paper we report on the first observation of the contribution of a soft mode to the Urbach tail in SbSBr. From this result we propose a phase transition mechanism of SbSBr in accordance with the so-called "pseudo-Jahn-Teller" effect, that is the phase transition is caused by the interaction of the two bands of different parities with transverse optic phonon (soft mode) at Γ point.

The transition temperature of SbSBr is $T_c=22.8$ K. The low T_c is advantageous in the study of the Urbach tail in the thermally less noisy condition above T_c. The crystal structure is highly anisotropic and it can be shown that only two B_{1u} optical phonons interact with excited electrons or an exciton. From the far-infrared spectroscopy one of B_{1u}s is the phonon with 220-270 cm^{-1} transverse-longitudinal-optical phonon splitting and the other is the soft mode with 40-90 cm^{-1} splitting at 300 K. The Urbach tail of SbSBr consists of two parts. One is due to 270 cm^{-1} mode and the other is due to the soft mode. The latter one makes the absorption coefficient of the lower energy part of the Urbach tail increase when the temperature approaches T_c from above and decrease below T_c. This behavior can be explained by the temperature dependence of the soft-mode frequency. The contribution of the soft mode to the Urbach tail is also observed in the measurement of the temperature dependence of the refractive index of SbSBr.

To understand the lattice instability of SbSBr in accordance with the pseudo-Jahn-Teller mechanism, we carried out the X-ray structural analysis at several temperatures. From the displacements of Sb and S atoms relative to Br atom at 11 K and the band-gap energy shift below T_c, the deformation potential due to the soft mode of SbSBr was estimated to be 1.9 eV/Å. This value gives the stable-limit frequency of the pseudo-Jahn-Teller mechanism and in SbSBr the paraelectric structure is stable only when the soft mode frequency is larger than 200 cm^{-1}, which is far larger than the soft-mode frequency of 40 cm^{-1} at 300 K. Then it is concluded that SbSBr has the structural instability due to the strong electron-phonon interaction.

LIGHT SCATTERING IN CuCl - EFFECT OF THE EXCHANGE INTERACTION

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The recent development of a new cw dye laser (polyphenyl) enabled us to study simultaneously resonant Raman scattering of CuCl in the Z_3-Z_{12} exciton region (3-3.4 eV) and the resonant Brillouin scattering near Z_3. The experiment is performed on as grown [111] platelets the surface quality of which can be ascertained by the observation of sharp Brillouin lines. The Brillouin shifts can be explained in the framework of the polariton theory applied for a two oscillator situation. A strong enhancement of the LO and LA scattering efficiencies is observed near Z_3, which is attributed to the Fröhlich mechanism. A comparable enhancement is also observed for the TA and TO phonons. It is interpreted as due to deformation-potential coupling. Such coupling should not give strong resonances near Z_3 in the absence of electron-hole exchange interaction. The strong resonance observed is attributed to exchange coupling. It provides a direct measure of this coupling.

The present experiment enables us to determine deformation potentials for acoustic and optic phonons. We confirm that these deformation potentials for CuCl are much smaller than in other zincblende-type materials because of cancellation between p- and d-electron contributions. The Fröhlich interaction is shown not to be very effective for the strongly localized 1s excitons of CuCl. Hence, the latter are expected to have a long lifetime. The variation of the exciton damping with energy is also discussed.

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TIME-RESOLVED RESONANT RAMAN SCATTERING AND HOT LUMINESCENCE AT THE 1s ORTHO-EXCITON IN Cu_2O

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The time dependence of one-phonon and two-phonon Raman modes resonantly enhanced at the 1s (Yellow) orthoexciton of Cu_2O is reported. The Raman modes are excited by a tunable picosecond dye laser and detected with subnanosecond time resolution by a time-delayed coincidence photon counting system.

The one-phonon mode is measured both in the selection rule allowed and forbidden configurations. In the allowed configuration a two-exponential decay with decay times: 0.7 nsec and 1.5 nsec is observed. In the forbidden configuration only a single exponential decay with 1.5 nsec decay time is determined. These results are explained in terms of hot luminescence from a 1s orthoexciton population which is initially polarized but becomes depolarized by cross relaxation among the triply degenerate orthoexciton states with time constant 0.7 nsec and finally decays into the paraexciton with lifetime of 1.5 nsec.

The decay of the two-phonon mode is found to change with the laser photon energy. This behavior is explained by the fact that the emission is again dominated by hot luminescence of the 1s exciton population. Since the exciton lifetime decreases with the exciton energy so the hot luminescence decay time also decreases as the laser photon energy is increased. The measured decay times are in good agreement with the exciton lifetimes calculated from exciton-acoustic phonon scattering in Cu_2O with no adjustable parameters.

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NEW RESULTS ON THE Si/SiO_2 INTERFACE

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We report on studies of Si/SiO_2 interfaces including samples grown on fully configured process lines and in research processing labs. The parameters varied include sample cleaning techniques, preoxidation steps, oxidation temperature, oxide thickness, post-oxidation annealing, and other post-oxidation steps compatible with spectroscopic analysis. Analytical techniques include X-Ray Photoemission Spectroscopy (XPS) coupled with chemical stop-flow etch profiling [1], etch rate analysis using ellipsometry and XPS, and electrical characterization.

We focus our discussion on the weak structures which fall in binding energy between elemental silicon and SiO_2 derived peaks in XPS spectra. We have previously identified these structures as originating from the Si^{+1}, Si^{+2}, and Si^{+3} incomplete oxidation states of silicon which comprise a submonolayer located at the Si/SiO_2 interface [1]. We find strong variation in the ratio of +1:+2:+3 suboxide intensity as a function of processing conditions and initial substrate material, and we associate these variations with step and dislocation distributions at the interface. In the case of Si(100) we expect the ideal interface to consist of +2 species alone, while the Si(111) ideal interface would consist of a monolayer of +1 or +3 species.

As support for these arguments we note that on the (100) surface the first oxidation results in a predominance of +1 and +3 intermediate oxidation states, while after several preoxidations the +2 state dominates. The +2 state is never seen to dominate a Si(111) interface, regardless of processing conditions. The specific ratios, and in particular the +3:+1 ratio, vary strongly with anneal conditions and substrate quality.

We find consistently that the incomplete oxidation states comprise between approximately .75 and .9 monolayers, and never more than 1 monolayer. We infer that the remainder of the interfacial layer consists of decorated defects, i.e. silicon species involving bonds to hydrogen and other contaminants. The only exception is oxides which are grown at temperatures higher than 1200°C, which apparently have disrupted interfaces. Finally, we note that etch rates are either suppressed or enhanced as the interface is approached, depending on anneal and oxidation temperatures.

Recent results of Hollinger and Himpsel [2] and Hattori and Suzuki [3] have suggested, respectively, that the (111) and (100) interfaces are substantially identical, and that the +3 state extends into the oxide layer. While we disagree with these conclusions, we demonstrate that their results are consistent with the above description of the interface.

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HYDROGEN ADSORPTION ON α-Sn AND InSb SURFACES STUDIED BY LEELS

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High resolution low energy electron spectroscopy has been applied to the study of hydrogen adsorption on InSb and the zero gap semiconductor α-Sn. Surfaces of InSb were prepared by Ar^+ sputtering and annealing in the standard manner. Films of α-Sn were heteroepitaxially grown by the MBE technique on top of substrates of InSb. Adsorption of hydrogen was induced by dissociation of an H_2 stream passing over a hot (∿2000°C) tungsten filament.

The spectrum of the $(\bar{1}\bar{1}\bar{1})$-Sb surface shows a vibrational loss at 1863 cm^{-1} (0.231 eV) which is close to that of the Sb-H stretching mode in amorphous[1] GaSb:H and to the mean value of the stretching frequencies of SbH_3. The (111)-In surface shows a loss at ∿1742 cm^{-1} (0.216 eV), this frequency being ∿40 cm^{-1} higher than the one obtained by Dubois and Schwarz[2] in adsorption measurements on InP. The (111) surface of α-Sn presents a weak and broad band centered ∿1790 cm^{-1} (0.222 eV), an intermediate value between those of In-H and Sb-H, as could be expected. This frequency also agrees with estimates based on the stretching mode of SnH_4. Comparison of the data for InSb with those of hydrogen adsorption on GaAs by Lüth and Matz[3] and those on InP and GaP by Dubois and Schwarz[2] reveal the same trend: Group-V-element hydrogen stretching mode in close agreement with the stretching mode of the respective hydride (SbH_3, AsH_3, PH_3) and group-III-element H vibration in agreement with the extrapolation[4] group V-H > group IV-H > group III-H for elements in the same row of the periodic table.

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THE THERMAL DESORPTION SPECTRA STUDY OF HYDROGEN CHEMISORPTION ON Si(100) CLEAN SURFACE

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The thermal desorption spectra of hydrogen chemisorbed on Si(100) clean surface have been measured by means of flash heating the sample after exposure to atomic hydrogen. The result shows that under low hydrogen exposure at room temperature exists only one desorption peak A at about 500° C , while a second desorption peak B with lower peak temperature appears as the exposure time increases. If the hydrogen exposures are carried out at elevated tempertures, the peak B does not appear in the desorption spectra when the exposure temperature is higher than 230°C, but the peak A still exists until the exposure temperature exceeds 530°C. Heat annealing after room temperature exposure can remove the peak B if the annealing temperature is higher than 350°C, and the peak A will also disappear at 530°C annealing. From all these features of thermal desorption, it is suggested that the peak A and B might relate to the desorptions of monohydride and dihydride phase on the Si(100) surface. The measured activation energies of desorption of these two phases are 52.9 Kcal/mol and 14.5 Kcal/mol respectively. It could be deduced from the peak asymmetry and the invariance of peak temperature with initial hydrogen coverage that the desorption of peak A occurs as a first order desorption process. The order plot has further confirmed $n=1$ for the desorption of monohydride. But if the measured activation energies of desorption are compared with the calculated binding energies of monohydride and dihydride by Verwoerd, it looks like that the monohydride phase is desorbed in the form of molecule which indicates that the mechanism of hydrogen desorption on Si(100) surface is different from the ordinary first order process.

7×7 RECONSTRUCTION OF Si(111) AND Ge(111)-Sn SURFACES
—— AN UNDERLYING MECHANISM FOR BINNIG ET AL'S MODEL ——

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A possible mechanism lying behind the adatom version of Binnig et al's model for the Si(111)-7×7 surface is proposed.[1,2] Based on the hexagonal Fermi surface of the 2-d ideal metallic surface band previously stressed by Tossati and Anderson, we introduce a symmetry-adapted RKKY type interaction among Si adatoms. Taking Fermi wave number for the nearly half-filled case, we calculate Ewald's sum of interaction energies for all kind of adatom arrangements in the n×n-type structure ($1 \leq n \leq 10$), finding that Binnig et al's model is energetically most stable. The present mechanism resolves both the problems of the long-range periodicity and of local arrangements in the surface unit cell. In a similar way, the coverage-dependent 7×7 → 5×5 transition on the reconstructed Ge(111)-Sn surface is explained by a small change in Fermi wave number caused by electronic charge transfer from Sn atoms to the Ge ideal surface band. An applicability of the theory to molecular-cluster versions of Binnig et al's model is also suggested.

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17th International Conference on the Physics of Semiconductors

Surface and Interface **TuP-PC5**

INTERFACIAL DEEP LEVELS RESPONSIBLE FOR SCHOTTKY BARRIER FORMATION AT SEMICONDUCTOR/METAL CONTACTS

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We present calculations that explain the main experimental facts concerning Schottky barriers at Si/transition-metal silicide and III-V/metal contacts. At Si/transition-metal silicide interfaces the Schottky barriers are due to Fermi-level pinning by interfacial dangling-bonds, a mechanism which accounts for the following facts: (i) The barrier heights are independent of transition-metal, to within ≈0.3 eV; (ii) On the 0.1 eV scale there are chemical trends in barrier heights for n-Si, with the heights decreasing in the order Pt, Pd, and Ni; (iii) Barriers form at low metallic coverages; (iv) Barrier heights are independent of silicide crystal structure or stoichiometry to ±0.1 eV; and (v) The barrier heights for n-Si and p-Si add up to approximately the energy of the band gap.

The following facts concerning III-V (e.g., GaAs, InP) Schottky barriers can be understood in terms of Fermi-level pinning by interfacial antisite defects (sheltered by vacancies) at semiconductor/metal contacts: (i) The barrier heights are almost independent of the metal in the contact; (ii) The surface Fermi levels are pinned at sub-monolayer coverages and the pinning energies are almost *unaffected* by changes of stoichiometry or crystal structure; (iii) At low metallic coverages the sums of the surface barrier heights for n-type and p-type semiconductors are, in many cases, less than the band gap energies; (iv) The concentrations of donors and acceptors responsible for Fermi-level pinning in GaAs are nearly equal; (v) Cleavage of GaAs appears to produce one type of defect and chemisorption another; (vi) Annealing of p-GaAs/metal junctions causes the Schottky barriers to disappear at the As_{Ga} annealing temperature (not at the vacancy annealing temperature), but the n-GaAs Schottky barrier remains; (vii) The surface Fermi energies of $Al_xGa_{1-x}As$ alloys overlaid with Au, Al, and In are slightly different.

The apparent dependence of barrier height on chemical reactivity in, for example, n-InP/metal contacts can be understood in terms of switching of the dominant Fermi-level pinning defects from antisites (for non-reactive metals) to vacancies (for reactive metals).

The complicated dependence of Schottky barrier height on alloy composition for (III-V alloy)/Au contacts is explained in terms of Fermi-level pinning by cation on anion-site defects.

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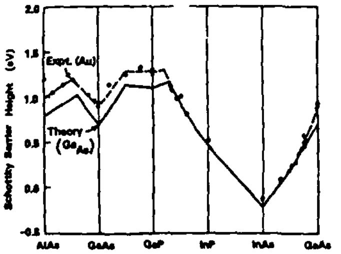

NOVEL POLYPHOSPHIDE SEMICONDUCTORS WITH GOOD INTERFACIAL PROPERTIES TO InP

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We are reporting, for the first time, on the surface and bulk properties of amorphous polyphosphide thin films and their interface properties with InP. These materials are derived from low symmetry crystalline compounds, MP_{15} (M = alkali metal) in which P atoms are arranged in pentagonal cross-section tubes and alkali metal atoms bridge parallel tubes.[1] The amorphous films have a microscopic structure based on units of P tubes which leads to low density of dangling bonds and the presence of intermediate range order. We have prepared polyphosphide thin films by vapor transport methods (MBE, CVD, Sputtering). By means of electrical and optical measurements we have determined that polyphosphides are high resistivity ($\sim 10^{10}$ Ωcm) semiconductors with a bandgap of $\sim$1.8 eV.

Amorphous polyphosphide films provide good passivation of the InP surface because of the chemical and physical continuity at the interface. By means of C-V characterization of MIS diodes, we have shown that the density of surface states on the <100> face of undoped ($\sim 2 \times 10^{15}/cm^3$) InP has been reduced to $\sim 10^{10}/cm^2$ eV at 0.2 eV below CBM. This is the lowest reported value for passivating layers.[2] The shape of the density distribution is consistent with the position of the pinned Fermi level on InP surfaces.[3] With measured dielectric constant of $\sim$10, and breakdown field of $\sim 10^6$V/cm, these structures provide possibilities for MISFET devices on InP.

We also demonstrated that by cosputtering with 0-2% Ni, the resistivity of polyphosphide films can be controlled over eight orders of magnitude. Reduction of the conductivity activation energy from 0.9 to 0.2 eV accompanied by $\sim$0.2 eV change in the optical gap, is an indication that the Fermi level has been unpinned. High current, up to 1A/cm^2 at 1V are achieved in metal-semiconductor structures. The I-V characteristics are strongly non-linear. This effect is attributed to a transport mechanism in an amorphous material in which the electronic coherence length is commensurate with intermediate range order.

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INVESTIGATION OF THE Si(111) SURFACE IN UHV: OXIDATION AND THE EFFECT OF SURFACE PHOSPHORUS

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The importance of controlling and characterizing the electronic properties of Si-SiO_2 and Si-metal interfaces has prompted great interest in the atomic-scale chemistry and physics of those interfaces. Recently, we have demonstrated that optical second-harmonic generation (SHG) can be an effective *insitu* probe of interfaces as thin as 1 or 2 atomic layers.[1] Here we report an investigation of the clean Si(111) (7x7) surface under oxidation and thermal annealing using SHG as well as Auger Electron Spectroscopy (AES) and Low Energy Electron Diffraction (LEED).

The Si(111) wafers (0.010" thick, n-type, $10^{15}/cm^3$ P-doped) were cleaned of oxygen in UHV (7×10^{-10} torr) by annealing at 1000°C for a few mins. and considered clean when the ratios of AES peaks were $0_{507}/Si_{92} < 5 \times 10^{-4}$ and C^{270}/Si^{92} = 1.5%.. The great sensitivity of SHG to surface electronic properties made it possible to follow the early stages of oxidation. For 10^{-6} torr 0_2 dosages, the SHG dropped to 50% of its clean surface value and saturated in ~100L upon the formation of the chemisorbed oxygen layer[2] at room temperature, to 40% and saturated in ~70L for thermal oxidation at 800°C. The 10% difference in SHG was correlated to the formation of 1 or 2 layers of subsurface oxide, presumably Si-0 intermediate complexes.[3]

The SHG for a nominally clean Si sample decreased as the temperature was raised. AES indicated that this change was due to the segregation of P to the surface at room temperature and its diffusion into the bulk at elevated temperatures. Because the sample contained $10^{15}/cm^3$ P impurities, the changes in SH could be due to no more than 2% of a P monolayer on the surface. While the diffusion and segregation of P on the clean Si surface was reversible for short heating cycles, it was not reversible to such cycles after the sample was exposed to 120L of 0_2, even when AES indicated that the heating cycle did not change the surface atomic composition. The latter indicated the formation of new SiP or SiP_xO_y complexes on the oxidized surface. Previous work on heavily ($10^{20}/cm^3$) P-doped Si shows evidence for a strong attractive surface potential for P.[4] The importance of P segregation on oxidation for Si with low levels of P-doping has not been appreciated previously.

Further oxidation and thermal annealing cycles caused the accumulation of P at the surface and in the near surface bulk. As the surface P concentration increased, the 7x7 LEED pattern became more difficult to see and gradually a sharp ($\sqrt{3} \times \sqrt{3}$) R30° pattern appeared (at room temperature). This is the first observation of such a LEED pattern. Because there could be no more than 2% of a P monolayer on the surface, the sharp ($\sqrt{3} \times \sqrt{3}$) R30° pattern is probably not due to a P overlayer but rather due to a P-induced reconstruction of the Si surface atoms. Similar impurity-induced surface reconstructions have been observed on Mo and W (001) surfaces.[5]

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IONIC CONTRIBUTION TO SILICON-METAL BONDING: Si(111)-Ca INTERFACE REACTIONS

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The low d-count of alkali earth metals and their small electronegativity compared to Si make them interesting test systems for the existing models of Si-metal interface bonding that rely upon the dominant interaction of metal d with Si-p states. We present a Synchrotron Radiation Photoemission study of interface reactions at the Si(111)-Ca junction. The interfaces were formed in situ through metal deposition on cleaved substrates at room temperature.

The earlier evolution of the interface (Ca coverage below 1-2Å) involves the removal of the intrinsic Si surface state emission, a large reduction (2 eV) of the semiconductor surface work function and the establishment of the equilibrium Schottky barrier. For metal coverages above 2Å, dramatic changes occur in the experimental lineshape of the Si 2p and Ca 3p core levels. Such modifications correspond to the emergence of two chemically shifted components in the Si 2p line and to changes in the intrinsic loss spectrum associated with the Ca 3p cores. The unprecedented magnitude of the Si 2p chemical shifts (1.4 and 2.1 eV) emphasize the substantial ionic contribution to the local chemical bonding for this interface. The changes in the collective loss spectrum associated with the Ca 3p excitation are consistent with the progressive modification of the electronic valence states within 2 eV of the Fermi level and indicate that two well defined reaction products appear sequentially at the interface for metal coverages above 2Å. The profound differences in the electronic structure of these two phases reflect the variation in local stoichiometry of two silicide-like interface compounds.

Resonant Photoemission as a Local Probe for Interfaces - An Application to Al-GaAs(110)

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Very recently, we reported1) the observation of resonant enhancement of photoemission cross-section from Al-GaAs surfaces in the vicinity of Al 2p core excitation threshold. The phenomena were successfully interpreted as Fano type resonances due to the interference between direct $2p(al)^6v(Al)^n$-$2p(Al)^6v(Al)^{n-1}c$, and indirect $2p^6v(Al)^n$-$2p(Al)^5v(Al)^n ex$-$2p(Al)^6v(Al)^{n-1}c$ processes. Here 2p(Al), v(Al), ex, c stand for Al 2p state, Al originated valence band state, Al 2p core exciton, and continuum state, respectively.

Because of the intrinsically localized nature of the Al 2p core exciton on the surface (interface), this type of resonant photoemission is expected to serve as a sensitive probe for chemical bonding status and electronic structure at surfaces and interfaces. We have exploited this resonance to detect changes in bonding state of Al atoms during Al-GaAs(110) interface formation in the range of Al coverage between 0.06 and 3.7 monolayers (ML).

Three stages were found in the course of the interface formation. Between 0.06 and 0.26 ML coverage, the resonance features extremely broad profile, indicating the occurence of rapid direct recombination of the core exciton. This suggests the exciton localization is very strong. Width of the resonance profile suddenly becomes narrow at the coverage of 0.37 ML, and at 0.62 ML it slightly increases but still much narrower than that in the first stage. When the coverage exceed 9.5 ML, a "metallic" state is distingulshable in the energy range between E_f and about 2 eV below E_f in the valence band photoemission spectra. The photoemission cross-section of this "metallic" state also exhibits weak resonance enhancment. The variation of intensities, peak positions, and lineshapes of Al 2p, Ga 3d, and As 3d spectra during the interface formation were found to correlate very well with the evolution of resonance proflie described above.

The present results supports three stage model for the Al-GaAs(110) interface formation, that is , successive occurence of the following stages.

i) nearly isolated Al chemisorption or very small Al cluster formation in the range below 0.26 ML.
ii) Al-Ga replacement reaction suddenly triggered at around 0.3 ML. Al atoms are supposed to be replaced with Ga atoms in the second layer, leaving the first layer unchanged.
iii) further progress of Al-Ga replacement reaction with accumulation of "free" Ga and "metallic" Al. The "free" Ga are very likely to be under the "metallic" Al.

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TuP-PC10

CRYSTALLOGRAPHIC AND ELECTRONIC STRUCTURE OF ION-CLEANED AND MBE-GROWN Si(001) SURFACES

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We have used a combination of reflection high energy electron diffraction (RHEED) and angle resolved photoemission to investigate the reconstruction and surface electronic bands of Si(001). Some surfaces were prepared by cleaning with low energy ($<$ 3 keV) Ne$^+$ ions and annealing below 650°C, while others were grown in-situ using an e-beam evaporation source, a technique now called "silicon MBE". In both cases the most commonly observed reconstruction was Si(001)-c(4x4), although with ion-beam cleaned surfaces it was possible to obtain a Si(001)-1x2+2x1 structure with low temperature annealing. The grown surfaces, obtained at a substrate temperature of $\approx$ 650°C, were c(4x4). We discuss these results in terms of Chadi's tilted dimer model for Si(001) surfaces[1], and attempt to relate them to the more usually observed Si(001)-2x1, which calculations show to be a higher energy form.

The photoemission measurements of the ion-bombarded and annealed as well as the grown surfaces show in all cases strong surface state emission in the energy region just below the valence band maximum, similar to published results[2]. We compare the spectra from the differently prepared surfaces and again relate our results to calculations based on the tilted dimer model. If this is taken as the basic unit, the observed surface structures can be derived from it by allowing for various degrees of one-dimensional surface disorder.

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TuP-PC11

A Unified View of Schottky Barrier Formation

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At a metal-semiconductor interface, there is generally a continuum of states of the metal which lie energetically in the semiconductor gap,[1] and decay exponentially within the semiconductor. Elsewhere,[2] in what may be viewed as a natural extension of work by Heine[1] and by Louie et al,[3] I observed that these "metal-induced gap states" give rise to a local density of states at the Fermi level (E_F) in the semiconductor which is sufficiently large that, for the first few layers, the semiconductor must be viewed as metallic. In the strongly metallic limit, the Fermi level in the semiconductor is therefore determined by local charge neutrality, as at any metal-metal interface. Local charge neutrality requires E_F to lie near that energy in the gap where the (evanescent) states cross over from primarily valence to conduction character. This energy represents a "canonical" Fermi level which is characteristic of the semiconductor, and which can be calculated directly from the bulk semiconductor bandstructure. Such metallic pinning of E_F is expected to occur at any metal-semiconductor interface, regardless of the detailed interface structure, and of the presence or absence of defects at the interface. (Structural factors may however effect the precise value of the barrier height.)

Here I present results of calculations for several semiconductors (including new results for InP and GaSb) which give "canonical" Fermi levels in good agreement with those determined by barrier-height measurements for interfaces with most metals of practical interest. In addition, results for a model metal-semiconductor interface are presented. In that case, the full electronic structure of the (ideal) interface is calculated selfconsistently. In accord with the discussion above, E_F falls near the valence-conduction crossover point in the semiconductor gap when the electronegativity difference between metal and semiconductor is small. Moreover, the dependence of barrier height on metal electronegativity is weak for small energy gaps (strong pinning): in that case the "canonical" Fermi level position accurately describes the barrier for all reasonable values of metal electronegativity. However for large-gap semiconductors the dependence of barrier height on metal electronegativity approaches the Schottky (unpinned) limit. This is the first *direct* calculation of the dependence of barrier height on metal.

These results provide the most unified perspective to date on Schottky barrier formation. In particular, elemental and III-V semiconductors are treated on an equal footing. Most important, barrier heights are predicted *quantitatively* on the 0.1 eV level, with no adjustable parameters, and no assumptions about interface structure or hypothetical defects. Trends with metal electronegativity and with semiconductor gap size are also in accord with experiment.

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$Si-SiO_2$ INTERFACE STRUCTURES ON Si(100), (110), AND (111) SURFACES

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The distributions of intermediate oxides(SiO_x, $0 < x < 1$) in ultrathin oxide films formed on (100), (110), and (111) surfaces were investigated by using nondestructive measurements of Mg Kα radiation excited Si 2p photoelectron spectra, synchrotron radiation($h\nu$ = 130 eV) excited Si 2p photoelectron spectra, and X-ray excited Si KLL Auger electron spectra. The oxide films were grown in dry oxidizing ambient at 600-1000 °C. The experimental observations can be understood as follows: (1) the abrupt interfaces are formed for three crystal orientations; (2) the interface formed on (100), (110), and (111) surface consists mainly of SiO, the mixture of SiO and Si_2O, and Si_2O, respectively; (3) the interface structures depend on the oxidation temperatures; (4) the interface structure on (100) surface are the same in the range of oxide film thickness 0-100 Å; (5) Si_2O_3 is distributed in the oxide films near the interfaces for three crystal orientations.

RECONSTRUCTIONS OF THE GaAs(100) SURFACE: CORE-LEVEL PHOTOEMISSION STUDY

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High resolution synchrotron radiation photoemission measurements and theoretical calculations are reported for three MBE GaAs(100) surface reconstructions of the As-rich c(4×4) and c(2×8) and the Ga-rich 4×6. Detailed comparison of Ga(3d) and As(3d) core lineshapes provide the first resolution of amorphous As capping layer from the features characteristic of atomic displacement in the ordered reconstructed surface. The As(3d) lineshape was least square fit by multi-gaussian peaks with the same FWHM. We measured the spin-orbit splitting, 0.7 eV, and the branching ratio, 0.66, using the As(3d) lineshape from bulk GaAs and from an amorphous As film. Core level decompositions were reproduced for three different experimental runs on the same reconstruction. The fitting of a lineshape taken with different photon energies showed a reproducibility within the experimental uncertainty of ±0.05 eV for the position and ±5% for the intensity.

The GaAs(100) surface As coverage (estimated from the surface peak intensities) increased, going from 4×6 to c(2×8) to c(4×4). In addition to the bulk As(3d), three doublets were necessary to obtain a best least square fit for the c(4×4) surface, while two doublets were sufficient for the 4×6 and c(2×8) surfaces. We attributed the extra c(4×4) feature at the higher binding energy to the formation of As-As bonds. From the intensities of the As(3d) components, we estimate the thickness of such an amorphous layer to be 0.25±0.1 of a monolayer. Larsen et al.[1] was unable to separate the intrinsic surface component at higher binding energy from this amorphous As at the surface.

Our findings provide a complete picture of the c(4×4) surface. The surface has an excess of a quarter of a monolayer of amorphous As which is more tightly bound than in the bulk GaAs. We attribute the other two surface As doublets to both symmetric and asymmetric As dimers.[2] Their intensities agree with calcu-lations of the GaAs(100) reconstruction. The energy positions are modified due to the formation of As-As bonds capping the c(4×4) surface. The GaAs(100) c(2×8) and 4×6 surface reconstructions exhibit one doublet on each side of the bulk one. The energy position and the intensity of these peaks are characteristic of the surface atomic rearrangement involved. The atomic rearrangement of the surface As is distinct enough to characterize the different GaAs(100) surface reconstructions.

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Surface and Interface TuP-PC14

DISLOCATION MEDIATED MELTING OF SILICON-METAL INTERFACES

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ABSTRACT

It is known that the silicide formation between silicon and transition as well as noble metals occurs at 0.3-0.4 of the melting temperature of silicon. It is proposed that the chemical reaction is preceded by an interfacial melting process due to dislocation generation via the Kösterlitz-Thouless mechanism. The overall softening of the Debye temperature at the interface leads to the low temperature chemical reaction observed. A softening mechanism due to screening of the silicon lattice by the metal overlayer is suggested(1).

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Column V Elements on III-V Compound Semiconductors: the InP(110)-Sb(ϑML) Interface

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The atomic structure and chemical composition of InP(110)-Sb(ϑML) interfaces ($0.25ML<\vartheta<20ML$), formed in UHV on cleaved InP, have been studied with low energy electron diffraction (LEED) and Auger electron spectroscopy (AES). These interfaces exhibit three distinct growth mechanisms. In the first stage ($\vartheta<1ML$), Sb forms an ordered (1x1) structure, in registry with InP. The Sb p-like electrons form directional covalent bonds with the substrate. The growth proceeds by 2-D nucleation in monolayer-height patches which exhibit a regular dimension in the $[\bar{1}10]$ direction and produce a characteristic splitting of the LEED spots. The overlayer structure preserves the symmetry of the InP(110) unit cell. These patches coalesce at 1ML and form a continuous and ordered (1x1) structure with two Sb atoms/unit cell. The presence of two inequivalent Sb has been confirmed by photoemission studies [1]. A LEED determination of the interface atomic geometry is presently being performed. This geometry is expected to be comparable to that of GaAs(110)-Sb(1ML). At this interface, the overlayer consists of Sb chains bound to the nearly unrelaxed substrate with atoms occupying sites close to those of the first missing GaAs layer [2]. In the second stage ($1ML<\vartheta<10ML$), Sb has a larger surface mobility and undergoes 3-D nucleation. This produces a sub-exponential attenuation of the substrate AES peaks as a function of coverage. The increase in mobility is probably due to the saturation of the first-layer Sb bonds by the substrate and neighbor Sb atoms. The passivity of the first Sb layer is also demonstrated by its high resistance to oxidation (as compared to bulk Sb). The third stage of the overlayer growth ($\vartheta>10ML$) begins when the 3-D Sb clusters entirely cover the first layer, as indicated by the disappearance of the LEED pattern. Beyond this point, Sb forms a continuous amorphous film.

In addition to these structural properties, we will discuss the abruptness of the interface and the absence of Sb-substrate reaction, expected from thermodynamic considerations. We will compare these results with earlier findings for Sb on GaAs and comment on the role of column V elements vs. column III elements in the epitaxial growth of III-V compound semiconductors.

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Surface and Interface **TuP-PC16**

MICROSCOPIC STUDY OF THE GaP-Si INTERFACE*

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The GaP-Si system is a prototypical semiconductor heterojunction interface due to the matching properties of its components. We investigated the fundamental interface parameters of this system, band discontinuities and built-in potential, using synchrotron-radiation photoemission as a microscopic probe. In particular, we performed for the first time parallel and correlated local measurements of the valence band and conduction band discontinuities using different photoemission techniques which enabled us to remove the most severe uncertainities affecting previous indirect photoemission measurements of the valence band discontinuity. To investigate the crucial question of the influence of local order and disorder on the interface parameters the experiments were performed on disordered Si overlayers deposited on GaP and then on the same overlayers ordered by annealing. The results unambiguosly demonstrated that the ordering did not affect the discontinuities within the experimental uncertainity of 0.1 eV. This and similar results recently obtained on ZnSe-Ge confirm the basic message of the Katnani-Margaritondo study,[1] i.e. the magnitude of microscopic contributions to the discontinuities does not exceed 0.15-0.2 eV. Therefore, they also confirm the first-order role of the bulk band structures of the components in determining the band discontinuities, as suggested for example by Harrison.[2] On the contrary, the substrate band bending and therefore the built-in potential was dramatically changed by the overlayer ordering process. Therefore, annealing processes can be used in heterojunction technology for a selective control of the built-in potential which does not severely affect the other fundamental interface parameters.

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ADSORPTION OF ALKALI METALS ON Si(111)SURFACE

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Adsorption of alkali metals at submonolayer and monolayer coverages on Si(111) 7x7 surface are studied. Second derivative electron energy loss spectroscopy (ELS) and Auger electron spectroscopy under ultrahigh vacuum conditions are employed. Coverage dependent ELS studies using 100 eV primary electron energy show a systematic reduction in all surface loss features. Sharp losses due to the formation of interface states are observed at ELS energies 1.9 and 3.5 eV. These losses are associated with the interactions of alkali s electrons with dangling bond surface states near valence band maximum (VMB) and with Si bulk π-bands 0.4 eV below VBM,respectively. With increasing alkali coverage, decreases of 0.86 and 1.1 eV are observed in the alkali s and p core level transition energies, respectively. Excitonic alkali p core transitions are associated with the ionic nature of the alkali bonds.

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CYCLOTRON RESONANCE ABSORPTION AND EMISSION BY HOT CARRIERS IN GERMANIUM IN STRONG ELECTRIC AND MAGNETIC FIELDS

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The work concerns with the cyclotron resonance physics of hot carriers in strong electric and magnetic fields at the energies high enough up to the intense electron and hole scattering by optical phonons. The very peculiar phenomena are observed at these conditions in germanium caused by deviations of the semiconductor bandstructure from a parabolic one, by intervalley and intersubband carrier transitions, by deformation and inversion of the carrier distribution functions and other effects, which appear at high carrier energies.

The classical theory of cyclotron resonance phenomena in crossed fields for the many valley's and warped bands under inelastic optical phonon-carrier scattering is developed for Ge as an exemple. The results of experimental investigations of the cyclotron resonance of hot electrons and holes in Ge in crossed fields are reported, which measured at liquid-helium temperatures at field E up to 2 kV/cm and H up to 25 kG in submillimeter range λ = 0,3 - 2 mm, corresponded to the conditions. The discovered effects (shift and suppression of the lines, appearance of the new lines and the observed cyclotron absorption and emission characteristic peculiarities) are adequatly explained in the frame of the developed theory as a result of the bandstructure complicity and the different dynamical behaviour of carriers on clossed and disclossed trajectories in active and passive p-momentum space regions in $E \perp H$ at $1/\tau \ll \omega_c < 1/\tau_0$ (ω_c - cyclotron frequency, τ and τ_0 - impulse relaxation times for acoustic phonon (impurity) scattering of carriers at $\varepsilon < \hbar\omega_0$ and for optical phonon scattering of carriers at $\varepsilon > \hbar\omega_0$, $\hbar\omega_0$- optical phonon energy).

ANISOTROPIC MOBILITY AND ELECTRON-PHONON INTERACTION IN BLACK PHOSPHORUS

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Black phosphorus is a layer-like narrow gap semiconductor with a direct gap of about 0.3 eV at point Z in the first Brillouin zone[1]. Measurement of mobilities and cyclotron effective masses of carriers in black phosphorus single crystals was reported for both of p and n types recently[2,3]. The results show that mobilities obay the $T^{-3/2}$ law typical for acoustic= phonon scattering in the temperature ranges from 50 to 200 K for p type samples and from 80 to 220 K for n type samples and the anisotropy of mobilities is remarkably different from that of the inverse effective masses, especially the mobility in the y direction parallel to zig-zag bonds in plane is larger than that in the z direction perpendicular to plane, while the inverse effective mass in the y direction is smaller than that in the z direction.

We have investigated the anisotropy of mobility in the temperature range where acoustic phonon scattering is predominant by using the deformation potential approach for electron-phonon interaction and by using lattice vibrations calculated in terms of the force constant model[4].

From a symmetry consideration, the carrier-acoustic phonon interaction is given by

$$\delta E = D_{xx}e_{xx} + D_{yy}e_{yy} + D_{zz}e_{zz}$$

where $D_{\alpha\beta}$ is the deformation potential tensor and $e_{\alpha\beta}$ is the strain tensor produced by phonon field.

The anisotropic mobilitiy has been calculated by solving the Boltzmann equation obtained by Taylor[5] in terms of the vector mean free path. The results show that it is difficult to explain the anisotropic mobility by using the anisotropic lattice vibrations due to the layered structure of black phosphorus alone and, to do so, it is needed to assume a large anisotropy in the deformation potential tensor.

In order to make the origine of such an anisotropic deformation potential clear, we have investigated the dependence of energy levels at point Z on changes in structural parameters produced by an accoustic phonon with small wave vector. As a result of it, it is shown that the strong anisotropy of the deformation potential comes from the fact that the decrease of the interlayer distance reduces the gap energy, while that of the bond length enlarges it.

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TuP-PD3

A.C. BAND CONDUCTIVITY IN COMPENSATED SEMICONDUCTORS EFFECT OF POTENTIAL FLUCTUATIONS

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In S.I. semiconductors, long range potential fluctuations drastically change d.c. (1) and a.c. conductivity because : i) local band carrier conductivity is fluctuating with the local potential, ii) ionisation of deep centers is no more uniform. We derive the macroscopic a.c. complex conductivity $\sigma_{ac}(\omega,T) + i\omega\varepsilon_{ac}(\omega,T)$ due to band carriers in presence of a gaussian distribution of fluctuations of standard deviation $\Gamma/\sqrt{2}$. σ_{ac} starts from σ_{dc}, grows as ω^{s} , $(s < 1)$, then tends to a limit σ_{∞} at very high frequency. The total carrier density $n_o = \sigma_{\infty}/q\mu$ is expressed as fonction of Γ, and of center density and energy. Comparison with experiment : 1) S.I. GaAs:Cr. Our data from 0.1 Hz to 2×10^{8} Hz between 240 and 410°K are accurately fitted with $\Gamma = 120$ meV ; moreover this leads to a perfect agreement between experimental $\sigma_{\infty}/q\mu$ and $n_o(T)$ calculated by considering ionization of EL2 and HL1 levels. 2) Interpretation of M.POLLAK and T.H. GEBALLE (2) data in X-Si (n° 13-8) at low temperature. A shallow donor (possibly nitrogen) is likely present, so the P level is not compensated and $N_d^{+} \propto \exp(-E_d/2kT)$. In n° 13 P ionization appears at $T_i = 20.5$°K (P.G. fig.5) where $N_d^{+} = 2.28 \times 10^{12}$ cm^{-3}, leading to $\mu = 178$ $cm^{2}/V.s$; in n° 8 $T_i = 12.5$°K at which $N_d^{+} = 6.6 \times 10^{8}$ cm^{-3}, and $\mu = 107$ $cm^{2}/V.s$. These mobilities are likely for band carriers (which were not considered by P.G.). Experimental σ_{dc}, σ_{ac} curves are very accurately predicted, considering $\Gamma = 4.06$ and 7.85 meV respectively. It is concluded that in X-Si, as in S.I. GaAs, band conduction predominates and completely hides hopping. 3) a-Si, a-Ge : ABKOWITZ (3) σ_{ac} data, our low temperature data on a-Si, those of LONG (4) on a-Ge may also be precisely accounted for, by considering band carriers, with mobilities of the order of 10^{-3} to 1 $cm^{2}/V.s$, associated with potential fluctuations. This suggests that, in amorphous semiconductors too, band conduction process is likely significant. Thus, in most semiconductors, observation of anomalous conductivity likely results from band conduction associated with potential fluctuations, rather than from hopping.

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QUANTUM HOT-CARRIER TRANSPORT IN INHOMOGENEOUS SYSTEMS*

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The limitations of the Boltzmann equation in describing carrier transport in semiconductors (especially in small devices) in the presence of high electric fields are well known, and lead to a need for more powerful methods to describe such a highly non-equilibrium situation. Here, we study hot-carrier transport in semiconductors induced by a strong, space dependent external electric field. We allow the system to be inhomogeneous in space and assume sufficiently high carrier concentrations to ensure the dominance of the carrier-carrier interaction over the carrier-lattice interaction. Starting from the Heisenberg equations describing the system microscopically we use the non-equilibrium operator technique to derive (macroscopic) balance equations for the electronic system. Our balance equations give the evolution of the local particle number, momentum, and energy to lowest order in the electron-phonon coupling and the thermodynamical forces due to the inhomogeneities in the system. The influence on the evolution of the system at one region of space due to other regions and by the previous history of the system is described by quantum correlation functions of pairs of operator densities at different time and space points. Although the carrier-carrier interaction is included in the approach via a local two-particle potential we suggest an alternative treatment of its overall effect in the spirit of the Vlassoo equation for simplicity. Consideration of new terms, not occurring in the Boltzmann treatment, shows that these effects can be significant in heterostructures.

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TuP-PD5

THE CONDITIONS OF RADIATION AMPLIFICATION BY HOT HOLES IN p-Ge UNDER E ⊥ B FIELDS

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The electric and magnetic field dependent cross-section for free carrier absorption in 40-500 μm wavelength range in p-type Ge is investigated theoretically. The absorption cross-section is calculated by integrating over the momentum space of the absorption probability weighted with the hot hole distribution functions. The probability of the acoustic and optical phonon as well as impurity ion assisted photon emission and absorption by the free holes are accounted for in the framework of a quantum-mechanical approach under an effective mass approximation. Hot hole distribution functions are obtained by the Monte Carlo simulation of a single particle history in the momentum space.

The radiation absorption by the light- and heavy-holes assisted by the optical phonon emission increases sharply with E and dominates under strong heating. The impurity ion assisted free carrier absorption decreases significantly as the hole heating increases. This contribution can become negative. The hole population inversion of the energy states involved in the direct intersubband optical transitions can lead to the amplification of the radiation corresponding to these transitions in the wavelength range $\lambda = 40 \div 200$ μm. The necessary conditions are considered.

ULTRAFAST TRANSIENT TRANSPORT IN POLAR SEMICONDUCTORS

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Calculations of transport coefficients have been based on Monte Carlo computer techniques or kinetic equations, which are founded on the use of some form of relaxation-time approximations, with thermodynamic variables and scattering frequencies taken as phenomenological parameters. However, all these quantities are dependent on the instantaneous thermodynamic state of the system, which is evolving due to the irreversible relaxation processes that develop in the media.(1) We construct a theory, based on the nonequilibrium statistical operator method,(2) to derive nonlinear and non-markoffian transport equation in highly photoexcited plasma in semiconductors. We obtain expressions for the time-dependent nonequilibrium mobility, $\mu(t)$, and diffusion coefficient, $D(t)$, in direct-gap polar semiconductors. It is shown that, under certain restrictions, a Einstein-like relation holds for the instantaneous values of these coefficients. Numerical calculations appropriate to the case of GaAs under high levels of excitation is done. We demonstrate that there exists two different regimes in the behaviour of $\mu(t)$ and $D(t)$: (i) for LO-phonon effective temperatures, T^*_{LO}, roughly above half their Einstein temperature, θ_o, μ and D increase monotonously in time as carriers cool down after laser pulse excitation, and (ii) for T^*_{LO} roughly below $\theta_o/2$ and high levels of electron excitation a mobility and diffusion "overshoot" occurs in the early stages of relaxation processes following optical pumping. A brief report on the time-evolution of the drift velocity of carriers in zone-centre valleys of GaAs is presented in A.R. Vasconcellos and R. Luzzi, Phys. Rev. B <u>27</u>, 3874 (1983).

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OSCILLATORY BEHAVIOUR OF THE HALL-FACTOR IN CROSSED ELECTRIC AND MAGNETIC FIELDS[*]

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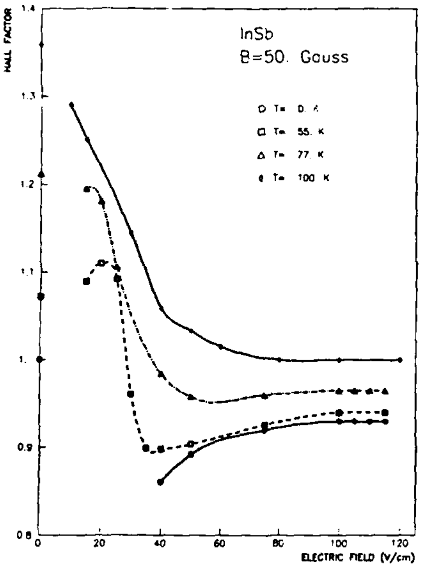
The Monte Carlo (MC) method is applied to find the Hall-factor (r_H), the drift mobility and the Hall angle for electrons in a parabolic band subjected to crossed electric (E) and magnetic fields and scattered by longitudinal optical phonons. A comparison is made with the results of 1) the "two-circle model", 2) the classical model of Komiyama et al. and 3) a drifted Maxwellian approach. We found that for sufficiently low temperatures (T<100 K), r_H shows pronounced structure as a function of the electric field (see figure) which is a result of the competition between 1) the streaming motion behaviour dominant at high E and 2) the confinement of the electron motion in velocity space due to the magnetic field (dominant at small E). Very recently Brazis et al.[1] predicted a similar oscillatory behaviour of r_H in GaAs.



The influence of non-parabolicity and other scattering mechanisms (i.e. ionized impurities and acoustical phonons) on the oscillatory behaviour of r_H is investigated. The experimental conditions for InSb under which such an oscillatory behaviour of r_H can be found is carefully examined.

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TuP-PD8

MAGNETO-TRANSPORT AND ELECTRONIC PHASE TRANSITION IN GRAPHITE IN HIGH MAGNETIC FIELDS

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Recently, a striking anomaly was discovered in the magnetoresistance of single crystals of graphite in high magnetic fields (applied parallel to the c-axis) at low temperatures. Yoshioka and Fukuyama explained the anomaly as being do to the electronic phase transition to a CDW state. To obtain a comprehensive picture of the phase transition, the magnetotransport properties of graphite were investigated in pulsed high magnetic fields up to the megagauss range at low temperatures. In non-destructive fields up to 45 T, it was found that with increasing temperature the amount of the resistance jump at the anomaly as well as the slope of the jump are increased. The a.c. magneto-resistance was measured at frequencies up to 150 MHz, and the anomaly was found to become less distinct at high frequencies. The measurement of the Hall effect revealed that no prominent anomaly is observed in σ_{xy} at the critical field where σ_{xx} shows the anomaly. These results are analysed based on the CDW model. To explore similar phase transitions which might occur at higher fields, the a.c. magnetoresistance was measured in megagauss fields. A kink was observed in the resistance v.s. field curve at 79 T, in addition to the anomaly reported above. Theoretical analysis of the Landau levels and the critical field for the CDW, SDW and the excitonic phase transition showed that the observed kink may be ascribed to the crossover of the n=0 spin up state at the K-point with the Fermi level.

TuP-PD9

ANOMALOUS TRANSPORT IN BORON CARBIDES*

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DC conductivity, Hall effect, Seebeck coefficient and thermal conductivity measurements on boron carbides between 300K and 1200K are inconsistent with conventional analyses of both itinerant and hopping transport. Most striking are Seebeck coefficients which are both large ($> 100\ \mu V/K$) and strongly increasing function of temperature ($\sim 0.1\ \mu V/K^2$) despite thermally activated conductivities (0.16 eV). We can understand all of these results in terms of the hopping of small-polaron holes between sites which are inequivalent in energies and electron-lattice coupling strengths. In this situation, in addition to the usual electronic (entropy) term, the Seebeck coefficient garners a contribution from the vibrational energy transferred with a carrier as it hops between inequivalent sites. With a broad distribution of site energies (relative to kT), this contribution increases monotonically with temperature. The Hall mobilities are low ($\sim 1\ cm^2/V$-sec) and often thermally activated. Under pressure (up to ~ 20 kbar) both the prefactor and the activation energy of the conductivity increase. These features are consistent with small-polaron hopping. We ascribe the basic site inequivalence to carbon atoms which reside in either icosahedra or in intericosahedral (CBC) chains. The amorphous-like thermal conductivites of compositions with less carbon than is required to fill both types of sites are consistent with the carbons being distributed among these sites. When all sites are filled, B_4C, the thermal conductivity is that characteristic of a good crystal. Thus, small-polaron hopping between inequivalent centers containing carbon (in icosahedra and CBC chains) provides a consistent explanation of our data. Furthermore, it is the inequivalence of the hopping sites which causes the anomalously large high-temperature Seebeck coefficients which makes the boron carbides prime candidates for very high temperature (1700K) thermo-electric devices.

