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This, the Final Scientific Report on AFOSR Grant # 86-0166, provides the highlights of the work accomplished under the project. While the details are to be found in the publications listed as part of the report, the major accomplishments are: (1) identification of growth kinetics optimized and reproducible growth, independent of machine parameters, of GaAs/AlGaAs and GaAs/InGaAs layered structures via the usage of real time reflection high energy electron diffraction in molecular beam epitaxical growth, (2) the first realization of high mobility inverted HEMT structures, (3) demonstration of the dominant scattering from band edge discontinuity fluctuations, rather than the commonly held view of well width fluctuations in high quality GaAs/AlGaAs quantum well structures, (4) demonstration of in-situ growth of laterally confined structures and, (5) demonstration of defect reduction in strained growth via growth on prepatterned GaAs substrates.

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FINAL SCIENTIFIC REPORT
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KINETIC ASPECTS OF LATTICE MISMATCH IN MOLECULAR BEAM EPITAXICAL GROWTH ON PLANAR AND PATTERNED SUBSTRATES

SUBMITTED TO

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
ELECTRONIC AND MATERIAL SCIENCES DIRECTORATE
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CONTENTS

ABSTRACT

This, the Final Scientific Report on AFOSR Contract No. 86-0166, provides the highlights of the work accomplished under the contract. The details are to be found in the publications listed as part of the report.

I. SALIENT ACCOMPLISHMENTS

Under the AFOSR Grant (No. 86-0166) a variety of significant results have been obtained and published. A list of these publications, conference presentations, and graduate student/post-doctoral associates trained is provided in subsequent sections. In the interest of brevity here we note the highlights of some of the major projects undertaken.

I.A. ESTABLISHING RHEED AS IN-SITU, REAL TIME MONITOR OF GROWTH CONDITIONS:

Under the present contract we undertook systematic and extensive studies of RHEED intensity behavior and demonstrated its power as a pragmatic, real-time, monitoring tool for establishing growth conditions reproducibly, without reliance on the MBE machine measuring instruments such as gauges and thermocouples. This also permits the only means of comparison between the results from different machines. Both these aspects are of crucial importance to scientific and pragmatic considerations of MBE technology.

Our approach was one of reliance on the intrinsic nature of the sample surface to establish whether the same growth *conditions* (*i.e. substrate temperature* (T_s), group III pressure, and group V pressure (P_V)) are obtained when desired. To this end we examined the RHEED specular beam intensity behavior of STATIC GaAs(100) and $Al_xGa_{1-x}As$(100) surfaces as a function of T_s and P_V covering the range of surface reconstructions exhibited (i.e. As(2x4), the transition region (3x1), and the Ga(4x2)) with particular emphasis on the behavior within the As(2x4) region commonly employed for growth. This behavior was also studied as a function of the **diffraction conditions**: the angle and azimuth of incidence. Characteristic signatures were thus obtained, including the demonstration of regimes of reversible and irreversible behavior.

Next, we examined the dynamics of the of the specular beam intensity during growth under group III controlled growth conditions - the commonly employed situation. The behavior of the oscillation damping, the average value, the steady state value, and the intensity recovery upon growth termination at various stages of deposition was examined as a function of T_s, P_V, and growth rate. This was also studied as a function of the diffraction conditions. Finally, group V (i.e. arsenic) controlled growth was studied to establish a direct calibration of the group V beam equivalent pressure (as read by the ion gauge) using the arsenic incorporation rate at various substrate temperatures. The characteristic features of the specular beam behavior both in the absence and presence of growth under the first out-of-phase diffraction condition with respect to As-to-As adjacent (100) atomic plane separation were together shown to provide a reliable means of ensuring reproducible growth conditions. Details may be found in publications 2,5 and 10 and the references to our earlier work given therein.

