FINAL REPORT

CONTRACT NO.: ONR N00014-89-J-1157

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I. OBJECTIVE:

To perform theoretical studies on the electronic, transport and magnetic properties of magnetic multilayers and metal-semiconductor superlattices.

II. APPROACH:

We perform both first-principle and empirical tight-binding calculations on the band structures of metal-metal and metal-semiconductor superlattices. The materials of interest include superlattices made of transition-metals [(Fe,Co)/Cu, Fe/Cr], rare earths (Gd/Y, Dy/Y, Er/Y) and semimetal-semiconductor combinations [(Er, Gd)As/(Al,Ga)As]. The conduction electron mediated indirect exchange interaction (RKKY interaction) between magnetic atoms in these superlattices is calculated. The transport properties of these superlattices have also been studied.

III. PROGRESS (1990-1993):

A. Electronic structures and exchange interaction of magnetic multilayers

We have performed calculations of Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions of Gd/Y superlattices by using a simple one-band model. Our predictions of ferromagnetic coupling for $(Gd)_{10}/(Y)_6$ and antiferromagnetic coupling for $(Gd)_{10}/(Y)_{10}$ superlattices are in agreement with experimental observation.

We have also calculated the RKKY interaction in transition metal/noble metal superlattices within a one-band tight-binding model. An accurate and efficient integration scheme in momentum space is introduced to calculate the RKKY exchange interaction in superlattices. This is accomplished by writing the superlattice states in terms of linear combinations of complex-band solutions in analytic form, and dividing the integration domain into many subregions according to the shape of the superlattice Fermi surface in order to take into account the singularities in one-dimensional density of states. The results are compared to those obtained from

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Re: Final Technical Report for N00014-89-J-1157

To whom it may concern:

Enclosed is the Final Technical Report for N00014-89-J-1157. The report was prepared by Principal Investigator, Professor Y.-C. Chang.

If you require additional information, please let me know.

Sincerely,

Carolyn J. Wright

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using the bulk wave functions of the spacer layer and apparent deviations due to the superlattice effect are noted.

B. Electronic structures of metal-semiconductor superlattices

We have performed the first theoretical calculation of electronic structures of semimetal-semiconductor superlattices made of GdAs and GaAs using by a second-neighbor tight-binding model. It is found that this semimetal-semiconductor superlattice is metallic with overlapping conduction and valence bands for GdAs layers as thin as two monolayers. This is in qualitative agreement with recent experimental observation, while in contrast with the prediction based on a simple effective-mass model. The superlattice states with energies near the Fermi surface consist of states derived from the GdAs valence bands and the lowest GdAs conduction bands with wave vectors near X. It is shown that near the X point one of the GdAs heavy-hole band turns into a conduction band along the X-K direction which prevents the superlattice from turning into a semiconductor.

C. Theory for excitons bound to isoelectronic Te traps in ZnSe quantum wells

Excitons bound to Te isoelectronic traps in ZnSe are responsible for the prominent feature in the photoluminescence spectra. These systems have potential application in light-emitting diodes in the blue region. Thus it is important to understand their optical properties. We have performed the first realistic calculation of excitons and holes bound to a single isoelectronic Te impurity in bulk ZnSe and centered in ZnSe/$Zn_{1-x}Mn_xSe$ quantum wells. We use the novel effective bond-orbital model for the holes in order to account for the complicated valence-band structure and the spherical effective-mass approximation for the electron. The mutual Coulomb interaction is included, and solutions for the two-body system are obtained using variational method in an iterative scheme. The strong lattice-relaxation effects are absorbed in the value for the localized potential at the site of the impurity which is determined by fitting the binding energy of the bound exciton to the experimental value. We predicted the binding energy of a hole bound to the isoelectronic trap and the oscillator strengths of an exciton bound to the trap.

D. Magneto-transport properties of the magnetic superlattices and granular solids

We have presented a new framework for dealing with magneto-transport in magnetic granular solids and superlattices. We have demonstrated that the unfilled d bands of magnetic grains play an essential role in the magneto-transport properties of the system. It was shown that both the remarkable GMR and the giant magneto-thermopower effects arise naturally from spin-dependent s-d scattering rates due to

the different density of states for majority and minority d bands of the magnetic entities. Explicit expressions for the GMR and the magneto-thermopower have been obtained. Our formulas relate the GMR and magneto-thermopower to the microscopic and geometric quantities. The size-dependence and the $(M/M_s)^2$ behavior of the GMR, the $1/\rho$ scaling of the magneto-thermopower, and the absence of the negative GMR in the rare-earth structures are all explained by our model.