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SURFACE-RECOMBINATION CONTROLLED SNDC AND CURRENT FILAMENTATION

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While the influence of boundary conditions upon current instabilities associated with N-shaped negative differential conductivity (NNDC) has been convincingly elaborated in the past, see e.g. [1,2], no similar systematic treatment has been available for the case of S-shaped negative differential conductivity (SNDC). We have made a theoretical study of generation-recombination (g-r) induced bulk SNDC, which occurs in: low temperature impurity breakdown [3]; amorphous chalcogenide films [4]; and pin-diodes [5]. The resulting current filamentation depends sensitively upon the boundary conditions, in particular on the lateral surfaces, which can be controlled by surface recombination. We have calculated the profiles of the current filaments, and determined their stability against small carrier concentration and field fluctuations for various boundary conditions. In the limit of vanishing surface recombination all filaments are unstable under constant voltage conditions. Pinning of the quasi-Fermi level by strong surface recombination, on the other hand, leads to stable current filaments for a range of the quasi-Fermi level, and device dimensions in the near-micron and submicron range, even when the uniform steady state has positive differential conductivity and is thereby locally stable. Thus, bistability between uniform and filamentary states can be induced. This results in S-shaped (and other more complicated) current-field characteristics markedly distinct from those of uniform states without surface recombination. As the quasi-Fermi level at the surface is raised towards the conduction band, the SNDC-range shifts towards lower values of the applied field. This provides for control of the threshold and holding fields of the switching transition. It is of particular importance for applications in submicron devices.

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EVIDENCE FOR MICROWAVE PHOTON - ASSISTED CDW TUNNELING IN NIOBIUM TRISELENIDE

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Nonlinear conduction has been observed in $NbSe_3$ at about 25 K with microwave fields of amplitudes an order of magnitude both above and below the threshold field for nonlinear dc conduction. The experimental method has been phase resolved harmonic mixing. It is the phase resolved type of measurements which allows to discriminate against background signals. Results of the temperature variation of the mixing signal as compared with the variation of the dc resistance will also be presented. The obervations can quantitatively be explained by Bardeen's model of tunneling charge density waves and are in contrast to the model of a classical overdamped oscillator. A detailed discussion of both models and their implications to our observations will be given.

FRACTIONAL QUANTUM HALL EFFECT IN MOCVD-GROWN GAAS/ALGAAS HETEROSTRUCTURES AT PULSED HIGH MAGNETIC FIELDS

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Fractional Quantum Hall Effect (FQHE) has recently [1] been reported for very high mobility ($\mu > 500\ 000\ \mathrm{cm}^2/\mathrm{Vs}$) MBE-grown modulation doped GaAs/AlGaAs heterostructures with low ($n \cong 2*10^{11}/\mathrm{cm}^2$) carrier concentration. We demonstrate that also in MOCVD-grown heterostructures with much lower mobility FQHE can be observed, provided the carrier concentration and the magnetic field are increased such that for a given filling factor the width Γ of the Landau levels is kept small compared to the spacing of the levels (Γ/ω_c is proportional to $n/\sqrt{\mu}$). We report on measurements of the Hall-resistance and magneto-resistance of MOCVD-grown GaAs/AlGaAs heterojunctions with a mobility of $\mu = 107\ 000\ \mathrm{cm}^2/\mathrm{Vs}$ and a carrier concentration of $n = 3.8*10^{11}/\mathrm{cm}^2$. We used pulsed magnetic fields up to 37 Tesla at a temperature of 1.3 K. The rise time of the field is about 5 ms; it decays to half the maximum value in about 20 ms. We observe structure in both the magneto-resistance and the Hall-resistance at magnetic field values corresponding to fractional Landau level filling factors of $\nu = 2/3$ and $\nu = 4/3$. This is observed during both the rise time and the fall time of the magnetic field.

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PHONON SCATTERING IN HETEROLAYER TRANSPORT

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Two-dimensional conduction in heterolayer systems is being studied in detail in several laboratories. The very high low-temperature mobilities obtained with modulation doping are principally limited by the elastic scattering (due to ions, etc). The phonon scattering has a significant role at low temperatures, however, which is the subject of the work reported here: (a) It gives a contribution to the ohmic mobility μ which is a calculable property of the heterolayer alone. (b) It determines the hot electron effects. (c) A substantial "hot phonon" effect is to be expected. For this degenerate two-dimensional carrier system, the phenomena are different in the Bloch-Gruneisen range ($T < \theta$, say) than in the classical "equipartition" range ($T > \theta$). Here θ should normally be 5~10 K.

(a) For $T > \theta$ the lattice scattering contribution to $1/\mu$ is αT , where α depends on the normal-direction carrier density function $\rho(z)$ for given sheet carrier density n. For electrons in a GaAs heterolayer the measured α is the same, at a given n, for dark (thermal equilibrium) and after illumination. The computed and measured $\alpha(n)$ agree well [1]. For $T < \theta$ the calculated lattice-scattering $\Delta(1/\mu)$ is (so long as ohmic conditions apply) proportional to T^7 (deformation-coupled part) and T^5 (piezoelectric-coupled part). (b) For the warm-electron effect one has (if hot-phonon effects may be disregarded) $e\mu E^2 = F(T_e) - F(T)$ where T_e is the Fermi-distribution electron temperature. The theoretical temperature dependence F(T) is similar to that of $\Delta(1/\mu)$ -- proportional to T, or to T^7 and T^5, for the two regimes. The feeble dissipation of the Joule heat for $T < \theta$ would, however, be expected to lead to T_e readily increasing to $\sim \theta$; one would then expect an observed $\Delta(1/\mu)$ displaced towards the equipartition value. For $T > \theta$ one calculates a substantial rise in electron temperature at fields $E \sim 1$ V/cm in high-mobility GaAs heterolayers. (c) Dissipating the Joule heat will increase the occupation numbers $N(\omega)$ of the participating phonons. A calculation gives substantial increases δN at low temperatures for E values of only a few V/cm. (A similar estimate for the optical mode indicates that substantial δN values could be attained at higher fields.) One of the expected consequences of this augmentation is a modification of (b) above. These phenomena are of interest in themselves and provide a means of investigating the heterolayer electron (hole) states.

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FIR-EMISSION FROM FREE CARRIER PLASMA IN GaAs/AlGaAs HETEROSTRUCTURES

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Three different mechanisms of far infrared (FIR) generation from the two-dimensional free carrier plasma in GaAs/AlGaAs heterostructures are investigated experimentally and theoretically.

The broadband FIR radiation from hot electrons /1/ is analysed for the first time in GaAs/AlGaAs heterostructures. We measured electron temperatures as a function of mobility and electric field in the absence of magnetic fields. The results on electron heating and its dependence on carrier concentration and input power are well explained by theory of piezoelectric scattering in two-dimensional systems including screening by the two-dimensional electron system.

Radiative decay of two-dimensional plasmons excited by hot carriers /2/ is studied by means of holographically produced grating structures. We have studied the linewidth and intensity of the narrowband FIR emission in order to obtain information on the different decay mechanisms of collective excitations (Coulomb scattering, electron-electron scattering, radiative decay). Deviations from the dispersion relation of two-dimensional plasmons due to nonlinearity of the plasma and due to size effects in short channel GaAs/AlGaAs FET devices are found theoretically.

Free carrier plasmas with high drift velocities (v_d) along periodic grating structures are well known to emit electromagnetic radiation (Smith-Purcell-effect)/3/. The possibilities of generating FIR radiation from high-mobility 2D systems in GaAs/AlGaAs heterostructures ($\mu \sim 10^5$ to 10^6 cm²/Vs, v_d up to 3.10^7 cm/s) drifting along sub-μm grating structures are investigated. The electron distribution function in high electric fields fields can be studied directly in such experiments.

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Heterostructures **TuP-PE4**

SIZE RESONANCE IN QUANTUM WELL WIRES

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In recent years, Molecular Beam Epitaxy and other sophisticated techniques have made possible the fabrication of semiconducting quantum well wires (QWW), which are thought to have potential device applications[1]. The quantum transport behavior, in the quantum limit, of electrons in QWW is found to be similar to those confined in a magnetic field[2]. A size resonance is expected when a QWW is exposed to an optical photon field with electric field polarized perpendicular to the length of the wire, and the photon energy is equal to the spacing between quantized subbands. A superoperator, theory, based on the solution of Liouville's Equation for the density matrix, is developed to study the temperature and size-dependence of the resonance linewidth. The resonance linewidth due to the acoustic-phonons scattering is found to be enhanced, and that due to the ionized impurity scattering is found to be suppressed under strong carrier confinement conditions. For sufficiently thin wires, the resonance linewidth is found to be proportional to $(h/\tau_b)(\lambda_D^2/A)$, where τ_b is the bulk relaxation time, λ_D is the thermal de Broglie wavelength, and A is the cross-sectional area of the wire. The peak value of the resonance is found to decrease under stronger confinement conditions.

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THE EFFECT OF HYDROSTATIC PRESSURE ON TRAPPING CENTERS IN STRAINED-LAYER SUPERLATTICE STRUCTURES*

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The application of hydrostatic pressure to a semiconductor can, through a change in lattice constant, affect the bulk electronic and optical properties of the material and those impurities or defects. In a somewhat analogous fashion, the thin layers in a strained-layer superlattice (SLS) accommodate the lattice mismatch by altering their lattice constants. This strain effect leads to the unique properties of SLS's: the ability to independently vary the energy gap, lattice constant and transport properties during growth. The parallel between pressure effects and the structural characteristics of SLS's implies that the application of hydrostatic pressure to an SLS will result in measureable changes in the SLS properties. We have compared the results of applying pressure to $GaP/GaAs_{.3}P_{.7}$ SLS structures, and to non-SLS alloys of similar composition. The technique of deep level transient spectroscopy (DLTS) was employed to determine the trapping level parameters of both intrinsic and irradiation-induced traps as a function of hydrostatic pressure to 8kbar. With increasing pressure, the two intrinsic electron traps in the non-SLS samples with emission energies of E = 0.23 and 0.28 eV, remained essentially pinned to the conduction band edge, whereas the one intrinsic electron trap present in the SLS sample shifted closer to the conduction band by approximately 30 meV in 8 kbar. This value was only approximate, however, because the trap signal was relatively weak. To facilitate the examination of similar traps with strong signals in both SLS and non-SLS materials, the samples were exposed to heavy ($5x10^8$ rads) gamma irradiation. As a result, two electron traps (E = 0.366 and 0.760 eV) were observed in the non-SLS material and three (E = 0.249, 0.320, and 0.705 eV) in the SLS samples. Both traps in the non-SLS material remained essentially pinned to the conduction band, while the emission energies of the three SLS traps at 8 kbar had decreased to 0.225 eV, 0.283 eV, and 0.605 eV, respectively. These results suggest that the variation with pressure of the coupling between the electronic energy and the lattice is not the same in SLS and non-SLS materials. This is not surprising in view of the strain already present in the SLS structure. Another interesting feature of the defect trap behavior is that the application of pressure causes greater recombination-enhanced annealing of the traps in both SLS and non-SLS samples. Since the rate of this type of annealing depends on the efficiency with which the non-radiative recombination energy is transferred to the lattice, this result also demonstrates that the coupling coefficient is sensitive to pressure. Taken together, the results show that the study of trapping levels as a function of hydrostatic pressure can provide valuable insights into the behavior of both SLS and non-SLS semiconductor materials

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EFFECT OF k-LINEAR TERMS ON ELECTRONIC PROPERTIES OF 2D SYSTEMS

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The dispersion law of charge carriers in inversion layers includes k -linear spin-orbit term $H_{S0} = \alpha[\vec{\sigma} \times \vec{k}]\vec{\nu}$, as follows from symmetry consideration, $\vec{\nu}$ is the unit vector normal to a layer. H_{S0} lifts two-fold band degeneracy and results in the dispersion law $E^{\pm}(k) = k^2/2m \pm \alpha k$, m is the effective mass. $E^{-}(k)$ reaches its minimum at $k_0 = \alpha m$, $E^{-}(k_0) = -\frac{\alpha^2 m}{2} = -\Delta$. We have determined for the first time the values of α and Δ for 2D systems from experimental data. The experimental data [1,2] obtained on GaAs - $Al_xGa_{1-x}As$ heterojunctions are used, as well as the theory [3].

The combined resonance (i.e., electro-dipole spin transitions) in n-GaAs inversion layers was investigated in[1]. For strong magnetic fields B the spin resonance frequency $\nu = \nu_0 + g\mu_B B$ with $\nu_0 \neq 0$. In [2] the cyclotron resonance in p-GaAs inversion layers was observed and two effective masses $0.38 m_0$ and $0.60 m_0$ were found. We attribute both these findings to the effect of the H_{S0} term. When it is taken into account, the spectrum in the magnetic field is

$$E_s^{\pm} = \omega \varepsilon_s^{\pm}, \ \varepsilon_0 = \delta, \ \varepsilon_s^{\pm} = s \pm \sqrt{\delta^2 + \gamma^2 s} \ \ (s \geq 1), \ \delta = \frac{1}{2}\left(1 - \frac{gm}{2m_0}\right),$$

where $\gamma = 2\sqrt{\Delta/\omega}$, $\omega = eB/mc$, g is the g-factor. The processing of experimental data gives $\alpha \approx 2.5 \cdot 10^{-10}$ eV·cm and $\Delta \approx 2.5 \cdot 10^{-6}$ eV for n-GaAs (sample 2 in [1]) and $\alpha \approx 0.5 \cdot 10^{-9}$ eV·cm and $\Delta \approx 10^{-4}$ eV for p-GaAs [2].

The peculiarities in oscillatory phenomena caused by two-branch dispersion law are discussed and the theory of magnetic susceptibility of inversion layers is developed.

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INELASTIC AND RESONANT TUNNELING IN GaAs/AlAs HETEROSTRUCTURES*

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We report the observation of inelastic and resonant tunneling in a study of electronic transport perpendicular to single or multiple AlAs layers sandwiched between GaAs layers. These heterostructures were grown by metalorganic chemical vapor deposition (MOCVD). The layer thicknesses were between 50 and 250 Å except for the initial and final GaAs layers which were several microns thick. The AlAs layers were doped p-type with Mg. The GaAs layers were either undoped or n-type and degenerate. Electron transport across the AlAs layers was studied by making I-V, first derivative (dI/dV), and second derivative (d^2I/dV^2) measurements on these samples as a function of temperature.

In samples with only one AlAs layer, the room temperature current was dominated by thermionic emission over the AlAs barrier. At low temperatures leakage currents dominated in samples with barriers thicker than 100 Å, while tunneling currents were dominant in the samples with thinner AlAs barriers. Structures corresponding in energy to the GaAs and AlAs longitudinal optical (LO) phonon energies were observed in the second derivative spectra for samples with 50 Å thick barriers. These were attributed to electron self-energy effects in the GaAs, and the inelastic-excitation of LO phonons in the AlAs. This is the first observation of these effects in the AlAs/GaAs system. Negative resistance regions were observed in the I-V curves of samples with multiple AlAs layers, indicating the presence of resonant tunneling effects. Differences between these results and the results of measurements on samples with n-type AlAs barriers will also be discussed.

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Heterostructures **TuP-PE8**

EXCITONS IN SEMICONDUCTOR DOPING SUPERLATTICES

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Theoretical and experimental results for the properties of excitons in semiconductor doping superlattices are presented. These systems, which are composed of alternating layers of n and p doping, are especially attractive for study because their electronic properties can be tuned by photoexcitation or by variations in doping. A (photoexcited) electron and hole are considered to move in the quasi two-dimensional subbands of the parabolic potential created by the ionized impurities of adjacent n and p layers. Their excitonic properties are studied variationally using a wavefunction of the form $\psi(\underset{\sim}{r}_e,\underset{\sim}{r}_h) = N\zeta_e(z_e-z_D)\zeta_h(z_h+z_A)\ \exp\{-[\alpha((x_e-x_h)^2 + (y_e-y_h)^2) + \beta(z_e-z_h)^2]^{\frac{1}{2}}\}$ where z_e, z_h are the electron and hole coordinates parallel to the superlattice axis, ζ_e, ζ_h are the subband wavefunctions centered at z_D, and $-z_A$, and α, β are variational parameters. Extensive calculations of the properties of these systems have been performed as functions of the distance between the centers of the n and p layers and of the doping concentrations. In the limit of high doping the carriers are strongly confined near the centers of the respective doping layers, and a quasi two-dimensional exciton is found.[1] For very low doping the three-dimensional result is obtained. The transformation between these two cases is particularly interesting. As the doping decreases from large values the difference between the expectation values of the electron and hole positions decreases. A particularly interesting feature is that for separations between layers ≤ the three-dimensional exciton Bohr radius the exciton binding energy at first increases for decreasing doping before decreasing to the three-dimensional value. For decreasing doping the electron-hole wavefunction overlap increases and the recombination probability increases dramatically. Calculations also have been made for cases in which the hole (electron) of the exciton is bound to a charged acceptor (donor) in its doping layer by using the above variational approach with ζ_i replaced by $\exp\{-[\alpha_i^{-1}\ \underset{\sim}{r}_i-\underset{\sim}{r}_o\ ]\}$, $i = h,e$, where $\underset{\sim}{r}_o$ is the location of the charged acceptor (donor), and α_i is an appropriate radius. In these cases the exciton binding is found to be relatively small and to be dependent on the electron and hole mass ratios. The overlap is once again strongly dependent on doping.

Photoluminescence studies have been made of doping superlattices in GaAs with varying excitation intensity. Typical parameter values are doping concentrations of $\sim 1\times10^{17}\text{cm}^{-3}$ and layer widths of ~400 Å which gives a band bending ~.05 eV. With increasing photoexcitation the band edge luminescence moves to higher energy. As it approaches the value corresponding to the bulk, a new feature is found to appear abruptly at somewhat higher energy (in the region of that for the bulk exciton). We argue that this feature may be attributed in part to recombination from electrons and holes whose overlap increases with increasing photoexcitation as described above. For them the recombination probably becomes high, and the energy has the appropriate value.

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Photoluminescence Decay Times in Multiple Quantum Well Heterostrucures Prepared by Molecular Beam Epitaxy

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Following the great interest in quantum well heterostructures for the fabrication of short wavelength lasers in the GaAs-(A1Ga)As materials system we have been involved in a photoluminescence study of the dominant recombination mechanisms in isotype multiple quantum well heterostructures. We have already shown (1) that the steady state PL spectrum is dominated by free exciton recombination even at room temperature.

We have extended our studies to include measurements of the PL decay times as a function of temperature. It has been shown that the decay time at temperatures in the range 100-300K can be as long as 25 nanoseconds in 55 angstrom wide wells and is controlled by the optical quality of the (A1Ga)As barriers. The effective interface recombination velocities in the best structures can be as low as 10 cm/sec. Deviations from this dependence on the optical quality of the (A1Ga)As are observed at lower temperatures when impurities in the GaAs region become important. Following our investigation we propose an alternative explanation of the unexpectedly short exciton lifetimes reported by other workers(2,3) at low temperatures.

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PHOTOLUMINESCENCE AND EXCITATION SPECTRA OF $GaAs_{1-x}Al_xAs$ STRONGLY COUPLED DOUBLE WELL SUPERLATTICE:

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We have studied the mini-subband structure of a system consisting of two outer 200A Ga(Al)As layers, two inner 45A GaAs layers separated by a thin Ga(Al)As 12A layer. The system forms a strongly coupled double quantum well structure analogous to the one grown by Voos and Co-workers (1).

Since recombination involves longer times than the electronic optical excitation, we have calculated all electron and hole mini-band structures as a function of parallel momentum within a 6 x 6 Hamiltonian effective-mass equation for the envelope wave function components with proper boundary condition[2] at a plane 100A away from the well edges. The model takes into account the non-parabolicity of subbands, and the finite height of the Ga(Al)As barrier. Due to the very large density of states of the heavy-hole band we have set the quasi-Fermi level of holes within the first heavy-hole mini-subband, corresponding to 10^{11} particles/cm^2.

The comparison of our results with the experimental photoluminescence and excitation spectroscopy of reference[1] suggests a very simple interpretation for both spectra. The excitation spectrum is composed of four peaks which we assign to transitions between an occupied state in the Valence mini-subbands and an empty state in the conduction mini-subbands. At low temperature the luminescence, according to our calculation, is due to the recombination of electrons at the bottom of the lowest electronic mini-subband and a hole at the top of the lowest heavy-hole mini-subband. As temperature increases, electrons in the filled Valence subband can be promoted to the empty part of the lowest heavy-hole mini-subband, therefore explaining the second luminescence peak observed in the reference[1] as well as the tendency of this second recombination process to overcome the low temperature luminescence peak.

In both luminescence and excitation spectra, the calculated transition energies never differs from the experimental resonances by more than 0.3%, which is smaller than every experimental line width.

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TuP-PE11

RECOMBINATION TIMES IN GaAs/$Al_xGa_{1-x}As$ QUANTUM WELL STRUCTURES

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Time-resolved photoluminescence measurements on MBE-grown GaAs/$Al_xGa_{1-x}As$ quantum well structures indicate a rapid $\tau \leq 1$ ns decay followed by a much weaker slow decay with $\tau \sim 50$ ns for an excitation fluence $\leq 1\ \mu J/cm^2$ at 300K. This behavior differs markedly from MOCVD quantum well structures we have previously studied, which have a slow decay component far stronger than that of the MBE structure.

Our MBE structure consists of 100 periods of undoped 87Å GaAs and 194Å $Al_{.26}Ga_{.74}As$ layers, sandwiched between two high bandgap confining layers. The substrate and 50Å cap are GaAs. The quantum well region is undoped. Excitation pulses $\sim$ 150 ps long at a repetition rate of 820 kHz are provided by a krypton ion laser system at 647 nm. The photoluminescence is passed through a 1/4-meter monochromator tuned to 847 nm to select the $n = 1 \rightarrow 1$ heavy hole transition. A cooled Hamamatsu 636-P photomultiplier tube combined with time-resolved single photon counting electronics allows the accurate determination of both short and long recombination times with wide dynamic range.

Both room temperature recovery times [1] and low temperature photoluminescence times [2] depend on exciton dynamics. At room temperature high phonon densities allow excitons to ionize as the photo-induced carriers are decaying to the lowest confined states in the wells. Room temperature photoluminescence dynamics thus represent primarily recombination between free carriers rather than excitons. Exciton saturation effects are likewise avoided. Recombination time measurements at 300K and 77K to demonstrate this difference are now in progress.

Trapping due to impurities, by holding up carriers in the barrier regions, may be responsible for the long decay times in different samples. We are now comparing recombination times for excitation photon energies above (647 nm) and below (752 nm) the band gap of the $Al_{.26}Ga_{.74}As$ barriers (but still above the $n = 1 \rightarrow 1$ transition energy), in order to place a lower limit on scattering rates into the well from the barrier region. Recombination time measurements as a function of carrier density will also be presented, and the role of diffusion in the slow decay mechanism will be discussed.

Acknowledgements

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TuP-PE12

INTRA- AND INTERBAND MAGNETOOPTICAL INVESTIGATIONS OF PbTe/$Pb_{1-x}Sn_xTe$ SUPERLATTICES

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IV-VI superlattices (SL's) exhibit striking new features as compared to III-V and II-VI systems due to the direct narrow gap at the L-point of the Brillouin-zone of their constituents. PbTe/$Pb_{1-x}Sn_xTe$ ($x=0.12$) SL's were grown by a hot-wall epitaxy method on BaF_2(111) substrates with individual layer thicknesses of 20...200 nm and up to 60 periods. The samples were characterized by X-ray methods (composition, periodicity, and strain in the constituent layers), the Sn-profile was controlled by sputtering and Auger electron spectroscopy and a SIMS analysis. The electrical properties of the SL's were determined by magnetoresistance measurements establishing quasi-two-dimensional properties of electrons or holes confined in the PbSnTe layers for PbTe layer thicknesses > 30 nm. Magnetooptical intra- and interband investigations were carried out with n and p-type SL's in Faraday and Voigt configuration for several superlattice periods and for various ratios of the constituent layer thicknesses. The experimental results were analysed with a SL band structure model calculation based on the envelope function approach considering strain induced terms. A semiempirical tight binding calculation yields a type I SL with valence band discontinuities about twice the conduction band steps as confirmed by experimental data. Due to the large dielectric constants ($\geq$ 1300 at 4.2 K) the charge transfer effects are negligible and the SL band structure even in the presence of a quantizing magnetic field for the (111) and the three oblique valleys was obtained without free parameters including k.p interaction with far bands. For interpreting the magnetooptical data not only the relevant transition energies but also the corresponding oscillator strengths were calculated. The numerous observed intra- and interband transitions and their systematic dependence on the varying SL parameters is in reasonable agreement with the model calculations.

MAGNETIC FIELD INDUCED METAL-NON METAL TRANSITION IN $Ga_{.7}Al_{.3}As/GaAs$ HETEROJUNCTIONS UNDER HYDROSTATIC PRESSURE

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An obvious advantage presented by the use of hydrostatic pressure for the study of $Ga_{.7}Al_{.3}As/GaAs$ heterojunctions lies in the possibility to obtain a very low density for the 2D electron gas [1] (by trapping of the electrons on a deep level in GaAlAs).
Carrier concentration lower than 5.10^{10} cm^{-2} can be obtained even in a rather doped sample. We use this possibility to investigate, for the first time, the problem of transport in the ultra quantum limit : we show that a magnetic field induced metal non metal transition occurs, associated to a large localization of the electrons. The remaining free carrier density is deduced from the σ_{xy} component of the conductivity tensor, assuming that the localized electrons do not participate in the Hall effect. In the low field limit, the behaviour of the resistivity as well as the carrier concentration is metallic.

For a given magnetic field (threshold field) the conductivity becomes activated as well as the free carrier density in the quantum well. At the transition the Mott's criterion is obeyed. In the activated regime, the activation energy increases linearly when the magnetic field increases ($\sim$ 0.1 meV/Tesla).
Different possibilities for the localization are discussed. In conclusion, the use of hydrostatic pressure and high magnetic field appears as a very convenient way to study the localization effects in $Ga_{.7}Al_{.3}As/GaAs$ heterojunctions, in relation with the conditions of growth.

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The experiments have been made in the Service National des Champs Intenses, Grenoble.

ELECTRONIC AND OPTICAL PROPERTIES OF MODULATION DOPED SEMICONDUCTOR QUANTUM WELLS*

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A multiband effective mass approach to the treatment of modulation doped semiconductor quantum wells is presented in which the kinetic energy of the spin 3/2 hole is described by a 4x4 $\vec{k}\cdot\vec{p}$ matrix and the well potential is treated by a finite square well plus an additional modulation doping potential. The method is applied to the GaAs/GaAℓ_xAs$_{1-x}$ system and results are presented. The hole band structure is found to be a complicated function of well width and modulation doping due to mixing of light and heavy hole bands. In the absence of modulation doping the first hole subband is direct with an effective mass which is insensitive to the variation of well width whereas the second hole subband is observed to undergo a transition from direct to indirect as the well width increases. When the second hole subband is indirect, the band structure along a given direction has a maximum at $\vec{k}_{\parallel}\neq0$ resulting in a negative effective mass at Γ. These findings are in agreement with similar results obtained with a 10 band tight binding calculation$^{(1)}$. These negative effective masses can qualitatively alter the absorbtion. When the hole mass at Γ is close to the negative of the effective electron mass, a sharp peak in the absorbtion spectrum will occur near the threshold of the valence subband to conduction band transition due to a von Hove singularity in the joint density of states at Γ. This novel phenomenon is predicted to occur in GaAs/AℓAs ($x=1$) quantum wells in the absence of doping for layer thicknesses aroung 50Å. The effect of repulsive modulation doping potentials is considered and is found to have important effects on the calculated band structure; in particular the mass of the hole subbands can be altered dramatically. For strong modulation doping, the hole wavefunctions are localized at the walls of the quantum well and give rise to degenerate pairs of direct bands associated with bonding and antibonding states. The bands with negative masses in the absence of doping which correspond to the antibonding bands undergo a transition from indirect to direct as the doping potential increases. This leads to dramatic changes in the optical properties due to the change in the doping potential.

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LOCALIZATION OF TWO-DIMENSIONAL EXCITONS IN GaAs-AlGaAs QUANTUM-WELL LAYERS

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An exciton moving in a weak random potential is, in principle, a promising model system for the study of localization effects. Its spectrum can be measured directly, and the Coulomb interaction, which complicates the interpretation of conductivity data, is not present at low exciton density. In a GaAs layer (quantum well) the exciton is two-dimensional and moves freely in the layer, but is scattered by the potential fluctuations produced by random variations in the layer thickness. These fluctuations broaden the exciton line into an inhomogeneous band. Excitons with energies low in this band may be localized at low temperatures. The short lifetime of this direct exciton makes direct observation of its motion difficult. However, since a delocalized exciton is strongly scattered, its homogeneous linewidth Γ should be much greater than that of a localized exciton, for which, at low temperature and low exciton density, Γ should equal the inverse radiative lifetime.

We have measured Γ by Rayleigh scattering(1) and by hole-burning, in GaAs layers 50 to 200 Å wide. The results obtained by the two methods agree where they overlap, but Rayleigh scattering is the only technique available at very low exciton density where the effects of localization are most clearcut. At high exciton density we have measured the exciton diffusion constant D by the transient grating technique,(2) with results in qualitative agreement with the measurements of Γ. We find that Γ and D increase sharply as the exciton energy increases through the line-center. Below the line-center Γ is thermally activated, with an activation energy approximately equal to the separation from the line-center. We conclude that excitons are effectively localized below the line-center and delocalized above it, as predicted by classical percolation theory.

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[*] Work done while at Bell Laboratories.

Heterostructures **TuP-PE16**

THEORETICAL STUDY OF POPULATION DYNAMICS OF TWO-DIMENSIONAL EXCITONS IN GaAs-AlAs QUANTUM WELL STRUCTURES

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The optical means such as the time-resolved photo-luminescence and the resonant Raman and Rayleigh scattering are quite promising to reveal the salient features of the two-dimensional excitons in quantum well(QW) structures. Recently Masumoto et al.[1] studied the time-resolved luminescence of 1s excitons(n=1, e-hh) in GaAs-AlAs MQW structures and found the anomalous behavior of the average energy of excitons which shows a non-exponential decay and whose decay rate is too small to be accounted for in terms of the kinetic energy relaxation process on the dispersion curve of the two-dimensional excitons with emission of acoustic phonons. In their experiment the GaAs layers are selectively excited by choosing the laser energy suitably and the AlAs barrier layers are sufficiently thick to rule out the possibility of inter-layer migration of excitons. It is well-known that the topological disorder of the interface produces sizable optical effects and an island-like structure of the QW interface with one monolayer height and a lateral size $\gtrsim$300A was proposed[2]. On the basis of this model we developed a theory to explain the anomalous behavior in terms of the intra-layer migration of excitons among islands with different thicknesses[3]. The exciton can be considered to be localized at some island since the lateral size of the two-dimensional exciton in the sample of Ref.[1] is estimated to be about 200A. After the photo-excitation the excitons migrate among the islands toward the lower energy sites with emission of acoustic phonons. The physics is quite similar to that of excitation transfer among paramagnetic impurities in solids[4] and of exciton transfer in mixed semiconductors[5]. Following the approach by Holstein et al.[4], the transfer probability of excitons among islands is calculated taking account of only the one-phonon assisted transfer process and using the interaction Hamiltonian of localized excitons in QW structures with acoustic phonons which is derived microscopically for the first time[3]. The transfer integral of excitons between two localized sites is calculated via the matrix element of the electron-electron interaction using the envelope function of localized excitons at each island. Using thus calculated transfer probability we set up a kinetic equation for the distribution function of excitons. Based upon this kinetic equation, the time-resolved energy distribution function is calculated and the non-exponential behavior of the average energy is obtained consistently with the experimental result. The decreasing rate of the average energy of excitons at the initial stage is quantitatively in reasonable agreement with the experimental value.

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The author would like to thank Dr. Y. Masumoto for many enlightening discussions.

OBSERVATION OF VERTICAL TRANSPORT IN A GaAs/GaAlAs SUPERLATTICE BY PHOTOLUMINESCENCE

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We shall report the first observation of vertical transport in a superlattice (S.L.) by luminescence. Photoexcited carriers created by the laser move in the conduction and valence bands of the S.L. and are trapped in purposely introduced enlarged wells then giving rise to luminescence. Even excitons are shown to move through the GaAlAs barriers. Photoluminescence Excitation experiments, power density variations as well as temperature dependance of the luminescence shape support this interpretation. Calculation of the mean trapping time in S.L. are performed at low temperatures with various scattering mecanisms (deformation potential, piezoelectric and ionized impurities) within a simple model. Impurity scattering calculations provide an interpretation to the variations of the S.L. and enlarged wells luminescence peaks intensity ratio with temperature, size of the enlarged wells and S.L. period.

OPTICAL BISTABILITY DUE TO BIEXCITONS IN CuCl

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Two-photon absorption to biexciton states gives rise to an anomaly of the dielectric function which leads to bistability. This effect has been experimentally observed at low temperatures, using CuCl platelets of 10 to 40 µm thickness as non-linear medium in a Fabry-Perot cavity (FP) and comparing the time shape of a dye laser pulse (3-4 ns FWHM) transmitted through the FP to that of the incident pulse.

This bistability is shown to be strongly resonant at half the biexciton energy ($E_B/2$). Switch-on times are very short. They could not be resolved by a GHz oscilloscope. They are inferior to 500 ps. The switch-off times are in the ns range when incident photon energies are equal to $E_B/2$, showing that energy dissipationsare then important, the radiative lifetime of biexcitons being of the order of 1 ns. When working with photon energies slightly off the biexciton resonance, the switch-off times become also very short, inferior to 500 ps. The biexcitons are then virtually excited, the dephasing time, important for this kind of transitions, being of the order of some ps.

Concerning switching intensities, we have shown the importance of the FP operating point with respect to the biexciton resonance. The lowest intensities have been obtained when a maximum of FP transmission corresponds to $E_B/2$. We have then measured a switch-on intensity of 15 MW/cm^2 and a switch-off one of 5 MW/cm^2. When changing the FP operating point, these values increase. We could even obtain differential gain without any switching.

This biexciton bistability can be accounted for by a non-linear dielectric function calculated by applying a matrix density formalism to a three level system (ground state, exciton, biexciton).

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TuP-PF2

RAMAN INVESTIGATION OF THE GROWTH INSTABILITY OF InGaAsP

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The growth instability of $In_{1-x}Ga_xAs_yP_{1-y}$ in certain composition range (miscibility gap) has been attracting much attention recently as a major drawback in its opto-electronic applications. Bulk thermodynamic theory has predicted phase separation into GaP-rich and InAs-rich phases but its applicability to epitaxial InGaAsP is dubious owing to possible substrate effects.

We made the first attempt to study the growth instability of epitaxial InGaAsP using Raman scattering. The samples used were VPE grown InGaAsP on GaAs (100) substrates and the spectra were taken in the backscattering geometry with the 5145 Å line of an Ar$^+$ laser. The spectra in the normal growth range consist of two main peaks with GaP- and GaAs-characters, respectively.
A salient feature characterizing the instability is the appearance of a new peak at 345 cm^{-1} with the rest of the spectrum remaining essentially intact, which cannot be explained by the bulk theory. Based on frequency and symmetry considerations, the new peak is identified as InP-like LO peak. We interpret its appearance as due to composition fluctuation along the lattice-matching line $y=2.1x-1.1$ with GaAs substrate. This is consistent with our x-ray studies which have shown no evidence of large lattice mismatch.
Strong substrate latching effect is also supported by the polarization analysis of the Raman spectra which has indicated orientational alignment of InGaAsP layer with substrate, Hence, we conclude that the growth instability is strongly dominated by substrate, which gives us hope to overcome the bulk immiscibility with the help of substrates.

PICOSECOND HIGH INTENSITY EXCITATION OF SILICON

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The interaction of ultrashort intensive laser pulses with silicon is studied by time-resolved optical and photoelectric measurements. The kinetics of the electron-hole plasma and the evolution of plasma and lattice temperature is investigated up to laser fluences such as required to melt silicon. The data confirm the dominance of thermal processes among the high excitation phenomena encountered in laser-induced phase transitions. Even on a time scale of picoseconds the energy is instantaneously transferred to the lattice phonons, giving rise to ultrafast heating and melting phenomena. More refined optical methods, including two time-delayed excitation pulses, reveal the role of impact ionization. Taking advantage of the high sensitivity of silicon films towards changes of the refractive index, the interplay between plasma formation and lattice heating is demonstrated directly in time-resolved signatures of reflectivity and transmission. Extending the range of probing wavelengths into the near infrared allows the experimental determination of the optical plasma susceptibility and conductivity. From them the optical reduced mass and the scattering times are deduced.

17th International Conference on the Physics of Semiconductors

Optical Properties **TuP-PF4**

SEMICONDUCTOR ON THE BASIS OF ACTIVE ZnO

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Active ZnO has not been researched as a semiconductive material so far. Active ZnO has been obtained by termic dissociation of the following zinc compounds: $ZnCO_3$, $ZnSO_4.7H_2O$, $ZnSO_3$, $Zn(NO_3)_2.6H_2O$, $Zn(OH)_2$, $ZnC_2O_4.2H_2O$, $Zn(CH_3COO)_2$ and by thermal oxidation of ZnS. The temperature and the temperature intervals for active ZnO obtained from different zinc compounds were precisely established.

The p-n transition was studied of the active ZnO obtained from the various Zn compounds. Experiments showed that active ZnO is obtained only when the maximum of the curve expressing the rectifying coefficient dependency on the tension applied has the permanent value of 1.0V. Specific electric conduction is determined for active ZnO $\sigma = 2{,}5.10^{-5}\Omega^{-1}m^{-1}$.

Photos of infra-red spectra of active ZnO were taken. It was found out that with the active ZnO the link between "Zn" and "O" is relatively weakened: its length is increased by $65cm^{-1}$ in *comparison with that of non-active ZnO.*

Moreover, active ZnO is of practical interest in electro-photography.

PULSEWIDTH DEPENDENCE OF THE NONLINEAR ABSORPTION, MELTING THRESHOLD, AND PHASE TRANSITIONS OF SILICON IRRADIATED BY 1 MICRON PICOSECOND PULSES*

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There is considerable interest in the picosecond deposition and redistribution of optical energy in silicon, primarily because of the interest in laser processing of materials and in nonlinear optical device applications. Here, we report the first pulsewidth study of (a) the nonlinear absorption, (b) reflection, (c) the melting threshold, and (d) the associated morphological changes and phase transitions of crystalline silicon that has been irradiated by pulses of 1 micron radiation from 4 - 300 ps in duration.

Specifically, we have measured the nonlinear transmission and reflection of Si over 4 decades in fluence, from the linear regime to beyond the melt threshold, for various optical pulsewidths. The Si transmission is observed to decrease by a factor of 6 at the highest fluences, but no pulsewidth dependence is detected. From this, we conclude, in contrast with previous results reported by other groups, that the nonlinear optical absorption is strictly fluence dependent and that two-photon absorption is unimportant. At high incident fluence, the transmission is dominated by free-carrier absorption and by increased indirect absorption caused by band-gap narrowing with increasing lattice temperature.

We have also measured a continuous reduction in the single shot melting threshold from 2.7 ± 0.3 J/cm^2 for 225 ps pulses to 0.6 ± 0.1 J/cm^2 for 6 ps pulses. A pulsewidth-dependent melting threshold taken together with a strictly fluence-dependent energy transfer from the optical pulse to the crystal suggests that significant energy transport is occurring on the time scale of the optical pulsewidths. Indeed, the carrier and thermal diffusion lengths for 10 ps are 200 nm and 40 nm, respectively (one absorption depth for liquid Si is ~10 nm). Moreover, the melt threshold exhibits roughly a square root dependence on pulsewidth, as would be expected for a transport-dominated process (where the diffusion length is proportional to the square root of time).

This pulsewidth dependence is also reflected in the surface morphology, where we consistently observe a crystal-to-amorphous transition using pulses of 10 ps duration or less, contrary to published expectations. By contrast, for pulses longer than 30 ps, bulk melting is followed by recrystallization. Periodic ripple patterns are observed for pulses as short as 4 ps. These observations are again consistent with energy that is transported an absorption depth on the time scale of approximately 15 ps.

Finally, we demonstrate how the measured nonlinear optical properties, together with the melt kinetics, can be used in a specific geometry to construct a picosecond optical energy limiter or regulator that has high transmission for low input energies but clamps the output at a low value for high input energies.

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TuP-PF6

PRESSURE EFFECTS ON THE LUMINESCENCE AND RAMAN SPECTRA OF HEAVILY DOPED CdS*

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Diamagnetic anomalies have been observed in heavily Cl-doped, pressure quenched CdS. The possible implications of superconductivity above 77K have shown the need to examine the role of impurities under pressure. We have previously shown that an excitonic superconducting mechanism[1] is possible if donors pressure ionize. We present here a study of the photoluminescence and phonon spectra of pure and Cl-doped CdS at 300°K, upto 42 kbar. This study has lead to some new and unexpected results which have a bearing on the pressure ionization of donors.

In pure and lightly doped CdS, the luminescence peaks shift at rates of 4.47 ± .02 and 4.24 ± .15 meV/kbar, respectively, following the band edge.[2] In heavily Cl-doped CdS, however, the shift is 5.35 ± 0.21 meV/kbar. The Fermi level E_F in this sample is close to or in the conduction band. If the donors pressure ionize, E_F will rise with pressure. A 50% increase in the number of free carriers would increase E_F by 0.03 eV at 25 kbar, which would account for the larger shift. This is the first observation of possible pressure ionization in CdS.

The 1- and 2-LO phonons should disappear at ~25 kbar, when CdS transforms to a rocksalt structure. We observe them, however, upto 42 kbar. The frequencies increase linearly with pressure, with a break between 24 and 26 kbar. Fitting the data to a segmented straight line, we obtain slopes of 0.56 ± 0.03 cm^{-1}/kbar ($P < 24$ kbar) and 0.42 ± 0.05 cm^{-1}/kbar ($P > 26$ kbar) for the 1-LO and 1.12 ± 0.04 and 0.80 ± 0.06 cm^{-1}/kbar respectively for the 2-LO. If the phonons arise from a small fraction of the wurtzite phase that is untransformed, their intensity should be correspondingly small, which is not the case. Possible mechanisms that could explain this anomalous behavior will be discussed.

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COEXISTENCE OF DIRECT AND INDIRECT ELECTRON-HOLE PLASMA COMPONENTS IN GaSe

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We report on our measurements of the spontaneous photoluminescence spectra, made at liquid He temperature and at high excitation levels. Special care was taken to insure that only luminescence coming from a homogeneously excited volume was detected: The samples had a thickness comparable to the penetration depth of the exciting light, and a pinhole was used to reduce effects of lateral inhomogeneities. At weak excitations, only direct optical recombinations are observable in the excitonic spectra. For carrier densities above the Mott value, the direct transitions merge to a wide band, and a second new band appears at lower energies.

We propose a new interpretation which deviates from earlier models [1]. In GaSe, the indirect conduction band minimum is only 25 meV lower than the direct one. Due to this, both direct and indirect conduction band valleys are populated. As suggested by their spectral positions, the two emissions at high excitation levels are zero-phonon recombination luminescence of direct and indirect electron-hole (e-h) plasma components. The phonon replicas of the indirect transitions are weakly observable at very high excitation densities only. From our luminescence spectra we extract the two normalized gaps. Making use of the now well developped theory of e-h plasmas [2,3], we find that the two gaps correspond to the same e-h pair density. Shapes and intensity ratio of the bands are strongly dependent on the carrier density. This indicates an increase of the ratio of indirect to direct electron population with pump intensity, and furthermore it excludes an interpretation in terms of phonon-assisted direct recombinations.

Our model is somewhat unusual, because the emission band at about 600 nm, corresponding to the indirect zero-phonon transitions, has optical gain (not very strong though, up to about 200 cm^{-1}) [1,4]. In GaSe however, due to the vicinity of the two gaps, indirect zero-phonon transitions are facilitated. Further, nonradiative recombination channels tend to saturate at high carrier densities. And the presence of an e-h plasma can increase the zero-phonon transition probability. In conclusion, our novel model explains the intense luminescence appearing up to three Rydbergs below the direct free exciton radiation in strongly excited GaSe.

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BAND EDGE SPECTRA OF HIGHLY EXCITED GALLIUMARSENIDE

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The optical spectrum of an optically excited semiconductor depends on the e-h pair density, the distribution functions f_e and f_h of the plasma-like excitations, and the degree of correlation between the particles, e.g. in lowest order the exciton effect. A sufficiently small density n_{e-h} of continuum e-h pairs will influence $\varepsilon(\omega, n_{e-h})$ only around the unperturbed gap energy E_g^o. The transition from discrete exciton line spectra to continuum edge pair spectra occurs in quasi-equilibrium at the Mott density of $n_{e-h}^{crit} \simeq 10^{15}$ cm^{-3} [1]. If only discrete e-h pairs (i.e. 1s excitons) of density n_{ex} are prepared initially, the edge spectrum looks substantially different: transient absorption spectra under resonant 1s pumping condition showed much less screening of the 1s exciton in the same density range and much larger $n_{ex}^{crit} \simeq 10^{17}$ cm^{-3} [2]. The present paper reports transmission spectra of 0.5 ... 2 μm GaAs platelets at 1.2 K with tunable psec laser excitation (i) above E_g^o and (ii) at the 1s exciton in a two-wavelength excite-and-probe configuration. We thus compare directly the effect of both the plasma (i) and the excitonic (ii) screening mechanisms on the absolute energy positions and widths of the 1s and 2s exciton. Bleaching of both lines occurred at densities 15 times higher in case (ii) compared to (i). In either case the bleaching of 2s required 10 times less density than bleaching 1s excitons. A substantial blue shift of the 2s line relative to 1s was found, the latter remained constant in energy up to complete bleaching. We also identified the influence of carrier cooling via e-h acoustic phonon coupling on the plasma screening behavior.

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TRANSIENT REFLECTIVITY AND FREQUENCY DEPENDENCE OF THE AMPLITUDE AND PHASE OF LIGHT REFLECTED FROM A CdSe CRYSTAL IN THE EXCITONIC REGION

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By an ellipsometric method (1), we studied with high resolution (0.1Å) the frequency dependence of the phase of light reflected by a thin CdSe platelet, cooled at 2°K. The results show a very fast variation of phase near the longitudinal exciton frequency. This variation is equivalent to an important delay in the time domain. We measured it in the following way : the source light is a CW dye laser pumped by an Argon laser ; it is sent into a Michelson interferometer. A linear polarizer parallel to the c axis of the sample is put in one arm and a crossed polarizer in the other one. The output light of the interferometer is sent to the CdSe sample and is reflected by the surface. We detect it after a linear polarizer on the direction of which the two polarization directions are projected. As the excitonic transition is allowed for the only polarization direction normal to the c axis, the corresponding beam is delayed and not the other one. By recording the enveloppe of the interferences while moving the mirror in one arm of the interferometer, one achieves the cross-correlation of the two electric fields. The shift of the maximum of the enveloppe gives the group delay of the wave-packet. In this way, we measured a delay as large as 12 ps near the longitudinal exciton frequency.

The results of amplitude measurement in transmission and amplitude, phase and delay measurement in reflection are in good agreement with a model taking into account an exciton-free layer of 100 A on the surface of the crystal. We explain the unusual large delay we observed by the combination of two effects. First, a significant delay (∿1ps) at the reflection between the dead layer and the bulk. This delay is due to spatial dispersion and has been calculated by Agrawal et al (2) in the case of a vacuum-sample interface (here, the permittivity of the dead layer increases it somewhat). Second, an enhancement of the delay by multiple reflections in the dead layer at the frequency where it acts almost as a Fabry-Pérot plate at the minimum of reflection.

Let us note, finally, that we were able to put into direct evidence the existence of the additionnal wave by recording at $\omega>\omega_L$ two reflected pulses in the case of a very thin sample (1μ). The delay between the two pulses shows without any ambiguity that one wave-packet has not been delayed and that the other one has travelled one way in the sample with a low speed and the other way with a high speed.

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K-DEPENDENT LONGITUDINAL-TRANSVERSE SPLITTING IN CuCl

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We start from the usual Hamiltonian for an electron (particle 1) in the spherical conduction band and a hole (particle 2) in the threefold degenerate valence band with the spin-orbit coupling ($I = 1$ and $S_2 = 1/2$)

$$H = H_{SO} + H' \quad \text{with} \quad H_{SO} = (2/3)\Lambda I \cdot S_2 \quad \text{and} \quad H' = T + V + W$$

Here the kinetic energy T consists of the relative and the translational energy operators, $T = T_r + T_t(\vec{K})$, $\vec{K}$ being the total momentum; V and W are the electron-hole Coulomb and exchange interactions, respectively. The spin-orbit term H_{SO} is diagonal in the coupled scheme $\vec{J} = \vec{L} + \vec{S}_2$ ($J = 3/2, 1/2$), and since it is usually much larger than other terms, we project the remainder onto the $J = 3/2$ and $J = 1/2$ subspaces to obtain effective Hamiltonians for $Z_{1,2}$ and Z_3 excitons (P and Q below are projection operators for $J = 3/2$ and $J = 1/2$):

$$\begin{aligned} H_{3/2} &= -\Lambda/3 + PH'P - \Lambda^{-1}PH'QH'P + \ldots \\ H_{1/2} &= 2\Lambda/3 + QH'Q + \Lambda^{-1}QH'PH'Q + \ldots \end{aligned} \tag{1}$$

Since H' contains simultaneously the exchange interaction W and the translational energy $T_t(\vec{K})$, the $\vec{K}$-dependent longitudinal-transverse (LT) splitting in CuCl comes out in a natural way from the cross term $\Lambda^{-1}Q(T_t(\vec{K})PW + WPT_t(\vec{K}))Q$ in the third term of (1).

With the aid of a newly-developed mathematical tool called angular-momentum algebra, the projection procedure can be carried out systematically to any order. Our result, when expressed à la Onodera, reads

$$\Lambda_{LT}(K) = \Delta_{LT}(0) + \frac{\alpha}{2} K^2 \qquad \text{with} \qquad \alpha = \frac{4}{3} \frac{2\Delta_0 + \Delta_{LT}(0)}{\Lambda} \times \begin{cases} B_2 & \text{for} \quad \vec{K} /\!/ 001 \\ B_3 & \text{for} \quad \vec{K} /\!/ 111 \end{cases}$$

Here B_2 and B_3 are mass parameters (equivalent of Luttinger's γ_2 and γ_3) for the translational motion $T_t(\vec{K})$, which, in turn, can be expressed in terms of the valence-band parameters L, M, and N. By taking Khan's values $L = 0.74$, $M = 0.54$, and $N = 0.04$, we obtain $\alpha = -0.05$ for $\vec{K} /\!/ 001$, which is to be compared with the experimental value $\alpha = -0.12$ by Mita, Sôtome, and Ueta.