I.B. DETERMINATION OF OPTIMIZED GROWTH CONDITIONS:

In addition, in conjunction with theoretical modelling and realistic computer simulations of MBE carried out largely under ONR sponsorship, the measured static and dynamic RHEED specular beam intensity behavior was shown to reveal the nature of the growth front and its evolution in response to the growth kinetics operative as a function of the chosen T_s, P_V and growth rate. Regimes of growth parameters for achieving optimized surface and growth front structural smoothness were thus demonstrated, making RHEED a powerful tool for achieving high quality interfaces. As a practical test of the reliability of RHEED behavior for determination of optimized growth conditions, a direct correlation between RHEED behavior and the optical properties (near-edge luminescence, Raman and Rayleigh scattering) of $Al_xGa_{1-x}As$ and $GaAs/Al_xGa_{1-x}As$ single and multiple quantum wells was demonstrated. Comparative studies between structures grown without and with growth interruption at the heterointerfaces under various RHEED determined growth conditions further substantiated the essential correctness and pragmatic value of the RHEED and optical behavior correlation established. The findings were reported in publications 1,3,4,6,8,13,18,20,21 and 22.

I.C. DEMONSTRATION OF BAND-EDGE DISCONTINUITY FLUCTUATIONS:

A study of the free-exciton photoluminescence (PL) line width dependence on the well width of $GaAs/Al_{0.3}Ga_{0.7}As(100)$ single quantum wells grown, without interruption, under RHEED determined identical and optimized growth conditions was undertaken. The well widths varied from 5 ML to 40 ML. The absolute linewidths were amongst the narrowest ever found testifying to the high quality of the samples. Of more fundamental physical significance, the linewidth (Γ_{PL}) was found to be nearly inversely proportional to the well width

(d_w). The observed $\Gamma_{PL} \sim d_w^{-1}$ relationship demonstrated for the first time that the commonly and routinely employed (though without any demonstrated basis) notion of well-width fluctuations which gives $\Gamma_{PL} \sim d_w^{-3}$ is not operative in high interfacial quality samples. Once again, through insights on the atomistic chemical nature of interfaces derived from the computer simulations, we proposed the view that the band-edge discontinuity fluctuations arising from the lateral variations in the alloy concentration on the exciton size length scale are responsible for the observed behavior. Calculations of Γ_{PL} versus d_w based upon this view were carried out and the dependence shown to conform to the experiments. The absolute magnitudes of the observed Γ_{PL} values required alloy concentration fluctuation amplitude of ~ 1% over a lateral correlation length of ~ 30°A. Details may be found in publications 3,6,9 and 15.

I.D. REALIZATION OF HIGH MOBILITY INVERTED-HEMT:

Having established a correlation between RHEED behavior and the optical properties of AlGaAs films and $GaAs/Al_xGa_{1-x}As$ interfaces in quantum well structures, we naturally addressed the issue of whether RHEED could be used to identify the growth conditions appropriate for the realization of good electrical properties as well. It must be recognized that the optical and electrical properties are not necessarily influenced to the same degree by the same scattering centers and consequently the choice of optimized growth conditions need not be the same. We focussed attention on the growth of the **inverted** (i.e. GaAs grown on $Al_xGa_{1-x}As$) HEMT as the more challenging problem since numerous previous attempts to realize high electron mobility in such structures had been unsuccessful. Through our work on the RHEED studies of the $Al_xGa_{1-x}As$ static surface and the growth of $Al_xGa_{1-x}As$ we had already identified the growth conditions needed for high quality inverted interfaces. However, for realizing high mobilities in the I-HEMT, the competing kinetics of Si dopant incorporation and out-diffusion had to be accounted for, apart from a means of minimizing the incorporation of the carbon impurity from the background and its tendency to surface-ride the $Al_xGa_{1-x}As$ growth front. We optimized between the competing need for high T_s to achieve high $Al_xGa_{1-x}As$ growth front smoothness and low T_s to reduce Si out-diffusion by introducing the following procedure: Grow UNDOPED $Al_{0.3}Ga_{0.7}As$ at an intermediate temperature of ~610°C at a slower growth rate (0.25 μm/hr) and at optimized As_4 pressure as indicated by RHEED. To maintain growth front smoothness and prevent accumulation of carbon, periodically stop the Al flux, permit growth of $\leq$ 1 ML of GaAs and then stop Ga flux to cause growth interruption and allow the faster migration kinetics of Ga to smoothen the growth front. Having grown the required thickness of the undoped AlGaAs in this fashion, lower the T_s to between 500°C and 550°C during doping of the AlGaAs layer, resuming T_s and the interjection of $\leq$ 1 ML of GaAs during growth of the AlGaAs spacer layer, ensuring no growth interruption at the inverted interface.

Following such RHEED optimized procedure we demonstrated dramatic improvement in the electron mobility over those obtained via conventional approaches. Absolute values of the LN_2 mobilities in excess of 10^5 Cm^2/V-Sec for carrier densities ~ 6-7x10^{11}/Cm^2 were thus demonstrated. In more recent times, using our new RIBER 3200 P MBE system, we have achieved the unprecedented values of LN_2 dark mobilities near 180,000 Cm^2/V-Sec at the extremely low carrier densities of ~ 4x10^{10}/Cm^2. We emphasize that all these extremely high mobility values have been achieved for the first time and that too without the usage of short period superlattices, unrealistically large spacer layers, and δ-doping. These results are to be found in publications 5,14,15,16 and 17.

I.E. GROWTH ON PATTERNED GaAs(100) SUBSTRATES:

In early Fall '87 we initiated work on the growth of $Al_xGa_{1-x}As$ and $In_xGa_{1-x}As$ on pre-patterned GaAs(100) substrates. The patterning was done via optical lithography and wet chemical etching. The work is motivated by our main focus on in-situ pre- and post-growth patterning and growth/regrowth on substrates with lateral pattern dimensions between 0.05μm to 2 μm. The range below 1 μm is to be achieved via a focussed ion beam (FIB) direct write system on order and to be UHV interconnected to the MBE growth chamber. While awaiting the arrival of this custom designed system as well as a plasma enhanced CVD (PECVD) system interfaced to the FIB and MBE systems (both ordered under this AFOSR contract), we undertook studies on ex-situ optically patterned and chemically etched substrates with lateral dimensions $\geq$ 1 μm since (a) this subject itself is in its infancy and much relating to growth kinetics, mechanism(s) and growth conditions needs to be examined, and (b) such studies provide a focus for identifying the issues that would have to be dealt with in moving the smaller lateral sizes.

For the lattice matched GaAs/AlxGa1-xAs system our investigations focussed on (i) the starting etched surface profile dependence on the chemical etching procedures, including the subsequent MBE substrate free etch and thermal oxide desorption, and (ii) the nature and role of the interfacet migration. These are reported in publication no. 23. Utilizing the nature of the interfacet migration, we demonstrated the first, all in-situ, fabrication of laterally confined structures.

For the strained InxGa1-xAs/GaAs system, growth on patterned substrates containing stripes of widths 1μm to 5μm or rectangular mesas of linear dimensions 10μm to 20μm were carried out as a function of In composition and growth conditions. Single epilayers of various thicknesses as well as multiple quantum well (MQW) structures, including InAs/GaAs short-period superlattices, were examined. A reduction in the defect density due to strain relief at mesa edges was demonstrated, along with interesting optical absorption modulation characteristics in thick ($\geq 1\,\mu$m) MQW structures with In content as high as 20%. Details may be found in publications 24, 26 and 27.

I.F. DESIGN AND ACQUISITION OF FIB AND PECVD SYSTEMS FOR IN-SITU PROCESSING:

A major effort was devoted towards the design and acquisition of a focussed ion beam (FIB) system and plasma enhanced chemical vapor depostion (PECVD) system interfaceable to the RIBER 32P MBE growth system. To our knowledge, this is the only system of its kind and enables, for the first time, exploration of many basic materials and device processing issues central to future semiconductor technologies, particularly opto-electronic integrated components and circuits.