TuP-PG4

Time-resolved Secondary Emission of Free Indirect Excitons in AgBr

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The dynamical behaviour of a hot exciton system optically created by picosecond laser pulses is studied in AgBr by measuring the time-resolved secondary emission. As excitation source we used a synchronously pumped dye-laser with Stilben 3 as laser dye (25 mW at 460 nm, pulse width 15 psec). The detection of the emitted light was performed using a fast channel plate photomultiplier and time-resolved single photon counting. The time constants derived from the experimental decay curves were obtained by deconvoluting the time dependent scattered intensity with the electronic excitation response (250 psec).

In case of indirect allowed excitons, the intensity of the secondary emission is proportional to the exciton distribution function The decay of the spectra therefore reveals the time evolution of the hot exciton system. This allows to evaluate the absolute transition rates for trapping at impurities, acoustic and intervalley phonon scattering, the relaxation processes known to be important in AgBr [1]. From our analysis we obtain an exciton lifetime of 950 psec and deformation potentials for acoustic and intervalley phonon scattering of $|E_c-E_v| = 0.84$ eV and $D_{iv} = 4.2$ eV, respectively.

The analysis of the experimental data indicates, that in case of indirect excitons in AgBr the SE is dominated by hot luminescence processes involving the lifetime of the intermediate state rather than by instantaneous Raman scattering.

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HIGH SENSITIVITY STUDY OF THE GREEN PHOTOLUMINESCENCE IN HIGHLY EXCITED SILICON

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It has previously been shown that the simultaneous recombination of two electron-hole pairs can lead to an extremely weak green luminescence at an energy near twice that of the indirect gap in silicon. This process was first reported for electron-hole-droplets,[1] and later for biexcitons and bound multiexciton complexes associated with the donor phosphorus.[2] Both of these previous studies were hampered by very low signal-to-noise ratios due to the extremely low intensities involved. A parallel spectrometer based upon an imaging photomultiplier tube has now been employed to study these processes in greater detail. This system collects 1024 spectral channels simultaneously, with a quantum efficiency of ~20% and a dark count per channel of ~1 per 3 minutes. Well resolved spectra due to electron-hole-droplets, biexcitons and bound multiexciton complexes associated with P, B and Li will be discussed. Systematic differences between the bound multiexciton complex spectra are in excellent agreement with theoretical expectations.

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IMPURITY BAND EFFECTS IN DILUTED MAGNETIC SEMICONDUCTORS†

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In CdMnSe large exchange enhanced g-factor makes it possible to study impurity bands under conditions that the spin splitting is comparable with the impurity band width in magnetic fields small enough that the orbital part of the wavefunctions are not appreciably perturbed. We have made studies of far infrared magneto-optical transmission in the 1 meV-12 meV photon energy range and the magneto transport on n-type single crystal $Cd_{0.9}Mn_{0.1}Se$ samples in the 2 K-20 K temperature range. Observations of bound electron spin resonance and conduction electron cyclotron resonance were published earlier.[1,2]

In the present work we report on studies of the background magnetotransmission spectra, which is related to impurity band effects. The absorption spectrum at zero field consists of a low frequency (1 meV-4 meV) broad peak followed by a monotonically increasing absorption at higher frequencies (5 meV-11 meV) which merges with the broadened 1s-2p transition (at 15 meV). As the field is raised the high frequency absorption has a blue shift while the low frequency part has a red shift. We attribute the higher frequency absorption to optical excitation of D^+D^-complexes, and the lower frequency absorption to photon induced hopping. The high frequency blue shift, the low frequency red shift and the negative magnetoresistance all have magnetic field dependences which scale (at different temperatures) the same as the electron spin-splitting energy.

These results can be understood consistently in terms of Coulomb exchange interaction effects between electrons in these relatively high donor concentration samples ($a_0N^{1/3} \sim 0.16$). We consider a molecular model in which electrons bound on a pair of neighboring donors have a splitting between the spin singlet and spin triplet levels that depends on their separation. At zero magnetic field the singlet state is lowest. As the magnetic field is raised the triplet states split and at a certain field the $S_z = -1$ state crosses the $S = 0$ level and becomes the ground state. Since the density of states of one of the $^3\Sigma$ triplet band is narrower in energy than that of the $^1\Sigma$ singlet state the hopping conductivity increases and the maximum of the absorption due to photon induced hopping shifts to lower energy. Also, photon induced formation of a D^+D^- complex from a donor pair in ground state would require a spin flip for the triplet, a process with small transition rate, greatly reducing the absorption due to the excitation of D^+D^- complexes. The transition of the ground state from the spin singlet to the $S_z = -1$ state occurs at somewhat different magnetic fields mostly due to different spacial separation between donors in a pair which leads to different exchange energy splittings of the $^3\Sigma$ and $^1\Sigma$ states at zero field.

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ACCEPTOR-BOUND MAGNETIC POLARON IN $Cd_{1-x}Mn_xTe$: A STATISTICAL MECHANICAL MODEL

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Our description of the bound magnetic polaron (BMP) in dilute semimagnetic semiconductors is based on the exchange Hamiltonian $H = -J\vec{s}.\sum_i b_i \vec{S}_i$. Here $b_i = |\phi(R_i)|^2$; the impurity envelope function ϕ is assumed hydrogenic. The partition function is deduced by treating the Mn^{++} spins $\vec{S}_i$ as classical vectors. The Gaussian approximation employed previously for the donor-BMP in CdMnSe is inadequate for the acceptor-BMP in CdMnTe, because the Bohr radius of the acceptor is much smaller and only a few (∿ 10) Mn spins are involved. We present a more accurate model for the acceptor-BMP, that describes both the low temperature saturation and the high temperature fluctuation regimes in a consistent manner. We consider a realistic arrangement of Mn ions over the cation sublattice, and cut off the sum at a finite distance R_c from the impurity center ($b_i = 0$, $R_i > R_c$). R_c is treated as an empirical parameter and interpreted as the distance where the hole-Mn exchange interaction becomes weak enough to be comparable to the antiferromagnetic Mn-Mn interaction. We assume the effective spin operator of the hole to be given by $s = 3/2$. The partition function is then calculated without further approximation. We compute the magnetic binding energy as a function of temperature and obtain an excellent fit of the experimental data of Nhung and Planel$^{(1)}$ on $Cd_{.95}Mn_{.05}Te$.

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TuP-PH3

THE FREE MAGNETIC POLARON IN $Pb_{1-x}Mn_xS$

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We report on the observation of the Free Magnetic Polaron in $Pb_{1-x}Mn_xS$ and give a model of the exchange interaction including the nondiagonal parts of the hamiltonian. After the observation of an unexpected zero-field splitting in the emission spectra of $Pb_{1-x}Mn_xS$-laser diodes [1] ($0=x=0.032$), we extended the measurements to the presence of external magnetic fields up to 12 Tesla. From the magnetic field- and polarization analysis we identify the emission lines as transitions between the spin-split Landau-levels of the CB and VB and additional impurity states. With increasing magnetic field the zero-field splitting merges into the classical field dependent splin-splitting. The field of this merge increases with the composition parameter x. For increasing temperature the zero-field spin-splitting decreases. The comparison of the evaluated high-field g-factor with that obtaines from intraband magnetoabsorption [2] makes clear that the dominant zero-field splitting is due to the VB corresponding to $Pb_{1-x}Mn_xTe$ [3]. It should be noted that similar phenomena are well known in magnetic semiconductors[4]. For semimagnetic (diluted) semiconductors, however, the established theory of KOSSUT-GALAZKA [5] does not reproduce these effects. We demonstrate by Green function technique that also for the diluted systems there is a zero-field spin-splitting in the density of states due to the contribution of the dynamic part of the interaction involving $S^{\pm}$..This splitting of the free-carrier states reflects the different quantum levels of the Free Magnetic Polaron. The adoption of this result to the k·p-model requires that the exchange interaction is not any more proportional to the macroscopic magnetization.

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OBSERVATION OF VAN VLECK-TYPE PARAMAGNETISM IN SEMIMAGNETIC SEMICONDUCTORS

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Van Vleck-type paramagnetism (VVP) is observed for magnetic ions with a singlet ground state. In the presence of magnetic field, such singlet mixes linearly with excited states, which leads to the temperature independent paramagnetism. We report the observation of the VVP in some new semimagnetic semiconductors: $Zn_{1-x}Fe_xSe$, $Zn_{1-x}Fe_xTe$ ($x \leq 0.05$) and highly doped GaAs: Mn. For the zinc-iron compounds the magnetisation measurements were performed at the magnetic field up to 15 T. The magnetisation of the crystals was found to be temperature independent between 2 K and 10 K, then it decreases with temperature. These results are interpreted on the base of the $Fe^{2+}(3d^6)$ electronic configuration. The ground state of the Fe^{2+} is a singlet A_1, which originates from the ^5E spin-orbit split orbital doublet. For GaAs: Mn a strong Faraday rotation was measured in the region of the fundamental absorption edge at the magnetic field up to 5 T, and was found temperature independent between 2 K and 300 K. This rotation is due to s-d type exchange interaction between the $Mn^{3+}(3d^4)$ ions and band carriers. The ground state of the Mn^{3+} in the strong crystal field case is an orbital singlet $^1A_1$, which mixes with $^1T_1$ orbital triplet All these magnetic and magnetooptical effects due to the VVP differ significantly from those reported up to now for the semimagnetic semiconductors.

ON THE QUESTION OF EXCITON LOCALIZATION IN (Cd,Mn)Te BY ALLOY DISORDER

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Recently, we have applied methods of picosecond spectroscopy to the study of the kinetics of a donor bound exciton in n-(Cd,Mn)Se (1). Large time-dependent spectral redshifts observed at low temperatures were interpreted in this work to be the signature of a photoinduced, dynamically developing bound magnetic polaron in the exciton volume. A more general question concerns the possibility for similar phenomena in the case of free excitons which might be localized by alloy potential fluctuations in such mixed crystals. Evidence of exciton localization in II-VI mixed crystals in the absence of a magnetic constituent has been published (2). We report here new results obtained from study of transient excitonic behavior by time-resolved experiments in the free exciton tail in the semimagnetic crystal (Cd,Mn)Te for differing alloy composition and as a function of temperature.

Our experimental approach has been to use transient photomodulation spectroscopy in the 5-1000 psec time domain, implemented by a pair of dye lasers in an excite-probe mode where both the excitation and probe energies can be independently tuned within the disorder broadened free exciton low energy tail. With good experimental sensitivity, the details of excitonic energy relaxation and thermalization can be studied in detail. For example, for (Cd,Mn)Te with x=.30 we see photomodulated spectral features below the free exciton peak which are characteristic of localized excitations, based on simple arguments. Time dependent shifts in these spectra on the order of 10 meV can be clearly seen at low temperatures (T=2 K) and appear to be a combination of thermalization and a dynamic energy normalization effects. Above 20 K the shifts are no longer observable. Throughout a wide temperature region, the well known neutral acceptor bound exciton (3) can be clearly identified in the photomodulation spectra but is well separated in energy from the free exciton tail so that its dynamics can be isolated and used to support arguments about energy exchange with partially localized free excitons. We have modelled the wide range of observed phenomena by considering the energy relaxation and trapping processes of free excitons by alloy potential fluctuations in the semimagnetic host and the role of shallow impurity states which may have merged with the bandedge states.

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PHONONS IN FLUORINATED AMORPHOUS SILICON ALLOYS

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A theoretical study of the F-induced vibrational excitations in amorphous silicon has been made in the rotationally invariant valence force field formulation for the cluster embedded into a Bethe lattice. The effects of the local environment on the strength of the Si-F bonds in the fluorosilane molecules $SiF_{4-m}H_m$ (M = 1,4) have been investigated by using the available infrared and Raman data. Further, the calculated phonon density of states lying within and outside the silicon bulk phonon band region arising from the simple SiF_n (n = 1,2,3) units and the interacting SiF_2 units is in excellent agreement with the available infrared data. It is concluded that the peaks at 214, 300 and 510 cm^{-1} seen in the infrared data originate from the isolated SiF and SiF_2/SiF_3 units. An unexplained peak at 650 cm^{-1} detected in the infrared data originate from the adjacent interacting SiH_2 units. The present results are in complete accord with those obtained by a similar analysis of the photoemission data by our group. Our work thus establishes the occurrence of the simple SiF_n units and the two adjacent interacting SiF_2 units in the a-Si:F alloys.

CARRIER DYNAMICS IN MICROCRYSTALLINE SILICON EXAMINED BY TRANSIENT GRATING METHOD

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The application of microcrystalline silicon (μc-Si) to solar cells has been expected because of the good electrical properties of a high dark conductivity and a high doping efficiency.

We separately and simultaneously determine the lifetime and the diffusion coefficient of photoexcited carriers in various μc-Si with different grain sizes (120-360 A) and volume fractions (0.02-0.70) by a novel transient grating method.[1,2] We clarify the carrier dynamics through the experimental results.

Under the condition of a constant grain size, the lifetime monotonically decreases from 30 μs to less than 10 μs with the increase of the volume fraction. On the contrary, the diffusion coefficient is constant under the volume fraction of about 0.2, but it increases gradually with the increase of the volume fraction to larger than 0.2. Under the constant volume fraction, the diffusion coefficient and the lifetime do not change significantly within the range of grain sizes from 120 to 360 A. Additionally, the tendency on the variation of the dark conductivity well correlates to that of the diffusion coefficient.

We propose a model taking account of the carrier recombination at the grain boundary regions and the carrier transport through a percolation path to understand the carrier transport in μc-Si. The calculated curves based on the model well explain our experimental results. These results indicate that the carrier recombination at the grain boundary regions and the percolation process are very important in the carrier dynamics of μc-Si.

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17th International Conference on the Physics of Semiconductors
Amorphous Semiconductors **TuP-PI3**

LOW FREQUENCY HOPPING CONDUCTIVITY IN AMORPHOUS GERMANIUM AND SILICON.

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The excess ac conductivity $\sigma_A(\omega) = \sigma(\omega) - \sigma(0)$ due to hopping processes in a disordered material is usually interpreted in terms of the ω^s law, $s < 1$, predicted by the pair approximation[1]. However, data on $\sigma_A(\omega)$ for amorphous germanium and silicon shows a roll-off behaviour for decreasing frequency in the region where the total ac conductivity $\sigma(\omega)$ becomes non-dispersive. $\sigma_A(\omega)$ falls off faster than ω^s below a characteristic frequency ω_c which exhibits a strong temperature dependence[2,3]. The pair approximation for a tunneling model cannot explain this phenomenon. Long has therefore questioned the validity of the assumption of tunneling between random sites in amorphous Ge and Si and has investigated alternative models of the hopping process. In this paper we show, on the contrary, that the roll-off is obtained when the **extended** pair approximation (EPA)[4] is applied to the tunneling model. It marks the *onset* of ac loss by subsets of sites contained in the infinite cluster determining $\sigma(0)$. Decreasing ω through ω_c changes s from less than unity to 2. To within a scale factor, the EPA gives a good account of the observed frequency dependence of $\sigma_A(\omega)$ and the temperature dependence of ω_c for evaporated germanium[2]. Data for sputtered germanium[3] is also explained well by the EPA predictions and the most recent data for sputtered amorphous silicon[5] is in extremely good agreement with the EPA predictions in the neighbourhood of ω_c with regard to the both frequency dependence and the ratio of the real and imaginary parts.

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MOLECULAR STRUCTURE OF MELT-QUENCHED $GeSe_2$ AND GeS_2 GLASSES COMPARED AND CONTRASTED

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New insights in the morphological structure of network glasses have emerged recently through the application of Mössbauer spectroscopy as a probe of chemical order of both cation and anion sites in indicated glasses (1). Probe of cation chemical order have made use of ^{119}Sn spectroscopy in melt-quenched ternary $(Ge_{0.99}Sn_{0.01})_xX_{1-x}$ glasses where X=S or Se. The spectra reveal two distinct and microscopically well defined sites (A,B) even at x=0.333. From the nuclear hyperfine structure the A sites are identified as the tetrahedral $Sn(Se_{1/2})_4$ sites while the B sites with Sn replacing one of the Ge sites in an ethanelike $Ge_2(X_{1/2})_6$ cluster. At x=0.333 the ratio of the site intensities $I_B/(I_A + I_B) = 0.16$ and 0.26 for X=Se and S respectively. The existence of a finite and reproducible intensity of the symmetry breaking nontetrahedral B-sites at x=0.333, we have *suggested (1,2) is better understood in terms of phase separation* of the glass network into cation-rich and anion-rich molecular clusters(3). In this approach, the degree of broken chemical order provides a measure of the physical size of the clusters. It specifically shows that the anion-rich cluster in GeS_2 is smaller in size than the one prevailing in $GeSe_2$ glass. Additional insights in the network structure are accessible upon contrasting the x-composition dependence of the Mossbauer site intensity ratios and Raman vibrational mode strengths in the Ge-rich phase ($x > 0.333$) of the present glasses.For example, a third type of a site (C) is seen (2) when $x > 0.37$ for X=Se, but already when $x > 0.333$ for X=S. The C site is attributed to a distorted octahedral GeX amorphous phase. Interestingly in Raman spectra of X=S glasses a new mode appears at 250 cm^{-1} when $x > 0.333$. The scattering strength of this mode scales with relative intensity of C sites in our spectra. This correlation strongly supports the original identification of the 250 cm^{-1} mode as belonging to an amorphous GeS phase (4). Its appearance at a lower x value for X=S than for X=Se glasses, can be understood in terms of a higher ionicity of the Ge-S bond which promotes a tendency to form *octahedrally coordinated structures.* These new Mössbauer and Raman results extend in a significant way previous understanding of the tetrahedral network structure of these stochiometric glasses based on previous Raman and diffraction measurements.

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TuP-PI5

EFFECT OF LIGHT ON THE THRESHOLD SWITCHING VOLTAGE IN AMORPHOUS THIN FILMS

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Smith and Henisch[1] and Henisch et al.[2] have shown that illumination of light on amorphouse chalcogenide alloy may increase the threshold current of switching tremendously, yet the threshold voltage is not changed much. This phenomenon may be explained by extension of Chiang's theory[3,4,5]. With the assumptions that two stable configurations (one with high conductivity, the other with low conductivity) coexisting in the films, the interconversion of these two configurations are governed by current excitation according to law of mass action or energy impact, a threshold switching equation is derived. With the appropriate parameters, the threshold voltage and threshold current may be calculated. During the illumination, more carriers are released and the conductivity of the configuration increases, therefore the threshold current increases; however, not all the extra released carriers are used in initiating the conversion from one configuration to the other, thus the effective threshold current is much less than the apparant threshold current. With this idea the calculated threshold voltage may maintain approximately the same value. Different effective threshold current corresponding to different conductivity (which may be produced under different illumination) has been calculated. The important issue as whether it is the field which is critical or whether it is the current which is critical as the determining factor for initiating the switching is also discussed.

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INFRARED SPECTRA OF B- AND P-DOPED a-Si:H FILMS

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The absorption spectra of several phosphorus and boron doped a-Si:H films,grown by an evaporation technique(1), are reported. The change of SiH_n stretching and wagging (or rocking) absortion bands, is studied as function of the dopant content determined by Auger analysis. A marked decrease of area of the stretching bands is also observed for P-doped samples, indicating a reduction of hydrogen content on increasing doping. The spectra of B-doped films are basically the same as those of P-doped samples showing a slight "transfer" of area between SiH_2 and SiH bands. A comparison of the results with the existing ones(2), gives strong support to the conclusion that the dopants in the a-Si:H matrix, affect the film morphology, by forcing them to grow with a different hydrogen bonding configuration and microstructure(3).In particular, has been noted that the residual fraction of the hydrogen content is essentially bonded as monohydride, indicating an overall decrease in the number of defects and consequentially an improvement of the network quality.

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Amorphous Semiconductors **TuP-P17**

Study of Neutron Transmutation Doping in a-Si:H

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Abstract

High doping efficiency of phosphorus (P) in hydrogenated amorphous silicon (a-Si:H) prepared by glow discharge has been achieved by neutron transmutation doping (NTD).

The doping process is based on nuclear reaction

$$^{30}\mathrm{Si}\ (n,\gamma)\ ^{31}\mathrm{Si} \xrightarrow{2.6\ \mathrm{hr}} {}^{31}\mathrm{P} + \beta^{-}.$$

This reaction converts the isotope ^{30}Si into ^{31}Si. The ^{31}Si isotope produced is unstable and decays through β^{-} emission to ^{31}P, which is expected to act as a donor impurity on Si sites.

Thermal neutron irradiation was performed at a flux density of approximately 5×10^{11} n/cm^{2}sec. The neutron irradiation doses were 1.8×10^{16} and 9.0×10^{16} n/cm^{2}. The annealing studies for electrical properties and radiation damage were performed in a vacuum at several temperatures.

ESR signals for as-irradiated films have been newly appeared on signals ($g=2.005$) for as-grown films, with a decrease of photo conductivity. Recovery of dark and photo conductivities has been observed accompanying a disappearance of the new ESR signals by the subsequent annealing near the growth temperature of a-Si:H films. Dark and photo conductivities for as-grown and NTD a-Si:H films as a function of annealing temperature are evaluated. These conductivities abruptly increase with the annealing temperature and show the recovery at about 220°C in agreement with growth temperature of a-Si:H films. The activation energies of 0.69 and 0.42 eV were obtained for transmuted P concentrations of 3.4×10^{12} and 1.7×10^{13} /cm^{3}, corresponding to neutron doses mentioned above, respectively. This phenomenon shows an excellent doping effect by NTD. Therefore, this doping efficiency by NTD is higher than one of the conventional gas-doping [1].

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PHONON DENSITY OF STATES AND RAMAN SPECTRA IN Si-BASED AMORPHOUS SEMICONDUCTORS

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Raman scattering spectra have been found to be sensitive to structural disorder in amorphous(a-) Si. We have found that the width of the TO-like peak due to Si-Si vibration increases with x in a-$Si_{1-x}N_x$ and a-$Si_{1-x}C_x$ and the density of the ESR spin due to dangling bonds increases with an increase in that width for a-$Si_{1-x}N_x$, a-$Si_{1-x}C_x$ and a-Si prepared by various methods. There is still confusion about what kind of disorder, such as bond angle fluctuation, bond length fluctuation etc. affects most importantly the shape of the Raman spectra. Especially it is almost unknown how the incorporation of N or C into a-Si changes the phonon density of states(PDOS) from theoretical viewpoint. In order to solve these questions, the calculation of the PDOS was carried out. We first constructed 110~133-atom clusters of a-Si, a-$Si_{1-x}N_x$ and a-$Si_{1-x}C_x$ with balls and sticks in which Si and C atoms are tetrahedrally coordinated and N atoms have three-fold planar coordination. These structures were relaxed by minimizing the Keating potential. Then we calculated the PDOS by using the Keating potential whose parameters had been adjusted for crystalline Si, SiC or Si_3N_4 to reproduce the observed PDOS. We found from the calculations of the PDOS for a-Si clusters with various structures that the observed broadening of the width of the TO-like peak is due to the bond angle fluctuation whereas the bond length fluctuation has a rather small effect on the PDOS. As for a-$Si_{1-x}N_x$ and a-$Si_{1-x}C_x$, it is found that the incorporation of N or C makes the bond angle fluctuation around Si atoms larger. This fluctuation is brought about because the bond lengths of Si-N and Si-C are considerably smaller than that of Si-Si. Calculations of the PDOS for these clusters show that the width of the TO-like peak increases with N or C contents. In conclusion, the incorporation of N or C atoms in a-Si makes the bond angle fluctuation around Si atoms larger, resulting in an increase of the density of dangling bonds.

EFFECT OF LIGHT ILLUMINATION ON THE DISTRIBUTION OF GAP STATE DENSITY IN P-DOPED a-Si:H

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A new method of obtaining the distribution of density of states (DOS) in the gap in lightly P-doped, hydrogenated amorphous silicon (a-Si:H) has been developed utilizing Staebler-Wronski effect. Samples were prepared by rf glow discharge decomposition of silane with appropriate amount of phosphine, ranging from 0.8 ppm to 200 ppm. Electrical conductivity was measured very accurately as a function of temperature after various degrees of illumination and doping. The room temperature ratio of annealed to light-soaked conductivities varied from zero for undoped samples to 10,000 for 8 ppm P-doped samples. The conductivity activation energy E_σ was observed to vary systematically with illumination dose and degree of doping. From the dependence of E_σ on the illumination time, DOS distribution in the gap was obtained. The result shows that, for lightly P-doped samples, deep minimum in DOS appears near 0.5 eV below E_c (conduction band mobility edge), followed by the sharp rise in DOS between 0.6 and 0.8 eV. This is quite contrary to the result of ICTS1) which gives DOS maximum at 0.5 eV below E_c, but agrees well with the results of DLTS2). The changes in E_σ and conductivity pre-exponential factor with temperature and doping were analyzed in terms of the dependence of Fermi energy on temperature and the distribution of DOS in the gap. Our results strongly indicate that the doubly occupied dangling bond state (D^-) should lie at about 0.85 eV below E_c.

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ELECTRICAL PROPERTIES OF NON-STOICHIOMETRIC AMORPHOUS $CdGeAs_2$

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The ternary system $CdGeAs_2$ is of particular interest because it is one of the few semiconductors with tetrahedral coordination which can be prepared in the glassy state by quenching from the melt. In tetrahedral amorphous semiconductors a number of quite generally observed transport properties still remain unexplained. In particular, the sign anomaly of the Hall effect is not well understood. Earlier work (1) on the amorphous $CdGe_xAs_2$ system with $0 < x < 1.0$ has shown that the Hall coefficient is negative for all compositions except for the stoichiometric compound $CdGeAs_2$, whereas the thermopower changes from p- to n-type with increasing Ge content

In this study measurements of dc conductivity, thermopower and Hall effect are reported for $CdGeAs_2$ glasses having a small excess or deficiency of the three elements compared to the stoichiometric composition. The experimental results can be summarized as follows:

(a) The conductivity measured in the temperature range 200 - 500 K differs only slightly for the different compositions. The data are best fit by smooth curves with gradually increasing activation energy

(b) The thermopower always indicates n-type conduction.

(c) The Hall coefficient is negative for $CdGe_{1-x}As_2$, $Cd_{1+x}GeAs_2$, and $CdGeAs_{2+x}$; and a positive sign is observed for $CdGe_{1+x}As_2$ and $Cd_{1-x}GeAs_2$.

(d) The Hall mobility is very small (between 0.015 and 01 $cm^2V^{-1}s^{-1}$ for the different compositions) and is nearly temperature independent.

The results will be discussed in the framework of the current theoretical concepts for conduction near a mobility edge. The applicability either of the Emin theory of small-polaron formation or of the Mott theory of localization in disordered systems will be examined. Although electron microscope observations did not yield convincing evidence for a heterogeneous structure, the glasses may consist of two amorphous phases. When interpreting the experimental transport data, the presence of a bi-phasic structure with different electrical parameters for each phase will be considered.

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PHOTOELECTRONIC PROPERTIES OF a-Si,Ge:H ALLOY FILMS

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We have achieved an important breakthrough in the deposition of a-Si,Ge:H alloy films through independent control of spatially separated Si-H and Ge-H plasma phase interactions. This is accomplished in a UHV base pressure dual magnetron sputtering system. We have previously established conditions for deposition of highly photoconductive intrinsic films of a-Si:H and a-Ge:H(1,2), and found that the pressures of H required are very different, 0.4mTorr for the a-Si:H and 4.0mTorr for a-Ge:H. For deposition of the alloy films, we have used a standard Si target, but have modified the Ge target so that the hydrogen pressure in the chamber produces a higher "effective" hydrogen pressure at at the Ge target. Proceeding in this way and using the power input to the individual targets as an additional deposition parameter, we have been able to control: (1) the ratio of Si to Ge atoms in the alloy, (2) the total hydrogen concentration, and (3) the fractional bonding of H to the Ge and Si alloy components. This represents a significant advance over previous attempts to produce high electronic quality alloys by either (1) glow discharge decomposition(GD) of silane and germane mixtures, or (2) diode sputtering from composite Si/Ge targets. In these two deposition schemes, the Si, Ge and H atoms are in a common plasma, and the resulting films display (1) an asymmetry in H-atom attachment in which Si-H bonds dominate and (2) relatively weak photoconductivity. In contrast, the intrinsic alloy films that we grown with approximately equal Si and Ge concentrations and band-gaps of about 1.4 eV, have photoconductivities that are more than an order of magnitude higher. We attribute this to a decrease in the density of recombination and/or trapping states that results in part from more nearly equal H compensation of potential Si and Ge dangling bonds. We have monitored the IR absorption and found that increases in the photoconductivity are correlated with the nature of the bonding of H to both the Si and Ge atoms, in particular to the appearance of weak features in the IR that come from dihydride bonding of both Si and Ge atoms (isolated Si-H_2 and Ge-H_2 groups). We attribute the differences in H-atom attachment in our films relative to the GD and diode sputtered films to the spatially separated generation of Si-H and Ge-H precursor molecules, and to the fact that in our system they are combined at a substrate in a region which is plasma free. Film characterizations include measurements of the photoconductivity, optical absorption and dark conductivity as functions of the alloy composition (by e-beam microprobe) and bonded H concentrations (by ir absorption).

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EFFECT OF OXYGEN ON THE STABILITY OF a-Si:H

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In this note the effect of oxygen on the stability of a-Si:H structure and on the light-induced effect has been studied by ir adsorption and conductivity measurements respectively.

The ir spectra of different temperature annealed a-Si:H show that the 2190 cm^{-1} peak and, particularly, the 2250 cm^{-1} peak is stable after annealing up to 600°C. This indicates that the Si:H configuration backbonded with more oxygen are more stable than that without oxygen as the nearest neighbors.

The Staebler-Wronski effect in a-Si:H doped with different amount of oxygen is measured by conductivity measurement. From the comparison of conductivity before and after illumination it is shown that the Staebler-Wronski effect is weaker in heavily oxygen-doped a-Si:H than that in undoped or slightly doped sample. Therefore, it is concluded that due to stabilization of Si-Si weak bonds with oxygen as bridging atoms the a-Si:H:O structure is more stable under illumination and the oxygen related centers could not be the origin of the light-induced effect.

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SOME PROPERTIES OF B-DOPED SILICON FILMS

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Some results of B-doped silicon films prepared by low pressure chemical vapor deposition (LPCVD) are reported. (1) The flow rate of gases is one of the important factors which affects the properties of the films, and there is an optimal flow rate. (2) The direct current conductivity (σ_d) of films is concerned in grown temperature. X-ray diffraction and scanning-electron-microscope experiments show that the B-doped silicon films prepared at about 635°C are of both amorphous and microcrystal structures possibly, and σ_d is above 10Ω-1cm-1 under room temperaure, and that the diffraction peaks in (111) (220) are found for the films prepared at about and above 670°C, but not for one below 635°C. (3) The activation energy of both are 0.026ev and 0.23ev, respectively. (4) No hydrogen is found from Infrared Absorption experiment.

A MODEL OF THE LOCAL STRUCTURE OF RANDOM TERNARY ALLOYS: EXPERIMENT VERSUS THEORY

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We have performed an Extended X-ray Absorption Fine Structure measurement of $Cd_{1-x}Mn_xTe$ solid solutions for various concentrations x in the single phase range $0 \leq x \leq 0.7$. The data have been collected on the Mn K, Cd L_{III}, and Te L_{III} edges. We have found well-defined different nearest-neighbor Cd-Te and Mn-Te distances almost independent of x. We have developed a model of the microscopic structure of the zinc-blende-type $A_{1-x}B_xC$ ternary alloys based on a random distribution of cations. The model describes the bimodal distribution of near-neighbor distances in terms of distortion of the anion sublattice using only the lattice constant of the alloy and the bond-stretching constant of the each binary component. We believe that the local distortion in zinc blende-like $A_{1-x}B_xC$ alloys described by our model is a universal feature of such alloys. Its application to $Cd_{1-x}Mn_xTe$ and $In_{1-x}Ga_xAs$ alloys proved to be in excellent agreement with the EXAFS results. Within the framework of this model we consider also the problem of the structural stability of $Cd_{1-x}Mn_xTe$.

TuP-PJ1

DOPING DEPENDENCE OF MUONIUM RELAXATION IN SEMI-CONDUCTORS

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Muonium in semi-conductors can be considered as a light isotope of hydrogen ($m(\mu^+) = 1/9\ m(H^+)$). Two muonium states, normal muonium (deep donar) and anomalous muonium (shallow donar) are observed. In this contribution the relaxation rate λ^* of anomalous muonium in silicon with different exceptors and different exceptor concentrations was investigated as a function of temperature. The behaviour of λ^* is very well describable by scattering of conduction electrons on anomalous muonium.

TuP-PJ2

OPTICALLY DETECTED MAGNETIC RESONANCE STUDIES OF DONOR-ACCEPTOR EXCHANGE INTERACTIONS IN II-VI SEMICONDUCTORS

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ODMR applied to donor-acceptor luminescence is now a well-established method for obtaining the EPR spectra of donors and acceptors . However, the optically detected EPR lines are usually very broad . We describe experiments which show that the line broadening is due to the D-A exchange interaction J_{DA} and provide information about this interaction in the range 10^{-3} - 10^{-1} cm^{-1} where it is much too small to be resolved optically .

We use a time-resolved ODMR technique that discriminates as a function of optical lifetime and therefore as a function of the D-A separation distance r_{DA} . Studying various II-VI compounds (ZnO, ZnS, ZnSe, ZnTe and CdS) we find, firstly, that very long-lived D-A pairs (those with large r_{DA}) give narrow ODMR lines corresponding to virtually isolated donors and acceptors. Secondly, as the timing is changed to emphasize emission from pairs with smaller r_{DA} , the lines become extremely broad. We attribute this to a statistical distribution of exchange splittings and discuss the relation between J_{DA} and the reciprocal lifetime for the different D-A systems studied .

For shallow donor - shallow acceptor pairs in CdS, where phonon broadening of the luminescence is small, we have achieved more precise selection of pairs of given r_{DA} by restricting observation to a narrow range of emission wavelength . The ODMR lines then show a resolved exchange splitting. Measurements of the splitting as a function of emission wavelength give the distance dependence of J_{DA} over two orders of magnitude . The results are explained by an exponential form of the donor wavefunction and provide a measure of the donor radius . The value of J_{DA} extrapolated to $r_{DA}=0$ is compared to the exchange splitting in the free exciton . Because of the relation between J_{DA} and the wavefunction overlap, the methods used in this work have potential for mapping shallow centre wavefunctions out to relatively large distances .

DEFECT-RELATED HOPPING TYPE CONDUCTION IN GaAs

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ABSTRACT

We have performed detailed experimental and theoretical investigations of defect related electronic transport mechanisms in GaAs. Different test vehicles are used, but particular attention is devoted to the leakage current between AuGe and AuGe/n^+ contacts with 10 µm to 150 µm separations and fabricated on the same semi-insulating substrate.

Two types of defects are studied : i) "surface related" defects introduced by chemical treatments or by a dielectric deposition and ii) more in-depth defects introduced by implanting boron ions at different doses (10^{10} to 10^{14} cm^{-2}), with kinetic energies up to 180 keV. The effect of isochronal (30 min) annealing at different temperatures ranging from 300 °C to 600 °C is also reported.

The I-V characteristics recorded in the voltage range from -40 to +40 V and for temperature ranging from 80 K to 400 K. The low voltage ($|V|<5V$) I-V characteristic is roughly ohmic and varies with temperature according to an electronic-hopping conduction - Mott type - law : $\exp-(T_o/T)^n$ where $n \approx 0.4$, T is the temperature in Kelvin and T_o a constant. Thus, all defects studied yield similar conduction mechanisms.

For higher voltages, a strong departure from ohmicity is observed. Furthermore this non-ohmic portion of the characteristic is found to be very sensitive to treatments affecting the first monolayers of the GaAs surface.

The similarity between surface and ion implantation defects is quite remarkable and is confirmed by Deep-Level Transient Spectroscopy (DLTS) and by photo-response investigations. The results of these investigations will be published elsewhere.

Our observations allow us to suggest a microscopic Quantum-Mechanical model treating in a unified manner ion-implantation and surface related defects. The electronic mechanisms are governed by multiphonon tunnelling between closely spaced (~200 Å) defects. It is to be emphasized that in the case of GaAs, the small Γ - conduction band effective mass greatly enhances tunnelling probabilities. We demonstrate, in particular, the key rôle played by the mid-gap level related to the As_{Ga} antisite defect. The differences in behaviour between this mechanism and those related to an inhomogeneous arsenic pile-up at the surface will be discussed.

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Impurities **TuP-PJ4**

HOT EXCITON KINETICS IN THE VICINITY OF THE NEUTRAL SHALLOW DONORS IN GaAs

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Free exciton (FX)-neutral donor (D^o) scattering in high-purity GaAs is considered to be one of the important processes for the hot exciton kinetics, because of the effective "pumping" of oscillator strength from FX towards donor bound exciton (BX). In order to clarify the hot exciton kinetics in the vicinity of D^o, we have investigated systematically the radiative and nonradiative recombination processes of FX and BX as a function of the exciton effective temperature T_X, from the observed excitation-level dependence of the photoluminescence spectra at 1.8 K and 4.2 K. By analyzing the emission intensities of FX, BX, and two electron (TE) satellite of FX as a function of T_X, we could determine for the first time the exciton-capture rate ($\gtrsim 4x10^{-5} cm^3/s$) as well as the partial Auger recombination rate ($\gtrsim 5x10^{-7}\sqrt{T_X}\ cm^3/s$) per a neutral donor.

The effective temperature T_X was determined by the emission from upper polariton branch (UPB) of FX, which was satisfactorily fitted with the calculated lineshape of UPB in a model of the exciton-electron inelastic collision1). The model describes the inelastic scattering of FX into photonic branches by hot electrons with the temperature $T_e=T_X$. As a function of photoexcitation density J_p ($1\ mW/cm^2 \lesssim J_p \lesssim 2\ W/cm^2$), we can observe ; (1) T_X increases from $\sim$2K to $\sim$ 34 K, (2) The TE satellite of FX shows a slight blue shift, (3) Intensity ratio of the TE satellite relative to the UPB emission intensity increases linearly with $\sqrt{2kT_X/M_X}$ (i.e., mean FX velocity), from which we conclude that the partial Auger recombination occurs as a result of the Brownian motion of FX in the vicinity of D^o with the geometrical cross section πR_o^2 ($R_o \sim 100$ A), (4) The emission from BX ground state broadens as T_X increases, (5) The intensity ratios of the BX ground state relative to the 2nd rotator state and to the UPB emission decrease rapidly as T_X increases up to 8 K, and gradually decrease up to 34 K. By fitting the intensity ratios with the calculated one based on the detail balance equations, it has been successfully shown that the BX is partially in thermal equilibrium with hot FX, and that the reemission of FX out of BX competes with the radiative recombination with $T_X > 8$ K. The observations (4) and (5) are more remarkable under the externally applied electric field.

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INVERTED ORDERING OF ACCEPTOR BOUND EXCITON STATES IN SEMICONDUCTORS*

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The j-j coupling scheme in acceptor bound excitons (A^oX) in Si, GaAs and InP is studied by a variational calculation within the multi-band effective mass approximation. We have included in our calculation the effects due to local strain and Stark fields, the short-range central-cell potential, the degeneracy and warping of the valence band structure, and most importantly the hole-hole correlation effect. The realistic valence band structure is taken into account by using a 6x6 $\vec{k}\cdot\vec{p}$ matrix for the kinetic energy term for the hole. The local strain and Stark field effect is included in a spin-axial interaction term proposed by Morgan(1). The trial wavefunctions for the two-hole product states have the crystalline symmetries described by the Γ_1, Γ_3, and Γ_5 irreducible representations of the T_d point group. Each single-hole state in the trial wavefunctions has the Γ_8-symmetry and is a linear combination of the $j = 3/2$ and $j = 1/2$ (for the spin-orbit split-off band) spinors multiplied by spatial orbitals with angular momentum ℓ=0 or 2. The above trial wavefunctions are allowed to couple with many two-hole product states whose Fourier transforms in $\vec{k}$-space are gaussian functions located at different $\vec{k}$-points surrounding the zone center. Thus the hole-hole correlation effect is included.

We find that the spin-axial interaction and short-range central-cell potential included in the single-hole Hamiltonian can modify the energy separations of the Γ_1, Γ_3, and Γ_5 two-hole states, but they cannot invert the ordering of these states in A^oX. Without including the hole-hole correlation, the ordering of these states are, starting with lowest energy, Γ_3, Γ_5, Γ_1. The inclusion of the hole-hole correlation tends to reverse the trend. For Si doped with Aℓ, Ga, and In and GaAs:Sn, the ordering is found to be inverted. The energy separations of these states are found in reasonable agreement with all available experimental data.

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TuP-PJ6

THE DIRECT OPTICAL OBSERVATION OF IONIZED ACCEPTOR STATE IN n-HgTe

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HgTe is a zero-gap semiconductor. In this material only acceptor impurities create localized states which are degenerate with the Γ_8^c conduction band. Even in purest n-HgTe crystals such states are present in the concentration about 10^{15} cm^{-3}. If the Fermi level energy is higher than the energy of acceptor states, all those states are ionized and the optical transitions from ionized acceptor states to the conduction band states above Fermi level can be observed.

The transmission measurements on n-HgTe samples with electron concentration $3 \div 5 \times 10^{16}$ cm^{-3} at LHeT using the Furier interferometer were done. The "transmission window" from about 6 meV to about 15 meV was observed. The low energy edge of this "window" is determined by the plasma edge, TO phonon and/or interband $\Gamma_8^v \rightarrow \Gamma_8^c$ transitions give the high energy "cut off". In between the two pronounced transmission minimas were observed. The first one is explain by well known photon - ionized impurity - plasmon processes and the second one is due to described above transitions from the ionized acceptor states to the conduction band. Energy of this state is estimated at about 3.0 ± 0.5 meV. This result is coherent with previous transport and magnetooptical estimation but is the first optical observation of this state when it is degenerate (resonant) with conduction band.

TuP-PJ7

ELECTRONIC STRUCTURE OF THE POINT DEFECTS GaP:V_P AND GaP:O*.

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The multiple-scattering Xα method within the framework of the Watson-sphere-terminated cluster model was used to carry out electronic structure calculations of a single neutral ideal phosphorus vacancy and an oxygen substitutional impurity replacing phosphorus in gallium phosphide. The results suggest that a relaxation away from the vacancy site is highly likely for the gallium atoms surrounding the vacancy. This result plays a fundamental role in determining the physical properties of the GaP:O center.

The calculations were performed by considering different electronic configurations for the oxygen 2p atomic state. The results are summarized as follows.

(i) For the unrelaxed lattice they can be interpreted in terms of the conventional "classical description" of Dean et. al.[1]; i.e., a singly occupied a_1 level in the gap and O derived 2p states in the valence band.

(ii) For the relaxed lattice (0.12Å displacement of the Ga nn away from the O), the one electron energies in the $2p^4$ shell lie below the valence band bottom. A hyper deep s-like state is also found. Both levels have wavefunctions almost entirely associated with O. The defect states resemble those of the vacancy, weakly perturbed by the impurity, in agreement with Morgan's recently proposed description[2].

(iii) The one electron energies for the $2p^5$ and $2p^6$ shells lie inside the valence band. We suggest that these configurations correspond to the on-center metastable weakly bonded defect state identified by Kukimoto et. al.[3].

The mixing of defect and host states in these configurations may lead to the strongly relaxed state of the defect[3].

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TuP-PJ8

MANY-ELECTRON LOCALISED STATES OF NEGATIVE IONS IN SEMICONDUCTORS

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It is shown that there is a new class of weakly localised bound states in semiconductors that are stabilised by correlation phenomena peculiar to systems with enfeebled sp^3 covalent bonds. In particular, numerical results based on large-scale pseudopotential calculations are presented for the excited states of GaP:O^- and for the ground state of GaPAs:N^-.Satisfactory agreement with experiment is obtained in both cases.

Bound states of negatively charged defects in solids, such as the states of substitutional chemical impurities and F-centres, are normally treated as two-particle states, by analogy with free ions. In some exceptional cases, e.g. GaP:O^-, the one-electron potential is so strong that a single bound state is predicted (1). However, as in the case of a free hydrogen atom with two electrons, no excited states can be generated by existing methods. This is in contrast with very recent experimental data which indicate that both spin-singlet and spin-triplet excited states of GaP:O^- may exist (2). The results presented in this study show that the existence of these states can be explained, if the effect of the electronic structure of GaP:O is fully taken into account, and the correlation contribution evaluated via configuration interactions. This enhanced correlation effect derives its strength from the one-electron electronic structure which arises because the impurity potential pushes the valence s-electrons at oxygen deep below the valence band. As a result, there are several resonances well localised in the vicinity of oxygen (3),which make a significant contribution to the correlation effect. A similar phenomenon is studied for the isoelectronic substitutional nitrogen impurity in GaPAs alloys. In particular, the present numerical results show that -in contrast to the one-electron results- the localisation of the many-electron ground state wave function as a function of alloy composition is compatible with the existing experimental data.

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HYPERFINE INTERACTION OF THE IRON IMPURITY NUCLEI AT THE TETRAHEDRAL INTERSTITIAL SITE IN SILICON

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The spin polarized electronic structure of an iron impurity at the tetrahedral interstitial site in silicon is calculated self-consistently using a Green's function approach[1] within a single-site impurity-centered dynamic basis set and the local spin density functional formalism, including an approximate self-interaction correction to the impurity orbitals[2]. The host silicon is described by the LCAO's formed from the 10 Slater orbitals (s,p,d,f). The impurity-centered local host orbitals are the same local orbitals used as basis functions in the host LCAO band structure, but they are impurity-centered. The impurity-centered local impurity orbitals are determined iteratively by solving the Schrödinger equation of an "effective impurity atom" in the field $V_H + \Delta V$, where V_H is the host potential and ΔV is the perturbation potential determined from the Green's function. We choose a valence basis set (3d, 4s, 4p, 4d, 4f) and a core basis set (1s, 2s, 2p, 3s, 3p), both of which changes in each iteration, responding to the impurity-induced perturbation. In the Green's function problem, we use the augumented Green's function which includes an added impurity 3d orbital term and the ordinary Green's function, according to the adspace idea of Williams et al.[3]. The bound t_2 and e states exhibit a hybridization which controls their exchange splittings[2]. The hyperfine field is evaluated from the contributions of the Fermi direct contact interaction, the core polarization of the filled s shells, and the contribution from the orbital magnetic moment. Because of the strong hybridization between the impurity 3d orbitals and the tails of the sp^3 hybrid orbitals of the surrounding silicon, we find a large reduction of the hyperfine field and the exchange splitting. The main contribution to the hyperfine field is the negative core polarization caused by the repulsive intra-atomic coulomb interaction between the core s elections and the 3d electrons. The effective 3d orbital occupation is very close to 8.0 (in the case of the atom, the 3d orbital occupation is 6.0), however, localized magnetic moment is reduced to $1.1\mu_B$ (in the atomic case 4.0 μ_B) by the strong hybridization. We also evaluate the nuclear spin-lattice relaxation time from the contribution of the orbital current and the Fermi direct contact interaction. These results are in good agreement with the recent experimental data[4].

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TuP-PJ10

ELECTRIC FIELD EFFECT ON MULTIPHONON CAPTURE AND EMISSION PROCESSES AT DEEP CENTRES

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We present new theoretical and experimental results on the effect of an electric field on multiphonon capture and emission processes at deep centres. The standard theory of multiphonon transitions is extended to the case of an applied electric field. The field effect is twofold. First it modifies the multiphonon processes by making them tunneling assisted. Second it opens a new transition channel by giving allowence for tunneling with and without phonon assistence. Only the latter process has been considered so far (Makram-Ebeid et al.). The first process is dominating, however, if field strengths are not large enough as in many practical cases. At higher fields the characteristic field and temperature dependencies of the two processes are identical. The field dependence deviates from the asymptotic low field expression considered so far. Measurements of the field and temperature dependence of emission rates of various deep levels in Si (Au acceptor, radiation defects) by means of DDLTS are reported. The experimental data can be fitted by means of our theory using common values of deep level energy, Huang-Rhys factor and phonon energy. Particular attention is paid to the anisotropy of the field effect due to different electron masses parallel to the electric field in different directions. Field dependent capture rates are derived from emission data by applying arguments of detailed balance. The controversial experimental data for the EL2 centre of GaAs (Makram-Ebeid, Kaminska, Li et. al.) are discussed on the base of our theory.

DEEP DEFECT LEVELS IN THE WURTZITE SEMICONDUCTORS: SiC , ZnSe , ZnTe

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The chemical trends in the energy levels of sp^3-bonded substitutional impurities and vacancies in the wurtzite semiconductors SiC , ZnSe and ZnTe are reported. The method used is similar to that employed for defects in zinc-blende materials and is discussed in the recent work of A. Kobayashi *et al.*[1] The Green's function formalism coupled with the empirical tight-binding method is employed. The band structure of the perfect host crystal is calculated in an sp^3-tight-binding model. The parameters are determined by scaling the parameters for the corresponding zinc-blende semiconductors. The defect potential matrix is constructed in the tight-binding basis and the problem is reduced to a multiband, single-site Koster-Slater impurity problem. A large number of anion- and cation-site impurities and vacancies are considered. The results show that the present empirical tight-binding model for defects in wurtzite semiconductors is quite successful in accounting for at least the observed chemical trends.

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TuP-PJ12

THEORY OF 3d-TRANSITION-METAL IMPURITY PROPERTIES IN CADMIUM II-VI COMPOUNDS

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The stable charge states, level energies, ground state spin configurations, and ("internal") excited state energies of all substitutional 3d-transition-metal impurities in CdS, CdSe, and CdTe are predicted. We have developed a spin-polarized and self-consistent tight-binding model which provides a simplified but global understanding of 3d-traps. It is shown that the spin-related properties of 3d-impurities are controlled by $3d_{x^2-y^2}$-states which remain atomic-like in the solid, whereas the gap states are predominantly delocalized vacancy-like states even for the light 3d-elements, in contrast to the widely accepted crystal-field picture of weakly perturbed 3d-ions. A stringent test for the theory is provided by the optical cross sections for ionization processes and "internal" transitions. We have calculated them in terms of the model and find good agreement with the experimental data. Including new optical data for CdSe:Ni, six 3d-elements - more than in any other compound - are now known experimentally to form donor levels in CdSe, in full accord with the theory. In addition, the chemical trends in the ionization energies and in the "internal" excitation energies, and the total spins are in excellent agreement with experiment.

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Impurities TuP-PJ13

THE NITROGEN ISOELECTRONIC TRAP IN GaAs

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We report the pressure-induced *formation* of the N isoelectronic trap in GaAs and $GaAs_{1-x}P_x$ (x=0.045, 0.115). Nitrogen traps are well known in GaP and AlAs and certain of their alloys. But for $x \leq 0.22$ in $GaAs_{1-x}P_x$ and for $x \leq 0.15$ in $Al_xGa_{1-x}As$, N_x states of isolated N vanish from the energy gap in photoluminescence (PL).[1] Consequently, the existence of N-doping and its possible role in the electronic structure of GaAs and GaAs-rich alloys had not been established. In this work we show from extensive PL and PLES that N impurities induce a "deep-trap resonance" above the GaAs conduction bandedge, which may be driven into the fundamental gap through applied hydrostatic pressure.

Experiments were performed at 5K *at up to* 80 kbar in a diamond anvil cell. For low pressures shallow direct-gap excitons dominate PL, giving a linear Γ_1-gap variation of 10.6 meV/kbar. The Γ_1-X_1 crossover occurs *near 40* kbar; *an* X_1-gap dependence of -1.4 meV/kbar is obtained. *In VPE samples prepared in* NH_3 atmosphere, N levels emerge from the Γ_1 conduction band and form luminescent N_X bound states in the gap above 22 kbar. Spectra closely resemble GaP:N -- A and B *excitons are identified*; optic and acoustic participation reflect the GaAs phonon density-of-states. Despite relatively small binding energies (< 135 meV), the N_X level varies under pressure as a "deep electron state," following no single conduction bandedge (Γ,X,L) and, unlike the edges, depending nonlinearly on P. Above 75 kbar the level strongly mixes with and forms a resonance within the X_1 band. From level dependences, the N_X state is predicted near 150 meV above the Γ_1 edge at atomospheric pressure. Our results indicate these resonances remain localized despite degeneracy with and coupling to the continuum.

Corresponding pressure studies in $GaAs_{1-x}P_x$:N show *strong alloy broadening* of N trap transitions. Disorder increases *rapidly* with x, causing a 100-meV-wide band at 0.115; implications for alloy microstructure will be discussed. Threshold pressures for N_X bound state formation decrease with x; level dependences *referenced to band states* are identical to GaAs:N. Results demonstrate that all lower conduction band structure participates in N_X level formation and that X_1 states significantly contribute.

We conclude that despite small or vanishing binding energies, N impurities behave as deep traps both inside and *outside* the gap of III-V materials. This illustrates that *traditional views of deep defects* as only those inducing levels well into the host gap can be misleading.

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HOPPING CONDUCTION IN N-TYPE EPI - GaAs AT HIGH FREQUENCIES AND HIGH MAGNETIC FIELD

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Thin (1-9μm) n^+nn^+ epitaxial mesa sandwich structures (diameter 0.1-1mm) are employed to study the temperature, frequency (0-15MHz) and magnetic field (0-20T) dependence of the hopping conductivity σ of n-GaAs. Because of the favourable geometry, the device resistance is low and easily measurable over a wide frequency range even when the resistivity is high ($\sim 10^8$ Ωcm under low temperature and high magnetic field conditions).

For $T>2K$, σ shows activated behaviour with $\varepsilon_3 = 0.4-0.5$ meV. For $0.5<T<2K$, variable range hopping predominates. At relatively low magnetic fields ($B \leq 5T$), both longitudinal (L) and transverse (T) magnetoresistance show an $\exp(\text{const} \times B^2)$ dependence. The magnetoresistance rises less slowly and appears to saturate at higher magnetic fields. The overall B-dependence is explained using Ioselevich theory (1) with the impurity binding energy suitably modified to take into account the magnetic field (2).

At high electric field, a non-ohmic behaviour is observed and its dependence on applied magnetic field (L and T) is discussed. The frequency-dependent conductivity ($0<f<15$MHz) follows the prediction of the extended pair approximation (EPA) (3) in contrast with previously reported experimental work on GaAs (4). A marked decrease in the magnetoresistance $\sigma(B,f)$ is observed at high frequencies ($\geq$ 1MHz). This behaviour is discussed in terms of EPA.

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CONDUCTIVITY RELAXATION IN THE ELECTRON GLASS

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In recent studies of metal-insulator transition in systems such as Si:P, it has been recognized that not only electron-electron correlations are important[1,2] but also some electronic properties resemble analogues in glasses and spin glasses.[3] For these reasons, the system on the localized side near the metal-insulator transition is referred to often as an electron glass.[4] Experimentally, for example, the ac conductivity has a frequency dependence that is similar to amorphous semiconductors and insulating glasses.[3] The slow relaxation behavior moreover bears a strong resemblance to spin relaxations in spin glasses near or below the spin glass freezing temperature. It has been shown that the electron glass problem theoretically is formally the same as the spin glass problem.

Random interactions and correlations of electrons (spins) give rise to an assembly of near degenerate levels. Relaxation of a single electron (spin) is necessarily followed by sequential relaxations of other electrons (spins) because of its correlation with the others. An effective way of accounting for these complex multi-particle processes is to calculate the evolution of the entropy of the level structure with time caused by the sequential transitions of the multi-particles. The spectrum of these excitations are determined by the level spacing distribution of a Gaussian orthogonal ensemble of random matrix Hamiltonian which mimics these interactions. Coupling of an electron to these level spacings generates the level spacing excitations and modifies the interaction of the electron with the norminal heat bath. The dynamics of the electron as controlled by its direct interaction with the norminal heat bath give rise to a simple rate equation with a constant transition rate. A calculation of the effect of the electron with the level structure interactions in the random matrix Hamiltonian form leads to a modification of the constant transition rate to a time dependent transition rate. This is best understood in terms of the environmental modification which serves to delay the relaxation process since the level structure excitations have maximum entropy and can lose entropy by its interaction with an already displaced electron. The overall entropy increases since it is dominated by the increase in entropy of the electron as it relaxes to equilibrium. This increase in entropy is only slowed by the presence of an environment that can have its entropy decreased by its interaction with displaced electrons. The calculation of the entropy evolution of the level structure excitations is the key of our procedure. The decrease of this entropy is logarithmic in time and yields the required results for a calculation of the conductivity relaxation of the electron glass. We use the electric modulus formalism to calculate the ac conductivity of the electron glass. Fair agreement with experimental measurements is obtained. Relations between the high frequency and the low frequency responses are made. Similarities of relaxations in electron glass and spin glass are brought out.

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Impurities **TuP-PJ16**

A STUDY OF THERMALLY ACTIVATED CONDUCTION, HALL EFFECT AND INFRA-RED ABSORPTION FROM THE IMPURITY BAND IN n-InP

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We shall report measurements of Hall effect and resistivity in n-InP epitaxial layers, with doping levels below the metal-insulator transition. These are compared with Far Infra-red absorption in magnetic fields, which can be used to determine independently the concentrations of carriers in the conduction band, and in the 1s donor ground state, by measuring the temperature dependence of the 1s-2p+ and cyclotron absorption intensities. The measured ground state occupancy is then used to determine the temperature dependence of the Fermi level, which can in turn be used to correct the thermally activated resistivity and Hall effect, in order to obtain the true threshold energy for conduction.

It is found that the threshold energy for conduction lies significantly above that deduced for electron population of the conduction band tail, both from Hall effect and from an analysis of the cyclotron resonance intensity. This discrepancy would lead to the assumption of a thermally activated mobility, on a simple effective medium picture. We ascribe the difference as due to long range potential fluctuations which localise the tail states and prevent conduction until a percolation threshold is reached. Hall voltage, on the other hand, requires only the establishment of a potential gradient, and thus occurs due to the population of isolated 'islands' of conduction band states, in the same manner as occurs in the Quantum Hall effect. Similarly cyclotron resonance is a local transition, which is unaffected by the long range potential.

MAGNETOIMPURITI OSCILLATIONS OF PHOTOCONDUCTIVITY IN n-GaAs.

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Oscillations periodic in the inverse magnetic field were observed in the photoconductivity of n-GaAs at low temperatures under infrared photoexcitation conditions. The oscillations were found to be due to inelastic scattering of electrons by neutral shallow donors that are initially in the lowest excited state $2p_{-1}$ and make transitions to the ground state in the scattering process. The probability of such a process has sharp maxima at the magnetic field values that satisfy the resonance condition, i.e. the distance between any two Landau levels is equal to the energy transmitted to electron from an excited donor.

In addition to magnetoimpurity oscillations several resonant lines of lower amplitudes in the high magnetic field region were observed that are due to inelastic scattering of electrons by neutral donors in excited states lying above the $2p_{-1}$ state.

Thus, we have been able to obtain the data on the spectrum of several low excited states and even on the chemical shift of donor ground state in GaAs in the magnetic field without utilizing any spectral device. A simple kinetic model is proposed to describe the influence of the inelastic scattering on the sample conductivity.

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Impurities TuP-PJ18

Na^+-INDUCED SURFACE STATES AT THE $Si-SiO_2$ INTERFACE

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The drifting of Na^+ ions close to the Si/SiO_2 interface provides one of the unique possibilities to induce a potential disorder at a semiconductor surface in a controlled and reversible way. *This physical system has been* extensively investigated recently in order to study the transport properties of 2D-amorphous materials (1).

The same physical system is well adapted to the study of gap states in semiconductors related to a potential disorder, using Deep Level Transient Spectrocopy. Indeed :

1. DLTS is not invalidated by the huge potential fluctuations which build up at the semiconductor surface.
2. It is not impeded by the bulk carrier freeze-out at low temperature as in bulk amorphous Si (2).
3. There is no deconvolution problems of spatial/energetic trap distribution, as in 3D-materials (2).

We have thus performed a systematic DLTS study of the influence of Na^+ ions at the Si/SiO_2 interface on the gap states in silicon of both types. In n type Si, the results clearly reveal the existence of a band tail between 75 meV and 300 meV from the conduction band. *These states can be annealed out by a* pumping of the Na^+ ions toward the metal gate. The introduction kinetics of these shallow traps as a function of Na^+ concentration is highly non-linear and universal, i. e., independent of the technological origin of the samples. No such states are observed in p type material, indicating the coulombic nature of these gap states.

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EEP ENERGY LEVELS IN SEMICONDUCTORS

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eep energy levels in semiconductors have attracted a great deal of ttention during the last decades and a great number of papers have een published on this subject. Any attempt to review even the most xciting results would be beyond the scope of this paper. Instead, an ttempt will be made to illuminate our present insight into the physial properties of deep centers by high-lighting the example of double onors in silicon.

halcogens give rise to various donor centers in silicon. These include solated, probably substitutional impurities, impurity pairs as well as ore complex centers. Most of these centers are double donors with exited states. Combining junction space charge techniques and ESR meaurements with high resolution IR absorption and photoconductivity pectroscopy considerable detailed information about the energy spectum of such centers is obtained. The IR spectra are discussed with emhasis on valley-orbit splittings of excited states which depend on the ymmetry of the centers and, hence, give information about the crystalographic site of the impurities. Excited states up to 7 $p_\pm$ have been tudied, and the binding energies of these levels were determined in ome cases with an accuracy of 0.01 meV. When a no-phonon excitation rom the ground state to the continuum interacts with a transition from he ground state to a bound excited state accompanied by emission of a honon, marked resonance structures are observed above the ionization imit. No-phonon transitions which are forbidden and, hence, not seen n absorption or photoconductivity line spectra have been investigated ia such Fano resonances.

ouble donors also exhibit unique properties regarding capture of free harge carriers. It will be shown that hole capture at neutral chalcoen donors is governed by Auger processes. The measurements also prove hat the two levels observed for most of the chalcogen-related center e indeed two different charge states of the same defect.

17th International Conference on the Physics of Semiconductors

Surface Structure **WeA-P2** **Plenary**

Scanning Tunneling Microscopy

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An overview of the status of Scanning Tunneling Microscopy (STM) is given. This includes recent experiments on adsorbate and surface structures, rise in the theoretical understanding, comparison with other surface diagnostic methods, and assessment of the STM potential in other fields of science and technology.

May 11, 1984

SOLID STATE PHYSICS ON A FEMTOSECOND TIME SCALE

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Recent advances in measurement techniques have made experimental investigations of dynamical processes in solids possible with femtosecond time resolution. In this talk, I will describe applications of femtosecond optical techniques to studies of optically excited semiconductors. Topics to be discussed include optically induced phase transitions in Si, and the evolution of nonequilibrium hot carriers in semiconductors and semiconductor multi-quantum well structures.

Present and Future Trends in Electron Microscopy of Semiconductors

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The applications of transmission electron microscopy (TEM) to semiconductor analysis can be classified in three categories; namely, structural analysis of semiconductor defects and interfaces, analysis of semiconductor reconstructed surfaces, and analysis of the electronic properties of defects and interfaces. Structural analysis of semiconductor-semiconductor and metal-semiconductor interfaces uses the atomic resolution capabilities of the transmission electron microscope to image interfaces on an atomic scale. Application of this technique to the AlAs-GaAs interfaces grown by molecular beam epitaxy will show that a hyperfine control of interface structure can be achieved by deposition on vicinal (100) GaAs surfaces. Application of medium energy (400 KeV) TEM instrument to atomic resolution interface analysis will be discussed.

New developments in TEM aimed at direct imaging of semiconductor reconstructed surfaces will be presented using as examples the Si (111) 7x7 and 1x1 surfaces and the GaAs (100) reconstructed surfaces. Trends in this new form of surface analysis have led to the development of new instruments which will be discussed.

Finally, the use of TEM to the analysis of some of the optical and electrical properties of defects in semiconductors will be illustrated with an analysis of microplasmas in avalanche photodiodes. The low temperature cathodoluminescence and electron beam induced current in conjunction with the scanning TEM have yielded new insight on the microplasmas generation and behavior. Future trends in this type of defect electronic analysis also require a separate type of microscopes which will be discussed.

Surface Structure **WeA-A3**

THEORY OF VOLTAGE-DEPENDENT SCANNING-TUNNELING MICROSCOPY OF A CRYSTAL SURFACE: GRAPHITE

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The newly developed technique of scanning tunneling microscopy (STM)[1], whose resolving power in real space is now widely appreciated, is also potentially very interesting for studying the energetic spectra of both occupied and empty electronic surface and bulk states. We demonstrate this possibility with an explicit calculation of the voltage-dependent tunneling current for an ideal STM experiment performed on graphite. Graphite is chosen as a particularly attractive test case since it has a surface whose structure is unambiguous and for which a fairly simple and reliable electronic study is feasible. Furthermore, it has recently been shown that this surface exhibits very interesting empty surface states[2,3]. Our starting point is a pseudopotential electronic structure calculation for a repeated slab geometry of n-layer graphite slabs. Pseudopotential atomic form factors were extracted so as to reproduce accurately the all-electron local density LAPW band structure[3] in the vicinity of the Fermi energy E_F. Slabs are considered of increasing thickness from $n = 1$ to 4 carbon layers which are separated by a vacuum region of width $d = 2c$ ($c/2 = 3.35$ A is the interlayer spacing in bulk graphite). The resulting charge density is well described on the average up to 3.5A out from the surface plane, corresponding to an exponential decay of 5 orders of magnitude. The voltage-derivative of the tunneling current $dJ(V)/dV$ is approximated as the local density of states in the region of exponential decay away from the surface, $\rho(x_0,y_0,z_0; E-E_F = V)$, where x_0,y_0,z_0 is the tip position above the surface. We present a detailed study of how both surface and bulk electronic states are reflected in the tunneling J-V spectra for various tip positions. In particular we show that, due to their slower decay in the vacuum region, empty surface states of graphite can be well discrimated against bulk-like structures by considering STM spectra at different tip-surface separations

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CONSEQUENCES OF THE ZINCBLENDE-DIAMOND ORDER-DISORDER TRANSITION FOR $(GaAs)_{1-x}Ge_{2x}$ AND OTHER ALLOYS

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Newman and Dow have proposed that the observed V-shaped dependence of the direct gap $E_0(x)$ of $(GaAs)_{1-x}Ge_{2x}$ alloys is due to a zincblende-diamond order-disorder phase transition that occurs at the minimum of the "V" [1,2]. In disordered Ge-rich alloys, the stable phase is one in which either Ga or As atoms can occupy nominal cation and anion sites with approximately equal probability; in ordered GaAs-rich material, Ga (As) atoms preferentially occupy nominal cation (anion) sites. The order parameter for this transition is defined as the difference in the average occupancies $\langle P_{Ga}\rangle_{\text{"Ga"}}$ for finding Ga atoms on nominal "Ga" (cation) sites rather than on "As" anion sites: $M \equiv \langle P_{Ga}\rangle_{\text{"Ga"}} - \langle P_{Ga}\rangle_{\text{"As"}}$. This order parameter is calculated using a three-component spin Hamiltonian and mean-field theory.

The electronic structure of $(GaAs)_{1-x}Ge_{2x}$ alloys is studied using a modified mean-field virtual-crystal approximation. Schematically, the alloy consists of virtual cations and anions $Ga_{(1-x+M)/2}As_{(1-x-M)/2}Ge_x$ and $Ga_{(1-x-M)/2}As_{(1-x+M)/2}Ge_x$, respectively. This approximation is used to predict the bowing of all $(III\text{-}V)_{1-x}IV_{2x}$ alloys, e.g., the alloy $(InP)_{1-x}Ge_{2x}$, if it can be grown, should have a minimum band gap of order 10 μm's [3]. Other interesting effects of this transition include predicted bifurcations as functions of decreasing composition of the "deep-trap" energy levels of substitutional impurities [4].

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Phase Transitions **WeA-B2**

RAMAN SCATTERING FROM METASTABLE $(GaSb)_{1-x}Ge_{2x}$ ALLOYS

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Metastable alloys of III-V compounds and group IV compounds produced by reactive ion sputtering are stable at room temperature and may be usefully contrasted with the more familiar ternary III-V on binary IV alloys. The metastable alloys $(AB)_{1-x}C_{2x}$ show more disorder since the group IV element C substitutes on both group III (A) and group IV (B) sublattices. The question of long-range zinc-blend-like versus diamond-like order, raised by Newman and Dow, as well as questions of shorter-range ordering have been addressed using Raman measurements in $(GaSb)_{1-x}Ge_{2x}$ for $0 \leq x \leq 1$. This system shows 2-mode behavior, and the widths of the Raman peaks are strong functions of x. For $0.4 < x < 0.7$ the widths of Ge-like and GaSb-like modes are both an order of magnitude greater than those of Ge or GaSb, and these widths in the crystalline alloy are close to those measured in amorphous alloys. In addition the assymetry Γ_a / Γ_b of half-widths for a given line is not the monotonic function of $\Gamma_a + \Gamma_b$ found by F. Pollak and coworkers for ternary III-V alloys. This implies that the short-range structure probed by Raman scattering cannot be described by a single correlation length. Γ_a / Γ_b for the GaSb-like mode shows an anomalous peak for $x \simeq 0.3$, perhaps a reflection of the Newman-Dow ordering transition.

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17th International Conference on the Physics of Semiconductors
Phase Transitions WeA-B3

HIGH PRESSURE SIMPLE HEXAGONAL PHASE OF SILICON*

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Recently experments on silicon under pressure have discovered a new simple hexagonal phase. The well known β-tin phase is stable only over a small pressure range of less than 50 Kbars and transforms to the simple hexagonal phase at ~130-160 Kbars[1,2]. We have performed self consistent *ab initio* pseudopotential density functional calculations on each these structures. We find the simple hexagonal structure to be stable at pressures >105Kbars, thus establishing the sequence of diamond ⇒ β-tin ⇒ simple hexagonal with increasing pressure. The hexagonal structure has 2 nearest neighbours and 6 next nearest neighbours, which become 8 nearest neighbours when the c/a ratio is equal to 1. We calculate the c/a ratio of the simple hexagonal structure near the transition to be ~0.95 in good agreement with the experimental values of 0.941[1] and 0.937[2]. We find that c/a increases with increasing pressure in agreement with reference 2. We analyze the contributions of different orbital angular momentum components of the wavefunctions to the total energy and stress in order to understand the relative stability of each of the phases.

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Phase Transitions WeA-B4

2-D MAGNETIC PHASE TRANSITIONS IN GRAPHITE INTERCALATION COMPOUNDS*

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By intercalating graphite with magnetic species, materials exhibiting a variety of two dimensional magnetic properties can be synthesized. The two-dimensional behavior is enhanced by increasing the stage index, thereby separating sequential magnetic layers by increasing numbers of non-magnetic graphite layers. The $CoCl_2$ intercalated graphite system is of particular interest because of the high intraplanar magnetic anisotropy that can be achieved and the wide range of well-staged samples that can be prepared. For high stage compounds, the magnetic transition is expected to be characteristic of the two-dimensional xy model from a free vortex state above the Kosterlitz-Thouless transition temperature T_{KT} to a bound vortex state below. Because of the finite size of the intercalate domains in the basal plane, the magnetic susceptibility is not expected to become infinite, as predicted by the Kosterlitz-Thouless theory for an infinite system. Experimentally, the peak in the magnetic susceptibility per mole of Co^{+2} increases to very large values (compared to a ferromagnetic sphere), as the stage index is increased from 1 to 6 and the system becomes increasingly two-dimensional. To model the experimentally observed behavior in the magnetic susceptibility, χ, the two-dimensional xy model has been extended to include finite size effects.

Below T_{KT}, the weak p-fold symmetry-breaking field h_p (arising from the crystal potential) seriously affects the magnetic behavior, as predicted by the theory of Jose, Kadanoff, Kirkpatrick and Nelson (JKKN), and may in fact dominate the experimental observation of the magnetic transition. To measure χ experimentally, two competing symmetry-breaking fields must be considered; in addition to the 6-fold crystal field h_6, a 1-fold symmetry-breaking field h_1 is also present, due to the externally applied probing magnetic field. According to the JKKN theory, the Kosterlitz-Thouless transition can only occur when $p \geq 4$, so that the application of an external magnetic field is expected to suppress the transition, as is observed experimentally. By extending the JKKN theory to include multiple symmetry-breaking fields, we are able to interpret the magnetic field dependence of the peak susceptibility to quantitatively determine the magnitude of h_6. Furthermore, by comparing measurements of $\chi_{\parallel}$ and $\chi_{\perp}$ (where the external magnetic field is applied parallel and perpendicular to the probing field), we are able to determine T_{KT} quantitatively. Also of interest is our study of the magnetic properties in the cross-over region from 2-D to 3-D behavior, which is found to occur experimentally for the $CoCl_2$ intercalated graphite system as the stage index decreases from 2 to 1. The magnetic measurements on the stage 1 compounds are consistent with ferromagnetic alignment of spins within each plane but antiferromagnetic coupling between spins on adjacent planes.

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Holes in Quantum Wells **WeA-C1**

ENERGY LEVELS OF TWO DIMENSIONAL HOLES IN GaAs - (AlGa)As QUANTUM WELL HETEROSTRUCTURES

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We present combined resonant inelastic light scattering and magneto-transport investigations of high mobility two dimensional hole gases confined in the quantum wells of multiple GaAs - (AlGa)As heterostructures. The 2D hole systems are shown to be rich in new phenomena related to the degeneracy and non-parabolicity of the valence subbands. Most unexpected is the evidence pointing to a lifting of the Kramers degeneracy of the ground valence subband at finite wavevector. This effect is apparent in the resonant light scattering spectra, in the form of spectral bands at energies lower than those of conventional intersubband excitations, and also in the multiplicity of the Shubnikov-de Haas oscillations. Lifting of the Kramers degeneracy has been previously reported only in single heterojunctions, were it is believed to be induced by the absence of inversion symmetry in the confining potential well. The removal of the Kramers degeneracy in the quantum wells is an intriguing effect because the potentials in GaAs - (AlGa)As superlattices are expected to have inversion symmetry.

The samples are modulation-doped multiple GaAs - (AlGa)As heterostructures. The 2D hole systems, confined in the ~100Å thick GaAs quantum wells, have low temperature mobilities in excess of 30,000 $cm^2/Vsec$ and densities in the range $2 \leq p \leq 6 \times 10^{11} cm^{-2}$. Magneto-transport measurements were carried out at temperatures $300mK \leq T \leq 2K$. Light scattering spectra were obtained with photon energies carefully chosen to be in resonance with the fundamental optical gaps and at the same time minimize the luminescence background. These are the first observations of resonant light scattering by 2D holes in a direct gap semiconductor.

Light scattering allows direct spectroscopic determination of the spacing between valence subbands. At energies greater than ~10meV we observe the scattering assigned to transitions of holes from states in the ground valence subband to higher lying light and heavy hole states that are confined within the quantum wells. The spectral lineshapes, very different from those of 2D electron systems, display clearly the non-parabolicity of the subbands. At energies below those of conventional intersubband excitations the resonant light scattering spectra show the presence of unexpected bands with lineshapes that depend strongly on temperature and on power density of incident light. Their presence in the spectra indicate the existence of elementary excitations that can be interpreted only in terms of hole transitions between ground valence subband states. Our observations point to a splitting of the Kramers doublet in the ground subband. This interpretation is consistent with the measurement of Shubnikov-de Haas oscillations indicating that the holes populate two subbands degenerate at $k=0$ and with a slightly field-dependent mass ratio of $(m_2/m_1) \approx 2$. A preliminary analysis of the low lying light scattering lineshapes gives agreement with this mass ratio using an average ground valence subband mass of $\sim 0.4 m_0$.

PHONON EMISSION AND CARRIER HEATING IN A 2-DIMENSIONAL HOLE GAS

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The enhanced electron mobility in modulation doped (MD) GaAs-AlGaAs heterostructures has stimulated a great deal of interest over the last several years. Recently[1] a larger mobility (μ) enhancement was observed for the case of 2-dimensional (2-D) holes for the first time in a p-type MD GaAs-AlGaAs heterostructure. The influence of electric fields on μ is of interest not only from a basic transport point of view but also because most high speed devices operate under the influence of such fields and there are efforts presently underway to fabricate FET's out of this novel material. Because of the valence band degeneracy and the vastly larger mass of holes relative to electrons, transport studies in such systems is also of interest. In this paper we report first measurements of the field dependence of the mobility for a p-type MD GaAs-AlGaAs heterostructure at low temperatures (~1.5K) and correlate the changes in μ with phonon emission produced by the relaxation of the hot carriers. The phonons were observed at the opposite side of the .5 mm thick insulating GaAs substrate by means of a thin superconducting bolometer and time of flight techniques. Using pulsed techniques the changes in μ were also measured. For field strengths in the range of about 10 to 70 V/cm the mobility changes rapidly while for higher fields the decrease is less rapid and eventually levels off at fields ~ 200 V/cm. Over this field range μ changed from a high value of 40,000 $cm^2/Vsec$ to a value ~ 400 $cm^2/Vsec$. By comparing these data with the temperature dependence of μ we ascribe a hot carrier temperature $T_h(E)$ to the hole gas. For $T_h \lesssim 30K$ we observe primarily low frequency transverse acoustic (TA) phonons probably connected with piezoelectric scattering. At [illegible]r temperatures we observe a slow pulse presumably generated during relaxation of optic phonons into higher frequency TA phonons. The field dependence of μ and the phonon emission is shown to be a much slower function of E than for electrons[2,3] presumably because of the differences in effective mass and phonon coupling strengths. These measurements provide important insight into the dynamics of carrier relaxation in 2-D systems in semiconductors.

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EFFECTIVE MASSES OF HOLES AT A GaAs-AlGaAs HETEROJUNCTION

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Magneto-transport and cyclotron resonance experiments on a two-dimensional hole gas at a GaAs-AlGaAs heterojunction show the existence of two cyclotron masses of $0.60m_0$ and $0.38m_0$, which have been interpreted as a consequence of the lifting of the Kramer's degeneracy of the lowest subbands.[1] We present a simple model calculation of the GaAs subband structure, the density of states masses, and the cyclotron masses as a function of magnetic field. The Luttinger Hamiltonian[2] is employed and the self-consistent interface potential is incorporated within the effective mass approximation. The double degeneracy inherent in the Luttinger Hamiltonian is removed in the hole subbands by the interplay of the lack of inversion symmetry of the interface potential and the strong spin-orbit coupling. The calculated cyclotron masses of the lowest heavy hole subbands are magnetic field dependent and much lower than experimental values, e.g., we obtain $0.38m_0$ and $0.22m_0$ for a field of 6T. Kohn[3] has shown that in a two-dimensional electron system with translational symmetry, the cyclotron mass is unaffected by the electron interaction. We show that Kohn's theorem is inapplicable to holes because their band structure lacks translational symmetry. This result coupled with the large r_s value ($r_s \sim 5$) for holes at 5×10^{11} cm^{-2} indicates the strong contribution of the hole-hole interaction to the effective masses. This effect is being investigated.

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FRACTIONAL HALL QUANTIZATION OF TWO-DIMENSIONAL HOLES IN GaAs-GaAlAs HETEROSTRUCTURES*

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We report magnetotransport measurements, for fields up to 23T, in high-mobility two-dimensional (2D) hole systems formed at the interface of GaAs-GaAlAs heterostructures. At low fields we have studied the temperature dependence (from 4.2K to 300K) of the mobility and carrier density. At high fields and low temperatures (down to 0.51K) we have observed quantization of the Hall voltage and magnetoresistance structures at new fractional values of the magnetic level filling factor ν, in addition to those reported previously.

The heterojunctions were grown by molecular beam epitaxy in which the acceptor species (Be) was introduced in the GaAlAs layer at a distance d from the GaAs interface. By varying d between 450Å and 100Å, 2D hole concentrations between $1.8\times10^{11}\mathrm{cm}^{-2}$ and $4\times10^{11}\mathrm{cm}^{-2}$ were obtained. The highest mobility at 4.2K was $8\times10^{4}\mathrm{cm}^{2}/\mathrm{Vs}$ (for a density of $2\times10^{11}\mathrm{cm}^{-2}$), the best value ever achieved. The hole mobility, measured between 300K and 4.2K, showed, in all cases, a monotonic increase with decreasing temperature. Of special significance was the large increase between 77K (the highest mobility was $6\times10^{3}\mathrm{cm}^{2}/\mathrm{Vs}$) and 4.2K. This is in contrast to the situation in two-dimensional electrons, where at low temperatures a saturation or decrease in mobility with decreasing temperature is frequently observed.

At very low temperatures (0.51K) the magnetoresistance and Hall voltage were studied for fields up to 23T. In addition to the quantization of the Hall voltage for integer values of the filling factor, accompanied by vanishing resistance, fractional quantization was also observed for $\nu = 2/3$ and 3/5. This is the first report of Hall quantization for $\nu = 3/5$, as well as of weak but distinct structures observed in the magnetoresistance for $\nu = 3/7$ and 6/5. As in the 2D electron system, magnetoresistance minima occurred at $\nu = 5/3$, 4/3, 2/3, 3/5, and 2/5, but, in contrast, no feature in the vicinity of $\nu = 4/5$ was observed. This absence is inconsistent with the notion that all the excitations corresponding to the different fractional ν with the same denominator are equally stable.

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SPIN-SPLIT INTERSUBBAND RESONANCES IN 2D-HOLE SUBBAND SYSTEMS

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In systems without inversion symmetry the degeneracy of quasi-spin-states is lifted for $k \neq 0$. Whereas this effect is extremely small in the bulk of zinc-blende-compounds, it was predicted in Refs.1,2, that it should be important for the energy spectrum of holes in 2D-surface space charge layers. The spin-splitting results from the asymmetry of the surface potential and the strong spin-orbit interaction of holes. We have observed the inherent spin-splitting - without external magnetic field - on Si-(110)-MOS-structures using parallel excitation of intersubband resonances, i.e. with the exciting field vector parallel to the surface. From our experiments we can deduce, that the spin-splitting increases with increasing quasi-momentum k and vanishes for $k=0$. The splitting is considerable, e.g. 6meV for k about $3 \times 10^6 \text{cm}^{-1}$. The observation of quasi-spin-states in hole intersubband spectroscopy becomes possible, because the transition matrix elements for parallel excitation depend strongly on k. This causes, that only transitions in a small regime of the 2D-k-space near the Fermi-contour contribute to the intersubband resonance.

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THEORY OF TRANSIENT QUANTUM TRANSPORT IN HETEROSTRUCTURES

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The reduction of transistors to sub-micron dimensions and the advent of a wide range of novel devices and structures, made possible by MBE, has exposed serious deficiencies in our ability to theoretically describe phenomena such as transport. Even if we were to disregard important new phenomena, such as the fractional quantum Hall effect, there are significant problems with the understanding of rudimentary transport processes. These include: the breakdown of Boltzmann transport; the description of quantum effects such as resonances/tunneling/multiple reflections; and scattering processes in the time-space transient domain where asymptotic quantum mechanics is inappropriate. Complications also arise from the extended quantum well profiles of many sub-micron systems. We report here detailed calculations for transport processes based on a new formalism for transport which replaces the classical Boltzmann distribution with the Wigner phase space distribution. We first describe the extreme of quantum ballistic transport where the concept of a unique barrier traversal time is shown to be inadequate to describe resonant tunneling barrier devices. The effect of a non-parabolic band structure is shown to significantly alter the transmission properties of such devices. Whereas quantum reflection at steps in repeated overshoot devices is potentially hazardous, this effect is shown to exist for zero bias but is substantially diminished in relatively weak electric fields. From computer studies of minimum wave-packet propagation through barrier potentials it is concluded that with appropriate profiling it should be possible to prepare highly monochromatic electronic states. The extension of the theory to phonon assisted tunneling in transient transport is described and discussed in the context of current-voltage characteristics for resonant tunneling structures. These, and effects such as wave retardation, are also briefly interpreted in terms of a recent quasi-classical ensemble interpretation of the Wigner transport equation(1).

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QUANTUM TRANSPORT IN THE CHANNEL OF A FIELD EFFECT TRANSISTOR

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With the continuing drive to faster and higher frequency semiconductor devices, the decreasing spatial scales and concomitant high fields being encountered are making the semi-classical Boltzmann equation approach to electronic transport increasingly suspect. The associated quantum mechanical effects, in terms of spatial quantisation and modifications to electron scattering, mark the onset of a new regime in semiconductor device physics requiring a quantum mechanical approach to describe electronic processes and transport properties in such structures. In this paper we present a quantum mechanical formulation of the electronic transport in a simple semiconductor device structure. The model under investigation is intended to simulate the channel of a FET, and comprises a uniform electric field along the channel direction and a confining parabolic potential well transverse to the electron motion. This 'sloping gutter pipe model' was conceived to describe a depletion mode GaAS MESFET, but the formalism can equally well be applied to model the accumulation region of a HEMT or MOSFET device.

The formulation of quantum transport has been adapted from the method due to Sawaki and Nishinaga(1,2) and Sawaki(3). Their approach to high field electron transport makes use of the stark ladder representation of the electron eigenstates for a one-dimensional electric field superposed on the crystal potential. The electron-phonon interaction is treated by perturbation theory. Certain classes of interaction diagrams in the infinite series can be summed exactly within the pole renormalisation approximation (Saitoh(4)) giving rise to self energy corrections to the eigenenergies.

Generally speaking quantum transport formalisms are far too complicated to be applied to real semiconductor device structures. However, we show that for the model potential described above a tractable formulation of quantum transport can be developed. An important aspect of the structure being investigated is the lateral confining potential, and particular attention is given to the modifications to the electron transport due to the quantum confinement. Within the formalism presented we can study low field band conduction processes, high field stark ladder hopping transport, the subband structure, intracollisional field effect, correlation effects in scattering, and the concepts of ballistic transport and velocity overshoot. The importance of the quantum confinement on these processes will be discussed. The formalism described should be powerful enough to enable us to assess the relevance of quantum effects to modern semiconductor devices and we present our conclusions in this paper.

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WeA-D3

BALLISTIC ELECTRON TRANSPORT DETECTED BY SEEBECK VOLTAGE MEASUREMENTS ON SEMICONDUCTOR MICRO CONTACTS

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Ballistic electron transport is demonstrated by thermoelectric measurements on microcontacts. These contacts are made of two adjoining n-type silicon wedges under highly controlled conditions in an UHV environment.

The existence of a regime of Knudsen flow is proved by the detection of an asymmetric heat distribution via Seebeck voltage measurements. The contact area between the two semiconductor species of like conductivity type is made small enough to be comparable with the mean free path of the majority charge-carrier. Under these conditions a traversing current produces heat predominantly within the downstream part of the wedge couple. The asymmetry grows with shrinking contact dimensions and an agreement with the theory is established.

We are currently preparing measurements on GaAs samples and anticipate to report these results.

RESONANT MAGNETOTRANSPORT MEASUREMENTS IN SHORT (0.25μm to 9μm) n^+nn^+ GaAs SANDWICH STRUCTURES

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This paper describes a series of resonant magnetotransport measurements in short sandwich structures of n^+nn^+ GaAs using magnetic fields up to 20T and over a temperature range from 100 to 300K. The small size of the active layer (0.25-9μm) allows us to apply very high electric fields (up to 25Kv/cm) Under these conditions we have observed novel features in the magnetoconductivity which have not been previously observed in more conventional large samples.

At low electric fields we observe maxima in the transverse magnetoconductivity, σ_{xx}, at magnetic fields B given by the normal magnetophonon resonance condition

$$N\hbar \frac{eB}{m^*} = \hbar\omega_L \quad N = 1,2,3, \ldots$$

where m^* is the electron effective mass and ω_L is the longitudinal optical phonon frequency.

However, as the electric field is increased these maxima change into minima at fields E_c given by the condition

$$E_c = \frac{(\hbar m^*)^{1/2}}{e} \left(\frac{\omega_L}{2}\right)^{3/2} \frac{1}{N^{3/2}(N+\frac{1}{2})^{1/2}}$$

We can explain this behaviour in terms of a novel mechanism of magnetoconduction in high electric and magnetic fields, elastic scattering between adjacent Landau levels. The relation above for E_c can be calculated exactly using the analytical solution of Schroedinger's equation for an electron moving in crossed electric and magnetic fields.

This process is observed over the temperature range 100K-300K and its temperature dependence will be discussed.

At electric fields much higher than E_c ($E \gtrsim 10$Kv/cm for $B \sim 10$T) the amplitude of the magnetophonon resonances decreases at all temperatures and eventually they disappear. Possible reasons for this behaviour (intra-collisional field effects, inter-valley transfer, ballistic transport) will be discussed.

Transport **WeA-D5**

MICROWAVE AND FAR-INFRARED LASER CYCLOTRON RESONANCE STUDY IN HIGH-PURITY ZnSe

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We report the first observation of millimeter and submillimeter wave cyclotron resonance (35, 692, 1364 and 1743 GHz) in high-quality ZnSe under intrinsic photoexcitation which exposes various new features of the photoexcited conduction electrons at liquid helium temperatures. The experiment enables us to make precise determination of the effective mass value and the collision rate of the photoexcited electrons. A strong anisotropy in absorption intensity has been observed in 35 GHz measurement.

An undoped ZnSe crystal grown by the modified Prior method was used in the present experiment. The residual impurity concentration was estimated to be less than 10^{15} cm^{-3}. A xenon flash lamp was employed for the carrier excitation. Two absorption lines, with much different strength, close to each other were observed for the 220 μm(1364 GHz) measurement. The stronger absorption line corresponding to the effective mass of $m^*=0.145\ m_0$ is attributed to the cyclotron resonance of electron. From the line width, the collision rate has been found to be $5.3\times10^{10}\ s^{-1}$. The decisive identification of the weaker line with $m^*=0.149\ m_0$ has not been made as of now, though a few possibilities occur to our mind, e.g., the light hole signal, the quantum line of electron owing to the non-parabolic energy band by polaron effect and so on.

The most peculiar part of the 35 GHz observation is the angle dependence of the absorption character. That is found when the magnetic field is rotated in a (110) plane. For the magnetic field direction perpendicular to a certain characteristic direction, we obtain the strongest resonance signal that lies on a broad plateau. The resonance peak gradually loses its height as the magnetic field is rotated and the completely dies down when the magnetic field is applied along that characteristic direction. Then only the broad plateau remains. The behavior could perhaps be explained by the presence of densely packed stacking faults.

SCHOTTKY BARRIERS IN COMPOUND SEMICONDUCTORS

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Detailed studies of metal contacts deposited on atomically clean semiconductor surfaces carried out over the last few years have shown that in many cases the interface is neither ordered nor atomically abrubt. Interdiffusion and chemical reactions of metal and semiconductor are common but only recently are the driving mechanism associated with these interactions beginning to be understood. In this talk we concentrate in particular on the interaction of a range of metals with GaSe, InP and CdTe cleaved surfaces and in particular on the kinetic and thermodynamical aspects of the interface formation. We consider the role of metal cluster formation which often appears to be intimately linked with exchange interactions across the interface.

The formation of Schottky barriers and ohmic contacts at metal - compound semiconductor interfaces is still relatively poorly understood although considerable progress has been made recently. In this talk we consider the relationship between the barrier formation and the chemical interactions at the interface and consider models where deviations from perfection have a dominating influence. We also describe experiments whereby the interface has been deliberately modified by 'doping' and where the corresponding Schottky barriers have been modified in a controlled way.

17th International Conference on the Physics of Semiconductors
Interface: Electronic Properties **ThA-A2** Invited

LONGITUDUAL AND TRANSVERSE ELECTRICAL TRANSPORT IN THE CRYSTALLINE THIN FILM SYSTEMS $CoSi_2/Si$ AND $NiSi_2/Si$

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Physically, the disilicides $CoSi_2$ and $NiSi_2$, which crystallize in the cubic, fluorite structure, are of considerable interest because from a bonding standpoint they are remarkably similar to silicon itself, i.e. tetrahedral bonding of Si's to Co or Ni via sp^3 hybridization, unlike any of the other common silicides.[1] (They may be viewed as a simple cubic, *metallic* phase of Si stabilized by Ni or Co in every other cube). Because they have the fluorite structure plus a close lattice match to Si, these compounds alone among the common metal silicides can be grown epitaxially as single crystal films of extraordinary perfection on Si substrates.[2] This provides a rare opportunity to examine the physical properties of a quasi-two-dimensional system with nearly ideal interfaces, i.e. planar and essentially perfect on an atomic scale. We have performed electrical transport measurements and studies of galvanomagnetic properties in fields up to 10 tesla of these systems as a function of temperature (<1 to 300°K) and as a function of film thickness ranging from 70Å to ~1000Å. We are able to observe departures from the canonical behavior of a 3D metallic system, *viz* on one hand the appearance of localization effects accompanying the transition to a quasi 2D regime, or on the other hand, size effects and evidence of a high degree of specular electron scattering from the interface in the opposite regime where the mean free paths far exceed the film thickness. Damage introduced into these films by bombardment with 2 MeV ^4He ions has a profound effect on electrical transport, the results showing a strong increase in residual resistivity but little change in phonon scattering - a graphic example of Matthiessen's rule. The uncommonly large susceptibility to damage is characteristic of the tetrahedral coordination. These studies are able to answer the important puzzle of why $CoSi_2$ and $NiSi_2$, while virtually identical morphologically and electronically, exhibit very different transport properties. As regards to conduction transverse to the silicide/Si interface we have measured[3] Schottky barrier heights using capacitance and I-V techniques. The results show that the barrier heights depend upon crystallographic orientation and interface atomic structure. The implications will be discussed.

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Interface: Electronic Properties ThA-A3

ELECTRONIC STRUCTURE OF INTERFACES BETWEEN CRYSTALLINE AND AMORPHOUS SILICON*

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Although a great deal of theoretical attention has been devoted to idealized interfaces between lattice-matched semiconductors,(1) relatively little effort has been devoted to the study of realistic interfaces between crystalline and amorphous semiconductors.(2) To illustrate the status of the crystal/amorphous interface problem, Pantelides and Long(3) recently constructed an atomic-scale model of the Si/SiO_2 interface by hand, the idea being to connect a continuous random SiO_2 network to a crystalline Si substrate without introducing any dangling bonds. Since their "hand-crafted" method of construction deliberately avoids the creation of dangling bonds, the resulting model does not include the types of structural imperfections that should occur at crystal/amorphous interfaces. In this paper we will describe computer-generated atomic-scale models of interfaces between crystalline and amorphous silicon in which structural defects such as dangling bonds occur naturally. Our theoretical approach is based on geometrical transformations between close-packed solids and covalent networks which have been used previously to generate models of bulk amorphous semiconductors.(4) To our knowledge, the present work represents the first application of these geometrical transformations to the construction of interfaces. Beginning with a random close-packed solid which is sandwiched between two crystalline close-packed solids, we carry out a transformation which produces an amorphous silicon region bounded by two crystalline silicon slabs. Assuming Keating-type interactions between atoms,(5) the entire structure is then relaxed. In this way structural defects, including dangling bonds, are generated. After describing the atomic structure of our model, we will discuss the results of electronic density of states calculations based on a tight-binding Hamiltonian and a mixed recursion-moment method. We will also indicate how the local atomic arrangements and the local electronic density of states vary with distance from the interface. Our method can be readily generalized to deal with more complex crystal/amorphous interfaces, such as the Si/SiO_2 interface.

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OBSERVING ONE INTERFACE TRAP: LATTICE VERSUS ELECTRON TEMPERATURE

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We have recently demonstrated [1] how to monitor directly the occupancy of a <u>single</u> interface trap. We fabricate special MOS transistors with narrow gate segments 0.1 μm wide by 1 μm long. These contain so few scatterers that changing one of them can produce a change in conduction of order one percent. We observe square-wave random switching sequences which depend strongly on temperature and gate voltage, caused by the fluctuating occupancy of a single trap. Analysis of the gate voltage dependence confirms that the electron traps are on the oxide side of the interface.

We have now made extensive measurements of the occupancy of a single trap over the temperature range 4-20 K, varying both lattice temperature and electron temperature. The latter is accomplished by applying a source-drain voltage of several mV per μm, and is measured using the temperature dependence of the conductivity to establish an electron temperature scale. We find that electron capture depends on both electron and lattice temperatures, but electron emission seems to depend only on lattice temperature. Implications of this data for trapping models will be discussed.

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PROGRESSES IN SYNCHROTRON RADIATION ELECTRON SPECTROSCOPY FOR THE STUDY OF CONDENSED INTERFACES: NEW METHODS AND SOME RESULTS.

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A whole new chapter in spectroscopy has been opened by the availability of Synchrotron Radiation (SR) as a tunable excitation source which allows a fuller exploitation of photoelectron (PES), Auger (AES) and X-ray absorbtion (XAS) spectroscopies, than possible in conventional laboratories. The high photon flux and extended monochromatic output range of modern SR beam lines permit important parameters entering the electron spectroscopy processes to be controlled, investigated in their own nature, and then exploited to obtain deeper information from electron emission measures. The possibility of choice of the final state for the emitted electrons allows to exploit the energy dependence of the electron mean free path and therefore to choose the amount of material to be sampled (5-25A). A more fundamental parameter that can also be exploited with SR is the hν dependence of the probability of photoionizing a particular subshell i.e. the photoionization cross section σ of core and valence states. The σ dependence on hν bears informations on the initial state wavefunction of the electron, being a function of the overlap of the initial state with the free electron final state. A relevant example is that of 4d and 5d transition metals (TM), which present Cooper minima(CM) at soft X-rays energies. By choosing hν values at different σ values for the electron states, it is thus possible to enhance the separation between the orbital contributions to the final state spectra, and therefore investigate the structure of the chemical bonding in condensed systems. - Also the measure of variations of the σ for electron states in atomic vs condensed, vs chemically reacted samples has been shown, for the favorable cases of TM and TM-Si systems, to provide a diagnostic for atomic-like vs band-like, vs hybrid band-like states, and, tentatively, bonding vs non bonding states.

The use of atomic-like σs for deep core level PES, allows a quantitative indication on the average compositions for different depths at interfaces.

Resonant photoemission and photon excited AES lineshapes are also SR "orbital-sensitive" techniques, for simple cases. Near absorption edge XAS measure the unoccupied DOS and it is advantageous when one-electron transition dominate; this is the case, for example, of $L_{2,3}$ XAS of near noble metal-Si systems, where XAS complements PES in the study of the d "partial" DOS. Techniques and results will be discussed.

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*Work mostly done while at Stanford Electronics Labs., Stanford University.

PHOTOELECTRON SPECTROSCOPY OF THE Si/Eu INTERFACE USING SYNCHROTRON RADIATION

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The spectroscopic study of the silicon/rare earth interface constitutes a next logical step in the study of reactive Si/metal interfaces to progress in the full understanding of the Si/metal interface in microscopic terms. This research also has technological implications arising from the stability and the low Schottky barrier height seen at these interfaces. We report here the first results on the Si/Eu interface, studied by synchrotron photoemission spectroscopy. The samples were fabricated in situ by deposition of incremental layers of metal (from 0.5 to 15 monolayers) on a cleaved Si(111) surface at room temperature, under UHV conditions. Electron energy distribution curves were taken after each evaporation of the Si 2p, Eu 5p and the valence band region, with photon energies ranging from 65 to 180 eV. Resonant photoemission was used around the Eu 4d photoexcitation threshold to enhance or to suppress the emission from Eu related states. Si LVV Auger spectra and XPS spectra of the Eu 3d core levels was collected as well.