Working together with the Riber Division of Instruments S.A. Inc. (manufacturers of our RIBER 32P MBE growth and metallization chambers), Alcatel (manufacturers of the PECVD system), FEI (manufacturers of the focussed ion gun and control system) and Thermionics Northwest (manufacturers of the FIB manipulator), we tackled many engineering and scientific issues relating to UHV integrity, sample transfer and manipulation, vibration isolation, appropriate pumping, safety requirements of the gases to be used in the PECVD, etc. The system has arrived at Alcatel facilities in San Jose (California) where it is under test. We expect it to be tested and ready for research by end of 1990.

I. AFOSR SUPPORTED PUBLICATIONS:

J.Y. Kim, F. Voillot, P. Chen, A. Madhukar, N.M. Cho and W.C. Tang, "A Photoluminescence Study of GaAs/$Al_xGa_{1-x}As$ (100) Single Quantum Wells Grown via MBE under RHEED Determined Optimized Growth Conditions for Continuous and Interrupted Growth", Jour. Elec. Materials, 15, 317 (1986).

P. Chen, A. Madhukar, J.Y. Kim and N.M. Cho, "The Nature of Surface Migration During MBE Growth of III-V Compounds: a Study via the RHEED Specular Beam Intensity Dynamics", Proceedings of the 18th International Conference of Physics of Semiconductors, (Stockholm, Sweden, Aug. 11-15, 1986) Ed. OLOF ENGSTROM (World Scientific Press, Singapore), Vol. 1, p.109 (1987).

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10. P. Chen, T.C. Lee, N.M. Cho and A. Madhukar, "RHEED as a Tool for Examining Kinetic Processes at MBE Grown Surfaces", Proceedings of SPIE Conference on Advances in Semiconductors and Semiconductor Structures, Mariott's Bay Point Resort, Florida, March 22-27, 1987; SPIE Vol. No. 796, 139 (1987).

11. A. Madhukar, P.D. Lao, W.C. Tang, M. Aidan and F. Voillot, "Observation of Phonon Modes through Resonant Mixing with Electronic States in the Secondary Emission Spectra of $GaAs/Al_{0.32}Ga_{0.68}As$ Single Quantum Well", Phys. Rev. Lett. 59, 1313 (1987).

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14. Anupam Madhukar, "Exploiting Kinetics in Molecular Beam Epitaxial Growth for Realization of High Quality Normal and Inverted Interfaces", Workshop on HEMT, Organized by U.S. Army Electronics and Device Technology Laboratory, Ft. Monmouth, New Jersey, Jan, 27-28, 1988.

15. Anupam Madhukar, "The Atomistic Nature of Compound Semiconductor Interfaces and the Role of Growth Interrup-tion", MRS Symposium Proceedings, Vol. 102, entitled, Epitaxy of Semicondcutors, (Eds. R.T. Tung, L.R. Dawson and R.L. Gunshor) p.3. (1988).

16. P.G. Newman, N.M.Cho, D.J.Kim, A.Madhukar, D.D.Smith, T.R.Aucoin and G.J.Iafrate, "Surface Kinetic Considerations for MBE Growth of High Quality Inverted Heterointerfaces", Proceedings of the 15th PCSI Conference, (Feb. 1-4, 1988; Asilomar, Ca.); Jour. Vac. Sc. Tech.B6, 1483 (1988).

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19. W.C. Tang, Pudong Lao, and A. Madhukar, "Optical Investigation of Resonant Mixing Between Electronic and Optical Vibrational Levels in $GaAs/Al_xGa_{1-x}As$ Single Quantum Wells", Proceedings of the SPIE Conference on "Advances in Semiconductors and Superconductors;

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23. S. Guha, A. Madhukar, K. Kaviani, L. Chen, R. Kuchibhotla, R. Kapre, M. Hyugaji and S. Xie, "Molecular Beam Epitaxical growth of $Al_xGa_{1-x}As$ on non-planar Patterned GaAs (001)", MRS Spring Meeting, Symposium on "III-V Heterostructures for Electronic/Photonic Devices", San Diego, CA (April 1989), Vol. 145, P.27 (1990).

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CONFERENCE PRESENTATIONS:

1. J.Y. Kim, F. Voillot, P. Chen, A. Madhukar, N.M. Cho and W.C. Tang, "A Photoluminescence Study of $GaAs/Al_xGa_{1-x}As(100)$ Single Quantum Wells Grown via MBE under RHEED Determined Optimized Growth Conditions for Continuous and Interrupted Growth", Electronic Materials Conference, Amherst, Ma. (June 1986).

2. P. Chen, A. Madhukar, J.Y. Kim and N.M. Cho, "The Nature of Surface Migration During MBE Growth of III-V Compounds: a Study via the RHEED Specular Beam Intensity Dynamics", Proceedings of the 18th International Conference of Physics of Semiconductors, Stockholm, Sweden (Aug. 11-15, 1986).

3. A. Madhukar, P. Chen, F. Voillot, M. Thomsen, J.Y. Kim, W.C. Tang and S.V. Ghaisas, "A Combined Computer Simulation, RHEED Intensity Dynamics and Photoluminescence Study of the Surface Kinetics Controlled Interface Formation in MBE Grown GaAs/$Al_xGa_{1-x}As$(100) Quantum Well Structures", International MBE Conference, York, U.K. (Aug. 1986).

4. P. Chen, T.C. Lee, N.M. Cho and A. Madhukar, "RHEED as a Tool for Examining Kinetic Processes at MBE Grown Surfaces", SPIE Conference on Advances in Semiconductors and Semiconductor Structures", Mariott's Bay Point Resort, Florida, March 22-27, 1987.

5. A. Madhukar, "Molecular Beam Epitaxial Growth Kinetics, Mechanism(s) and Interface Formation: Computer Simulations and Experiments", Proceedings of the NATO Advanced Research Workshop, Glasgow, Scotland, Sept. 9-11, 1986, entitled "Thin Film Growth Techniques for Low-dimensional Structures".

6. P.D. Lao, W.C. Tang, A. Madhukar and F. Voillot, "Resonant Mixing between Electronic and Optical Vibrational States of a Quantum Well Structure", 3rd International Conference on "Modulated Semiconductor Structures", Montpellier, France, (July 1987).

7. Anupam Madhukar, "The Atomistic Nature of Compound Semiconductor Interfaces and the Role of Growth Interruption", MRS Symposium on Epitaxy of Semicondcutors, Boston, Ma. (Dec. 1987).

8. P.G. Newman, N.M.Cho, D.J.Kim, A.Madhukar, D.D.Smith, T.R.Aucoin and G.J.Iafrate, "Surface Kinetic Considerations for MBE Growth of High Quality Inverted Heterointerfaces", 15th PCSI Conference, Asilomar, Ca. (Feb. 1-4, 1988).

9. Pudong Lao, Wade C. Tang, A. Madhukar and P. Chen, "Alloy Disorder Effects in Molecular Beam Epitaxically Grown $Al_xGa_{1-x}As$ Examined Via Raman and Rayleigh Scattering and near Edge Luminescence", Proceedings of the SPIE Conference on "Advances in Semiconductors and Superconductors: Physics and Device Applications", Newport Beach Mariott Hotel, CA (13-18 March, 1988).

10. W.C. Tang, Pudong Lao, and A. Madhukar, "Optical Investigation of Resonant Mixing Between Electronic and Optical Vibrational Levels in GaAs/$Al_xGa_{1-x}As$ Single Quantum Wells", SPIE Conference on "Advances in Semiconductors and Superconductors; Physics and Device Applications", Newport Beach Mariott Hotel, CA. (13-18 March, 1988).

11. W.C. Tang, P.D. Lao, and A. Madhukar, "Atomistic Nature of Molecular Beam Epitaxically Grown GaAs/$Al_xGa_{1-x}As$(100) as Revealed in Luminescence and Raman Spectroscopies", SPIE Conference on "Lasers and Optics; Superlattices and Quantum Wells", Los Angeles, Ca. (Jan. 1989).

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