The spectroscopic results can be summarized as follows:

i) Several different stages of interface formation with reactive inter mixing between Si and Eu atoms were detected for incremental depositions between 0.5 and 5 monolayers (ML). A strongly shifted Si 2p peak (1.6 eV to lower binding energy) appears at 2 ML, clearly indicating a change in the Si bonding configuration.

ii) No evidence of mixed valence or valence change was detected. The Eu atoms remained divalent in the reacted phase formed at the interface as well.

iii) At a total deposition of 5 ML Eu, the interface formation is complete. Subsequent deposition forms metallic Eu on the surface.

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Interface: Electronic Properties **ThA-A7**

SURFACE BARRIER FORMATION ON (110) GaAs STUDIED WITH RAMAN SPECTROSCOPY

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The band bending behavior close to the (110) surface of UHV-cleaved n-GaAs crystals is investigated during formation of semiconductor/metal and semiconductor/semiconductor interfaces. The measurements have been performed by means of electric field induced Raman scattering. Close to resonance, the intensity of the symmetry forbidden LO-phonon line of GaAs is proportional to the square of the surface electric field and consequently reflects directly the surface or interface barrier height. The typical light penetration depth of the order of 100 Å offers the unique possibility to measure barrier heights at internal surfaces or to follow in situ the formation of Schottky barriers and heterostructures from submonolayer coverages to relatively thick overlayers. We have used this method recently to investigate the band bending behavior during crystalline and amorphous growth of Ge on GaAs /1/.

In the present communication we report on results obtained for both metal and semiconductor overlayers and chemisorption of gas molecules. Starting from well cleaved (110) GaAs surfaces, which exhibit approximately flat band condition, we find in all cases that the surface barrier height is increasing rapidly already at low, submonolayer coverages. This is in qualitative agreement with photoemission experiments /2/. For metal or semiconductor overlayers larger than a few monolayers, however, a different behavior is observed. While a crystalline Ge overlayer leads to a strong decrease of the interface barrier, room temperature evaporation of Ag and Au results in a further relatively sharp increase of the Schottky barrier height at a coverage of about 10 monolayers. These effects have been missed in the work of /2/, probably because of the limited electron escape depth and the possibility of Ga and As segregation that leads to core-level signals which, however, are not correlated with the core-level shifts of interface atoms. The new results show strong evidence that the idea of Fermi level pinning on (110) GaAs due to chemisorption induced defects is not generally applicable.

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ANGULAR RESOLVED PHOTOEMISSION AND INVERSE PHOTOEMISSION STUDIES OF LAYERED TRANSITION METAL DICHALCOGENIDES

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Angular resolved UV photoemission with high energy and angle resolution using synchrotron radiation and resonance lines combined with inverse photoemission provides detailed information on the electronic band structure of occupied and unoccupied states. By applying both methods we have studied several layered transition metal dichalcogenides in the vicinity of the Fermi level E_F in order to relate their electronic structure with the intriguing transport properties often observed in connection with phase transitions which may manifest themselves in superlattices and metal-semiconductor transitions.

In particular, we have investigated in detail the interesting and still controversially discussed case of 1T-$TiSe_2$ which develops a $2a_0 x 2c_0$ superlattice around 200 K associated with a marked change in resistivity. At room temperature $TiSe_2$ has been considered to be a semimetal or a degenerate semiconductor. — 1.) The high resolution EDCs show new fine structure at the top of the Se p valence bands around Γ which can be attributed to spin orbit splitting. 2.) An overlap of the top of the Se bands and the minimum of the Ti 3d derived lowest conduction band at the zone boundary M(L) has not been confirmed yet with certainty even by studying $k_\perp$ effects with continuous synchrotron radiation. 3.) Below the transition temperature the characteristic highly asymmetric d-emission at E_F near the zone boundary splits into two components indicating a reduction of the Fermi surface which corresponds with the observed increase of resistivity. 4.) Adsorption of molecules carrying an electric dipole moment (H_2O,CO) makes the d-emission visible over the entire Brillouin zone (Γ-M) which can be explained by dipole induced band bending pulling the lowest unoccupied d-states below E_F.

By inverse photoemission we have identified the unoccupied e_g- and t_{2g}-like non overlapping subbands. Their dispersion and splitting are smaller than predicted by theory . This indicates stronger localization of the Ti 3d electrons and possible non negligible correlation effects.

INDIRECT TRANSITIONS IN PHOTOEMISSION OF SEMICONDUCTORS

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Angular resolved photoemission has been extensively used in the last few years to obtain the "experimental band structure" of many metals and semiconductors. One electron theory and free electron final state have given very good results in the case of Cu, Ag, Au, GaAs, GaP, InSb.

All these results have been interpreted in the framework of the direct transition model, excepted in the case of the lead salts for which non direct structures have been observed at normal emission(1,2). We show that for semiconductors or metals with low Debye temperatures, strong phonon-assisted indirect transitions are likely to appear, even in the UPS range and at moderate temperatures. In this letter, we report on angular resolved photoemission measurements on PbS (100) and PbTe obtained at various temperatures between 20°K and 300°K. In the main part of photon energy range used for band structure determination (25 - 120 eV), both indirect (phonon-assisted") and non direct ("surface-assisted) transitions are observed. Indirect transitions are dominant at room temperature and only the low temperature data allow an accurate determination of E(k).

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INVESTIGATION OF ELECTRONIC STATES IN GERMANIUM AND SILICON BY SPIN DEPENDENT PHOTOEMISSION

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Optical spin orientation of photoelectrons represents a promising and increasingly active field of spin polarized photoemission. The spin polarization is obtained by excitation with circularly polarized light. It is fully determined by the symmetry properties of the initial and final state wave functions. Therefore, band hybridization may be measured directly, as illustrated by the example of the upper valence bands in germanium. In addition, the sensitivity to symmetry is shown by comparing polarization spectra of crystalline and amorphous Ge: although the short range order of amorphous Ge is still tetrahedral, the polarization vanishes completely. By its very nature as a differential quantity the measurement of the spin polarization increases the resolution of the photoemission experiment considerably. For instance, the 40 meV spin-orbit splitting of the valence band edge in silicon is readily resolved. The optically spin oriented electrons are also a fascinating subject for study in their own right: the observed depolarization by paramagnetic moments adsorbed on the surface opens for the first time the possibility to measure exchange constants of hot electrons as function of their energy.

ELECTRONIC BAND STRUCTURE OF RHOMBOHEDRAL ARSENIC STUDIED BY HIGHLY-ANGLE-RESOLVED ULTRAVIOLET PHOTOELECTRON SPECTROSCOPY

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Angle-resolved ultraviolet photoemission spectra of a rhombohedral arsenic (r-As) single crystal have been first measured in the very high angular resolution (less than 1.5°) with the He I resonance line as an exciting source. The experimentally determined band structure of r-As has been compared with the self-consistent pseudopotential calculation performend in this study as well as with four others presented mainly by the group of Falicov. The present photoemission measurement has directly identified the location of the electron pocket at the L point and the hole pocket near the T point in the Brillouin zone as predicted by the early band calculations.[1,2] However, it has been found that contrary to the calculations[1,2] only one band goes across the Fermi level into the occupied states near the L point, forming a pocket for electrons. Some stationary points with high symmetry and/or almost no dispersion along the interlayer, (111), direction have been successfully assigned in the experimentally determined band structure.

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THE USE OF HYDROSTATIC PRESSURE AS AN ADDITIONAL VARIABLE IN INFRARED MAGNETO-OPTICAL STUDIES OF III-V COMPOUNDS AND ALLOYS

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The development of simple pressure cells enabling magneto-optical experiments to be performed at liquid helium temperatures has opened up new possibilities for studies of impurities and band structure in semiconductors.

The hydrostatic pressure has the following effect:
i) By increasing the direct energy gap the i-effective mass increases, deepening the donor states concerned; ii) For some of the shallow donors, the states arising from the same impurity but originally lying deep within the conduction band can be brought into the forbidden energy gap, passing through resonance with the Γ-associated donors. Close to this condition, hybridisation of the states occur, dependent on the symmetry and admixture of the bands concerned. When the higher band states are moved deep into the forbidden gap, the Γ-associated components in the spectrum disappear completely iii) The sample resistance can be increased by many orders of magnitude when these states are placed deep into the gap, thereby improving the sensitivity of photoconductive detection. iv) A pronounced narrowing of all the donor lines is frequently associated with this increase in resistance. v) Some of the states which can be introduced into the forbidden energy gap experience a strong lattice relaxation and are metastable. Once these states become occupied, the pressure can be removed and the increase in resistance obtained on applying the pressure maintained. In this case any line narrowing is also retained. vi) Associated with the increase in band gap the static dielectric constant decreases with increasing pressure.

A preliminary report of effects (i) - (iv) in InSb was made at the previous semiconductor meeting. We can now report (v) and (vi) for InSb and (i)-(iv) and (vi) for GaAs. In addition experiments have been extended to the alloy systems $InAs_{1-x}P_x$ and $InAs_{1-x}Sb_x$. Remarkably sharp lines are found in both systems ($\omega\tau>20$ for the cyclotron resonances) enabling alloy disorder effects to be studied precisely over a wide range of energy gap.

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ThA-B6

PHOTOTHERMAL SPECTROSCOPY OF PLASTICALLY DEFORMED GaAs

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The role of plastic deformation on electrical and optical properties of GaAs samples has recently been investigated by EPR, photo EPR and photoluminescence [1]. It was concluded that observed signals induced by deformation could be correlated to As_{Ga} antisite defects created during dislocation motion. The hypothesis was put forward that such defects might be part of the "killer" centers for near band gap emission [1]. Following recent proposals for dislocations studies in semi-conductors by photoacoustics and photothermal spectroscopy [2] [3], we present here the first direct evidence of the existence of dislocation induced near-gap non radiative centers is GaAs using photothermal spectroscopy with the mirage effect technics [4]. In our case, an excitation beam at various wavelength is shined outo GaAs samples before and after plastic deformation. Non-radiative transitions are detected by the corresponding slight temperature rise which, due to the correlated refraction index gradient in surrounding medium, deflects a Ne-He laser probe beam. Comparing results obtained for instance for samples with $10^4 cm^{-2}$ and $10^8 cm^{-2}$ surface concentration of etch pitches gives a reproducible non-radiative transitions excitations spectra peaked at 1.4eV at room temperature (Fig.1). Varying modulation frequency of the excitation beam allows for depth profiling investigation through thermal length scanning.

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STRUCTURAL AND CHEMICAL DISORDER IN a-GaAs

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Electron spin resonance (ESR) and nuclear magnetic resonance (NMR) measurements have been performed on films of a-GaAs. The two films studied were prepared by different means, molecular beam deposition (MBD) for the first, and DC sputtering for the second; both on SiO_2 substrates. Photoluminescence, raman, and x-ray measurements were successfully employed in characterizing the samples as amorphous. The ESR spectra of both materials indicate high concentrations of As_{Ga} antisite defects, roughly 10^{17} cm^{-3} for the MBD film, and 10^{18} cm^{-3} for the sputtered film. The observation of As_{Ga} thus provides direct and unambiguous evidence of chemical disorder or "wrong-bonds" in a-III-V materials. The sputtered GaAs exhibits, in addition, an intense feature at $g \sim 2.0$ which may be attributable to dangling bond-type defects. ^{69}Ga, ^{71}Ga, and ^{75}As NMR linewidth measurements on both samples demonstrate conclusively the presence of second-order quadrupole broadening. Charged defects (whether impurities or native defects) are known to result in first-order quadrupole broadening in crystalline GaAs.[1] The observed magnitude of the quadrupole interaction in a-GaAs is thus attributable to slight deviations from crystalline bonding parameters which results in the loss of perfect tetrahedral symmetry. Nuclear spin-lattice relaxation times (T_1) of a-GaAs are an order of magnitude shorter than crystalline GaAs T_1's, which reflects a general property of disordered materials.[2]

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BANDGAP WIDENING IN HEAVILY Sn-DOPED In_2O_3

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The optical properties of evaporated films of doped semiconducting In_2O_3 in the 2-6-eV range, i.e. around the fundamental bandgap, have been investigated. The study serves two purposes: to elucidate basic properties of heavily n-doped semiconductors, and to improve our understanding of a technologically important material which is widely used when transmittance of visible or solar radiation needs to be combined with good electrical conduction or low thermal emittance.

Films of pure and Sn-doped semiconducting In_2O_3 were prepared by reactive e-beam evaporation. The direct optical bandgap (E_g) was measured by spectrophotometry in the 2-6-eV range. E_g increases with electron density (n_e) approximately as $n_e^{2/3}$ for $n_e \lesssim 10^{21} cm^{-3}$. This result is interpreted within an electron gas model for n-doped semiconductors above the Mott critical density. A degenerate electron gas is assumed to occupy the bottom of the host conduction band. The model accounts for a Burstein-Moss shift as well as electron-electron and electron-impurity scattering treated in the random phase approximation. Experiments and theory were reconciled by assuming a parabolic valence band with an effective mass $\sim$ 1.5 m.

ThA-B9

BAND GAP ANOMALY IN TERNARY CHALCOPYRITE SEMICONDUCTORS AND OPTICAL BOWING IN BINARY SEMICONDUCTOR ALLOYS.*

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Ternary chalcopyrites ABC$_2$ (A=Cu, Ag; B=Al, Ga, In, and C=S, Se, Te) and ternary pnictides (A=Zn, Cd; B=Si, Ge, Sn; C=P, As, Sb) form a large group of novel semiconductors, some of which have recently become useful in a wide range of opto-electrical devices, including solar cells (above 10% efficiency for polycrystalline CuInSe$_2$). To a large extent this resulted from the fact that the band gaps of the ternary chalcopyrites (e.g. CuGaSe$_2$) are anomalously small (by 30%-80%) relative to their binary counterparts (e.g. ZnSe), placing the former band gaps in the center of the solar spectrum, whereas Zinc binaries (II-VI) are transparent to sunlight. While the ABC$_2$ ternaries are structurally isomorphous to the binary zincblende semiconductors, they show, in addition to the band gap anomaly, also an interesting structural anomaly in the form of anion displacements (the C atom is closer to A than to B, hence the system shows "bond alternation"). Turning to quite different systems-random alloys of III-V compounds [e.g. $(InP)_x (GaP)_{1-x}$]—it has been known for a long time that the band gap of the alloy is smaller than the concentration-average gap of the constituent semiconductors ("optical bowing"). In this talk I show that the two, seemingly unrelated band gap "anomalies"—in ternary crystalline semiconductors and in random alloys of binary systems—share a common physical origin, namely bond *alternation*. Using self-consistent band structure techniques, I will analyze the electronic structure of ABC$_2$ semiconductors CuAlS$_2$, CuGaS$_2$, CuInS$_2$, CuAlSe$_2$, CuGaSe$_2$, and CuInSe$_2$, and discuss the band gap anomaly in terms of a chemical factor (p-d hybridization and cation electronegativity) and a structural factor (bond alternation). I will apply the same approach[1] to binary alloys (GaP-InP, ZnS-ZnTe) and show that bond alternation accounts for much of the optical bowing and hence disorder contributions may be smaller than hitherto accepted.

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Multiple Quantum Wells **ThA-C1** ***Invited***

HgTe-CdTe SUPERLATTICES

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We report magneto-absorption investigations done at 2 K in new superlattices (SL) fabricated from II-VI compounds by molecular beam epitaxy, i.e. HgTe-CdTe structures. Far infrared magneto-optical transitions are observed in the range 2-30 meV in such a SL where the HgTe and CdTe layer thicknesses were 180 and 44 Å, respectively. They extrapolate to an energy ~ 0 at zero magnetic field and are interpreted in terms of transitions between Landau levels of the ground valence (H_1) and conduction (E_1) subbands. The data are fitted to theoretical calculations done in the envelope function formalism and, from these investigations, we deduce the SL band structure in the k_z direction, where k_z is the wavevector along the growth axis. We show, in particular, that the system considered here is a zero-gap semiconductor, and we obtain also the first determination of the offset Λ between the valence bands of HgTe and CdTe. Additional magneto-optical transitions observed around 350 meV are interpreted from the calculated band structure, and are due to interband transitions from a valence subband derived from the Γ_6 HgTe states up to E_1. Finally, knowing the value of Λ allows us to calculate at different temperatures the band structure of HgTe-CdTe SL's along k_z as a function of the thickness d of the layers. These calculations show that a semiconductor-semimetal transition may be expected as a function of d. They show also that the interesting cut-off wavelengths for infrared detectors (8-12 μm) are obtained at 77 K with reasonable layer thicknesses, i.e. $\sim$ 50-70 Å. Optical measurements on such SL's are now performed to confirm these calculations.

HgTe-CdTe SL's are new two-dimensional heterostructures whose properties are only beginning to be investigated and present unusual features. More generally, SL's made from II-VI compounds should present a great fundamental interest and might have, in some cases, important applications. For example, from the point of view of basic physics, $Hg_xMn_{1-x}Te$-CdTe superlattices might be very interesting since they might lead to two-dimensional spin glasses. On the other hand, from the point of view of applied physics, in addition to the possibility of making infrared detectors around 10 μm from HgTe-CdTe SL's, one can also expect to be able to use $Hg_xCd_{1-x}Te$-CdTe SL's to make, for instance, detectors at 1.3 and 1.5 μm which are important wavelengths.

RESONANT RAMAN SCATTERING IN GaSb-AlSb SUPERLATTICES

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Resonant Raman Scattering (RRS) is used to analyze the E_1 transitions in GaSb-AlSb superlattices (SL). Resonance can be produced both by changing the frequency of the incident light or by modulating the gap by temperature variations. Measurements are performed in several polarization configurations in order to study either the allowed (deformation potential and electro-optic) or the forbidden (Frölich) scattering mechanism. As expected, a much sharper resonance is found for the forbidden scattering than for the allowed one, which in turn behaves in a way similar to other techniques used for this problem[1]. Moreover, in the proper configuration we observe interference between both mechanisms[2]. By performing experiments on different SL we estimate the decrease of E_1 with the increase of the SL period.

In order to analyze these results, we have computed the band structure of these systems by means of a perturbative procedure in a tight-binding framework including spin-orbit interaction. The valence band offset ΔE_v (top of GaSb minus top of AlSb) is the only free parameter in the calculation. This magnitude is very important here because when $\Delta E_v < 0.26$ eV, holes at L are confined in AlSb, and when $\Delta E_v > 0.26$ eV, they are in GaSb. This affects the behaviour of the SL because electrons at L are always confined in GaSb. From our results of RRS a type I behaviour of the SL states at L is deduced, so that ΔE_v must be greater than 0.26 eV.

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Multiple Quantum Wells **ThA-C3**

OPTICAL PROPERTIES OF ZnS-ZnSe SUPERLATTICES PREPARED BY A HWE

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After the first proposal of superlattice (SL) by Esaki and Tsu[1] many interesting works for SLs of III-V compound semiconductors (CSs) have been carried out. In these years our grouphas made efforts in making SLs of IV-VI CSs by a hot wall epitaxy (HWE)[2] and in investigating their properties[3] Recently we tried to make ZnS-ZnSe SLs on GaAs (100) substrates by a modified HWE system and observed their quantum size effects. For ZnS-ZnSe heterojunction lattice mismatch is somewhat large (4%). Considering, however, their electronic affinities (ZnS : 3.90 and ZnSe:4.09 eV) and energy gaps (ZnS:3.64 and ZnSe:2.81 eV), ΔE_c (0.19 eV) and ΔE_v (0.64 eV) are rather large and a large variation of energy gaps of the SLs or confinement of carriers into quantum wells is expected even for the SLs with a thin ZnS layer (barrier layer $\sim$ 50 Å). This thin layer may be able to absorb the lattice mismatch; i.e. it will be easily strained. Photo luminescences (PLs) of the SLs excited by a Hg lamp were measured at 77 and 4.2 K and strong PLs of free excitons were observed. Their peak energy (Eex) was varied from 2.8 to 3.0 eV by changing the SL structure (for examples; 2.90 eV for the ZnS (58Å)-ZnSe(35Å) SL and 2.99 eV for the ZnS (51Å)-ZnSe(23Å) SL.). PLs associated with defects were observed also and their energies were shifted to high energy side with Eexs. These facts would enhance the blue light emissions in EL devices. Experimental results of PLs and photo reflectances are analyzed and discussed using the Kronig-Penney model.

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COLLECTIVE ELECTRONIC EXCITATIONS IN SEMICONDUCTING SUPERLATTICE STRUCTURES.

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The bulk and surface or interface excitations of a number of different semiconducting superlattice structures have been investigated. The superlattices are treated as periodic arrays of two dimensional free carrier layers embedded in a material of appropriate background dielectric constant. The structures studied include infinite and semi-infinite type I and type II superlattices, non-Bravais superlattices, and superlattice sandwich structures. The spectrum of electronic collective modes is rich and varied. Bulk plasmon bands, acoustic and optical surface plasmons, and wave guide type modes of sandwich structures are found. Because of their possible usefulness in integrated optical electronics, the dispersion and damping of these modes and their dependence on sample geometry is of considerable interest. Analytic formulae will be presented for the frequencies of both bulk and surface or interface modes as a function of wavevector and the material parameters of the sample. Numerical results for several cases of particular interest will also be presented.

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NOVEL SELECTION RULES IN RESONANT RAMAN SCATTERING FROM GaAs QUANTUM WELLS

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We have discovered that the phonons active in resonant Raman scattering from GaAs quantum well heterostructures are actually the optical vibrations of a thin ionic slab. The slab modes, although occurring at the same frequencies as in the bulk material, are characterized by selection rules for the polarizations of incident and scattered light which are strikingly different from those of the infinite crystal. The observation of scattering by optical phonons at transverse and longitudinal frequencies allows, for the first time in heterostructures, the study of the deformation potential electron-phonon interaction, as well as its comparison with the forbidden Frohlich interaction. It is shown in a microscopic analysis of these mechanisms that the unique electronic structure of this quasi-two dimensional system plays an important role in Raman processes.

The light scattering measurements are made on heterostructures where many alternating layers of GaAs and AlGaAs, each ~ 100 Å thick, are enclosed by two ~1μ AlGaAs cladding layers. The unique advantages of this type of structure are twofold. First the cladding acts as a waveguide, permitting light to propagate in the plane of the layers. This allows the first light scattering study from heterostructures in which the wavevectors of incident and scattered photons are at right angles. Phonon displacements both perpendicular to and in the layer plane are active in this geometry. Vibrations in the layer plane occur at the bulk transverse optic frequency, whereas those perpendicular to the plane occur at the bulk longitudinal optic frequency. In addition, the multiple thin layers have a profound effect on electronic properties. Confinement of electrons in the GaAs layers causes a large increase in exciton behavior. The narrow quasi-two dimensional exciton states provide the strong resonant enhancement necessary to observe the light scattering.

Our experiments display evidence that the electron-phonon interaction in quantum wells is significantly different from that in bulk GaAs. The observed polarizations for light scattering at the transverse optic frequency indicate that the deformation potential in these heterostructures couples light and heavy holes. Theoretical analysis shows that this interband process can be traced to the reduced symmetry of the layered system, and that it is described by a Raman tensor which is non-symmetric. On the other hand, scattering at the longitudinal frequency seems to be mostly via the forbidden Frohlich electron-optical phonon interaction. In addition to the usual forbidden Raman scattering, in which the wavevector dependence of the interaction yields parallel incident and scattered polarizations, we also observe forbidden scattering in crossed polarizations. This surprising result appears to be a further consequence of the broken symmetry in this system.

INTERBAND MAGNETO-OPTICAL STUDIES OF GaAs-$Ga_{1-x}Al_xAs$ QUANTUM WELLS

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Excitation spectroscopy experiments on thin, undoped GaAs layers sandwiched between $Ga_{1-x}Al_xAs$, (thicknesses between 30Å and 150Å) at 1.8 K in high magnetic fields show the ground state and up to ten excited states of the free excitons of different two dimensional subbands in a magnetic field (B<23T). Several of these transitions can clearly be resolved using left and right circular polarization of the exciting light. The higher excited exciton states at high magnetic fields are strongly field dependent and extrapolate to zero field at higher energy than the ground state, which itself shows only a weak field dependence. These observations can be explained by the fact that higher excited exciton states are very weakly bound and can effectively be described as free electron and hole interband transitions between Landau levels, while the more strongly bound ground state just shows a diamagnetic shift. The magnetic field dependence of the excited states is analyzed with detailed bandstructure calculations as described in ref. 1.

From the different behaviour of the ground states with respect to the higher excited states the binding energies at zero magnetic field are obtained for different subbands in a very direct manner. It is found that the binding energy for thin layered samples (<100Å) is much larger than the three dimensional exciton binding energy in GaAs and that it decreases with increasing layer thicknesses. At the same time the magenetic field dependence of the ground state is found to be much weaker than that in bulk GaAs in these samples. For thicker samples (d>150Å) the magnetic field dependence approaches that of the bulk GaAs exciton, even though the subband structure is still essentially two dimensional. This general trend is in accordance with simple calculations of the binding energy and of its magnetic field dependence in a hydrogenic model using an exact numerical solution for the two dimensional case and the adiabatic approximation for the case of a finite thickness.

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A NEW QUANTUM STATE IN MULTIPLE QUANTUM WELL STRUCTURES

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Photoluminescence studies of undoped AlGaAs-GaAs multiple quantum well structures under selective and high intensity excitation (>10 kW/cm^2) reveal a new intrinsic luminescence line with energy lower than the ground state (heavy hole) excitons. We observed the following characteristic properties of this feature: i) Upon its emergence, the line is as narrow as the exciton line, ~1 meV in one sample, and separated from the exciton by an energy ΔE which varies from 6.0 ± 0.5 meV in 160 Å well, to 11 ± 2 meV in 85 Å well structures; ii) Its integrated intensity grows more rapidly than the square of the exciton luminescence; iii) At higher excitation intensity I_{ex}, the line is slowly red-shifted as $\ln(I_{ex})$, and a low energy tail slowly develops; iv) The line decreases in intensity as temperature varies from 1.9 K to 45 K with a corresponding increase in exciton luminescence; v) Magnetic fields (up to 10 T) induce significant quadratic Zeeman effect and raise the excitation intensity threshold for the observation of this lower state. Observation of this new phenomenon has never been reported. In view of these properties, the interpretations of phonon[1] or plasmon replica, molecular exciton[2] and biexciton reactions,[3] and band-gap renormalization do not apply. Since the phenomenon does not appear to have an analogue in bulk GaAs, we tentatively interpret the feature as evidence of a new ground state of 2-dimensional quasi-particles interacting via electron hole plasmons. The 2-dimensional electron-hole plasma system with exchange and correlation effects is also considered.

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ThA-C8

Fermisurface Study of a Semiconductor Superlattice

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In contrast to extensive works perfomed on two-dimensional systems, little work has been done on "semiconductor superlattices", in which the electron wave tunnels through barrier layers and extends over many periods of alternating heterostructures. In the present work, we systematically investigate the dispersion relationship of a superlattice by Shubnikov-de Haas measurment. In this work we use superlattices consisting of 50A GaAs and 20A $Al_{0.3}Ga_{0.7}As$, for which the width of the first miniband is calculated to be 48meV and the minigap between the first and the second band is predicted to be 145meV. We prepared the superlattice samples of that structure with different electron concentrations: 1.8×10^{11} cm^{-2} per layer for sample "A", 3.8×10^{11} for sample "B", and 2.9×10^{12} for sample "C", by MBE. Since the calculated Fermi energies E_F for sample "A" and "B" are 18meV and 28meV above the bottom of the first miniband, respectively, the Fermisurfaces of these samples are expected to be closed and "somewhat distorted" ellipsoids with the longer axis lying along the superlattice direction kz. In contrast, the Fermi energy E_F of sample "C" is 128meV and located in the minigap; therefore the Fermi surface is open and will look-like a "somewhat distorted" cylinder with the axis parallel to kz. To reveal the predicted differences in the topology of Fermi surfaces, we have measured the anisotropy of Shubnikov-de Haas oscillations of these samples by applying the magnetic field, either normal($\theta=0°$) or parallel ($\theta=90°$) to the layer. We determined the Fermisurface cross section S from the measured period $1/B(=2\pi e/(\hbar S))$. The ratios of the cross section $S(\theta=90°)/S(\theta=0°)$ seen from the two direction are found to be 1.1 for sample "A", 1.2 for sample "B" and infinity for sample "C". This agrees with the theoretical prediction and gives the firm evidence of the predicted formation of minibands and minigaps in superlattice structures.

BOUND EXCITON RECOMBINATION IN HIGHLY Cu-DOPED ZnTe

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Abstract

Novel properties of excitons bound to complex defects are studied in the high doping regime for Cu-doped ZnTe, where a large number of such defects of both neutral (isoelectronic) and acceptor type give rise to a rich structure of bound exciton spectra. The possible identity of these defects is discussed in relation to Zeeman data at 10 T. The bound exciton lines in luminescence are associated with strong electronic satellites which are explained by an interaction process at high doping, leading to final state excitations on acceptors far away from the site carrying the bound exciton in the initial state. The phonon coupling to such bound excitons is found to be strongly nonadiabatic with a remarkably enhanced coupling strength in absorption.

SYMMETRY DETERMINATION OF COPPER-RELATED CENTRES IN GALLIUM PHOSPHIDE

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Photoluminescence bands arising from exciton recombination at Cu-related centres in GaP have been the subject of intense study over the last few years[1]. The two most distinct spectra have sharp zero phonon lines (ZPL's) at 1.911 eV and 2.177 eV respectively. Zeeman spectroscopy has shown that the ZPL's arise from the recombination of spin triplet bound excitons (BE). However, the observed splittings were isotropic, presumably due to the quenching of the valence band orbital angular momentum in the local strain fields of the presumed axial centres. Therefore, the symmetries of the centres could not be determined directly from these measurements.

In the present work, piezo-spectroscopy at low temperature is employed to determine the symmetries of the Cu-related centres from study of the BE recombination lines. The 1.911 eV system is found to exhibit uniaxial stress splitting characteristic of recombination at a centre with rhombohedral I symmetry. The splittings observed are consistent with lifting of orientational rather than electronic degeneracy. The symmetry deduced here agrees with the results of ODMR for this centre.

The 2.177 eV centre shows very different behaviour. It is found to have both orientational and electronic degeneracy. The piezo-spectroscopic results can be explained by the splitting of an E to A transition at a centre of trigonal symmetry. The behaviour of the E state is consistent with the electron in the BE being in a valley-orbit E state, and reflects the fact that the multi-valley degeneracy of the conduction band is not lifted by trigonal distortions. The previously mysterious paradox of the absence of ODMR for the 2.177 eV centre can now be understood as arising from broadening of the initial E state by coupling to random strains in the crystal.

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PERSISTENT PHOTOLUMINESCENCE QUENCHING EFFECT OF 0.77-eV EMISSION IN UNDOPED SEMI-INSULATING GaAs*

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Three broad featureless photoluminescence bands at 0.63, 0.68 and 0.77 eV are present at 4.2K in undoped semi-insulating GaAs bulk materials. The 0.63-eV band was assigned to a center related directly or indirectly with O. The 0.68- and 0.77-eV bands are commonly present together with sample dependent relative intensities. The 0.68-eV band is due to a main deep intrinsic donor EL2 and shows a persistent photoluminescence quenching effect[1]. Such anomalous photoquenching phenomena associated with EL2 have been observed by photocapacitance, photoconductivity, absorption and photoelectron paramagnetic resonance.

The present study shows that the persistent photoluminescence quenching effect also occurs on the 0.77-eV emission. The dependence of the persistent emission on below band-gap excitation has been measured. The magnitude of the quenching depends on the below band-gap energy in the range of 0.9-1.4 eV. The maximum of the photoquenching occurs at ~1.15eV. The quenching-vs-energy relation yields two absorption peaks which can be attributed to the intracenter transitions of the center responsible for the 0.77-eV emission. The quenching effect is eliminated by a thermally activated process with increasing temperature to ~140K. The effect can be explained by the presence of both normal and metastable states. The metastable state is initiated by the intracenter electron transitions which appear as the two maxima of the quenching-vs-energy relation curve. The determination of the Frank-Condon shift of the 0.77-eV emission yields the energy of the levels of the intracenter transitions.

This analysis of the quenching-vs-energy relation implies that the center responsible for the 0.77-eV emission may be due to the anion antisite double donor As_{Ga}. This assignment is consistent with the photoelectron paramagnetic resonance experiment[2] and recent theoretical calculation[3]. The quenching behaviors of the 0.77-eV emission are compared with those of the 0.68-eV emission.

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* Work performed at AF Avionics Laboratory, Wright-Patterson Air Force Base, Ohio 45433, under Contract F33615-84-C-1423.

INVESTIGATION OF ROLES OF AMPHOTERIC IMPURITY IN $Pb_{1-x}Sn_xTe$

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Indium atoms in $Pb_{1-x}Sn_xTe$ have both donor-like and acceptor-like characters, and pin the Fermi level at low temperatures. A huge and "persistent" photoconductivity (PC) has been observed which is regarded as the most important key to elucidating the role of the amphoteric indium impurities. We have measured the far-infrared reflectivity ($60cm^{-1}$-$460cm^{-1}$, 20K-300K) by a Fourier spectrometer and the submillimeter magnetoplasma absorption (λ=337μ m, 4.2K, H<3.5T) for the first time, in $Pb_{1-x}Sn_xTe$/In (x=0.25;0.30) films on BaF_2 substrates as well as their transport properties. The plasmon-LO-phonon coupled mode frequency determined from the reflectivity spectra increases abruptly below 40K due to a gigantic increase of photo-carrier concentrations. The peaks of the dielectric anomalies in the magnetoplasma spectra become smaller and their positions shift to lower fields as a result of decrease of carrier concentrations with attenuating room temperature radiation level. The cyclotron mass is determined, under a low illumination, as $m_t=0.0155m_o$ and $m_l=10.5m_t$ for semi-insulating specimens (x=0.25). In spite of a small content (~1%) of indium impurities, the measured m_t is found to be larger than that expected for the undoped $Pb_{1-x}Sn_xTe$. A large magnetic field dependence of the Hall coefficient (R_H) has been observed near the p-n inversion temperature of R_H. This can be explained only when we take into account the coexistence of thermally excited electrons and holes through a small energy gap caused by a valley splitting among the <111> valley and the others which arises from the strain of the film. A kind of "semimetallic state" may exist in some specimens at low temperatures.

DEFECT IDENTIFICATION : EL2 IN GaAs.

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The short review of experimental methods for defect identification together with the recent achievements in the determination of defect nature in semiconductors will be presented. The case of the technologically important midgap EL2 defect in GaAs will be discussed more widely. Specially, the external field measurements, which establish for the first time that EL2 has tetrahedral symmetry and is, therefore, an isolated point defect will be shown. The combination of these data with technological and theoretical works allows to relate EL2 to an arsenic antisite defect.

EL2 IN GaAs - REEVALUATION OF OPTICAL DATA

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In order to promote a better understanding of the physics behind the EL2 level in GaAs we will in this paper present new optical data which are obtained by using a novel technique for selective measurements. This technique, which utilizes the quenching effect of the EL2 level, is fairly simple, but gives nevertheless new information. A reevaluation of optical data obtained by absorption, photoluminescence (PL) and photoluminescence excitation (PLE) measurements is therefore necessary. The low temperature absorption data obtained with this technique shows properties which exclude the previously suggested interpretation of the σ_n^0 -spectra as being caused by the density of states in the conduction band [1]. Instead the data support the recently suggested excistence of an excited EL2-state [2,3]. New PL and PLE data clearly show that the 0.63 eV luminescence band, which previously has been directly connected with EL2 [4,5], is not related to EL2. The reason for the earlier misinterpretation of this luminescence band will be discussed.

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SYMMETRIC RELAXATION AROUND INTERSTITIAL 3d IMPURITIES IN SILICON

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Transition metal (TM) atoms form a unique class of impurities in silicon. Having highly localized d orbitals, unmatched by the sp bonded host crystal, they form deep impurity states that couple literally to hundreds of host bands and, in sharp contrast to isolated TM ions, they can sustain many stable spin and charge states in a relatively narrow energy range[1] (the Si band gap). Under normal preparation conditions, all TM appear in Si in the tetrahedral interstitial site, retaining the cubic site symmetry of the host crystal. Using our recently developed Quasi Band Crystal Field (QBCF) Green's function method[2], we have calculated self-consistently the electronic structure of all 3d impurities in silicon[3] within the local density formalism. We will discuss the chemical trends in the electronic structure and bonding in this series. Using the self-consistent density displacement, we further calculated the impurity-induced forces on host atoms. The breathing mode distortions of the 8 shells of Si atoms surrounding the impurity are then calculated (assuming an empirical Si force field, fit to the phonon spectra, to reprresent interactions of unperturbed Si atoms) by relaxing the atomic positions with an automatic Jacobian Update technique. For all 3d impurities, we find that the first shell of nearest neighbors (containing 6 Si atoms) moves away from the impurity, whereas the second near neighbor shell (containing 5 Si atoms) moves towards the impurity. This deformation pattern tends to equalize all 10 Si-TM bonds, producing an uncommon species of an approximately 10-fold coordinated 3d atom. Interestingly, all 3 metallic bulk disilicides types ($TiSi_2$, $CrSi_2$, and $MoSi_2$ structures) are known to avoid the conventional close packing (coordination of 12) and exhibit a variety of unique stacking sequences that result in a 10 fold coordinated TM. We will discuss the mechanism leading to this special relaxation pattern and its relationship to the physics of bulk silicides.

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Deep-Level Impurities **ThA-D8**

NO LARGE LATTICE RELAXATIONS AROUND THE ARSENIC ANTISITE DEFECT IN GaAs

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The As antisite defect in GaAs has received a lot of attention in the last two years as a likely candidate for the EL2 center.[1,2] Large lattice relaxations and the existence of a metastable state due to strong electron-lattice coupling were invoked to explain the quite peculiar behavior of EL2 e.g. upon illumination (quenching of the photocapacitance[3] and of the photoabsorption[4]).

Our self-consistent, parameter-free calculations of the lattice relaxations around the As antisite defect in GaAs for all charge states indicate that this center is a rather well behaved point-defect with tiny breathing relaxations associated to it ($\lesssim 1\%$ of the perfect crystal bond length).

From this finding we are lead to strongly suggest that the isolated As antisite defect cannot by itself be identified with the EL2 center in GaAs.

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ThP-A1

INELASTIC TUNNELING CHARACTERISTICS IN Bi-GaS-Bi AND Pb-GaS(Se)-Bi JUNCTIONS

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Tunneling junctions have been made for the first time with a pair of evaporated films of Bi sandwiching an extremely thin ($\sim$30 Å) piece of crystalline GaS of layer structure with its c-planes facing the Bi electrodes. Bi film is preferably oriented with its face parallel to the trigonal plane. Procedures for fabricating the junction and the method of assuring the absence of structural defects (e.g. contacts through pinholes in GaS) are described in the present paper. At 1.8 K the tunneling current, I, vs. bias voltage, V, shows a nonlinear increase around $V \cong \pm 70$ mV, saturates around $V \cong \pm 250$ mV and then exhibits a negative incremental resistance of -4 kΩ for the junction area of ~ 0.018 mm^2 up to $V \cong \pm 400$ mV where a sharp increase in I sets in. Such anomalies in tunneling characteristics can be explained quantitatively in terms of extrema in the density of hole states at the T- and Γ-points and of electron states in midway between Γ and T, as deduced from the theoretical calculation by Golin.$^{1)}$ The inelastic spectrum of dV^2/dI^2 vs. V shows structures at $V = \pm 11$ mV and ± 13 mV corresponding to the extrema in the density of states at T and L points of phonon dispersion in Bi.$^{2)}$ The phonons of a semimetal electrode with their finite wavevectors have never been identified in a symmetric tunneling junction. In a similar manner, the asymmetrical junction of Pb-GaS(or Se)-Bi shows inelastic tunneling peaks associated with the maxima in the density of states of phonons in GaS and GaSe. The near-zone-edge phonons of GaS(GaSe) have been identified in comparison with neutron data.$^{3)}$ In short, the inelastic tunneling spectroscopy proves to be a powerful means of identifying the maxima in the phonon density of states with their wavevectors extending up to the zone-edge. An appreciable asymmetry in the d^2V/dI^2 vs V spectrum for $|V| \lesssim 20$ mV is observed in the Pb-GaS(Se)-Bi junction. Their characteristics may be interpreted in terms of the self-energies due to electron-phonon interactions in electrode metals.

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TIME-RESOLVED PHOTO-EXCITED PHONON TRANSPORT IN GaAs*

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It has recently been proposed[1] that the thermalization of optically excited carriers in GaAs leads to the excitation of long-lived, near-zone-edge transverse-acoustic (TA) phonons. The experiments in GaAs by Ulbrich et al.[1] showed broad TA phonon pulses which were interpreted in terms of the transport of highly dispersed short-wavelength (~10-20 Å) phonons. Other studies[2] have not reproduced these results, but generally exhibit a sharp onset near TA followed by a long tail.

We have performed optically-excited phonon transport experiments in GaAs that substantially clarify this situation. We report, for the first time, a dramatic dependence upon phonon propagation direction of the phonon pulse shape. We also find that for pulsed laser excitations near the gap (~1.52 eV) dramatic changes are observed in the time-resolved phonon signal as the excitation wavelength is varied. In addition, we will present the first evidence for substantial changes in the ballistic phonon pulse shape due to irradiation with CW, low-level, below gap light. We propose that these results can be understood on the basis of an anisotropic scattering mechanism which leads to the effective thermalization and down-conversion of high frequency TA phonons for certain phonon propagation directions in GaAs.

We have measured optically excited phonon transport in <100> cut LEC GaAs using a novel superconducting NbN bolometer.[3] This bolometer makes it possible to examine the effect of thermal scattering over a wide temperature range (1.8 to 5K) using a single sample with a single bolometer. For phonon propagation along the <100> direction, we observe a sharp onset in the bolometer response near the expected low frequency LA and TA phonon transit times, followed by a long tail. The relative contribution of delayed TA phonons to those near the sharp TA onset depends significantly on temperature, laser power and excitation wavelength. For phonon propagation along <110> and <111> directions we observe only a broad pulse lineshape. The peak position of the broad pulse scales linearly with phonon propagation length, as observed previously.[1] These anisotropic phonon propagation effects may be related to defects in GaAs. We have some preliminary evidence which suggests that the native EL2 defect in GaAs may be involved: Irradiation of the sample with low-level light at 1.1 μm quenches the photoconductivity (PC) in our GaAs sample (using the NbN as a detector of PC). There is a concomitant measurable change in the phonon pulse shape which suggests that irradiation at 1.1 μm has increased the thermalization process from high to low frequency phonons.

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TRANSPORT PROPERTIES OF TERAHERTZ PHONONS IN GaAs

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Recent experiments in GaAs have unambiguously shown that TA phonons with $\nu = 1...2$ THZ are long-lived with an energy relaxation time $\tau_E \geqslant 1\,\mu\text{sec}$ [1,2]. The observation of anomalously long mean free paths of > 1mm for these phonons, however, has become subject of a controversy [3,4]. We report further experimental evidence supporting the original interpretation [1]: (i) dispersive focussing patterns in highly angular-resolved time-of-flight measurements with Pb detectors ($\nu \gg 0.7$THZ) after pulsed laser excitation of either bulk GaAs or constantan films, and (ii) comparison of three different phonon detection schemes (Al bolometer, high-quality Pb junctions, and shallow ionisation by phonon absorption with $\Delta E \geqslant 4.4\text{meV} \triangleq 1.06$THZ).

The most striking features are sharp focussing patterns along $\langle 1,0,0 \rangle$ with <u>no</u> diffuse, i.e. undirectional background for the whole leading portion of $\sim 30\%$ of total signal area of the Pb-2Δ detector signals over r=1.2mm, which we report here for the first time. Furthermore, we observe considerable broadening, but still no undirectional background in the focussing patterns for later arrival times $t \approx 1.2...3\ t_o$, where t_o is the TA phonon onset time. We attribute this to TA phonons above 1THZ which have propagated unscattered over 1.2mm.

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THEORY OF BRILLOUIN SCATTERING FROM SURFACE WAVES IN SEMICONDUCTOR SUPPORTED FILMS AND LAYERED STRUCTURES

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It has been proved in the past few years that Brillouin scattering in non-normal incidence is an accurate tool for the direct measure of the density of states of surface acoustic waves in both the discrete spectrum (e.g. Rayleigh and Lamb waves) and in the continuous spectrum (bulk waves projected on the surface and modified by the surface boundary conditions) /1/.

By taking into account the elasto-optic interaction and the light scattering from the interface ripples caused by the surface waves in thermal equilibrium, a general theory of Brillouin scattering from a film supported on a semiinfinite substrate has been developed /2/.

Various systems of interest are investigated such as: different surfaces of GaAs, silica on crystalline silicon, GaAlAs on GaAs. The main results are: the interpretation of a structure appearing in the spectra as a new leaky surface mode (or resonance) of longitudinal character; the possibility of deriving the elasto-optic tensor from a quantitative comparison between theory and experiment.

Theory and calculations have been extended to the case of repeated layered structures of GaAlAs and GaAs. The behaviour of the velocity of the surface waves versus the film composition and thickness has been studied and a comparison with the available experimental data is presented.

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ThP-A5

Calculations of the Elastic Properties of Si, Ge, and GaAs*

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Theoretical calculations based upon density functionals and *ab initio* pseudopotentials have been shown to predict accurately energies, forces, and other properties of semiconductors.[1-3] We have recently derived a "stress theorem" to also determine the stress tensor directly from the electronic ground state for any crystal structure with arbitrary strains and atomic displacements.[3] The simultaneous calculation of stress, force, and energy makes it possible to determine stress-strain relations including all microscopic internal strains of the atoms. Here we describe results of *ab initio* calculations for Si, Ge, and GaAs, giving the equilibrium lattice constant (where pressure =0), the full set of linear elastic constants C_{11}, C_{12}, and C_{44}, and many higher order elastic constants. Agreement with experiment for macroscopic elastic constants of all materials is within a few percent, as found before for Si.[3] The microscopic internal strain parameter differs from currently accepted values, as discussed in Ref. 3, in ways crucial for properties such as band deformation potentials and the piezoelectric coefficient of GaAs.

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CPA LATTICE DYNAMICS OF III-V MIXED CRYSTALS: THEORY AND EXPERIMENT

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We present a Coherent Potential Approximation (CPA) model of the lattice dynamics of III-V ternary and quaternary alloys. We show that theoretical predictions agree with our Raman scattering results on $Ga_{1-x}Al_xAs$ and $Ga_{1-x}In_xP$ alloys. A continuous evolution from two-mode to one-mode behavior is demonstrated. The starting point of our study is a series of shell models for the III-V compounds. (Experimental frequencies are well reproduced, and predictions of eigen-displacements agree with ab initio calculations whenever available.) In particular, model parameters vary slowly from one compound to another, thus allowing interpolations across the periodic table; this is why the dynamical matrix of the alloy can be successfully handled by an appropriate virtual crystal interpolation; the mass disorder is then treated within the CPA approximation. This powerful calculation, which provides total, spectral and local densities of states, includes correctly from the beginning the long range forces. We first analyse, in the case of two-mode behaviour alloys like $Ga_{1-x}Al_xAs$ or $In_{1-x}As_xP$, the emergence of new disorder activated zone center modes, the frequency shift and asymmetrical broadening of the zone center optical modes and compare these predictions with previous calculations and with our detailed Raman scattering experiments on $Ga_{1-x}Al_xAs$ epitaxial layers. We also determine the "thick" dispersion curves and use them to explain our Raman scattering results on GaAs/GaAlAs superlattices; the more complicated behavior of In_{1-x}GaxAs and in1-xGaxP alloys is then analysed, as well. Concerning the latter one, our theory well accounts for the quasi-local resonant mode of Gallium in InP observed by Raman scattering and attributes this feature to the weakness of the mass perturbation compared to the longitudinal transverse splitting. As the mass defect is varied, the zone center density of states continuously evolves from a two-mode behavior (in the case of strong mass defects) to various behaviors more or less close to the one-mode bahavior (for weak mass defects).

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ThP-A7

INITIAL PROCESS IN SELF-TRAPPING OF EXCITONS

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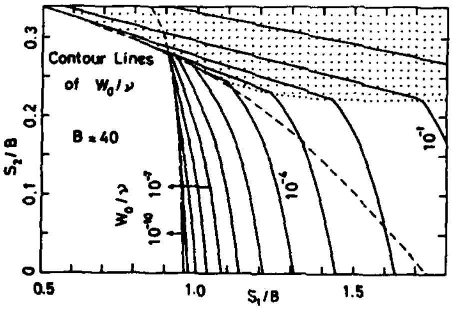
Excitons are self-trapped into a localized state with strong lattice distortion in various crystals. In the course of self-trapping, however, it seems probable that a free exciton does not make a transition directly to the shrinked self trapped state, but first a state of nucleation less localized than the final shrinked one is formed and then it shrinks by inducing lattice distortion further more in order to stabilize itself. The relaxed self-trapped state has a symmetry of one-center (monomer) type in some crystals but of two-center (dimer) type in others. However the self-trapping process is a symmetry-breaking process in which the symmetry of the self-trapped state cannot be anticipated from the symmetry of the lattice. Therefore, it is possible that the symmetry of the nucleation state for self-trapping is different from that of the relaxed lowest self-trapped one.

We can calculate a rate of nonradiative transition to an assumed nucleation state with appreciable lattice distortion from a free state without it. It enable us to analyze the self-trapping rate of 4.2K and the temperature dependence of the quantum yield of free-exciton luminescence both of which have been observed in RbI and KI. It is deduced that the nucleation state should have a symmetry of one-center type with spatial extension of the order of a lattice constant in RbI and KI where a self-trapped state of two-center type exists as a relaxed state.

When the nucleation state is of one-center type in alkali halides, we are led to two possibilities; (1) A cross over of the self-trapped state from one-center to two-center types occurs during lattice relaxation; or (2) Both types of self-trapped states coexist as relaxed states. When 1s free exciton is excited in alkali iodides, we observe so called E_x luminescence different from σ and π ones emitted from the self-trapped state of two-center type. The symmetry of a state emitting E_x luminescence has not been known. Then it seems reasonable to predict that it is emitted from a self-trapped state of one-center type in the case (2).

A rate W of transition to the nucleation state ψ is a function of the symmetry and the extension ℓ of ψ for a given set of the half width B of the exciton band, the site-diagonal and off-diagonal exciton-phonon interaction energies S_1 and S_2 and the phonon energy $\hbar\omega$. The symmetry and ℓ are so determined as to maximize W a each temperature. Energies and W are respectively scaled in units of $\hbar\omega$ and $\nu=\omega/2$ W takes W_0 either at 0 or 4.2K. The figure below shows contour lines of W_0/ν for B=40 in the $(S_1/B, S_2/B)$ plane. ψ has a symmetry of two-center type in the dotted region, while in the right half of the remaining region it has a symmetry of one-center type although exciton cannot be self-trapped in its left half. Experiments show that W_0/ν equals $10^{-4} \sim 10^{-3}$ in RbI and KI with $\hbar\omega \simeq 7.5$ meV. Then the region of the figure allowed for ψ of two-center type is much narrower than that allowed for ψ of one-center type although either type is still possible to reproduce the observed W_0/ν. Next we can show that the temperature dependence of W is much more rapid in the former region than in the latter one. The observed temperature dependence of the quantum yield of free-exciton luminecence can be fitted much better by W obtained in the latter region than in the former one.



ThP-A8

DIRECT EVIDENCES OF FREE MOTION OF POSITIVE HOLES AND EXCITONS BEFORE SELF-TRAPPING IN $AgCl_XBr_{1-X}$ ($X \geq 0.45$)

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Direct evidences of potentially free motion of positive holes and excitons before self-trapping in $AgCl_xBr_{1-x}$ ($x \geq 0.45$), where self-trapped states are eventually stable[1)2)], have been obtained, for the first time, by the measurement of the Hall angle Θ at crossed high electlic and magnetic fields and subnanosecond luminescence spectroscopy, respectively.

First, two components of the transient photocurrent, Q_x and Q_y in $AgCl_xBr_{1-x}$ were studied in detail at 4.2K up to the electlic field $E_x \doteq 3$kV/cm and the magnetic field $H_z \doteq 96$kOe by using a fast pulse technique with blocking electrodes[3)]. The Hall angle Θ is defined by $\Theta \equiv Q_y/Q_x$. The measurement of the magnetic field dependence of the Hall angle of $AgCl_xBr_{1-x}$ has been performed at various values of electlic field. The value of Θ can be plotted as a function of the quantity $\zeta \equiv v_{LO}/v_y$ where $v_{LO} = (2\hbar\omega_{LO}/m^*)^{1/2}$ and $v_y = cE_x/H_z$. Namely, Θ increases linearly with increasing ζ when $\zeta < 1$. This indicates the existence of *streaming motion of polarons* . On the other hand, Θ increases abruptly with increasing ζ when $\zeta > 1$. This phenomenon is caused by *the polaron accumulation* in the k-space. Normally in the crystals($x \geq 0.45$), main carriers are electrons. However, free positive holes also can accumulate in the k-space. Positive hole accumulation reduces Q_y and thus suppresses the increasing rate of Θ as for pure AgBr[3)]. Our new data of $AgCl_{0.64}Br_{0.36}$ exhibit a kink at $\zeta_e = 1$ for electrons but become saturated at higher H_z. This reveals an unexpected transient contribution to Q_y and an advent of accumulation of free positive holes. Absolute values of Θ are of intermediate grades between AgCl and AgBr under similar condition. The difference between behaviours of Θ on ζ for AgCl and $AgCl_{0.64}Br_{0.36}$ are due to the difference of potential barrier height between free and self-trapped state.

Secondly, new time-resolved luminescence spectra from free exciton(FE) state in $AgCl_xBr_{1-x}$ ($x = 0.53, 0.64$), have been observed, for the first time, in addition to self-trapped exciton(STE) states eventually stable[2)], by using subnanosecond spectroscopy technique ($\doteq 10$MW/cm^2, pulse width $\doteq 3$nsec). At the gate time of about 300psec in the rising part of laser pulse, *the luminescence near by absorption edge is enhanced* . The intensity of this luminescence band depends super-linearly on the excitation power of laser pulse. The decay time of this band is of the same order with the duration of laser pulse. The relaxation time from FE state to STE state is considered to be of the order of picosecond. Therefore, luminescence from FE state can be hardly observed at usual level of excitation. However, radiative recombination life time of FE, if any, in $AgCl_xBr_{1-x}$ ($x = 0.53, 0.64$) can be estimated to be several 10μsec extrapolated from the experimental value when $x < 0.45$. Thus, at high level of excitation, the effect of collision between excitons can yield also appreciable amount of luminescence due to FE. This collision process competing with self trapping process well stands out at high level of excitation because of the intensity dependence of the new luminescence band on the laser power irrespective of the short decay time. The enhanced region of luminescence band near by absorption edge at the gate time before the laser peak is tentatively ascribed to radiative recombination of free excitons in relaxation process.

We conclude that the results in transport phenomena definitely indicate *the potentially free motion of positive holes* even in these mixed crystals ($x \geq 0.45$) *before self-trapping* and also the new time-resolved luminescence band of $AgCl_xBr_{1-x}$ ($x = 0.53, 0.64$) at high levels of excitation is due to *free exciton before self-trapping* perhaps sustained via exciton-exciton collision both irrespective of self-trapping mechanisms of picosecond order.

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INVESTIGATION OF AMORPHOUS SILICON WITH SYNCHROTRON RADIATION

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The information about the electronic and structural properties of amorphous silicon (a-Si) obtained using high resolution photoemission and partial yield spectroscopy is reviewed. Strain in the amorphous network of unhydrogenated a-Si leads to local variations of the valence charges as witnessed by the broadening of the Si 2p core levels. These charges are reduced by the strain-relieving incorporation of hydrogen. The amount of hydrogen bonded to Si and the bonding configurations are deduced from the chemical shifts induced by H in the Si 2p core level spectra. Utilizing the variations in sampling depth with photon energy the core level spectra reveal an enrichment of hydrogen at the surface that is specific for the different Si-H_x configurations. The enrichment is accompanied by variations in the position of the valence band edge and of the Fermi level as monitored by valence band spectra.

Employing partial yield spectroscopy the transition from Si-Si to Si-N antibonding states has been followed with nitrogen concentration in a-SiN_x:H. The onset of localization of states at the conduction band edge in a-SiN_x:H could be identified spectroscopically by the autoionization of transitions into these states.

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Amorphous Semiconductor **ThP-B2**

VALENCE-BAND DENSITY OF ELECTRONIC STATES IN AMORPHOUS SILICON

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Differences between the x-ray photoemission (XPS) valence-band spectra of crystalline and amorphous silicon are generally explained by analogy with differences in the calculated densities of valence-band states for two crystalline forms of silicon, diamond cubic and ST12, where it is believed that the crucial aspect of the ST12 structure is the occurrence of odd-membered rings. We present new experimental data and new theoretical results which together suggest an alternative explanation. Our XPS valence-band spectra for *in situ* cleaved crystalline and hydrogenated amorphous silicon are qualitatively similar to earlier data,[1] but differ quantitatively such that the usual interpretation based on odd-membered rings is less attractive. We are exploring further the origin of the experimental discrepancies, but it is apparent even now that an understanding of these spectra requires a proper calculation of the density of electronic states of amorphous silicon, one in which neither the structural model nor the electron-atom potential need be oversimplified. To that end, we have applied to amorphous silicon a new theoretical framework for calculating the electronic properties of disordered materials.[2] Preliminary results suggest that dihedral-angle disorder alone is sufficient to account for the principal differences between our XPS valence-band spectra of crystalline and amorphous silicon.

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ENERGY DEPENDENCE OF THE OPTICAL MATRIX ELEMENT IN HYDROGENATED AMORPHOUS SILICON

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Although many measurements of the optical absorption of hydrogenated amorphous silicon (a-Si:H) have been performed, they have been difficult to interpret since neither the conduction band density of states (DOS) nor the energy dependence of the optical matrix elements are known independently. The energy dependence of the optical matrix element, in particular, should be different from that of crystalline semiconductors because the states involved in the dominant optical transition change from extended to localized states. We have measured on the same film the valence band DOS using x-ray photoemission and the conduction band DOS using inverse photoemission. From these spectra, we have calculated the joint density of states and compared it with the ε_2 spectrum measured directly by ellipsometry and with published ε_2 spectra determined from Kramers-Kronig analysis of reflectivity data. The ratio of the measured ε_2 to the joint density of states gives the dependence of the average matrix element squared, $|P(E)|^2$ on photon energy, E. Our measured energy dependence of $|P(E)|^2$ for a-Si:H is quite similar to that calculated[1] for a simple tetragonal cystalline form of silcon known as ST-12. This form of Si contains bonding configurations similar to those believed to occur in a-Si i.e., odd-member rings and bond angle variations. In both ST-12 and a-Si:H, $|P(E)|^2$ exhibits an asymetric peak at an energy of 3.5±.4 eV and with a width of ~2.0 eV. For energies below the peak, $|P(E)|^2$ decreases more or less linearly. Proceeding to energies above 4 eV, $|P(E)|^2$ decreases roughly as 1/E. The results indicate that ε_2 spectra at high energies dominated by the energy dependence of $|P(E)|^2$ rather than the energy dependence of the joint density of states. The implications of these results for interpreting optical spectra will be discussed.

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Amorphous Semiconductor **ThP-B4**

CALCULATIONS OF THE ELECTRONIC AND TRANSPORT PROPERTIES IN Si-Ge-H ALLOYS

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We have calculated the densities of electronic states for a series of Si-Ge and Si-Ge-H alloys, using the tight-binding-coherent-potential approximation model which we applied previously[1] in a-Si:H.

We have found that the energy gap for the Si-Ge alloys shows a monotonic decrease from Si to Ge as expected. The addition of hydrogen increases the energy gap in agreement with what is known from experiments in hydrogenated a-SiGe alloys.

We have also used the Kubo-Greenwood formalism within our multi-band model, to calculate both the dc and ac conductivities. From the dc conductivity and the density of states we derive a value for the mean free path and thus relate our results to the localization properties of these materials. From the ac conductivity we obtain the absorption coeffiecient from which we determine the Si and Ge conscentrations that give the optimum gap for photovoltaic conversion.

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ANOMALOUS PRESSURE-DEPENDENCE OF LUMINESCENCE IN c-As_2S_3 AND a-As_2SeS_2: IMPLICATIONS FOR DEFECT STRUCTURE

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The effect of hydrostatic compression (at 13K) on native-defect photoluminescence (PL) is studied for the first time in crystalline (c-) As_2S_3 and in amorphous (a-) As_2SeS_2 to 110 kbar and 17 kbar, respectively. The goal of this work is to probe defect structure. Pressure accomplishes this by shifting the local bond-equilibria at a defect in such a way as to trace out the relevant configuration coordinate (cc) potentials. The experiments require special cryogenic diamond-anvil-cell techniques, in which solid argon is the hydrostatic pressure-transmitting medium. For c-As_2S_3 it is found that the initially (at $P=0$) mid-bandgap PL-peak E_{PL} shifts to higher energy at the rate + 1.2 meV/kbar. Simultaneously the band edge E_g, and the PL excitation peak (which remains tied to the edge) shift to lower energy at −14 meV/kbar. Hence, the Stokes shift decreases drastically under compression, and by 110 kbar the PL peak is partially reabsorbed in the approaching band edge. The results for a-As_2SeS_2, though limited due to photo-induced PL-fatigue, indicate a similar behavior for this chalcogenide glass. The observed PL pressure-response is quite anomalous since it violates the well established (at $P=0$) mid-bandgap rule, viz. $E_{PL} \approx E_g/2$, that holds for native-defect PL in c- and a-chalcogenides of widely varying composition.[1] Consequently the effects of applying pressure and varying composition are definitely not equivalent for PL in As-chalcogenides. The relatively small changes in the Stokes shift induced by temperature are also considered; it is found that they can not be simply explained by thermal expansion. The present results are contrasted to earlier work on a-Si:H.[2] The pressure dependence of the Street-Mott[3] defect energy-level scheme is deduced from the observations on c-As_2S_3. It is found that if the Stokes shift decreases for one defect species, it must remain approximately constant for the other. To explain this dependence a new cc-model based on layer inter-linking defects is developed. This treatment succeeds because it invokes both soft inter-layer phonons and stiff intra-layer phonons to describe the ground and excited states, respectively, of the PL defect-center. The reduction in Stokes shift then follows from the large decrease in inter-layer spacing, which is known to be the dominant effect of pressure on this molecular crystal. It is concluded for c-As_2S_3 that the PL-defects exist on the surface of the layers, and that they loosely couple adjacent layers in the ground state but tightly couple them in the excited state. The preceeding analysis can be adopted to explain the similar PL pressure-response in As_2SeS_2 glass, if layer-like clusters now play the role of the crystalline layers. A model of this type has recently been proposed.[4] An evaluation of the present results in terms of this and other current models[3,5] suggests that the detailed defect structure could be obtained from a calculation of realistic cc-potentials, guided by the PL pressure-response.

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17th International Conference on the Physics of Semiconductors

Amorphous Semiconductor **ThP-B6**

A STRUCTURAL MODEL OF AMORPHOUS SILICON WITH PERIODIC BOUNDARY CONDITIONS

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We describe a novel systematic method for the generation of realistic structural models of amorphous silicon with periodic boundary conditions. We have relaxed one such model containing 216 atoms using Weber's adiabatic bond charge potential.[1] This is the first application of Weber's method to the relaxation of amorphous structures. The results are compared with those obtained by relaxing with a Keating potential using a relaxation procedure described by Steinhardt et al.[2,3]

Our approach is to start from the diamond structure with periodic boundary conditions built in from the start.[4] We then progressively rearrange the structure while always maintaining the original tetrahedral coordination and periodicity. The process consists of randomly switching bonds on adjacent atoms in such a way as to be physically reasonable. This allows the generation of a sequence of increasingly randomized models by a process somewhat akin to melting. In the process, bond lengths and angles are increasingly distorted and the topology is changed to include 5 and 7-fold rings.

Having obtained a random structure, the bond switching mechanism is continued, but a new restriction is included: Each new arrangement of bonds must lead to a lower total strain energy. Depending upon the degree of randomizatin produced in the "melting" process, resolidification yields either a perfect diamond structure or a stable amorphous structure. All amorphous structures produced in this manner are essentially the same as determined by the radial distribution function, ring statistics, and density. The agreement with experiment is very good. Weber's adiabatic bond charge model introduces long-range Coulomb forces. Their effect is to increase bond angle distortions by tenths of a degree and to decrease bond length distortions compared with the results obtained with Keating forces alone.

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LONG RANGE STRUCTURAL AND ELECTRONIC COHERENCE IN AMORPHOUS SEMICONDUCTORS

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We have computed the electronic states and optical absorption spectrum for amorphous Si (a-Si) within a novel lattice model. Until recently it was believed that the continuous random network models, which adequately describe the structure of a-Si and other semiconductors, contain no remnant of long range order. However, the optical absorption and its pressure dependence in a-Si suggests that such order does exist, and we use curved space polytope lattices to describe it. One of the polytopes, "polytope 240," which contains 240 atoms arranged in 6-fold boat-like rings, is a particularly promising model. It contains a channeling axis associated with a local screw symmetry which can be found in previous amorphous network models by visual inspection (Polk's model and Chaudhari's model have been examined). Its presence implies that even in the "random" network models electronic eigenstates possess phase coherence over many bond lengths. The identification of coherence allows us to compute a "band structure" within the polytope model which is associated with the screw symmetry and which bears a resemblance to the surface band structure of a semiconductor. Remnants of a selection rule are implied for the optical absorption spectrum at the band threshold. We discuss other symmetry properties of the polytopes and their possible relation to observables in a-Si, and we also elucidate the connection between the present application of non-euclidean models and recent similar work on other condensed matter systems, e.g., metallic glasses.

EVIDENCE FOR EXISTENCE OF TWO-LEVEL TUNNELING STATES IN a-Si

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In amorphous tetrahedral semiconductor a-Si, no evidence for the existence of two-level tunneling states (TLS) has been found so far. In this paper we report the first clear observation of the existence of TLS in a-Si by means of surface acoustic waves (SAW) propagated along polished 128° Y-cut $LiNbO_3$ SAW devices. Amorphous Si films with ~6 μm thickness were sputtered from a Si target in an O_2-free Ar atmosphere of 10^{-2} Torr (background pressure: 10^{-6} Torr). Variation of SAW velocity and attenuation was measured down to 0.1 K at 330 MHz.

A logarithmic increase in SAW velocity with temperature, which is a direct consequence of the resonant interaction between TLS and SAW, was observed below 4 K for all the samples prepared. In a film of thickness h, SAW velocity v ($\simeq 4\times10^5$ cm/sec) is given by[1] $\Delta v/v = (n_0 M^2/\rho v^2)K[1-\exp(-2h/\lambda)]\ln(T/T_0)$, where n_0 is the density of states of TLS, M their coupling constant to SAW, ρ the mass density ($\simeq 2$ g/cm^3), λ SAW wavelength (= 12 μm), K a constant ($\simeq 0.03$), and T_0 an arbitrary reference temperature. The slope of the logarithmic variation gives the coupling parameter $n_0 M^2 = (3.5-5.2)\times10^7$ erg/cm^3 at 330 MHz, which is an order of magnitude smaller than that ($\simeq 2\times10^8$ erg/cm^3) found in a-SiO_x.[2] Oxygen impurities have been thought to be very effective in forming TLS in a-Si.[2] Oxygen content of the present samples, however, is of the order of 10^{19} cm^{-3} which is three orders of magnitude smaller than in a-SiO_x. If oxygen impurities form TLS, $n_0 M^2$ should be as small as 10^5 erg/cm^3, which is not the present case. In addition, the temperature variation of SAW attenuation exhibited a shoulder at 10 K which is ascribed to a relaxation of TLS.

In conclusion, keeping these experimental results in mind, we believe that there exists TLS in four-fold coordinated a-Si and a-Ge with a small density as well as two-fold coordinated a-SiO_x and a-GeO_x.[3]

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INFRARED ABSORPTION IN α-Si:H: FIRST OBSERVATION OF GASEOUS MOLECULAR H_2 AND Si-H OVERTONE

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The incorporation of molecular hydrogen in α-Si:H has been speculated[1] and deduced[2,3] from the proton spin-relaxation time near 30K and from thermal calorimetry indicating coversion of orthohydrogen to parahydrogen in solidified hydrogen at T ≈ 0.1 - 3K. We report here the first observations of collision induced infrared absorption of the fundamental vibrational band of molecular hydrogen incorporated in microvoids in heavily hydrogenated amorphous silicon. These results provide the first direct evidence of high pressure gas (~2000 atm.) occluded in α-Si:H. We also report the observation of the overtone absorption spectrum of Si-H bond in α-Si:H indicating that, despite large inhomogenities in the Si-H environment, the anharmonicity of the bottom of the SiH potential well is not substantially modified from the gas phase value. Temperature dependence data indicate that large anisotropic relaxations may be responsible for the high pressure encountered in this material. Preliminary results dealing with the gas/solid phase transition of the trapped H_2 will also be presented.

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BAND MIXING IN GaAs-(AlGa)As HETEROSTRUCTURES

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We report experimental and theoretical results that reveal unexpected behavior of the eigenstates at the energy gap of GaAs-(AlGa)As quantum well heterostructures. In such superlattices, the direction normal to the layers, being the structural "unique axis" is also believed to be the axis of quantization of angular momentum for states near $k=0$. Our experiments are specifically designed to probe this fundamental property as a function of wavevector in the range $0 \lesssim k \lesssim 2\times10^{6}\text{cm}^{-1}$. This is achieved by investigating the polarization of optical transitions between conduction and valence subbands. These experiments show important changes in the components of angular momentum in the ground valence subband. This surprising behavior is analyzed in terms of the effective mass calculations that make use of K.P. perturbation theory.

The samples of special design were fabricated by growing n-type modulation doped GaAs-(AlGa)As multiple quantum wells between two "cladding layers". The waveguide thus created propagates light emitted in the plane of the layers. This allows the measurement of "novel" plasma luminescence with optical polarization along the normal to the planes, as well as "conventional" spectra with in-plane polarization. The capability to measure spectra with normal polarization reveals directly the mixing between $|3/2 \pm 3/2\rangle$ and $|3/2 \pm 1/2\rangle$ states. The absence of hydrogenic exciton structure offers the unique possibility of observing optical transitions from the photon wavevector $\sim 3\times10^{5}\text{cm}^{-1}$ out to the Fermi wavevector of the 2D plasma ($K_F \simeq 2\times10^{6}\text{cm}^{-1}$).

The luminescence spectra measured with optical polarization parallel and normal to the interfaces exhibit drastic differences in relative intensities and in line shapes. This behavior is interpreted in terms of mixing of heavy and light hole character of the ground valence subband. Thus the natural choice of the "unique axis" as being the direction of quantization of angular momentum breaks down. Most surprisingly, we find that for $k \lesssim 3\times10^{5}\text{cm}^{-1}$ there is about 20% mixing, with the heavy hole character dominant. However for $k \sim 2\times10^{6}\text{cm}^{-1}$ a completely mixed $|3/2 \pm 3/2\rangle$ and $|3/2 \pm 1/2\rangle$ character is obtained. This dependence has been estimated within the effective mass approximation. The Luttinger hamiltonian together with a symmetric superlattice potential does not explain the observed 20% mixing although qualitative features are reproduced. Asymmetry in the quantum well potential and final state interactions cause finite mixing at small k. Rough estimates based on these two effects are found to be too small by one order of magnitude to account for the observed mixing. These are the first experimental results to reveal the changing character of the eigenstates of the GaAs-(AlGa)As multiple quantum wells.

HOT ELECTRON RELAXATION AND TRAPPING IN MODULATION-DOPED GaAs-AlGaAs MULTI-QUANTUM WELL HETEROSTRUCTURES

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We have observed the photoluminescence from modulation doped GaAs-AlGaAs multi-quantum well heterostructures grown by molecular beam epitaxy, with time resolution in the picosecond range. Most of the luminescence is strong and intrinsic, and the instantaneous intensity at a given energy can be related directly to the electron density at a corresponding energy. Luminescence decay rates depend then on energy as well as on carrier density, and can be interpreted to give information about 1) carrier energy relaxation rates, 2) transient bandgap renormalization, and 3) carrier trapping. 1) Energy relaxation proceeds most efficiently by LO-phonon emission, but we find that the electron- phonon interaction in our case is significantly reduced: we obtain a scattering time "tau sub zero" of approximately 7 ps, compared with 0.5 ps in bulk GaAs at a similar carrier density.(ref. 1) 2) At high excitation density, the luminescence just below the bandgap shows a rapid (~ 200 ps) decay which we interpret as disappearance of the large (~15 meV) gap renormalization as the carrier density decreases. 3) At low photoexcited carrier density, there is clear evidence of relatively long-lived luminescence from shallow traps. Finally, we find a risetime for luminescence arising from recombination of electrons near the bottom of the lowest subband of about 100 ps, even when only the GaAs quantum wells are excited. A similar risetime was reported in a previous experiment (ref.2), when only the AlGaAs barrier was excited, and it was attributed to carrier transit time in the barrier. This interpretation must now be reexamined.

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PHOTOLUMINESCENCE STUDIES OF LANDAU TRANSITIONS IN GaAs/AlGaAs MULTIPLE QUANTUM WELLS.

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The photoluminescence of n-type modulation-doped GaAs/AlGaAs MQW heterostructures has been studied in the presence of external magnetic fields up to 20T. Spectra were recorded at temperatures of 2K and 70K, using a variety of laser excitation sources, namely 4880A (Ar^+ion), 6328A (He-Ne) and the 8000-8700A range using an Ar^+ pumped tunable IR dye laser.

The main luminescence feature at zero field is due to conduction to valence band (CB → VB) transitions and occurs at approximately 12250cm^{-1} (1.519eV) at 2K and shifts to about 12195cm^{-1} (1.512eV) at 70K. In the presence of a magnetic field this broad feature breaks into discrete components which are attributed to radiative transitions between Landau levels of the conduction and valence bands with $\Delta\ell=0$. These components vary linearly with field.

Significant changes occur when the sample temperature is lowered to T = 2K. Using a swept field technique in the 0 - 6T range the number of Landau transitions observed dramatically increases. The field dependence indicate a 1:3:5... ratio for $\Delta E/\Delta H$. The lines emanate from a common origin at 12165cm^{-1} (1.508eV), which is well below the zero field energy gap in GaAs. This rigid downshift of the electron distribution is probably related to exchange effects. Numerical fitting to the Raman and luminescence Landau data reveal electron and heavy hole masses for these MQW heterostructures of $0.068m_e$ and $0.50m_e$ respectively.

In addition, at higher fields the energies of the lower Landau luminescence transitions deviate from the linear behaviour observed at 70K, with a marked decrease in the slopes. Furthermore the lines split into two strongly circularly polarized components (σ_+ and σ_-) associated with the two spin states in each Landau level. However, the corresponding g-factors are considerably enhanced over the accepted values for bulk GaAs.

Finally, by exciting with a laser energy only a few meV above the Fermi level, it is possible to keep the electron temperature at a minimum. Under these conditions, at the quantum limit, only the lower spin component is observed, and between 1/4 and 1/3 the quantum limit a new step-like anomaly is observed in the transition energy versus field, which we suggest is related to enhanced exchange energy.

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Multiple Quantum Wells **ThP-C4**

HOLE HEATING AND HOLE-PHONON INTERACTION IN MODULATION DOPED 2D HOLE SYSTEM

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We report in this paper the first measurements of the hole distribution function and the hole mobility in a 2D hole system in the presence of an externally applied electric field. Analysis of our data lead to the striking conclusion that the low temperature optical phonon scattering rate for the holes is a factor of 25 larger than that determined earlier [1] for electrons in modulation doped 2D systems. These measurements represent the first direct comparison between hot electron and hot hole behavior and provide a fundamental understanding of carrier-phonon inteactions in this important class of semiconductors.

Our measurements were made on a p-type modulation doped, multiple quantum well GaAs/AlGaAs sample [2] with a low field mobility of 36,000 cm ^{2}/V-sec at 2K. Luminescence and conductivity were measured simultaneously with the lattice at 2K for electric fields up to 300 V/cm applied parallel to the layers. Analysis of these data allowed us to determine the distribution function and the mobility for the 2D holes as a function of electric field. In addition to the striking difference in the hole and electron coupling to the optical phonons, our data show that the hole distribution function is Fermi-Dirac type with the carrier temperature T_C larger than the lattice temperature T_l. For 265 V/cm, T_C has increased to ≈ 50K while hole mobility shows a large decrease. Power input/hole, P, and T_c are found to be related by $P=P_o\exp(-hw_o/kT_o)$ showing that optical phonons of energy hw_o dominate the hole-phonon interaction above 30K. We determine that $P_o \cong 1\times10^{-7}$ Watts/hole, which is equivalent to an effective average scattering time of 0.06 psec. This result is intriguing because similar measurements on 2D electrons yield a much longer effective average scattering time of 1.5 psec.

These results provide important new insight into field induced carrier heating, carrier-phonon interaction and carrier relaxation processes in the modulation doped 2D systems.

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Picosecond Carrier Dynamics in GaAs/$Ga_{1-x}Al_xAs$ Single and Multi Quantum Well Structure

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Picosecond time resolved photoluminescence was examined under various wavelengths, temperatures and external magnetic fields for single and multi quantum well structures by using a picosecond time resolved photon counting technique. The single quantum well structure (SQW) of $Ga_{.7}Al_{.3}As/GaAs/Ga_{.7}Al_{.3}As$ and the multi quantum well structure (MQW) of $(Ga_{.5}Al_{.5}As/GaAs/Ga_{.5}Al_{.5}As)_n$ were obtained by a MBE technique.

Carriers excited in the barrier region are captured in the quantum well in a time less than 100 ps at liq. He temperature. The decay time of the luminescence for SQW is about 100 ps and is much faster than that observed in a bulk crystal (~1 ns) and MQW (~400 ps). An effect of induced emission is neglected in our experimental condition of a single photon counting. The decay time for SQW is independent of the wavelength of the luminescence. However, the decay time for MQW varies with the wavelength. The shorter the wavelength is, the faster the decay time is. We discussed the electron capturing and emission process in the quantum well. We explained our results by an enhancement of the recombination by the localization of carriers in the quantum well and the fluctuation of the well width of MQW. We also report that the decay time of the photoluminescence from the quantum well under the external magnetic field perpendicularly applied to the quantum well is shorter than that observed without the magnetic field. The wavelength of the luminescence under the magnetic field shifts to shorter wavelength. Two dimensional free electrons in the quantum well are localized in a limited region under the magnetic field by the electron cycrotron motion and the electron-hole recombination probability increases by this electron localization. Our experimental results including the temperature dependence of the decay time of the luminescence are well explained by this localization effect. Details of the picosecond dynamics of the photo-excited electron will be discussed in the conference.

SLOW ENERGY RELAXATION OF EXCITONS IN GaAs-AlAs MULTI-QUANTUM-WELL STRUCTURES

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We present for the first time the systematic study on the picosecond energy relaxation processes of excitons in GaAs-AlAs multi-quantum-well (MQW) structures. Dephasing as well as energy relaxation processes of excitons in two-dimensional disorder systems provide one of the most important open problems in semiconductor physics. Excitons in GaAs-AlAs MQW are suitable for this study because of their excellently well-characterized two-dimensional disorder nature. By using a dye laser synchronously pumped by a mode-locked argon laser and a synchroscan streak camera, the energy- and time-resolved luminescence of 1s excitons (n=1, e-hh) in GaAs-AlAs MQW is studied in the picosecond time domain.1) Dynamical population changes of excitons are directly visualized in the energy-time coordinates. Results indicate that excitons lose their energy in the exciton band at the rate of an order of 10^6 eV/s in all the samples whose well thickness ranges from 53 Å to 108 Å . This rate is much slower than the calculated kinetic-energy-loss rate and is ascribed to the disordered nature of the well. In fact the theory developed on the basis of the localized exciton transfer model2) explains the observed energy relaxation rate.3) In addition to the energy relaxation, the dephasing relaxation is studied by means of the non-degenerate four-wave mixing in the frequency domain. The study of the dephasing relaxation is important, because the dephaing relaxation directly reflects the microscopic relaxation mechanism of excitons. The obtained dephaing relaxation time is discussed in connection with the localized exciton transfer model.

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Multiple Quantum Wells **ThP-C7**

Electron - Hole Relaxation and Recombination in GaAs/GaAlAs Quantum-Well Structures from Picosecond Photoluminescence

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We describe time resolved measurements at 10 K of spontaneous emission on a picosecond timescale to study relaxation and recombination of an optically excited electron-hole plasma and of excitons in GaAs/GaAlAs quantum well structures. Optical excitation occurs by picosecond lightpulses from a cw Dye-laser (Rhodamine 6G, emission wavelength 605 nm), which is synchronously pumped by a modelocked Kr-ion laser. For time resolved detection of the luminescence a $LiIO_3$ light gate, a 1m-monochromator and a photomultiplier tube are used. Two different GaAs/GaAlAs quantum well structures were grown by MOVPE with a well thickness of 5 nm. Excitation occurs either directly in the quantum well or in both the quantum well and the GaAlAs barrier layers. In both cases a value of about 750 ps for the exciton life time of the lowest subband is found. This value is much longer than previously reported by others. In case that both the quantum well and the GaAlAs barrier layers are excited, it turns out that reabsorption in the quantum well of luminescence radiation from the barriers dominates the generation of carriers in the subbands of the well.

ThP-C8

INVESTIGATION OF CARRIER DYNAMICS IN AlGaAs/GaAs QUANTUM WELL STRUCTURES BY PICOSECOND LUMINESCENCE SPECTROSCOPY

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Time resolved luminescence spectra of MBE grown single and double quantum well AlGaAs/GaAs heterostructures with different well thickness L_z between 5-15nm have been studied with picosecond time resolution using a synchronously pumped dye laser and a synchroscan streak camera for excitation and recording of the luminescence, respectively. A 0.25m grating monochromator inserted in front of the streak camera serves for spectral selection of the investigated luminescence band. The excitation pulses are almost completely absorbed in the top AlGaAs layer. The experimental data reveal an efficent and fast trapping of the carriers into the quantum wells and a distinct recombination enhancement for carriers in the quantum wells compared to bulk GaAs. The carrier lifetime decreases with well thickness L_z from 1ns for L_z=14nm to 300ps for L_z=5nm, due to the increased overlap of the electron and hole wavefunctions caused by the stronger carrier location.

The transient spectra for different time delays after picosecond pulse excitation display the relaxation of the photoexcited carriers from AlGaAs extended band states into the n=2 and finally n=1 GaAs quantum well states. Remarkable band filling of the quantized states is attainable at the moderate energy of our excitation pulses.

The transient spectra can be fitted on the base of the 2D joint density of states taking into account excitonic enhancement as well as carrier heating. Time resolved luminescence spectra for direct excitation of carriers into the n=1 and n=2 subbands are presently under study.

SILICON SELF-INTERSTITIAL MIGRATION: MULTIPLE PATHS AND CHARGE STATES

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Total energy calculations performed to study the migration of silicon self-interstitials reveal an amazing complexity of migration paths. Si(++) and Si(0) each migrate along more than one path and different paths from each other. Some paths involve interchange with bulk atoms. Electron assisted transport is found to occur for the Si(++) stable tetrahedral site in all directions. Si(0) is found to have several almost degenerate lowest energy configurations. Of these the lowest is a newly discovered "Exchange" configuration which also has the possibility of being a Si(-) (negative) interstitial.

Migration of Interstitials in Silicon

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We calculate total configurational energies for interstitial Aluminum and Silicon in silicon. The calculations, based on the self-consistent Green's function technique, are done for a selective migration path along the "empty" channel in crystalline silicon. Short- and long range structural distortions are found to be sizable and strongly varying along the migration path. Carrier capture is possible along the migration path resulting in a drastic dependence of the migration barrier on the nominal charge state of the defect. For aluminum migration in p-type silicon we find a barrier of $V_B = 1.3 \pm 0.5$eV, which in n-type material can be lowered by $\Delta V_B = 0.8 \pm 0.4$eV due to carrier capture. Both numbers agree well with experiment. Assuming a similar migration path for interstitial silicon the calculated values are $V_B \approx 0.4$eV± 0.5eV and $\Delta V_B \approx 2.0$eV± 0.4eV. In addition, the heat of tetrahedral formation of interstitial Si is evaluated to be $\Delta H_I \approx 4.7$eV.

ATOMIC DIFFUSION IN SILICON*

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This talk will describe results of self-consistent Green's-function total energy calculations which, for the first time, provide a firm theoretical framework for understanding the microscopic mechanisms and paths of atomic diffusion, especially the motion of Si atoms in Si under a variety of experimental conditions.

Si atoms, when dislodged from their normal positions by irradiation, have been found to have a remarkable mobility even at 4 K. This athermal migration contrasts with high-temperature (1200-1400 K) self-diffusion data according to which Si atoms diffuse thermally with an activation energy of about 5 eV. Until now, it has not been possible to achieve detailed microscopic understanding of these two observations or to reconcile the apparent conflict between them. A variety of mechanisms have been proposed to explain the high-temperature data where diffusion is likely to be mediated by thermally created defects, but no consensus has been reached, largely because of the lack of reliable theories and the scarcity of direct experimental evidence. Instead, most arguments in support of particular mechanisms are based on interpretations of related experiments, relying on assumptions about entirely different phenomena.

The new theoretical results reveal a very rich structure and a rather remarkable behavior by the self-interstitial in Si. We find that athermal migration is possible along several paths, predict that self-interstitials mediate self-diffusion by a large variety of paths, and reconcile the low- and high-temperature data by showing that nearly all the thermal activation energy is needed to create interstitials while the migration barriers are very small.

In finer detail, our results are as follows. The interstitial exists in three different charge states and the equilibrium site depends strongly on the charge state. At T=0 K, the interstitial exhibits negative-U behavior in the sense that only ++ and neutral are stable charge states for all positions of the Fermi level. Athermal migration is possible under irradiation conditions because capture or emission of excess carriers lead to a change in charge state and hence to motion to a different site (Bourgoin-Corbett mechanism). At high T, all charge states are created thermally with a formation energy in the range 5-8 eV depending on Fermi-level position), but migration barriers along several paths are surprisingly small (0-0.5 eV). We distinguish between simple paths, traced by a single interstitial, and interstitialcy paths, which involve exchange between interstitial atoms and atoms at normal atomic sites. The latter are necessary for tracer self-diffusion to occur at high temperatures. We find that interstitialcy paths exist and the net activation energy for tracer self-diffusion is within the range of experimental values.

In addition to the self-interstitial, our calculations for the vacancy reveal that the net activation energy for self-diffusion via the vacancy mechanism is also within the range of experimental values. We conclude that both mechanisms contribute to self-diffusion. Finally, the multitude of paths for the interstitial, some of which involve substantial lattice relaxation, account for the observed large entropy of diffusion. The results are also useful in analyzing a variety of other experiments that relate to self-diffusion (the gold-diffusion data, oxidation-induced stacking faults, etc.)

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ThP-D4

REASONANT POLARON EFFECT IN NON-POLAR SEMICONDUCTOR BLACK PHOSPHORUS

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Black phosphorus is an elemental narrow-gap layer-structure semiconductor. The effective masses of carriers have been shown to be considerably anisotropic along the three principal crystal axes [1].

We have measured the far-infrared absorption spectra in n- and p-type single crystals of black phosphorous by using a Michelson interferometer and found several absorption peaks related to shallow donor or acceptor states. Assignment of the peaks is successfully made by calculating energy levels of impurity states based on the effective mass approximation. The excited states are found to be highly anisotropic, reflecting the large mass anisotropy.

We have also found the absorption due to optical phonons at Γ point [2]. When the Zeeman effect of acceptor is investigated, reasonant coupling between the 1s→2p transition and the Γ_3^- (B_{1u}) optical phonon is observed. To our knowledge this is the first observation of the polaron effect in non-polar crystals. In the usual polar crystals, strong Reststrahl absorption prevents observing the reasonant effect in the region where polaron pinning occurs. On the contrary we can observe the reasonant effect distinctly in the entire pinning region, owing to the weakness of phonon absorption because black phosphorus contains no ionic bonds. Therefore it is thought to be one of the most suitable materials for investigating the polaron coupling mechanism. The non-degenerate nature of the valence band edge also makes the theoretical analysis favorable.

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POSITIVELY CHARGED ACCEPTORS WITH $(1s)^3$ AND $(1s)^4$ CONFIGURATIONS

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We have discovered several multilevel acceptors (Ge:Be, Ge:Zn, Ge:Cu) which can bind an extra hole [1]. A fascinating aspect of the triply charged double acceptors and the quadruply charged triple acceptors is that the three or four holes can all simultaneously occupy the single particle ground state orbital. Because of the fourfold degenerate top of the valence band of Si and Ge, we can model acceptors with pseudo atoms having 3/2 spin electrons. The Pauli principle allows in this case up to four particles in a (1s) orbital.

Positively charged beryllium double acceptors in germanium (Ge:Be$^+$) have been observed at temperatures < 3.5 K in single crystal samples of Ge:Be ($7 \times 7 \times 3$ mm^3, $[Be] \approx 10^{15}$ cm^{-3}). The samples are irradiated with broad band continuous black body radiation which leads to single ionization of Be acceptors ($Be^0 \rightarrow Be^-$). Some of the free holes are trapped by neutral beryllium leading to Be$^+$. The very shallow Be$^+$ centers are detected using photoconductivity and a far infrared Fourier transform spectrometer. The Be$^+$ spectrum shows a continuum with a sharp onset at $\nu \approx 40$ cm^{-1} (~ 5 meV). The following experimental findings show that the shallow center is unambiguously due to positively charged beryllium acceptors. i) When the photon energy range was limited with cold filters ($T < 3.5$ K) to $E < 6.25$ meV so that neither shallow acceptors nor beryllium acceptors could be ionized to produce free holes, no Be$^+$ could be observed; ii) when the same filters were used warm ($T \approx 300$ K), Be$^+$ reappears because the black body radiation ionizes shallow and deep acceptors; and iii) when a uniaxial stress is applied along [111] the Be$^+$ centers disappear because the fourfold degeneracy at the top of the valence band is lifted and acceptors can no longer be described with pseudo atoms with spin 3/2 electrons.

Calculations using different approaches [2,3] verify that in germanium the third hole binds to a neutral beryllium double acceptor as well as the fourth hole to a neutral copper triple acceptor. The theoretical results are in good agreement with the experimental data.

A further interesting phenomenon is the extraordinary strength of absorptions in the Be$^+$ continuum which are caused by ground state to bound excited state transitions of shallow residual acceptors inside the Ge:Be samples. A simple estimate using doped single crystals as absorbers in front of the Ge:Be samples and comparing the absorption peaks from shallow levels in these samples with the internally caused absorptions leads to effective absorption cross sections which are one to two orders of magnitude larger for the internal acceptors than the values determined by transmission experiments. Mechanisms which may lead to the strongly enhanced absorption will be discussed.

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BOUND EXCITON AND BOUND-DOUBLE-EXCITON COMPLEX IN ZINC DOPED GERMANIUM

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Time-resolved far-infrared (FIR) magneto-absorption measurement is combined with near-band-gap photoluminescence (PL) to explore the unique excitonic problem in "compensation free" zinc-doped germanium crystals. Investigation in three specially grown crystals, with $N_A = 10^{14} - 10^{16}$ cm^{-3}, led to unexpected new features about the exciton binding by zinc, a rarely treated double acceptor

(1) Existence of a bound exciton (BE), an exciton bound to a neutral double acceptor, is confirmed in both PL and FIR magneto-absorption. So far we have only one report on a double acceptor BE in GaSb with unidentified acceptors and no reports in Ge or Si.[1] Our double acceptor BE has an electron loosely bound to an A^+ center, that consists of a doubly ionized acceptor plus three holes. This donor-like structure gives spectra of FIR magneto-absorption similar to $1s \rightarrow 2p_\pm$ absorption spectra of a shallow donor
(2) A bound-double-exciton complex (BDEC), two excitons bound to a neutral double acceptor, is first identified in PL measurement. This new complex has four holes and two electrons in the surroundings of a doubly ionized acceptor. The BDEC center in Zn doped Ge is quite unique, since the first hole shell is closed by all of the four holes according to the shell model of a bound multi-exciton complex proposed by Kirczenow.[2] The surprisingly high relative PL intensity of BDEC may be explained by the so much stability owing to the just closed hole shell structure.
(3) Time-resolved FIR magneto-absorption measurement of BE and a free exciton was performed. We obtained, at 4.2 K, the lifetime of BE to be 0.75 μs and the capture cross-section of an exciton to a neutral acceptor 1.2×10^{-15} cm^2.
(4) The dissociation energies of BE and BDEC are so determined as to be 5.7 and 3.2 meV, respectively. The deepness of Zn acceptor is responsible for such a large dissociation energy of BE. It even causes reversal of order in energy between BE and BDEC as compared with the bound multi-exciton complex in Si.
(5) The ionization energy of BE to make an A^+ center is estimated to be 5.4 meV, while the binding energy of a hole to a neutral acceptor, or the hole affinity to make an A^+ center, to be 4.5 meV.

Dependence of excitation intensity on PL intensity and FIR magneto-absorption intensity confirms the assignment of BE and BDEC. BDEC has not been observed in FIR absorption hitherto. Further important features to be presented and discussed will be the PL observation of BDEC in magnetic fields.

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ThP-D7

MAGNETOOPTICAL STUDY OF SHALLOW DONORS IN InSb UNDER HIGH PRESSURES

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Five intra-impurity transitions between the states associated with the lowest Landau level were studied as a function of magnetic fields up to 19T and hydrostatic pressures up to 1.4GPa in pure n-InSb samples. The observations were performed by photoconductivity measurements in the 5cm^{-1}-50cm^{-1} spectral region using optically pumped infrared lasers and a Fourier spectrometer. Three of the transitions involving the /000/ ground state reveal a distinct central cell structure /chemical shift/, the remaining two are between the excited states. As the latter transitions have no central cell structure they may be used to test the theoretical calculations for a screened Coulomb potential within the effective mass method. This, in turn yields the theoretical values for the transitions involving the ground state and thus enables us to determine the chemical shifts for the observed donors. A comparison with recent theoretical calculations of Trzeciakowski et al. /this conference/ shows excellent agreement, allowing to determine the pressure- and magnetic field variation of the static dielectric function as well as the matrix elements of the localized potential which causes the observed chemical shifts.

S-LIKE EXCITED STATES OF THE 78-meV ACCEPTOR IN GaAs*

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Recently there has been much interest in determining the origin of the 78-meV acceptor which occurs in liquid encapsulated Czochralski (LEC) GaAs grown from a Ga rich melt. A determination of the valence of this acceptor would aid in understanding its nature. We observed two excited states of this level in two different samples using techniques sensitive to the detection of *s*-like excited states: selective excitation luminescence (SEL)and electronic Raman scattering (ERS). These techniques involve using a tunable dye laser as a source of below bad gap light for sample illumination, and the observation of the resultant luminescence in energy loss. They complement each other since the former can detect acceptor excited states in compensated material, while the latter works with *p*-type material. The SEL experiment revealed excited states with excitation energies of 62.5 meV and 66.5 meV above the ground state, while the ERS experiment gave values of 62.9 meV and 66.9 meV. By comparing the data with spectra from other acceptors measured by these techniques, we deduce that both of these levels are probably due to transitions from the ground state of the acceptor to *s*-like final states. Calculations based on a simple model predict a splitting of the first *s*-like excited state of a double acceptor in GaAs to be 2.6 meV. We therefore conclude that these two levels could correspond to transitions from the $1s^2$ ground state to the split $1s^1 2s^1$ excited state of a double acceptor.

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A NOVEL NEAR-INFRARED VIBRONIC SERIES IN IRRADIATED SILICON

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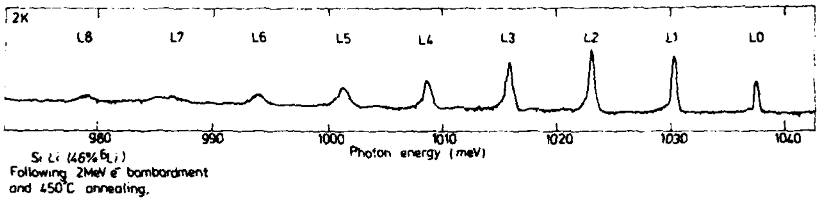
Despite the important technological discovery by Vavilov et al (1) in the early 1960's that lithium impurity could "deactivate" radiation damage in silicon, it is only in the last 3 years that significant progress has been made in developing specific models for the Li-associated complexes responsible.
It is now known, for example, that 4 Li atoms complex with an isolated vacancy to form a C_{3v} molecular isoelectronic trap (2). However the microscopic nature of the Li-divacancy, Li-Si_I interactions and so on have not yet been established. Detailed studies of the lithium-saturated vacancy have been made possible by the sharp zero phonon line structure of its associated 1.045 eV vibronic band (3). When this band disappears upon heat treatments at $\sim$450^{o} C a variety of new luminescence features emerge, including the unusual vibronic series L0-L8 shown below, with a zero phonon line at 1037.3 ± 0.1 meV.



Si Li (46% ^{6}Li)
Following 2MeV e^- bombardment
and 450°C annealing.

Whereas most vibronic bands in irradiated Si exhibit appreciable coupling to a wide range of phonon energies, it can be seen that at 2 K this band only contains a quantum of $\sim$7 meV. In addition, the luminescence system shown above exhibits other unusual properties.
All the relatively sharp features shift to higher energy when samples are doped with ^{6}Li rather than ^{7}Li. i.e. they exhibit a NEGATIVE ISOTOPE SHIFT. We thus have the comparitively rare situation where mode softening is predominantly in the ground state of the electronic transition. The magnitude of this isotope shift is appreciable for the zero phonon line (0.5 ± 0.1 meV). In contrast the vibrational quantum is almost independent of the Li isotope, being typically about 1% larger for the lighter isotope.
For a given isotope the phonon frequencies increase along the vibronic series. For example, from 7.10 ± 0.06 meV for n=1 to 7.32 ± 0.06 meV for n=6, where n is the number of phonons created and the frequencies correspond to ^{7}Li spectra at 2 K. i.e. the vibrational potential, at least initially, HARDENS with increasing n.
Despite the steady increase in halfwidth towards lower energies, phonon replicas to n=11 have been observed, providing an unusually convenient set of phonon-assisted features for study with uniaxial stress and Zeeman perturbations.

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QUANTUM HALL EFFECT: FRACTIONAL QUANTIZATION

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The quantum Hall effect refers to the new physical phenomena recently discovered in the transport of two-dimensional (2D) charged carriers, realized in semiconductors, in the presence of a quantizing magnetic field. It is characterized by the experimental fact that the Hall conductance is quantized to $G_H = ie^2/h$, where e is the electronic charge, h is Planck's constant, and i, the quantum number, are odd-denominator fractions as well as integers. In the case of integral quantization, i are integers identified with the number of filled Landau levels. The quantization results from the existence of localized states in the energy gap, separating the empty from the filled Landau levels, which gives rise to a dissipationless current-carrying state when E_F is in the localized region. This effect has now been seen in several well defined 2D systems. The fractional quantization, on the other hand, is observable only in extremely high mobility 2D systems in the extreme quantum limit, when the lowest Landau levels are fractionally occupied. To date, i = 1/3, 2/3, 4/3, 5/3, 1/5, 2/5, 3/5, 2/7, 3/7, and 4/7 have been observed and they are identified, respectively, with the fractional fillings of the Landau levels. The effect represents the first unambiguous, experimental observation of a fractional quantum number in physics. It is presently explained as resulting from the formation of a highly correlated electron fluid, which is separated by an energy gap from its fractionally charged excitations. This talk will review recent experimental developments with an emphasis on the fractional effect from work on GaAs-$Al_xGa_{1-x}As$ heterojunction thin-films structures.

THEORY OF THE FRACTIONAL QUANTUM HALL EFFECT

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The Fractional Quantum Hall Effect is caused by the formation of a new type of electron condensate when a 2-d electron system is placed in a strong *magnetic field. My theory describes* this condensate with the variational ground state wavefunction

$$\Psi_m = \prod_{j<k}^{N} (z_j - z_k)^m \; e^{-\frac{1}{4}\sum_{\ell}^{N} |z_\ell|^2} \quad ,$$

where $z_j = x_j - iy_j$ is the location of the j^{th} electron expressed as a complex number, m is an odd integer, and the magnetic length $(\hbar c/eH_0)^{1/2}$, with H_0 the magnetic field strength, is taken to be 1. Ψ_m is a liquid of electrons locked in a density $\sigma_m = (2\pi m\, a_0^2)^{-1}$. The elementary excitations of Ψ_m, the quasielectrons and quasiholes, are made with a thought experiment in which the liquid is pierced at some location with an infinitely thin magnetic solenoid through which is adiabatically passed a flux quantum $\Delta\phi = hc/e$. The solenoid is then removed by a gauge transformation, leaving behind an exact excited state of the many-body Hamiltonian. These excitations are *particles carrying electric charge ±e/m*. They behave physically like electrons of charge e/m confined to their lowest Landau level. My theory proposes approximate wavefunctions for these particles of the form

$$S_{z_0} \Psi_m = e^{-\frac{1}{4}\sum_{\ell} |z_\ell|^2} \prod_{i}^{N} (z_i - z_0) \prod_{j<k}^{N} (z_j - z_k)^m \quad ,$$

and

$$S_{z_0}^{\dagger} \Psi_m = e^{-\frac{1}{4}\sum_{\ell} |z_\ell|^2} \prod_{i}^{N} \left(2 \frac{\partial}{\partial z_i} - z_0^{*}\right) \prod_{j<k}^{N} (z_j - z_k)^m \quad ,$$

for a quasihole and quasielectron, respectively, *residing at* z_0.

SURFACE VIBRATIONAL STUDIES OF CHEMISORPTION ON SILICON

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In the past few years the semiconductor research has been much enriched by the extensive use of several surface-sensitive techniques. There are, however, only very few examples of the use of surface vibrational spectroscopy which is one of the most powerful probes of chemisorption processes. We present here the first vibrational studies of interface formation between silicon and a simple metal, together with similar studies of the highly unusual properties of chemisorbed benzene on cleaved Si(111). Thin (0.5 - 1 monolayer) Al overlayers deposited on Si(111)7x7 surfaces were studied with the high-resolution surface electron loss spectrometer of the CRISS facility at Montana State University. We found that the Al deposition on room-temperature Si does <u>not</u> remove the Drude-like tail of the Si(111)7x7 vibrational spectrum which is removed by other adsorbates, e.g. hydrogen. The Drude-like tail is instead removed from the Si-Al spectrum by annealing which also produces one of the following LEED patterns: pseudo-7x7, 1x1 and $\sqrt{3}\times\sqrt{3}$-R30°. The different patterns correspond to different positions of the main vibrational peak of the Si-Al spectrum in the region 50-70 meV. We shall discuss the implications of these results on (i) the metallic or non-metallic character of the surface, and the consequences on the models for Fermi-level pinning at the Si-Al interface, and (ii) the chemisorption geometry and in particular the possibility that different chemisorption geometries correspond to the different LEED patterns. The experiments on benzene clarified the origin of a <u>five</u> orders of magnitude difference in the sticking coefficient between cleaved Si(111) and other Si, Ge and GaAs surfaces. In particular, we found evidence for establishment of Si-C bonds and ruled out a "flat" chemisorption geometry.

SURFACE ELECTRONIC STRUCTURE CHANGE BY Cs ADSORPTION ON Si(111)2x1*

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We have observed in photoemission spectra that the intrinsic surface states of Si(111)2x1 are still present after one monolayer Cs adsorption. Similar behavior of empty surface states was reported in the case of Pd adsorption on GaAs(110) with partial yield measurements$^{1)}$, but the survival of the clean surface states is considered to be due to the peculiar structure of the GaAs(110) surface. On almost all the semiconductor surfaces transition and noble metal overlayers remove intrinsic surface states entirely. The present case is not due to structural characteristics but due to a peculiar nature of the chemisorption. The study employs photoelectron spectroscopy of the valence band and core levels with synchrotron radiation. Angle-integrated photoemission spectra have been measured with increasing Cs coverage up to one monolayer at room temperature. We find in the difference spectra of the valence band region that (1) a new peak (-0.4 eV) due to Cs 6s electrons appears at about a half of the saturation coverage and its intensity increases with increasing the coverage, and (2) the intrinsic surface states of Si(111) 2x1 at -0.8 eV are still present even at the saturation coverage with a small shift (0.3 eV) toward higher binding energies and the Fermi level is pinned at the empty surface states of Si. From these findings we conclude that (1) at about 50% of the saturation coverage the insulator-metal transition takes place in the Cs monolayer, and (2) after the transition the Cs metal interacts with Si weakly and the Cs monolayer lie on the Si surface without covalent bond formation. The adsorption energy is originated from dipole attraction between partially ionized Cs monolayer and partially negative charged surface Si atoms.

* The experiments were performed at BL-2 of the SOR-RING at the Institute for Solid State physics, The University of Tokyo.

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Adsorption on Surfaces **FrA-A3**

GaAs(110) + Sb,p(1x1): AN ADATOM CASE STUDY OF ADSORPTION ON COMPOUND SEMICONDUCTOR SURFACES

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The problem with determining the behavior of adatoms on compound semiconductor surfaces is approached by selecting a model system for detailed studies. *Sb on cleaved GaAs(110) is chosen* because well ordered epitaxial layers form at room temperature and several related experiments have been performed, e.g., LEED. A broad spectrum synchrotron photoemission study has been performed at the Wisconsin Synchrotron Radiation Center. The study included polarization-dependent angle-resolved measurements of the interband transitions, high-resolution core level shift analysis, and photoelectron diffraction measurements. The new valence features that are induced by the Sb adsorption are subtle, not being present in all spectra. However, several features are observed in different portions of the surface Brillouin zone, including emission features attributed to the lone pairs formed on the surface of the Sb overlayers. Several other valence band effects are observed: 1) the extinction of surface states, 2) the extinction of specific substrate interband transitions, and 3) most significantly, shifts in the substrate interband transition energies. The shifts have different magnitudes for different values of the perpendicular wave vector. The latter means that the bands do not uniformly shift in the band bending observed for Ge overlayers on GaAs(110), and this study suggests that the phenomenon is rather general. High-resolution studies (total experimental resolution of approximately 125 meV) of the Sb 4d, Ga 3d, and As 3d were performed at various coverages and were analyzed with a peak fitting program. *The results show a single, narrow pair of spin orbit lines for a thick Sb layer and two* pairs of Sb lines at the monolayer level. This result directly infers that there are two kinds of Sb sites on the surface, which is consistent with overlayer models suggested by detailed LEED analysis. The coverage-dependent data show that the two kinds of Sb sites exist at very low coverages. The As line, on the other hand, for the cleaved surface shows the well known shift corresponding to emission from surface atoms. This shift disappears after absorption of Sb, indicating that the bonds of the As atoms at the interface are essentially like the bulk As bonds. The observation of a single type of As atom is consistent with the suggestion that the surface relaxation found in the clean surface is healed by adatom Sb overlayers. Measurable photoelectron diffraction features are observed and their complex nature characterized. Model calculations for these systems are currently in progress.

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Adsorption on Surfaces **FrA-A4**

CHEMISORPTION OF Ag, Cu AND Au ON Si(111) and Ge(111) SURFACES

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A systematic study on the chemisorptions of Ag, Cu and Au on Si(111) and Ge(111) is of both practical and fundamental importance, since the results obtained might give some insight to the understanding of the nature of binding, the electronic states and the noble metal/elemental semiconductor interfaces. (1)

In the present work, the noble metal chemisorptions on elemental semiconductors are studied using the cluster model and the charge self-consistent extended Huckel method (EHT). The results obtained can be compared with the experimental work for low coverages (Ø<<1). The adsorbed site is determined by minimizing the total energy of the cluster. It is found from the present work that all three metals adsorb on the threefold hollow site of both Si(111) and Ge(111) surfaces. For Ag and Cu, the most stable sites lie below the surface which agree qualitatively with recent experimental results given by SEXAFS and ISS. It is quite possible that the interface formed is not abrupt. For Au/Si(111), there exist more than one stable site underneath the surface; this might account for the fact that there exist more than one type of gold silicide. From the local density of states obtained, it can be seen that the d states of noble metals are very much localized and the interfacial states are formed by d states of noble metals and the p_z and s states of silicon. The binding is very weak between Ag and the silicon, stronger for Cu, whereas the binding between Au and the silicon substrate is the strongest.

For noble metals on Ge(111), stable positions below the surface are also found, therefore no abrupt junctions can be formed either. However, for Au on Ge(111), only one position of energy minimum is found which is different from that for Au/Si(111). From the local density of states obtained, the binding between Au and Ge substrate is found to be strongest, the binding of Ag seems to be stronger than that of Cu, whether this is true or not remains to be proved by experiments.

The surface reconstructions of Si(111) and Ge(111) have not been taken into account throughout the calculation. Since chemisorption usually tends to reduce the reconstruction, the result obtained for non-reconstructed surfaces might be used as a qualitative guide for understanding the interfaces.

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17th International Conference on the Physics of Semiconductors

Adsorption on Surfaces **FrA-A5**

LASER INDUCED CHEMICAL REACTIONS AT THE Al-III-V SEMICONDUCTOR INTERFACE

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We have used pulsed laser annealing to produce highly localized chemical reactions at the interface between Al and various III-V compound semiconductors, resulting in contacts with strongly modified chemical and electronic properties. We have used Auger electron spectroscopy (AES) and soft x-ray photoelectron spectroscopy (SXPS) to monitor atomic movements and changes in chemical bonding configuration at successive stages of these laser-enhanced reactions on a microscopic scale as well as the chemical structure of the extended interfaces. We have found that in all cases a finite range of laser energy densities exists such that the chemical reaction is promoted without disrupting the surface morphology. In our experiment, 20-50 Å thick Al layers were evaporated onto (110) surfaces cleaved in ultrahigh vacuum and exposed to the light of a XeCl excimer laser (305 nm wavelength, 5nsec pulse duration) in the same vacuum. Energy densities up to 0.7 J/cm^2 per pulse were applied. The Al-semiconductor interface shows some evidence for chemical reaction and diffusion prior to annealing,[1,2] but this reaction is localized to within a few monolayers. During the annealing, in all semiconductors investigated (GaP, GaAs, GaSb, InP, InAs, InSb) the Al overlayer can be converted completely from a metallic bonded to a covalent bonded state, as indicated by a Al2p core level shift of 1.2 eV and a shift of the Al-LVV-Auger electron energy by 4 eV. Simultaneously, Al diffuses into the bulk of the semiconductor, the cation segregates to the surface but, in contrast to other annealing studies, no significant amount of anion is lost. Each of the materials exhibits a characteristic energy density threshold for the reaction ranging from .12 J/cm^2 for InSb to .26 J/cm^2 for GaP. This threshold fits extremely well to a linear correlation with the semiconductor heat of fusion, as opposed to a weak or anticorrelation with the semiconductor of heat formation or the heat of reaction associated with formation of metal anion compounds. Analogous to qualitative threshold studies for laser annealing of metals on Si,[3] these threshold correlations for Al on III-V compounds suggest that the activation barrier for an extended reaction can be overcome by the simultaneous melting of the overlayer and the substrate and that the chemical reaction mainly proceeds in the molten phase of the substrate. Since the melt depth during laser annealing can be varied very accurately, the reaction can be controlled to produce new, ultrathin compound layers with new dielectric properties. As an example for the case of Al on InP, we have found that this laser-reacted interlayer alters the electrical behavior of a metal semiconductor contact quite significantly: Al on UHV-cleaved InP-surfaces form quasi ohmic contacts, and laser annealing of the InP UHV-substrate does not alter this behavior. In contrast, the system Al- (laser-reacted Al-InP) - InP exhibits a rectifying contact with an effective barrier height of .55 eV. Thus chemical reactions promoted and localized near the microscopic metal-semiconductor interface by pulsed laser annealing can be used to modify and control the chemical and electronic properties of metal-compound semiconductor interfaces in well-characterized stages.

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CALCULATION OF OPTICAL GAPS IN SILICON WITH A SCREEENED EXCHANGE APPROACH

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Many approaches for calculating excitation energies in semiconductors are currently being investigated by various groups. It is conceptually and computationally simplest to remain close to a one particle picture. Phillips proposed a generalization of Koopman's theorem where the most important contribution to the quasiparticle energy corresponds to replacement of the exchange operator in Hartree-Fock by a dynamically screened exchange operator.[1] The quasiparticle energies are given by the eigenvalues of the screened exchange Hamiltonian, within the approximation that relaxation effects are negligible. Neglecting local field effects and using a static approximation for the screening, this is equivalent to considering the electron self energy in the screened exchange and Coulomb hole approximation[2] since the Coulomb hole contribution then gives a constant shift in the band energies. Our approach follows along the lines discussed by Kane who calculated matrix elements of the self energy operator in this approximation using empirical pseudopotential wavefunctions.[3] We use wavefunctions calculated self-consistently in the density functional formalism with the ab initio pseudopotential to calculate the screened exchange operator where screening for a semiconductor is included by use of the Levine-Louie dielectric function. These same wavefunctions are used to expand the quasiparticle wavefunctions and compute matrix elements of the screened exchange Hamiltonian. We find that off diagonal matrix elements are negligible at symmetry points which shows that the density functional wavefunctions give a good approxmation to the quasiparticle wavefunctions. The resulting quasiparticle energies are then easily obtained from the diagonal matrix elements. As suggested by others, we find that even with the approximation of static screening, the direct gaps calculated with this approach agree better with experiment than the usual density functional calculation for the prototypical semiconductor Si. However, the indirect gap is not improved. This and the band dispersions may depend on physical effects not included here. The effect of dynamical screening can be included by extension of the present work.

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EXCHANGE-CORRELATION POTENTIAL FOR ONE-ELECTRON EXCITATIONS IN A SEMICONDUCTOR

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Recently, new arguments have been given[1] why the local-density approximation (LDA) for the exchange-correlation potential underestimates the band gap of non-metals. One approach, suggested to rectify this situation[2], obtained the one-electron excitations from the Dyson equation within the homogeneous electron gas limit, empirically introducing a gap in the single-particle spectrum and the screened Coulomb interaction. We present a) a quantitative calculation of the electronic quasiparticle states for Si within the time-dependent screened HF approximation, which aims at a first-principle understanding of single-particle excitations in a proto-type semiconductor and b) an analytical, energy- and local-density ($\rho^{1/3}$-) dependent model for the self-energy of non-metals in general, which is found to work with reasonable accuracy both in semiconductors (Si, GaAs) and insulators (C, LiF, MgO). In the numerical work we have employed, for the first time, a dynamical screened Coulomb interaction which fully takes into account the charge inhomogeneities due to tetrahedral bonding as well as local-field and excitonic many-body effects. The dynamical correlation is found to be predominantly local in r-space and to scale with energy away from the gap. Band gaps, band widths and quasiparticle damping times are in very good accord with experiment.

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1s CORE SHIFTS AND THE GAP OF TETRAHEDRAL SEMICONDUCTORS.

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Relativistic effects result in a significant downward shift of the 1s core level even for moderately light elements (137 eV for Z=33). Due to orthogonality, the higher s-states are also shifted down (although by smaller amounts), while the averages of p- and d- doublets remain almost unchanged. The s-p energy difference is thus increased within a given principal quantum number in the atom, and the direct gap is decreased in s-p bonded tetrahedra semiconductors, as compared to non-relativistic values. Representative results for GaAs (from first principles, using the local-density approximation) confirm this picture and giv some useful insight in the nature of the energy gap. They also suggest that future tests of improved exchange-correlation functionals /1/ should treat core electrons in a consistent fashion, since the 1s states are mostly affected by the existing improvements over the straight LDA /2/

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17th International Conference on the Physics of Semiconductors

Electronic States : Theory FrA-B4 Invited

THEORY OF STRUCTURAL PROPERTIES OF ELEMENTAL SEMICONDUCTORS

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We demonstrate that not only the static structural properties but also the crystal stability, pressure-induced phase transitions, and lattice dynamics in crystals can be accurately described using an ab initio pseudopotential method within the local-density-functional formalism. Using atomic numbers of constituent elements and a subset of crystal structures as the only input information, the calculated structural properties of Si, Ge, and C are in excellent agreement with experiment.

Breakdown of the Quantum Hall Effect

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ABSTRACT

We wish to report our experimental results on the breakdown of the quantum Hall effect in GaAs-$Al_xGa_{1-x}As$ heterostructures, obtained from several samples at temperatures from 6 to 0.5 K and in magnetic fields up to 28 T. The breakdown manifests in the onset of dissipation, which shows sudden onsets in some samples but gradual in others. In the case of a sudden onset, the current at which dissipation occurs is the same for the $i = 1,2$ and 4 Hall plateaus. This critical current, being sample dependent, is approximately two orders of magnitude lower than that expected from breakdown through Zener tunneling [1]. However, it is suggestive of a phonon emission mechanism, where dissipation results from the onset of the emission of phonons when the electron drift velocity exceeds the sound velocity in GaAs.

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ENERGY DISSIPATION PROCESSES IN THE QUANTUM HALL REGIME

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From the theoretical point of view, the quantized Hall effect (QHE) is characterized by a dissipationless Hall current. This condition is not realized experimentally:

a) All QHE-experiments are based on measurements on devices with Hall geometry. The boundary conditions (equipotential lines at the source and drain contacts) lead to singularities in the current distribution and to an energy dissipation of $R_H I^2$ (R_H = quantized Hall resistance, I = source-drain current). Experiments on GaAs-$Al_xGa_{1-x}As$ heterostructures demonstrate that hot electrons can easily be generated close to the drain and source contacts, connected with the emission of CR radiation. Measurements on devices with Corbino geometry (which are not useful for QHE experiments) do not show this "heating" effects.

b) A finite energy dissipation in QHE-experiments is found even in measurements on Corbino devices. The corresponding scattering processes depend on temperature and current density. The electronic system becomes unstable at a critical Hall field.

The analysis of the experiments on high-quality silicon MOS devices (μ > 20 000 cm^2/Vs) demonstrate that some of the energy gaps in the Landau level spectrum, which determine the amount of thermally excited carriers in QHE-experiments, show an anomalous magnetic field dependence, which may be connected with the formation of a new groundstate.

QUANTUM - HALL EFFECT EXPERIMENTS ON A SUB - MICROSECOND TIME SCALE

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A sharp transition from the quantized Hall resistance state to the classical one can be induced in $GaAs/Al_{0.3}Ga_{0.7}As$ by the application of currents of the order of 0.1-1 mA. It is sharpest when the Fermi level is midway between two Landau levels. A detailed study of this phenomenon is of great interest for the general understanding of transport processes related to the quantum Hall effect as well as for the application of two-dimensional electronic systems, e.g. as far - infrared emission sources or as switching devices.

We report experiments with electrical pulses on a sub-μs time scale as well as in tilted magnetic field orientations. Previous pulsed experiments in the Hall plateau regime were limited to rise times of about 100 μs due to the high dynamical resistance of the potential probes ($\sim 25.8\ k\Omega/i$) and by parallel capacitances. This can be circumvented by using a two-terminal contact arrangement. Then the current-voltage characteristic consists of a superposition of the characteristic of the longitudinal voltage drop ($\propto \rho_{xx}$) and the Hall voltage ($\propto \rho_{xy}$) [1,2].

This allowed us to perform measurements 200 ns after the begin of the electrical pulses. On a sample with $n=2\times10^{11}\ cm^{-2}$ and $\mu(4.2K)=100\ 000\ cm^2/Vs$ the following results were obtained (i=2 plateau):

(1) At low currents ($\leq 5\mu A$) the Hall voltage shows no time dependence down to 200 ns.

(2) The transition from the quantized to the classical state occurs on a time scale shorter than 200 ns after the begin of the pulse.

(3) Tilted magnetic field geometry: (a) The critical current for the transition is independent of the tilt angle θ between B and the normal to the interface. (The plateaus are shifted to higher field according to $B_{\bullet}\cos\theta$),

(b) When changing the polarity of the current or the magnetic field no asymmetry of the current-voltage characteristic particularly also in the transition region is observed. (In the tilted geometry there is also a component of the Lorenz force perpendicular to the interface).

Results (1) means that delocalisation |3| around the maximum of the density of states in the Landau level occurs - if at all - faster than 200 ns. Results (2) and (3) show that the electron gas behaves purely two-dimensional in the transition region. There are particularly no traps involved whose concentration is usually different on the two sides of the interface. Possible mechanism responsible for the transition will be discussed.

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LENGTH SCALES AND THE QUANTISED HALL EFFECT

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We have extended earlier measurements (1) on the frequency dependence of the quantised Hall resistance in Silicon inversion layers to higher frequencies and magnetic fields. The frequencies reduce the transport length scale to less than ~ 1000Å resulting in a collapse of the role of localisation on the quantisation. The plateaus disappear to be replaced by peaks and we report on the competition between the length scale and the disorder.

We discuss the role of the electron interaction, which becomes important as the length scale is reduced. Results are presented showing the appearance of fractional quantisation when the disorder has little influence. Finally, we discuss the self-consistency of disorder and interactions in giving fractional and integer plateaus and the circumstances governing the conversion of the plateaus into peaks.

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Quantized Hall Effect **FrA-C5**

TEMPERATURE DEPENDENCE OF 1/3 and 2/3 FRACTIONAL QUANTUM HALL EFFECT IN GaAs/AlGaAs HETEROSTRUCTURES

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The fractional quantum Hall effect observed in two-dimensional (2D) electron system is one of the most attractive topics at present.

We have investigated ρ_{xx} and ρ_{xy} of a 2D electron system formed at a GaAs/AlGaAs heterojunction interface when the Fermi level lies in the lowest Landau level, i.e. $\nu < 1$ where ν is the filling factor of Landau levels. The sample used is a modulation-doped GaAs/AlGaAs heterostructures grown by molecular beam epitaxy and has high mobility of 1.1×10^6 cm^2/V·s and electron density of 1.2×10^{11} cm^{-2}. Measurements have been done in a magnetic field (B) up to 15.5 T and at tempeartures between 1.0 K and 0.1 K using dilution refregirator.

The activation behaviour of ρ_{xx} was observed at both 1/3 and 2/3 fractional occupation of the lowest Landau level in a single sample. The activation energy (W) at $\nu = 1/3$ or at B = 14.6 T, which was determined by observing ρ_{xx} minimum, is W(1/3) = 2.7 K and that at $\nu = 2/3$ or at B = 7.45 T is W(2/3) = 0.93 K. This result shows us an important fact that the energy gap at $\nu = 1/3$ and $\nu = 2/3$ are not identical. In other words, there is no symmetry in the electronic states at $\nu = 1/3$ and those at $\nu = 2/3$. The activation energy W(1/3) is in good agreement with theoretical prediction of 4 K at 15 T by Yoshioka, Halperin and Lee[1] and Laughlin[2]. The activation energy W(2/3) is close to the value 0.83 K observed at 9.25 T by Chang et al [3].

We also observed the ν-dependence of the activation energy at around $\nu = 1/3$ and $\nu = 2/3$. The results around $\nu = 2/3$ show a symmetric behaviour similar to that reported by Chang et al. [3]. However, the activation energy around $\nu = 1/3$ behaves not symmetric against ν. In the region $\nu > 1/3$, W(ν) decreases with the increase in ν in a similar rate as that around $\nu = 2/3$. However, in the region $\nu < 1/3$, W(ν) decreases with the decrease in ν more steeply.

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FRACTIONAL QUANTUM HALL EFFECT IN 2D-ELECTRON SYSTEM OF Si (001) MOS STRUCTURE

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Quantization of the Hall resistance ρ_{xy} and diagonal resistivity ρ_{xx} of 2D electron system of Si(001) MOS structure under magnetic field B=8 ÷ 11T and T=1.7K has been investigated (electron mobility in inversion layer was about $4 \cdot 10^4$ V/cm·sec). The peculiarities in the dependencies of $\rho_{xy}(V_g)$ and $\rho_{xx}(V_g)$ on the gate voltage V_g at rational fractional filling factors ν have been observed, namely at ν equal: 2/3, 4/3, 5/3, 7/3, 8/3, 6/5, 7/5 (see Figure). These observations indicate on appearance of additional gaps in the energy spectrum at fractional filling factors in 2D electron system of Si MOS structure. Speculations about origin of these gaps are discussed.

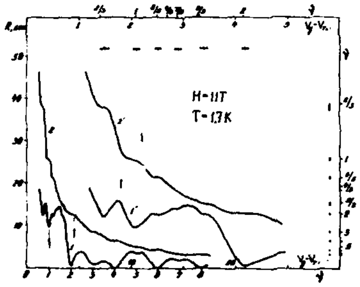

Figure
The dependences of ρ_{xy} (curves 2 and 2') and ρ_{xx} (curves 1 and 1') on the gate voltage V_g at H=11T and T=1.7K. The vertical scale for curves 1 and 1' is gained by factor two.

17th International Conference on the Physics of Semiconductors

Deep Level Impurities **FrA-D1** **Invited**

MUONIUM IMPURITY CENTERS IN SEMICONDUCTORS

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Although microscopic information about hydrogen impurity centers in crystalline semiconductors is rare, a great deal of information now exists about the analogous centers formed by implanting positive muons in semiconductors. This talk will review the experimental data on two types of muonium centers observed in Group IV and III-V crystals by muon spin rotation techniques, a form of magnetic resonance of muon spins. These data show remarkable deviations from the behavior of atomic muonium or hydrogen. Theoretical explanations will be advanced for the structure of these centers.

ELECTRONIC AND VIBRATIONAL STRUCTURE OF ISOELECTRONIC Cu-Li CENTRES IN GaP

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We present detailed magneto-optical photoluminescence (PL) and optically detected magnetic resonance (ODMR) measurements on three different sharp-line spectra observed in GaP upon codoping with Cu and Li. It is found that the usual Cu-related bound exciton (BE) spectra in GaP disappear after the subsequent Li doping. Instead several new PL emissions appear, the strongest ones with lowest electronic lines at 2.306 eV, 2.242 eV and 2.172 eV. A common feature of these spectra is the singlet-triplet configuration in the excited BE state of the system. The electronic structure resembles that of the Cu-related centres in GaP, but has smaller exchange splitting, typically 1 meV. The Cu-Li spectra are interpreted as BE recombinations at isoelectronic associates of Cu and Li. The sign of the axial crystal field created locally at the defects is deduced to be compressive. The electronic structure is found to agree with the general scheme of hole attractive central cells in a crystal field exceeding the exchange interaction in the BE state. The symmetry of the defects binding the Cu-Li excitons cannot be revealed from conventional Zeeman measurements. Because of the strong crystal field the BE states have pure spin character with isotropic magnetic splitting. ODMR measurements determine the symmetry of the 2.306 and the 2.242 eV centres as trigonal with <111>-oriented defect axes. The 2.172 eV centre shows well-resolved ODMR data in agreement with <110> symmetry axis. Isotope doping with Li has revealed the presence of Li in the centres through substantial shifts of the very strong and sharp local phonon modes present for all centres. These modes couple equally strongly to both the forbidden triplet transition and the allowed singlet one. As a contrast the singlet and the triplet couple very differently to the X- zone boundary phonons of GaP. The phonon coupling in relation to the defect symmetry is discussed for all three Cu-Li centres.

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Deep Level Impurities **FrA-D3**

Optical and ODMR Investigation of Antisite Defects in GaP

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Optical and ODMR studies on GaP:Zn are reported. Two luminescence bands at 0.95eV and 1.27eV (see fig.) are observed due to recombination of the doublet donor PP_4 and the triplet donor PP_3, respectively. They could be excited with light below band gap energy. From the excitation spectrum the positions of the two donor levels in the band can be determined. The linear dependence of the 1.27eV triplet luminescence on excitation light intensity reveals that the PP_3 antisite is not the excited state of the PP_4 doublet state as was suggested earlier[1], they are independent defect states.

The ODMR spectrum observed via the 1.27 triplet emission shows - in addition to the triplet signal - an acceptor resonance closely linked to the triplet resonance. It follows that the PP_3 donor and this acceptor form one complex. g-factor and angular dependence of the ESR indicate that Fe^{3+} is the acceptor. So it proposed that the triplet donor is a PP_3Y_P-Fe^{3+}-complex. with the Fe^{3+} in a well defined - probably interstitial- neighbouring position. Arguments are given that Y_P is a Ga replacing the 4th nearest neighbour Phosphor. So the ground state would be a $(P_{Ga}Ga_P)^-$-Fe_i^{2+} complex which by optical excitation is transformed to a $(P_{Ga}Ga_P)^{2-}$-Fe_i^{3+} donor-acceptor pair.

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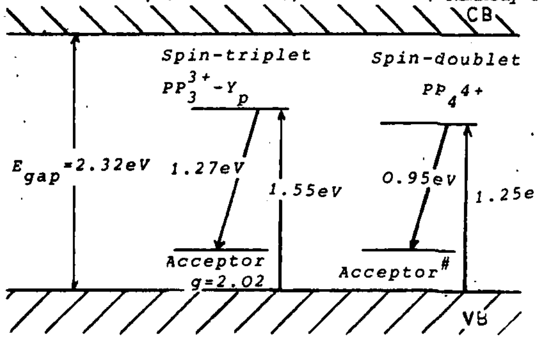

Figure:
Level scheme of spin-triplet and spin doublet antisite defects in GaP:Zn.

RAMAN STUDY OF NEUTRON IRRADIATED GaAs

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Neutron irradiated GaAs which has been shown by EPR to contain $\sim 8\times10^{17}$ cm^{-3} of As-antisite defects has been studied by Raman scattering. In addition to disorder induced acoustic phonon modes that have previously been observed in ion-implanted GaAs, a new Raman peak is observed at 227 cm^{-1}. This peak is relatively sharp (FWHM < 10 cm^{-1}) and has a Γ_1 symmetry. Using EPR techniques Wörner et. al. have shown that in neutron irradiated GaAs the As-antisite defect concentration exhibits a drastic decrease when the sample is annealed above 400 C. We find that the 227 cm^{-1} peak remains unchanged when the neutron irradiated sample is annealed to $\sim$220 C. However, this peak disappears when the sample is annealed above 400 C. Based on this annealing behavior and on the observed symmetry, we tentatively identify this peak as due to the As-antisite defect. We note that the frequency of this mode is very close to the 230 cm^{-1} optical phonon mode observed in amorphous As.

A comparison between the results for neutron irradiated GaAs and Cr doped GaAs will also be presented.

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17th International Conference on the Physics of Semiconductors
Narrow Gap Semiconductor FrA-E1

THE FIRST OBSERVATION OF TEMPERATURE DEPENDENCE OF FREE CARRIER ABSORPTION BY PHOTON-IONIZED IMPURITY-PLASMON PROCESSES IN SEMICONDUCTORS

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The free carriers can absorbe a photon with energy greater than plasma energy by exciting the collective (plasma) oscillation. Such process is possible in presence of ionized impurities. One can expect this absorption only in energy region where plasmons are well defined that mean for wave vectors smaller than critical one (q_c). At q_c the collective oscillations crosse the single particle excitation boundary and decay by exciting an electron of the Fermi sea.

It was shown previously for HgSe (zero-gap semiconductor which is always n-type) at 10K that such mechanism gives a significant contribution to the total free carrier absorption. In this paper new transmission data for HgSe in energy range 35 - 75 meV at 10K, 80K and 295K are presented. The measurements were done both below and above plasma energy ($\hbar\omega_p$) what permit us to extract the free carrier absorption by photon-ionized impurity-plasmon processes (PIIPP). The detailed analysis of experimental data is made on the basis of dynamic dielectric function (DDF) formalism. The contribution to DDF due to valence band-conduction band transitions characteristic for zero gap materials is taking into account in Kane [illegible] of HgSe band structure. The free carrier contribution to DDF without PIIPP is taken from classical Drude-Zener theory and well describe the transmission below the plasma energy.

The PIIPP absorption at low temperature (10K) has a sharp edge at photon energy equal to $\hbar\omega_p$ then slowly decline up to energy corresponding to q_c. Above this energy the discussed absorption decline faster. This behaviour is observed at all temperatures. However the maximum absorption due to PIIPP decrease with increasing temperature and the slope of the low energy edge also decrease. The physical origin of these phenomena is discussed.

17th International Conference on the Physics of Semiconductors

Narrow Gap Semiconductor **FrA-E2**

NONLINEAR OSCILLATIONS, BIFURCATION AND CHAOS IN n-InSb

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A wide variety of physical systems exhibit chaotic behavior. The prediction of the behavior of these dynamical physical systems as they approach chaos is of much interest today. Here we present the results of a study on nonlinear oscillations in n-InSb that demonstrate bifurcation and chaotic behavior due to impact ionization of shallow donor impurities. To our knowledge this is the first time bifurcation and chaotic behavior has been seen in a narrow gap semiconductor.

High purity samples (at 77 K, $N_d-N_a \approx 10^{14}\text{cm}^{-3}$) of n-InSb show marked nonlinear behavior of the electrical properties (conductivity and Hall coefficient) at 4 K. With an increasing applied magnetic field, the nonlinear behavior increases, and even negative differential resistance behavior is observed. The sample exhibits a series of nonlinear oscillations under nonohmic dc current conditions. The amplitude, period, and harmonic content depend upon the current, magnetic field and lattice temperature. At high currents all oscillations disappear. We demonstrate that the nonlinear oscillations, bifurcation, and chaotic behavior are due to impact ionization from shallow, tellurium impurity levels. Magnetic freeze out effects greatly influence the instabilities, oscillations, bifurcation, and chaos present in the InSb samples. We explain these oscillatory instabilities with a model based upon impact ionization of charge stored on these shallow donor levels and space charge injection. Additional interesting features observed and presented are (1) quenching of the oscillatory instabilities by the creation of free electrons by two-photon absorption from a CO_2 laser; (2) period doubling of the nonlinear response of the sample with sinusoidal driving currents.

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HIGH-PRESSURE FAR-INFRARED STUDIES OF PbTe AND INDIUM-DOPED $Pb_{1-x}Sn_xTe$*

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Hydrostatic pressure in the few kilobar range can cause large relative changes in the band gap, effective mass, plasmon and phonon frequencies in narrow-gap semiconductors. We have studied these effects by far-infrared reflectivity measurements from 20-250 cm^{-1} of samples of bulk PbTe and epitaxial films of indium-doped $Pb_{1-x}Sn_xTe$ (x=.21 and .25). In PbTe at 80 K we have measured a 38% increase in the transverse optical phonon frequency and a 12% increase in the carrier plasma frequency under 8 kbars of pressure. The effect of pressure on the plasma frequency is in good agreement with the shift calculated from a two-band model using the known pressure dependence of the energy gap. The Gruneissen's parameter calculated for the TO phonon, however, is 19.6--much larger than the values of around 3 typical of lattice anharmonicity effects in materials with the rock-salt structure. We have estimated the effect of the phonon softening through the pressure dependence of the paraelectric Curie temperature (T_c), but this can account for only about half of the discrepancy. The residual effect may be due to a large underestimate of the effect of pressure on T_c, or it may be related to the changes in the electronic structure through electron-phonon coupling.

In indium-doped material we observe at all pressures a large increase in the plasma frequency at temperatures below 30 K. At zero pressure the plasma frequency increases from 150 to 1200 cm^{-1} when the temperature decreases from 30 to 8 K.[1] This agrees well with DC measurements of persistent photoconductivity at low temperatures. Pressure has relatively little effect on the persistent photoconductivity, increasing the plasmon frequency at 10 K by only 10%--comparable to the pressure-induced shift at 80 K and considerably less than the effect of cooling from 15 to 10 K. Since the position of the indium level with respect to the band edge is known to be very sensitive to pressure, we conclude that the persistent photoconductivity is not related to the indium level approaching or entering the band. Since T_c is also sensitive to pressure, these results apparently also rule out the ferroelectric phase transition as the cause of the persistent photoconductivity. We believe that the strong dependence of the photoconductivity on temperature and the weak dependence on pressure can be explained if indium is a large-lattice-coupled impurity.[2] In this case there can be a configurational barrier between the band state and the impurity level and deexcitation from the band is thermally activated. Since the band state is only weakly dependent on the local lattice relaxation, the barrier is not greatly changed as the indium level is pushed above the band edge by pressure.

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MAGNETO-OPTICAL STUDIES OF In DOPED $Pb_{1-x}Sn_xTe$

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Indium doped $Pb_{1-x}Sn_xTe$ exhibits insulating dark resistivity at low temperature and persistent photo-conductivity for wavelengths as long as 5 μm. We report on far-infrared (9 μm - 170 μm) magneto optical studies of this material. Transmission, absorption and photo-response measurements have been made at 4.2 K - 70 K and for fields up to 100 kG. Under our experimental conditions the samples (n type $Pb_{0.79}Sn_{0.21}Te$:In) are in the metastable conducting state (i.e. degenerate semiconductor having 2×10^{16} cm^{-3} carriers at 4.2 K). Cyclotron resonances have been observed over the whole temperature range for 80 - 170 μm laser lines, and they split into doublets below 15 K. The angular dependence of the resonance field in Voigt geometry is slightly broken from cubic symmetry. The behavior is very similar to that of the ferro-electric phase transition in $Pb_{1-x}Ge_xTe$ and suggests that $Pb_{1-x}Sn_xTe$:In is in a ferro-electric phase, which has only been reported in the insulating state [1].

We have observed oscillations of infrared (9.2 - 10.6 μm) photo-conductivity and photo-Hall-voltage with magnetic field. The oscillations, however, do not depend on the photon energy as expected from direct interband Landau transitions. The oscillations, therefore, are of the Shubnikov-de Haas type. Also, d.c. magneto-resistance and carrier density show small oscillation at low magnetic fields, and the carrier density (or inverse Hall coefficient) increases linearly at high field. This result suggests that the Fermi level is pinned [2] in the conducting state. Another possible interpretation is that the recombination time is magnetic field dependent.

We have found that the decay time of photo-conductivity depends strongly on magnetic field. When laser light is turned off, the Hall coefficient and electrical resistivity increase (typically 50%) toward the steady state with only room temperature radiation, with decay time of 10 seconds. The decay time of the resistivity increases when magnetic field is applied (3 minutes at 60 kG). Sudden steps are sometimes observed in relaxation curves of resistivity. Such steps have been reported only in decay toward nonconducting state in dark [3], and are considered as instantaneous reconstructions of ferro-electric domains. Our results suggest that the samples have ferro-electric phase even in the metastable conducting state at low temperature.

We will report the first observation of ferro-electric phase in the conducting state of $Pb_{1-x}Sn_xTe$:In.

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17th International Conference on the Physics of Semiconductors
Narrow Gap Semiconductor **FrA-E5**

RAMAN SCATTERING IN THE NARROW GAP ALLOY $Hg_{1-x}Cd_xTe$.

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$Hg_{1-x}Cd_xTe$ besides being a leading IR detector material is also an important alloy system for the study of various basic interactions. Despite the importance of $Hg_{1-x}Cd_xTe$ and the utility of Raman scattering (RS) in probing fundamental interactions, only two studies on this material have been reported[1,2]. Mooradian and Harman[1] used RS to study the compositional dependence of TO and LO phonons and Amirtharaj et al[1] investigated the polarization dependent RS from <100> and <111> faces of p-$Hg_{0.8}Cd_{0.2}Te$.

We have measured the polarization dependent RS from <100>,<110> and <111> surfaces of HgTe (zero-gap) and $Hg_{0.8}Cd_{0.2}Te$ ($E_g \approx 100$ meV). All spectra were recorded at 77°K in the back scattering geometry using several lines of an Ar+ laser; the 5145 Å line is nearly resonant with the E_1 gap in $Hg_{0.8}Cd_{0.2}Te$. The polarization dependence of the zone center TO and LO phonon peaks from all the faces in both HgTe and $Hg_{0.8}Cd_{0.2}Te$ (mixed mode behavior) could be explained by including not only the deformation potential interaction but also effects due to linear q terms, or surface electric fields. From the <100> surface in both HgTe and $Hg_{0.8}Cd_{0.2}Te$ we have seen a symmetry forbidden TO feature which may possibly be due to internal strains. In addition to the zone center TO and LO phonon peaks, we have observed other features in RS from both HgTe and $Hg_{0.8}Cd_{0.2}Te$, several of which are related to deviations from "ideal" crystal behavior. They are: (a) a strong peak at ∿ 136 cm^{-1} in all $Hg_{0.8}Cd_{0.2}Te$ samples, having a Γ_1 symmetry, possibly originating from a vacancy; (b) a weak peak at ∿ 108 cm^{-1}, seen both in HgTe and $Hg_{0.8}Cd_{0.2}Te$, having TO phonon character possibly due to an anti-site defect[3], the amplitude of this peak was sample dependent and hence it is not intrinsic. (c) The RS of HgTe contained features on the low energy side of both the TO and LO phonon peaks with Γ_{15} symmetry, which may also be related to defects. In addition, an exteremely surface sensitive feature was observed in $Hg_{0.8}Cd_{0.2}Te$ and has been tentatively assigned to a coupled LO phonon-inter subband transitions in the naturally occuring surface inversion layer[2];

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Semiconductor: Structure

FrP-A1

Invited

SOLIDS IN LIMBO: STRUCTURE AND PROPERTIES OF NON-CRYSTALLINE SEMICONDUCTORS

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Two broad classes of non-crystalline solids, amorphous and glassy, are macroscopically distinguishable by their mechanical and thermal properties. Thus glassy solids when heated at ~10K/min melt near $T = T_g$ into supercooled liquids (e.g., g-As_2Se_3) while amorphous solids (e.g., a-Si:H) crystallize explosively at $T = T_R < T_g$. Amorphous solids accumulate substantial internal stress and are generally evaporated as thin films, while glasses are nearly stress-free and can be prepared in bulk. These macroscopic material properties have microscopic molecular analogues which explain the composition dependence of the glass-forming tendency and chemical trends in electronic properties (such as dopability of a-Si:H). Mathematicians have developed Ptolemaic geometrical descriptions of non-crystalline solids, while I have recently developed a physical or Newtonian topological model. Non-crystalline semiconductors provide the most exacting tests of competing theoretical models of these extensive non-equilibrium systems through recent Raman and Mössbauer experiments.

STRUCTURAL AND MICROSTRUCTURAL DETERMINATIONS OF CRYSTALLINE AND AMORPHOUS FRACTIONS OF MICROSCRYSTALLINE Ge: A COMPARISON

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Recent EXAFS measurements have shown that microcrystallinity in deposited Ge films nucleates in the form of small regions about 10-20Å in size.(1) These crystallite sizes are too small to be resolved by X-ray or neutron diffraction techniques, but also fall within the detectability province of visible - near uv spectroscopic ellipsometry (SE).(2) In this work we report the first direct comparisons of crystalline (c-) and amorphous (a-) volume fractions of the same microcrystalline (μ-) Ge films by these two qualitatively different techniques. EXAFS is a structural probe that senses microcrystallites via increased ordering of the second-nearest-neighbor atoms, while SE is a microstructural probe that responds to critical point features in optical spectra that results from Bragg reflection of electronic wavefunctions at lattice planes. We find good agreement between c-Ge volume fractions determined by the two techniques for a number of μ-Ge films with c-Ge fractions from 0 to 50% and microcrystallite sizes up to 50Å. Our results can be interpreted in terms of uniformly-sized nucleation centers embedded in the a-Ge matrix.

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17th International Conference on the Physics of Semiconductors

Semiconductor: Structure **FrP-A3** **Invited**

ATOMIC-SCALE STRUCTURE OF ZINCBLENDE ALLOYS

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Extended x-ray absorption fine structure (EXAFS) measurements(1) have been used to study the atomic-scale structure of representative zincblende random solid solutions. In particular, the nearest neighbor cation-anion distances have been obtained as a function of alloy composition. The results indicate that the nearest-neighbor distances remain closer to the respective distances in the pure binary compounds than to the average cation-anion distance defined by the lattice constant measured by x-ray diffraction. For example, in $Ga_{1-x}In_xAs$,(2) the Ga-As distance varies from 2.445 A in pure GaAs to 2.485 A as an impurity bondlength in InAs, in which the In-As distance is 2.622 A, while the In-As distance as an impurity in GaAs is 2.578 A. Atomic displacements from the ideal sites of the average (or virtual crystal) zincblende lattice are required to produce two different cation-anion distances at a given alloy composition. Analysis of the second neighbor EXAFS spectra indicate that the mixed sublattice (cations in $Ga_{1-x}In_xAs$ and anions in $ZnSe_{1-x}Te_x$) approaches the FCC sublattice positions of the virtual crystal, whereas the common sublattice (As and Zn in the above examples) contains the predominant distortions, with atomic displacements up to 0.1 A from the virtual crystal lattice sites. Bond angle distortions from the ideal tetrahedral angle of 109.5° result from these atomic displacements. The observed alloy structural features are similar to those inherent in the chalcopyrite crystal structure, which is based on a doubled zincblende lattice, except that in the alloys there is no long-range cation ordering. Similarities between the local structure of $Ga_{0.5}In_{0.5}As$ and the "cubic" disordered chalcopyrite $ZnSnAs_2$ are described, and these similarities are extended to alloy compositions other than 50:50. The equilibrium alloy structure is viewed in terms of the balance between the bond angle distortions which result from the atomic displacements from the ideal lattice positions and the bondlength deviations from the "ideal" ones which occur in the pure binary end members. A simple force constant model is proposed, from which the bond strain energy can be readily calculated as a function of alloy composition. It is shown that the strain enthalpy compares favorably with the experimentally measured solid solution interaction parameter. The use of the experimentally measured alloy atomic-scale structure in calculating the electronic properties(3) of zincblende solid solutions is also discussed.

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BOND LENGTHS AND AVERAGE LATTICE CONSTANT OF $Ga_xIn_{1-x}As$: A MICROSCOPIC THEORY

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Abstract

Recent EXAFS experiments 1) in $Ga_xIN_{1-x}As$ have revealed that over the whole composition range i) the average lattice constant obeys the Vagard's law, ii) the cation sublattice is close to that of the virtual crystal, iii) the anion sublattice is strongly distorted with Ga-As and In-As bond lengths nearly unchanged.

We have studied the equilibrium structural properties of the systems with x=0, .25, .75, and 1. Alloys are simulated by periodic simple-cubic crystals with 8 atoms per unit cell. The self-consistent calculations of the total energy are based on "ab initio" pseudopotentials 2) and the local density approximation. The total energy is minimized with respect to the lattice constant (verification of Vegard's law) and with respect to the anion displacements from the ideal zincblende positions (calculation of the bond lengths).

For x=0 and x=1 we have reproduced within 2% the experimental lattice constants of InAs and GaAs. Results for crystals with compositions x=.25 and .75 are in agreement with Vegard's law and provide anion displacements corresponding to Ga-As and In-As bond lengths which are close to the values reported in Ref. 1.

Microscopic analysis of these results in terms of electronic charge densities is used to show how the distorsion of the anion sublattice is induced by the electronegativity difference between the two cations.

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STABILITY AND FORMATION OF THE CLUSTERS WITH TETRAHEDRAL UNITS IN GERMANIUM-TIN-SELENIUM GLASSES

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The knowledge of the structure of the glass is of primary importance for the understanding of the physics, such as glass forming tendency, electronic properties, etc.. The germanium-tin-selenium alloys form typical good glasses even under a slow quenching from the melt.[1] We have explored the composition dependence of the infrared response spectra in the glasses, where the (Ge,Sn)(Se, or S)$_{4/2}$ clusters play a leading part. Each of the clusters is surrounded by chalcogen clusters in a wide composition range. The splitting between the longitudinal (LO) and transverse (TO) peak at the high energy F_2 band increases with increasing germanium compositions in g-$Ge_{1-x}Se_x$ and mostly levels off at x less than 4/5 and more than 2/3. The LO-TO splitting of the $SnSe_{4/2}$-F_2 band is examined as functions of tin compositions with various fixed selenium compositions, where tin atoms have been incorporated only into $GeSe_{4/2}$ clusters. The growth rate of the splitting is practically the same for g-$(Ge,Sn)_{1-y}Se_y$ at y less than 4/5, and becomes small at y more than 4/5. These trends suggest us that the cluster size is standardized in the glasses between x = 4/5 and the stoichiometric composition x = 2/3. An onset of a super-linear increase of the Raman peak position of the $GeSe_{4/2}$-A_1 mode occurs also at x = 4/5 with increasing germanium compositions. The stability and the formation of the clusters is discussed in connection with the glass forming tendency, based on our infrared and Raman works, combined with the topological theory.[2]

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17th International Conference on the Physics of Semiconductors
Optical Properties **FrP-B1**

MAGNETO-ELECTRIC AMPLIFICATION OF LIGHT IN InSb

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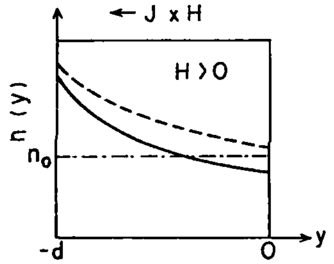
We report the first observation of a cooperative phenomenon involving a magnetoconcentration caused by the J x H force and photo-excitation which leads to amplification of ~ 5.3 μm radiation in InSb at temperatures from 80 to 300 K. In a semiconductor, having a narrow energy gap E_g and a thickness d, where electrons and holes coexist under the influence of the J x H force acting along the y-direction, the electron concentration n(y) will be increased near the surface (y = -d), as shown by the solid curve in Fig. 1, deviating from the thermal equilibrium value n_o, and a depletion region will be left over near the back surface (y = 0). The similar population will be realized for the hole concentration p(y), resulting in a population inversion, $np > n_i^2$, around the light emitting surface (y = -d), n_i being the intrinsic carrier concentration. Now, the depletion region will be removed by irradiating the region with a light having shorter wavelength than $\lambda_o \simeq ch / E_g$, and the population inversion will be realized through the whole volume of the sample, as shown schematically by the dashed curve in Fig. 1. Then, there will no longer be absorption of photons with wavelength λ_o and only the emission of the photons will occur. Thus, intensification of the light emission can be expected through the cooperation of the magnetoconcentration and the photo-excitation. We carried out such an experiment on n-InSb under suitable Ar^+ laser irradiation, from which ~ 5.3 μm infrared emission could be expected, and found anormalous intensification of the emission. The observed nonlinear dependence of the emitted intensity with respect to the irradiation power and the current intensity indicates that a light amplification for photons with wavelength $\lambda_o \simeq 5.3$ μm does take place through the induced emission in the inverted population region realized by the cooperation of the above effects.



17th International Conference on the Physics of Semiconductors

Optical Properties **FrP-B2**

EXCITONIC EFFECT IN THE OPTICAL SPECTRUM OF SEMICONDUCTORS

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The electron-hole interaction affects the optical spectrum of many a semiconductor not only in the bound exciton region in the energy gap but also throughout the continuum. In particular, it controls the strength of the E_1 and E_2 peaks in groups IV, III-V and II-VI semiconductors.[1] The band structure contributions to E_1 and E_2 are approximated by simple models near L and X points.[2] The electron-hole interaction is evaluated by means of linear combinations of plane waves instead of local orbitals as in Ref. 3. Solution of the Bethe-Salpeter equation yields the absorption spectrum in Si (and also in Ge) which accounts for the discrepancy between the measured strength in E_1 and E_2 and the calculated strength using the one-electron band structure. The electron-hole states which contribute to E_2 also form a bound state below the E_2 edge, which is broadened by interaction with E_1 continuum.

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LIGHT SCATTERING DUE TO INTERVALLEY ELECTRON DENSITY FLUCTUATIONS IN n-Si

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This type of electronic light scattering was predicted in 1965[1] and first observed in 1977 for n-Si.[2] The theory of Ref. 1, however, is not able to explain the observations. This fact has been attributed to the extremely short mean free path of electrons in n-Si, which requires the use of response functions for the collisions limited case.[3] We present an extensive experimental study of scattering by such fluctuations for a wide range of electron concentrations ($8\times10^{18} \leq N_e \leq 10^{20}$ cm^{-3}), temperatures ($77 < T < 473$ K) and laser frequencies, performed with a Raman ($\omega > 20$ cm^{-1}) and a Brillouin spectrometer ($\omega < 20$ cm^{-1}). The results indicate that the scattering mechanism is diffusion induced intravalley scattering. This mechanism is able to explain the observed scattering efficiencies and other details of the phenomenon, such as its dependence on T and N_e and the polarization selection rules. Failure to observe the scattering in ion implanted and laser annealed samples will also be discussed.

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THEORY OF SPECTRAL HOLE BURNING IN p-TYPE GERMANIUM BY A FREQUENCY-DOMAIN TECHNIQUE

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Frequency-domain techniques at CO_2 laser frequencies can be used to study the ultrafast relaxation of hole carriers in semiconductors. By performing saturation spectroscopy of the direct free-hole transitions in p-type germanium, one can measure the subpicosecond scattering rates with laser pulse durations which can exceed a nanosecond.[1] We report a theoretical study of the interaction of a high-intensity CO_2 laser beam with a wavelength of 10.6 µm and a low-intensity probe beam which is tunable in the 9-11 µm region in p-type germanium. The dominant absorption mechanism of the optical beams is direct intervalence-band transitions between states in the heavy- and light-hole bands. At low light intensities the relaxation mechanisms maintain the hole distribution near equilibrium. However, for pump intensities of the order of 1 MW/cm^2, scattering can no longer maintain the distribution at the equilibrium value, and the occupation probabilities for states near resonance with the pump beam decrease in the heavy-hole band and increase in the light-hole band. When the material is simultaneously irradiated with both the pump and probe beams, there is a nonlinear response which produces a component in the hole population difference between the heavy- and light-hole bands which oscillates at the beat frequency. Here, the population difference of the nonequilibrium excited states has a preferred orientation in k-space due to the polarization of the laser and the anisotropy in the momentum matrix elements. This periodically modulated component in the hole distribution acts as a moving excited-state grating which mixes the two beams. The maximum amount of mixing of the two beams occurs for parallel polarizations and decreases by about a factor of five for the case of orthogonal polarizations. The absorption of the probe beam is modified by both the saturation of the intervalence-band transitions and by the oscillating population difference, which can scatter pump photons into the direction of the probe with the frequency shifted to that of the probe. Calculations of the probe absorption as a function of the frequency difference between the two beams are presented, and good agreement is found with experiment. In addition to modifying the probe absorption spectrum, the oscillating population difference leads to a current density component which oscillates at the pump frequency plus the beat frequency. If the pump and probe beams are nearly phase matched, the excited-state grating can generate a new optical beam that oscillates at the pump frequency plus the beat frequency. The intensity of this generated wave is estimated as a function of the beat frequency and the probe intensity.

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OPTICAL INVESTIGATION OF PHASE TRANSITIONS AND "ANOMALIES" IN $Ti_{1-x}Hf_xSe_2$ CRYSTALS.

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The effect of phase transitions on the optical properties of metallic and semimetallic layered compounds 2H-$TaSe_2$, 1T-$TiSe_2$ has been studied in the past by several groups. More recently the attention has been focussed on mixed layered systems where disorder and Anderson localization of free carriers appear to play an important role.
In this communication we refer about thermoreflectance measurement both in the infrared and in the visible -UV up 6 eV on $Ti_{1-x}Hf_xSe_2$ ($0 \leq x \leq 0.5$) crystals (where $TiSe_2$ is a semimetal which exhibits a structural phase transition at 200K and $HfSe_2$ is a semiconductor). The evolution of plasmons and structures associated to low energy interband transitions versus stoichimetry yields new information on: magnitude of the gap induced by the phase transition, magnitude of the overlap between conduction and valence bands, precursor effects and mechanism responsible for the phase transition, disorder, etc.
Furthermore, thermoreflectance in the visible and UV measurement make it possible: i) to establish a correlation between the structures of interband spectra of $TiSe_2$ and $HfSe_2$ with a resolution which is much better than in previous conventional reflectance spectra, ii) to look at the stoichiometry dependence of the main structures of such spectra for $0 \leq x \leq 0,5$.
In order to explain the results, either a possible bowing effect in a semimetallic-semiconducting system or a perturbation of electronic properties due to impurities at intermediate stoichiometries are required.

Observation of Anomalous Faust-Henry Coefficients in the Hyper-Raman Scattering from II-VI Semiconductors

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The hyper-Raman (HR) effect is a three-photon process by which two incident photons are simultaneously annihilated and one scattered photon is created in the spectral region around the second harmonic of the exciting light.[1] We have measured the HR spectra of CdS, ZnS, and ZnSe at room temperature for various scattering configurations, using a Q-switched Nd-YAG laser with a peak power of about 10 kW and a pulse repetition rate of 5 kHz. The LO phonon lines turn out to be almost 500 times more intense than the corresponding TO phonon lines and thus indicate an order-of-magnitude difference between the electro-optic and deformation-potential coupling coefficients. We confirm our experimental results by pseudopotential calculations of the appropriate deformation potentials responsible for TO-scattering and the matrix element of the interband Fröhlich interaction responsible for LO-scattering. We also give an experimental as well as theoretical estimate of the absolute HR cross section and compare the HR effect with the two-step process consisting of second harmonic generation and subsequent normal Raman scattering.

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OPTICAL OBSERVATION OF CLUSTERS IN DISTRIBUTION OF Cd AND Hg IONS IN CATION SUBLATTICES OF $Cd_{1-x}Hg_xTe$

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In the IR lattice vibration reflection spectra of $Cd_{1-x}Hg_xTe$ mixed crystals at T=85 K the fine structure of CdTe-like band is definitely apparent. To interpret this structure by classical dispersion theory, additional weak oscillators (besides two main lattice oscillators characteristic of two-mode behaviour) were introduced with the frequencies from the LO-TO splitting of the main CdTe-like mode. The additional vibrational modes were also observed directly, using Raman spectroscopy in *resonant conditions*. It is supposed that additional oscillators are due to manifestation of clustering effect in $Cd_{1-x}Hg_xTe$ alloys when Cd and Hg distribution in cation sublattice is not random. The probability to find a Hg atom next to another Hg atom in cation sublattice is $P_{HH} = x + \beta(1-x)$ where in our case, according to model calculation, $\beta = 0.6$ ($\beta = 0$ corresponds to random cation distribution). I.e., in one volume with linear dimensions of the order of some atomic parameters the excessive (comparing with the mean x) Hg concentration is observed, in another - the excessive Cd concentration.

The effect of like ion clustering in cation sublattice of quasi-binary solid solution CdTe-HgTe observed is explained by the specific "fish"-like form of its phase diagram T-x. Such a shape *leads to a noticeable variation of* composition in the volume of alloy with the small fluctuations of temperature on crystallization front.

MELTING TEMPERATURE AND DYNAMICS DURING PULSED LASER IRRADIATION OF AMORPHOUS SILICON

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Pulsed laser irradiation of silicon has raised several important issues concerning the thermodynamics and kinetics of the amorphous to liquid transformation. Recent measurements of the enthalpy of crystallization for amorphous Si [1] predicts a melting point for the amorphous phase which is depressed several hundred degrees from the crystalline value. We have used a transient conductance technique [2] to directly observe the liquid-solid interface motion during 50 ns pulsed ruby laser (694 nm) irradiation of amorphous Si layer. Due to the difference in the melting temperatures of the crystalline and amorphous phases, the interface motion is delayed at the amorphous-crystalline interface. Measurement of this delay, coupled with numerical model calculations, have indicated a melting point depression of 200±50 K for the amorphous phase. Below incident laser energy densities sufficient to completely melt the amorphous layer, the transient conductance measurements show the existence of explosive crystallization within the remaining amorphous layer. This explosive crystallization is mediated by a thin (10 nm) liquid layer which propagates due to the latent energy released in the amorphous to crystalline transformation. This liquid layer propagates through the amorphous layer at a velocity of 10-20 m/s, resolidifying as fine grain poly-crystalline Si.

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SYMMETRY BREAKING MECHANISM AT THE MELTING THRESHOLD OF LASER IRRADIATED SILICON

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Coexisting liquid and solid regions have been observed close to the melting threshold of laser irradiated silicon. Spontaneous periodic surface structures, or ripples, with periodicity of the order of the optical wavelength, suggest that the observed pattern is due to interferences effect. To produces the observed ripples, this initial perturbance must grow, so that one must find an instability mechanism which amplifies any small perturbation.

Although the reflectivity of liquid silicon is larger than the solid one, the energy deposition is larger in the liquid than in the solid, as the laser penetration depth strongly decreases at melting (the important physical quantity being the heat deposition per unit volume rather than per unit surface). This allows the formation of stable liquid regions sligthly hotter than the melting temperature, for laser power sligthly above the threshold for melting. But in order to compensate for the decrease of absorbed energy a lateral heat flow is necessary from the neighbouring solid regions to the back of the liquid ones.

We illustrate this mechanism by solving analytically a 2-dimensional heat equation. We show that, starting with an homogeneous irradiation, a periodic set of liquid and solid stripes is a stable solution. We can determine the range of possible pattern sizes. As for any instability, the pattern effectively observed results from external boundary conditions which have to be added to the basic mechanism (as for example interference between the incident beam and diffracted waves travelling waves along the surface).

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Laser Annealing **FrP-C3**

SUPERSATURATED SUBSTITUTIONAL-NITROGEN IMPURITIES IN NANOSECOND-PULSED LASER ANNEALED SILICON

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It was clarified recently by Electron Spin Resonance (ESR) mesurement /1,2/ that substitutional nitrogen (N) impurities can be introduced into Si crystal by N_2^+ or N^+ ion implantation and subsequent pulsed laser annealing. Unlike the other group-V donor impurities (P,As,Sb,Bi) in Si, electronic states of substitutional N impurities, N_s , in Si have not been investigated in detail because N_s cannot be doped by the conventional techniques of crystal growth.

In order to investigate how N impurities with a high concentration of $1x10^{18}/cm^3$ are incorporated into the substitutional sites, how deep is the localized level of neutral N_s and whether or not negative charge states of N_s exist in the Si band gap, we have done ESR and photoluminescence (PL) measurements of various kinds of Si samples including N impurities (Si:N systems). In this conference, we report on the ESR and PL results and on the effect of shallow phosporus (P) donor doping into Si:N system.

The substitutional N impurities can be introduced effectively by nanosecond (or picosecond) pulsed laser annealing of N implanted Si, but neither by cw-laser annealing of N implanted Si nor by Si crystal growth with a special doping of N impurities. The high effectiveness of pulsed laser annealing for introducing N_s in Si is mainly due to extremely high velocity (2 - 3 m/sec) of recrystallization and extremely rapid cooling (faster than 10^9 C/sec)/3/ after recrystallization which have been clarified by some time -resolved measurements/3,4/.

With increment of doping P concentration, spin density of N_s was found to decrease above a critical P-implantation dose. This is interpreted in terms of formation of diamagnetic, negative charged N_s as a result of trapping of P donor electrons by neutral, deep N_s levels. Other possibilities can be ruled out, of pairing of P and N_s and strong spin-spin interaction between localized spin of N_s and degenerated donor electrons originated from P impurities. It was also found from PL study that there is a correlation between N_s and both 0.767- and 0.746-eV PL lines. These results suggest that the substitutional N impurities have a deep, neutral level and a shallow, negative-charge level in the band gap of Si.

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Laser Annealing **FrP-C4**

TIME-RESOLVED STUDIES OF ULTRARAPID SOLIDIFICATION OF HIGHLY UNDERCOOLED MOLTEN SILICON FORMED BY PULSED LASER IRRADIATION*

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In this paper we report extensive results of nanosecond-resolution time-resolved optical reflectivity measurements, during pulsed excimer (KrF, 248 nm) laser irradiation of amorphous silicon, which, together with model calculations and post-irradiation TEM measurements, have allowed us to study both the transformation of amorphous (a) silicon to the highly undercooled liquid (l) phase and the subsequent ultra-rapid solidification process. Preliminary results[1], obtained using these techniques and pulsed Nd (532 nm) laser irradiation of implantation-amorphized a-Si layers on crystalline (c) substrates, demonstrated that:

(1) Measurements of the precise time of the onset of melting of a-Si, during an incident laser pulse, provide a powerful constraint, fixing the value of the thermal conductivity of a-Si.

(2) Since the melting temperature (T_a) of a-Si is apparently ~250 K below T_c (1683 K) for c-Si, molten l-Si that is undercooled by hundreds of Kelvins can be prepared by pulsed laser melting of a-Si. Our preliminary results[1,2] suggested that bulk nucleation occurs in this highly undercooled liquid silicon and a nucleation temperature (T_n), with $T_a < T_n < T_c$, was estimated.

In our current studies, these techniques have been applied and extended to study the melting and subsequent solidification of a-Si layers of several different thicknesses (approx. 100, 220, and 500 nm). The use of ultraviolet excimer laser radiation minimizes differences in the optical properties of the a-, l-, and c-phases of Si, while also providing much higher precision in two different types[1] of time-resolved reflectivity measurements. As a result, the new measurements provide information about the heating of a-Si while still in the solid phase, prior to melting, and provide data on the thermal properties of a-Si and l-Si. The new measurements also provide, for the first time, in-situ time-resolved optical evidence of the onset of bulk nucleation and crystal growth near the molten surface, while melt-front penetration into the a-Si layer is still in progress. This time-resolved optical monitoring of nucleation and growth, with nanosecond resolution, can be correlated with post-irradiation TEM micrographs of the nature (fine- or large-grained) and depth scale of polycrystalline regrowth. Calculations of temperature profiles in the undercooled Si will be discussed, together with new estimates of the nucleation temperature T_n and its relation to T_a.

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Laser Annealing **FrP-C5**

ULTRAFAST SPECTROSCOPY OF VERY DENSE AND HOT ELECTRON-HOLE PLASMAS IN CRYSTALLINE AND AMORPHIZED SEMICONDUCTORS.

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The physics of very highly excited semiconductors has recently attracted a lot of attention. One avenue of research is concerned with the picosecond [1] or femtosecond [2] processes that accompany ultrashort pulse melting. In this paper, we focus on the picosecond dynamics of very dense ($n \geq 10^{20}$ cm^{-3}) and very hot ($T_e \geq 2000°K$) laser-induced electron-hole plasmas (EHP) in crystalline and amorphized Si and GaAs.

In most of our experiments, we have used a novel experimental technique in which a visible psec laser pulse creates a very dense EHP at the surface of the sample and a subsequent infrared psec pulse brings the sample to melting point. Efficient coupling of the IR pulse to the solid occurs via free-carrier absorption (FCA) : as the delay between the pulses increases, recombination and diffusion decrease the EHP density and thus more IR energy is required to melt the sample. By comparing the measured joint melting thresholds at various time delays and for different relative intensities, to the predictions of a theoretical model that describes the temporal evolution of the EHP density and temperature, and the lattice temperature, we can measure the EHP relaxation and recombination times, and the FCA cross-section

All our experimental results to date, obtained on a wide variety of Si and GaAs samples (from crystalline to fully amorphized) display similar qualitative features indicating the presence of a short-lived dense and hot EHP. For example, in one type of disordered Si, we obtain a good fit by assuming a 100 fsec hot carrier relaxation time, a 10 psec recombination time, and a FCA cross-section that is twice that of c-Si [3]. In very heavily damaged Si layers, the influence of FCA is reduced. In intrinsic Si, the presence of the very dense and hot EHP makes σ larger than at low excitation regimes. In fact, we have strong evidence that interconduction band transitions become important and we will present data that support a model where $\sigma = \sigma(T,n,T_e)$. In GaAs, another important process, two-photon absorption (TPA) in the IR, must be included to obtain agreement between theory and experiments.

We are continuing these experiments and will present further results obtained using our two-color excitation technique, with emphasis on the differences and similarities between Si and GaAs, and between crystalline and disordered materials.

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FREE CARRIERS DENSITY DEPENDENCE OF THE MELTING TEMPERATURE OF AMORPHOUS GERMANIUM

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Recently there has been considerable interest in the physics of pulsed laser annealing and laser induced phase transition in solids. Although the mechanisms involved in the melting of covalent semiconductors are not well-known, Combescot and Bok derived the decrease of the melting temperature T_m of Si and Ge which depends on the electron-phonon coupling [1]. Wautelet showed that near the melting point, the concentration of intrinsic defects is enhanced when an electron-hole plasma is present and this induces melting [2].

In the laser annealing experiments, the coupling of the laser beam energy with the lattice is described by diffusion equations for lattice temperature T and carriers concentration N. N is determined by the generation rate G produced by the laser and depending on the laser parameters (pulse duration, wavelength), the recombination rate (which under strong excitation is governed by the Auger recombination) and the carriers dissipation rate. This dissipation rate is depending on the ambipolar diffusion and on a non-linear effect such as plasma expansion.

In this paper, we report a series of experiments in which thin amorphous Ge films were irradiated in situ in a TEM microscope by YAG laser (λ = 1.06 m, λ = 0.53 m) with the pulse duration t = 10-40 ns. We have used unsupported a-Ge films of variable thicknesses (250-1000 A) which are of the order of the free-carriers diffusion length and smaller than thermal diffusion length. This allows more exact calculations of the temperature rise induced in these films and of the free-carrier density.

We measured the energy threshold for melting as a function of the pulse duration and the laser wavelengths. We observed for the first time the decrease of T_m with increasing n of free-carriers created by laser irradiation. The reduction of Tm we found ~ 150^{O}K for N varying from 1.3 to $1.5.10^{20}$ cm^{-3} is in qualitative good agreement with calculations reported in [1]. A melting mechanism corresponding to these excitation conditions is discussed.

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Laser Annealing **FrP-C7**

X-RAY DIFFRACTION STUDY OF SELF-IMPLANTED SILICON

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Damage and lattice disorder in self-ion implanted silicon crystals before and after thermal annealing are analyzed using a high resolution X-ray diffractometer. We have measured 333 Bragg reflection profiles for different implantation doses between 5×10^{13} and 5×10^{15} 180 keV Si^+ ions/cm^2. The strain distribution and the atomic displacements as a function of depth are obtained using a semi-kinematical approach of the dynamical scattering theory (1). The weak oscillations of the reflection coefficient at lower scattering angles observed in ion-irradiated crystals disappear completly after a two step annealing at 560°C and 1000°C. However, it be noted that the reflection coefficient and the half-width of the main peak change only slightly after the annealing process. This means that vacancies and interstitials are still present in the implanted region and lead to a smoothly varying lattice constant of the order of 10^{-5} a_o. The X-ray diffraction results are compared with electrical and photoluminescence data.

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Recombination and Spin-Dependent Properties **FrP-D1**

RECOMBINATION HEATING INDUCED DELAYED ENERGY RELAXATION OF NONEQUILIBRIUM CHARGE CARRIERS

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Recombination and electron-phonon-interaction are thought to reestablish independently of each other thermal equilibrium number and temperature of nonequilibrium carriers, respectively. It is shown here for the first time and in detail that recombination of parts of an ensemble of charge carriers may lead to an appreciable change of the temperature of the remaining carriers: Mostly heating occurs, sometimes there is cooling.

Sign and size of the recombination induced temperature change depends on the difference between the mean energy of recombining carriers and the mean carrier energy. This energy difference in turn depends on the carrier distribution function and the $\vec{k}$-dependence of the recombination rate τ^{-1}. If the recombination rate decreases with energy for both nondegenerate and degenerate statistics the temperature of the remaining carriers increases at a normalized rate $\frac{d(k_BT)}{dt} / k_BT \approx 1/\tau$. Detailed calculations for the medium injection limit in direct gap materials where e-h-recombination dominates shows that e.g. in GaAs at 1.7K recombination heating and energy dissipation via (unscreened) electron-acoustic phonon interaction are equal ($\approx 2 \times 10^6$ eV/s) at 38K in bulk material ($\tau \approx 10^{-9}$s). In GaAs multiple quantum wells ($\tau \approx 10^{-10}$s) recombination heating balances the considerably stronger hole-acoustic phonon interaction at ≈30K - ($dE/dt \approx 2 \times 10^7$ eV/s).

Heating at a normalized rate τ^{-1} also occurs for any recombination rate and degenerate statistics if the density is time dependent (e.g. a e-h-plasma). If the recombination rate is $\vec{k}$ independent or increases with $\vec{k}$ no effect or a cooling effect, respectively, results in the case of Maxwell statistics. The latter effect is quite similar to evaporation induced cooling of a liquid. Experimental results on the energy dissipation in GaAs, GaAs quantum wells, electron-hole drops in Ge and AlAs illustrate the different cases. The crossover temperature of the total energy dissipation rate (electron + hole) and the recombination heating rate presents a minimum temperature above the lattice temperature an electron-hole system reaches and keeps as long as the recombination process itself does not change its quality.

Recombination and Spin-Dependent Properties

FrP-D2

DETERMINATION OF THE ELECTRONIC STRUCTURE OF Si DANGLING BONDS AT THE Si/SiO_2 INTERFACE

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One of the most important intrinsic defects at the Si/SiO_2 interface is the P_b center. Recent ESR measurements of the ^{29}Si hyperfine structure of this defect have firmly identified it as a <111> paramagnetic dangling bond on a three-fold coordinated silicon atom.[1] We have shown by spin-dependent DLTS measurements[2] that this defect is responsible for the band of interfacial hole traps centered at 0.35 eV above the top of the valence band. In this paper we will present a model of the electronic structure of this dangling bond defect. We have used data from spin-dependent DLTS, spin-dependent recombination, DLTS, CV, and ESR vs. bias voltage to show that the band of singly occupied dangling bond states is centered at E_v + 0.28 eV with the doubly occupied states centered at E_v + 0.41 eV. The average effective correlation energy is therefore positive and equal to 0.13 eV. This result is in disagreement with other models for this defect which propose a much larger correlation energy of -0.6 eV.[3]

We are lead to our model by the following observations. First, the spin-dependent part of the broad DLTS hole-trap peak corresponds to only the upper half of the spectrum, i.e. a band of hole traps centered at E_v + 0.41 eV. We can show that it is the hole emission (as opposed to hole capture) process that is spin dependent, therefore the transitions near E_v + 0.41 eV must be due to the excitation of the second electron from the valence band to the dangling bond. A second observation is the large (10^{-4}) spin-dependent photocurrent effect at room temperature which implies a trapped electron-hole pair mechanism.[4] This in turn requires that some of the dangling bond centers be doubly occupied when the surface Fermi level is in the vicinity of E_v + 0.4 eV. Finally, our model is consistent with the ESR vs. bias voltage data of Johnson, et al.[3] According to our analysis of these data, there appears to be two classes of dangling bonds: a dominant component with a small correlation energy (consistent with our data), and a smaller component with a larger correlation energy (consistent with their model[3]). We will discuss these results as well as their relationship to other dangling bond centers in both amorphous and crystalline silicon.

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Recombination and
Spin-Dependent Properties

FrP-D3

STIMULATED RECOMBINATION AND THE DYNAMIC MOTT TRANSITION IN GaTe

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The dynamics of photoexcited carriers in direct gap semiconductors can now be measured directly by time-resolved spectroscopy using intense ultrashort laser pulses. In this paper we report measurements of the III-VI layered compound GaTe using time-resolved absorption and luminescence techniques. This material exhibits strong excitonic behaviour at low temperature ($E_G = 1.80$ eV; $E_X = 18$ meV). The exciton lifetime measured under conditions of weak illumination is 120 ps in our samples, and is due largely to trapping. At high excitation density we observe a bleaching of the exciton absorption due to a dynamic Mott transition. The temporal recovery of this absorption has been measured as a function of photoexcited carrier density: for $n \gtrsim n_c$ ($\sim 10^{18} cm^{-3}$) the recovery time is approximately 50 ps, but it shows two-component behaviour, the long component being due to exciton decay: for $n \gtrsim 5\ 10^{19} cm^{-3}$ we observe a dramatic reduction of the recovery time to $\sim$ 15 ps. This fast depletion of carriers is due to stimulated recombination: complementary luminescence measurements reveal the onset of stimulated emission at the renormalized band edge E_G' $(t \sim 0) = 1.76$ eV.

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Recombination and Spin-Dependent Properties **FrP-D4** **Invited**

CONDUCTION ELECTRON SPIN PRECESSION IN THE BAND BENDING REGION OF GaAs(110)

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Spin-polarized photoemission experiments from (Cs,0) activated GaAs(110) photocathodes show that the photoelectron polarization vector $\vec{P}$ experiences precessional rotations of up to θ_p=23°. These results can be explained by the splitting of the conduction band due to the spin-orbit interaction in conjunction with the lack of inversion symmetry in III-V compounds. Such splitting is equivalent to an effective internal magnetic field acting on the spins, whose direction depends on the direction of the momentum. The magnitude of the spin-orbital splitting of the conduction band (the precession frequency) is given by

$$\hbar\vec{\Omega} = \alpha\hbar^3(2m_{eff}^3E_g)^{-1/2}\vec{\chi}$$

where $\vec{\chi}$ is a vector with components $\chi_x=k_x(k_y^2-k_z^2)$, $\chi_y=k_y(k_z^2-k_x^2)$, $\chi_z=k_z(k_x^2-k_y^2)$, E_g is the band gap, and α is a dimensionless coefficient. Thus in general a non-zero spin precession is expected except for electrons propagating with $\hat{k}\,\|\,\langle 100\rangle$ and $\langle 111\rangle$. For $\hat{k}\,\|\,[110]$ we find the precession of $\vec{P}$ (optically oriented parallel to $\langle 110\rangle$) to be clockwise about the $[1\bar{1}0]$ direction /1/ in accord with theoretical expectations /2/. In the frame of the three-step photoemission model we conclude that the main contribution to spin precession arises within the band bending region for ballistic electrons. The precession angle is expected to be dependent on the doping level of the crystal as well as on the band-bending parameters. Therefore this experimental study opens a novel way to investigate the electronic properties of this important interface region.

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Recombination and Spin-Dependent Properties **FrP-D5**

STUDY OF PHOTO-MAGNETIC EFFECT IN PHOSPHORUS-DOPED SILICON WITH A SQUID-MAGNETOMETER: THE KINETICS OF D^- CENTERS

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A new method for observing a change in magnetic moment induced by photo-irradiation has been developed using a SQUID-magnetometer, and has been applied to investigate the kinetics and life-time of the D^- centers.

The SQUID-magnetometer is able to follow a small and rapid change in magnetic moment. When doped semiconductors are irradiated with an appropriate light in a magnetic field, a detectable change in magnetic moment may be induced due to the orbital diamagnetism of shallow traps or the spin reversal associated with relaxation processes of photo-generated centers. The relation between the amplitude of the photo-magnetic signal and the photon energy is used to distinguish various centers.
The temporal variation of the signal after switching-on and -off the light would give information on the relevant relaxation processes. The present purpose is to demonstrate such an example.

The samples were silicon doped with phophorus in the low concentration region, and the light was in the infrared(IR) and far-infrared(FIR) region. The IR light stimulates the following second-order reaction: $2D^0 + h\nu_{IR} \rightleftharpoons D^- + D^+$. Therefore, the diamagnetic signal is expected because the D^- centers have a large electron orbit.

Observation shows that the signal is diamagnetic and the decay form is non-exponential. The signal is occurred by the light in the photo-ionization range of the neutral donor D^0. Furthermore, the noticeable results obtained are as follows. (1) The relation of the amplitude and the decay form with the light intensity is described well in terms of the second-order reaction. (2) The signal amplitude leads to the estimation that several percents of the D^0 are converted to the D^- centers for the sample of $9\text{x}10^{16}$ P/cm^3. The steady D^- concentration depends on the IR intensity, temperature, and the doping amount. (3) The half-decay time is ranging in 0.9 to 0.1 sec at 1.7 K for the above sample, depending on the intensity of background IR irradiation such as room-temperature radiation which controls the recombination rate of the D^- and D^+ centers. These values are quite different from the previous obtained by the photoconductive measurement.[1] (4) The simultaneous irradiation of the FIR laser (170 μm) and IR light increases the signal amplitude, contrary to the prediction that the FIR light diminishes the number of the D^- centers. This fact may be resolved by assuming the coexistence of various kinds of D^--like centers, each of which is composed of an excess electron trapped in multiple donor impurities. These results will be discussed in detail.

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Recombination and Spin-Dependent Properties

FrP-D6

PHOTOELECTRON ENERGY DISTRIBUTION AND SPIN POLARIZATION MEASUREMENTS FROM GaAs WITH NEGATIVE AFFINITY

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We present high resolution energy distribution and spin polarization measurements of photoelectrons emitted from the (100) face of p-doped GaAs with negative electron affinity. A 20 meV resolution electrostatic electron spectrometer and a Mott polarimeter are used.

For a photon energy $h\nu$ of the order of the bandgap, we are able to obtain very narrow energy distribution curves : 110 meV at room temperature and 50 meV at 120K. This leads to interesting applications of GaAs photocathodes as intense monochromatic electron sources. When the photon energy is increased, electrons are excited higher in the conduction band, and the energy distribution curve (EDC) reflects both hot electron processes and details of the band structure. A $\vec{k}.\vec{p}$ calculation of the coupled conduction and valence bands, for electron kinetic energies up to 1 eV in the Γ minimum, accounts very well for the observed structures. The subsidiary L and X minima are shown to play an essential rôle in the thermalization processes.

The polarization energy distribution curve (PEDC) presents well defined structures enhancing those of the EDC.[1] The importance of hot electron spin relaxation is evidenced from the high energy part of the PEDC : the maximum polarization, measured at creation energy, ranges from 50% to 20% for $h\nu$ varying from 1.65 to 2.60 eV. The low energy part of the EDC and PEDC, which is the major contribution to the photoemission current, is due to electrons thermalized in the band bending region near the surface.

These detailed studies lead to a partial reexamination of the conclusions drawn in James and Moll's pioneer work[2] on EDC. Furthermore spin polarization analysis provides a more precise understanding of photoemission mechanisms.

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(*) Groupe de Recherche du Centre National de la Recherche Scientifique.

17th International Conference on the Physics of Semiconductors

Magnetic Semiconductors **FrP-E1** **Invited**

RAMAN SCATTERING BY MAGNETIC EXCITATIONS IN DILUTED MAGNETIC SEMICONDUCTORS*

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A diluted magnetic semiconductor (DMS), $A_{1-x}Mn_xB$, ($A \equiv$ group II element and $B \equiv$ group VI element) exhibits striking magnetic phenomena. A variety of unusual magnetic excitations--localized as well as collective--manifest themselves in the Raman spectrum of a DMS.[1] The Mn^{++} ions distributed on the group II lattice have an unfilled 3d^5 shell with $S = 5/2$ and hence a large magnetic moment. At sufficiently high temperature or small x the alloys are paramagnetic; in this magnetic phase $\Delta M_S = \pm1,\pm2$ transitions within the Zeeman multiplet of the $S = 5/2$ ground state of Mn^{++} appear in the Raman spectrum. The selection rules for this Raman-electron paramagnetic resonance and the microscopic models for its origin are discussed. Coupled modes of the EPR transitions and the zone center LO phonons are observed in the Raman spectrum. As the temperature is lowered, the DMS undergoes a phase transition into a magnetically ordered low temperature phase and the Raman-EPR line transforms into the high frequency component of the one magnon Raman line. Yet another magnetic excitation of a DMS accessible by Raman scattering is the spin flip of band electrons (holes) and of electrons (holes) bound to donors (acceptors). The fascinating case of electrons bound to donors in DMS in large, effective mass orbits exhibiting "bound magnetic polaron" features will be illustrated with extensive results in $Cd_{1-x}Mn_xTe$ and $Cd_{1-x}Mn_xSe$.[2,3]

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* Work supported by the National Science Foundation and the Office of Naval Research.

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17th International Conference on the Physics of Semiconductors
Magnetic Semiconductors **FrP-E2**

OPTICAL SPIN ORIENTATION OF EXCITONS IN (Cd,Mn)Se*

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This paper describes the first optical pumping experiments in diluted magnetic semiconductors. We have studied this effect in $Cd_{1-x}Mn_xSe$ crystals with $x = .05$ and $x = .10$, and see polarizations in the range of 0.01 to 0.02 in the luminescence from the donor bound exciton, while pumping with circularly polarized light incident along the c-axis. Comparison of our results with the optical pumping signal from pure CdSe[1] yields information on the hole - Mn^{++} spin interaction time and the spin dynamics of the bound magnetic polaron system. We estimate the spin exchange scattering time of the hole off the Mn ions to be 20 - 30 pSec before the formation of the bound exciton. The spin relaxation time of the hole in the bound exciton system is measured directly by studying the spin dephasing upon application of an external magnetic field perpendicular to the c-axis. We have also studied the optical pumping signal as a function of pump power and wavelength, looking for evidence of Mn^{++} spin alignment due to spin exchange scattering of the holes;[2,3] however, we find that the Mn^{++} spin relaxation time is too small to permit a significant spin alignment.

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*Work supported by the Office of Naval Research.

†Supported by the National Science Foundation through its Division of Materials Research.

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Magnetic Semiconductors **FrP-E3**

MAGNETIC POLARON EFFECTS ON BOUND EXCITONS

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Extensive photoluminescence experiments have been performed on undoped $Cd_{1-x}Mn_xTe$ as a function of x, the temperature T and the magnetic field H, in Faraday and Voigt configurations. For x up to about 7%, the luminescence is dominated by the A°X line. In the region of intermediate T (5-15°K) the behaviour of A°X is consistent with a model where the exchange between Mn ions and bound particles is considered as a perturbation. Simplified calculations starting from the best A°X wavefunction (1) have been performed, in the two limiting cases of a magnetization map fixed either by the initial A° state, or by the transitory A°X state. The best fit for the line energy correspond to the second case : Mn spins have time to react to the excited electronic state.

The model assumes that two lines, corresponding to the recombination of the electron with the two holes in different spin states, should be emitted : indeed two broad components are revealed by polarization properties when a magnetic field is applied. For x)3%, when H increases, the two lines disappear just when the upper component crosses the lower free exciton line : this is the point where A°X is destabilyzed by exchange effects. Moreover, the model suggests that A°X might become unstable at H=0 for x)7%. This can explain the rather abrupt disappearance of A°X at the benefit of excitons localized by fluctuations (2) (of chemical and magnetic nature) near that composition.

In the framework of this model, no strong magnetic polaron shift is predicted for D°X, because both electron and hole orbits are large. D°X should also be destabilyzed by a magnetic field. Available data in $Cd_{1-x}Mn_xSe$ will be discussed.

* On leave from the Institute of Experimental Physics, University of Warsaw, POLAND.

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Magnetic Semiconductors **FrP-E4**

HOPPING MAGNETOABSORPTION IN SEMIMAGNETIC SEMICONDUCTOR $n\text{-}Cd_{1-x}Mn_xSe$

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Hopping absorption in a partialy-compensated semiconductor consists in the photon-induced transition of a carrier from a neutral impurity to the ionized one [1].The hopping rate is determined by the difference between the ground state energies of the two impurities and by their wave functions overlap.In usual semiconductors the energy difference is due to the Coulomb potentials of the ionized compensating impurities. Overlap integrals are weakly magnetic-field dependent.In semiconducting alloys the energy difference originates predominantly from the composition fluctuations.In a semimagnetic semiconductor there is also a contribution from the magnetization fluctuations,via the exchange interaction of the carrier with the magnetic ions.Moreover,in wurtzite-structure n-type semimagnetic semiconductor,like $Cd_{1-x}Mn_xSe$ there exists a strongly magnetization-dependent mixing of spins and of s- and p-type electron wave functions of the donor[2].We show that this results in a very strong decrease of the overlap integrals with increasing external magnetic field.

In this paper the hopping magnetoabsorption of a semimagnetic semiconductor is calculated for the first time.The magnetization-dependent donor ground-state density is determined.The Fermi level is given as a function of compensation.The wave function of the donor ground state in a wurtzite-type semimagnetic semiconductor is calculated more accurately then in [2],including all terms of the second order in the uniaxial part of the Hamiltonian.The magnetization-dependent overlap integrals are obtained.Finally,the magnetoabsorption coefficient is calculated.

We present for the first time the measurements of magnetotransmission of $n\text{-}Cd_{1-x}Mn_xSe$, $0.05 \leq x \leq 0.20$,at LHeT in the broad wavelength region 0.1 to 2.5 mm,at the magnetic fields up to 6T.The comparison of the results with our theory is presented.

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DETERMINATION OF THE ANTIFERROMAGNETIC EXCHANGE COUPLING CONSTANT BETWEEN THE Mn^{++} ION PAIRS WITH $S = 5/2$ IN $Cd_{0.95}Mn_{0.05}Se$[*]

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We report the determination of the exchange coupling constant between the nearest-neighbor Mn^{++} ions in $Cd_{0.95}Mn_{0.05}Se$. Each Mn^{++} ion pair has a half-filled 3d shell, giving rise to total spin angular momentum $S = 5/2$. On application of a modest magnetic field, relatively isolated Mn^{++} ions interact strongly through exchange interaction with the conduction and valence band electrons of the host semiconductors, exhibiting unique optical, electrical and magnetic properties of semimagnetic semiconductors. Band electron - Mn^{++} ion exchange constants have now been determined for several materials including $Cd_{1-x}Mn_xSe$. These effects show modified Brillouin-like saturation when the isolated Mn^{++} ions and far-off neighbors are fully aligned. It turns out, however, that only ~60% of the total Mn^{++} present in $Cd_{0.95}Mn_{0.05}Se$ can be accounted for. Presumably, the rest are locked in antiferromagnetic pairs.

The Hamiltonian for the Mn^{++} pairs antiferromagnetic interaction is of the form

$$H = 2J\,\vec{S}_1\cdot\vec{S}_2 \tag{1}$$

which, for $S_1 = S_2 = 5/2$, may be written in the form

$$H = J\left[S(S+1) - \frac{35}{2}\right] \tag{2}$$

where J = pair exchange interaction and S = total spin of the pairs from $S = 0$ to $S = 5$. Thus, the ground state with $S = 0$ contributes no magnetic moment on the application of a modest magnetic field ≤ 9 T. However, on increasing the magnetic field, one Zeeman component of the $S = 1$ state begins to approach the magnetically-insensitive $S = 0$ state. At zero temperature we would expect to observe a step increase in magnetization when the lower energy Zeeman component of the $S = 1$ state crosses the $S = 0$ ground state. Extending this argument further, we expect a total of 5 steps with increasing magnetic field. Finite temperature will cause broadening of these steps. We have observed the first step at ~12 T and a second step at ~24 T (somewhat less conspicuously). The third, fourth and fifth steps should occur at 36 T, 48 T and 60 T, outside our present range. From our present measurements we deduce a value of $J \simeq 0.7 \times 10^{-3}$ eV or 7.5°K.

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[**] Supported by the National Science Foundation through its Division of Materials Research.

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Magnetic Semiconductors **FrP-E6**

OPTICAL PUMPING IN $Cd_{1-x}Mn_xTe$

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A first observation of spin orientation by optical pumping with non-resonant excitation is reported in $Cd_{1-x}Mn_xTe$ of low Mn mole fraction (below 0.01). It is detected by photoluminescence circular polarization measurements in the band gap region, mainly of bound exciton lines. A strong enhancement of the effect is observed under influence of a longitudinal magnetic field of a few Teslas.
An interpretation is proposed based on a simplified model assuming the carrier-magnetic ion interaction as a principal mechanism of carrier spin polarization decay.

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POST DEADLINE ABSTRACTS

NEW TYPE OF IMPURITY DEFECTS IN SEMI-INSULATING GaAs

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Rayleigh light scattering by optical inhomogeneities in semi-insulating gallium arsenide crystals was investigated in this work. As we use for a probe beam the CO_2-laser radiation (λ = 10.6μm), this method is sensitive for registration of large regions (a ~10 μm) with enhanced concentrations of dissolved electrically-active impurities.

The typical scattering diagrams by GaAs can be approximated by scattering at optical inhomogeneities with characteristic sizes: a_1~5 to15 μm. Decreasing of the sample temperature from 300°K to 77°K leads to disappearance of light scattering by 5%7 mm inhomogeneities. The initial scattering diagram was restored due to increasing of the sample temperature to the room one. The scattering intensity was not increased due to increasing of the sample temperature up to 400°K. These experiments show that inhomogeneities with a ~ 5 to 7 μm are the regions of charged impurity high concentration centres (and with high free carrier concentration of ~10^{16} cm^{-3}). It was established that the impurity agglomerations have spherical symmetry and the scattering intensity by the agglomerations is much higher in the samples with low ~ 102cm^{-2} dislocation density then in those with high ~ 105cm^{-2} density.

These experiments and the results of investigations on the influence of high ~ 900°C temperature annealing on light scattering help us to understand the nature of the impurity agglomerations. We think that a mechanism of their formation is a dissolution of impurity inclusions at high temperatures, subsequent diffusion of neutral impurities and finally interaction of neutral impurities with fast-diffusing impurities.

PD-2 TuP-PJ20

DIRECT EXPERIMENTAL EVALUATION OF THE ELECTRON IMPACT EXCITATION CROSS SECTION OF Mn^{2+} IN ZnS

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Some years ago the impact excitability of Mn^{2+} in ZnSe has been proven /1/ and a rather high cross section has been found to be probable. The success of the ZnS:Mn thin film electroluminescence devices introduced by Inoguchi /2/ boosted the interest in the details of this clearly electron impact excited emission process. Theoretical estimates /3/ of the impact cross section σ of the ground state $^6A_1 \rightarrow$ first excited (crystal field split) state $^4T_1$ were not far from the geometrical cross section of the $3d^5$ electron of the Mn^{2+} ion. In a careful analysis of the basic processes involved in the excitation/emission process of a.c. driven MISIM structures of the Inoguchi /2/ type we have managed for the first time to evaluate directly σ. This was possible by introducing the concept of partial efficiencies /4/ factorizing the (measured) efficiency which can easily be given in photons/transferred electron. These partial efficiencies characterize the independent elementary processes involved: excitation of Mn^{2+} by (at least 2.5 eV hot) electrons $-\eta_{exc}$; radiative deexcitation of the excited Mn^{2+} $-\eta_{lum}$, and optical outcoupling of the photons produced $-\eta_{opt}$. The plausible assumptions $\eta_{exc} = \sigma \cdot [Mn^{2+}]$; $\eta_{lum} = \tau_{meas}/\tau_{rad}$; $\tau_{opt} = 1 - \sqrt{1-1/n^2}$, with τ_{meas} being the measured luminescence decay time, τ_{rad} the radiative lifetime of the Mn^{2+} excited state; n the refractive index at the emission wavelength, can be justified experimentally. The procedure outlined results in a value $\sigma = 4.10^{-16}$ cm^2 ($\pm$ 20 %) which is about a factor of 2 higher than the theoretical estimate.

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The expert preparation of the MISIM structures by Dr. Gericke and J.v.Kalben is gratefully acknowledged.

THE INFLUENCE OF V, Nb AND Hf IMPURITIES ON THE OPTICAL AND ELECTRONIC PROPERTIES OF TiS_2 AND $TiSe_2$

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Single crystals of the degenerate semiconductor TiS_2, the semimetal $TiSe_2$, and the mixed solid solutions $Ti_{1-x}M_x(S,Se)_2$ with M = V, Nb and Hf have been grown by chemical transport reactions.

The optical spectra (Polarisation: $\vec{E} \perp \vec{c}$, spectral range: 5 meV - 3.75 eV) display features which are attributed to a polar phonon of E_u symmetry, to a collective oscillation of the free carriers (plasmons), and to interband transitions which occur for energies > 1 eV.

Through the analysis of the optical properties in terms of a dielectric function $\varepsilon(\omega)$ composed of the above mentionned elementary excitations we get a new insight into the physics of these high polarisable two dimensional materials.

The lattice vibrations are discussed taking into account the correct local field for the polar modes of crystals with layered structure. From the optical data we deduce the Born effective charges, the Szigeti charges and the contribution of the long-range forces to the energies of the E_u TO modes.

The study of the influence of impurities on the optical behaviour of the free carriers is complimented by transport measurements. The most pronounced effects are observed in $Ti_{1-x}V_xS_2$ and $Ti_{1-x}V_xSe_2$, where at low V concentrations a localisation of charge carriers occurs, thus yielding non-metallic phases. These results will be discussed in relation with angular resolved photoemission measurements where the existence of a localised impurity band has been observed in connection with V^{3+} and/or V^{2+} impurity centers.

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QUASI-ELASTIC LIGHT SCATTERING FROM SILICON AND DIAMOND

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We report a detailed study of light scattering from silicon and diamond crystals in the frequency range 0 to ±200 GHz and as a function of wavevector transfer (Q) and temperature (T). At elevated temperatures the spectra for both materials contain strong quasielestic, central components in addition to finite frequency peaks associated with acoustic vibrational modes.

In silicon, a single central component is observed. Analysis of the results suggest that it arises from second order phonon difference scattering processes involving phonons on the same dispersion branch, contributions from optic branches being dominant.

In contrast, the spectra for diamond contain two central features, one which is broad (~100 GHz) and non-Lorentzian the other relatively narrow (i/2p e 10 GHz) with Lorentzian shape. The broad component is qualitatively consistent with two-phonon difference scattering by acoustic modes. the narrow component is not observed at low temperature, but becomes dominant at high T and low Q where it acquires the characteristics of scattering by entropy fluctuations, i.e. i e DTQ2 where DT is the thermal diffusivity.

These results demonstrate clearly for the first time the manner in which a two-phonon difference spectrum in the collision-free regime (low T and large Q) develops into entropy fluctuation scattering in the collision-dominated regime (high T and low Q).

SOLUTION TO THE PROBLEM OF RECOMBINATION VIA DEEP IMPURITIES: THE DECISIVE ROLE OF FREE EXCITONS

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The physical nature of the carrier capture process into deep impurity levels in silicon is not sufficiently understood up to now. In this paper we present conclusive experimental evidence for Coulomb-enhanced Auger recombination at deep impurity levels. A complete and quantitative description of the recombination lifetimes of silicon containing deep impurities is now possible.

The new concept of an excitonic Auger process at deep levels becomes evident from the following time resolved photoluminescence measurements in Si:Cr, Si:Fe, and Si:Au:

- The temperature dependence of the carrier lifetime is analogous to the thermal ionization of free excitons, i.e. constant in the range 4 - 60 K (capture cross section $\approx 10^{-13}cm^2$) and *linearly* increasing above 60 K.
- An additionally applied electric field capable of ionizing the excitons leads to a considerable increase of the carrier lifetime.
- Screening of the excitons at high excitation levels near the "Mott-density" increases the lifetime strongly.
- We have direct evidence for the highly excited Auger particle generated by the recombination.

Our new model assumes an Auger recombination via deep impurities, which is strongly enhanced by the attractive Coulomb interaction between electrons and holes, leading to the formation of free excitons. For example, an ionized donor-like trap captures the electron from the exciton, whereas the hole is excited into the valence band. The efficiency of this process itself is independent of temperature. The calculated capture cross sections are of the order $10^{-13}cm^2$. Ionization of the excitons results in a decrease of the enhancement and therefore in an increase of carrier lifetime. In our experiments this is demonstrated by thermal ionization, by impact ionization within an electric field, and by screening of the Coulomb interaction at high excitation densities.

In summary, we have shown experimentally by three different methods that the recombination rate via deep impurities depends strongly on the Coulomb correlation of the carriers. Our new model gives a consistent interpretation of the experimental facts.

ICPS NAME INDEX