E. Resonant tunneling of Si-based double-barrier structures

Resonant-tunneling characteristics of electrons in Si/Ge strained-layer double-barrier structures are investigated within an antibonding-orbital model. The model is capable of describing the low-lying conduction bands accurately throughout the entire Brillouin zone. I-V curves for some selected Si/Ge strained-layer double-barrier structures for three different crystallographic orientations are studied. Negative differential resistances are found for these structures grown along [001] and [111] directions, but not along the [110] direction.

We have also developed a two-band effective-mass model to study the resonant tunneling effect for a structure in which a heavy-mass state interacts with a light-mass state, leading to a Fano type interference effect. By analyzing the interference structure in the resonant-tunneling spectra, one can obtain a direct measurement of the strength of band mixing occurred in semiconductor heterostructures.

E. Development of a new first-principle method by using planar orbitals

We have recently developed a first-principle pseudopotential method based on a new planar-like basis. Unlike conventional methods in which three-dimensional plane waves are used as the basis, we use the products of two-dimensional plane waves and one-dimensional Gaussian functions (along the growth axis) as our basis. The new basis has the advantage over the conventional basis in that the layer-like local geometry which appears in the heterostructure is naturally built in. This would not only make the computation much more efficient but also lead to better analysis of interface properties in terms of localized functions, such as layer-resolved local density of states. We have successfully applied the new method to study the electronic structures and work function of Si (001) 2×1 surface with symmetric dimer reconstruction with and without hydrogen passivation. We have also calculated the hydrogen dissociation energy and the result is in accord with previous experimental findings.

In the future, this method will be applied to transition-metal superlattices to obtain the electronic structure and exchange interactions.

F. Quantum Monte Carlo Studies of Polyexcitons and bound mult-exciton complexes in Semiconductors

Variational Monte Carlo method was used to calculate the binding energies and ground state wavefunctions of two, three, and four multiexciton complexes, in the spherical effective mass approximation. The method is capable of predicting accurate binding energies of highly correlated systems, and we apply it to the polyexciton systems for the first time. The binding energies of these systems have recently been measured and no theoretical calculations beyond two-exciton complexes are available. For three- and four-exciton complexes in Si, we predict that the binding energy with respect to the smaller complex with one less exciton is about $2.2meV$, in fair agreement with the experimental value of $2.5meV$.

We have also calculated the rate of radiative recombination of an exciton bound to a shallow impurity in direct-gap semiconductors. The electron and hole excitations of the crystal are described in the spherical mass approximation, in which the nature of the bound exciton is parametrized by the electron-hole mass ratio, σ, and donor and acceptor bound excitons are treated on an equal footing. The overlap integral of the initial and final states of the crystal is calculated for various values of σ.

G. Raman Spectra in GaAs-AlAs Superlattices

We have performed theoretical studies on Raman scattering of GaAs-AlAs superlattices. Both effects of superlattice phonons and electronic structures are included in our calculation. For phonons in superlattices, we used a rigid-ion model which takes into account the long-range Coulomb interaction properly. Combining it with a bond orbital model for the electronic states in superlattices, we have studied nonresonant Raman scattering of GaAs/AlAs superlattices for both optical phonons and acoustic phonons. For optical phonons, we have considered both $z(xy)\bar{z}$ and $z(xx)\bar{z}$ geometries. Our calculations are compared with the available experimental data with favorable agreement.

Publications of Yia-Chung Chang supported by ONR-N00014-89-J-1157 (Nov. 1, 1990 – Oct. 31, 1993)

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2. **Electronic Structures of GdAs-GaAs Metal-semiconductor Superlattices** , J. B. Xia, S. F. Ren, and Y. C. Chang, Phys. Rev. **B43**, 1692-8 (1991).

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4. **Optical Phonons in GaAs/AlAs Quantum Wires**, S. F. Ren and Y. C. Chang, Phys. Rev. **B43**, 11857 (1991).

5. **Theory of Excitons Bound to Isoelectronic Te Traps in ZnSe Quantum Wells**, G. T. Einevoll, D. S. Citrin, and Y. C. Chang, Phys. Rev. B **44**, 8068-8083 (1991).

6. **Optical Phonons in GaAs/AlAs Quantum Wires**, S. F. Ren and Y. C. Chang, Phys. Rev. **B43**, 11857 (1991).

7. **Theory of Optical Properties of Quantum Wires in Porous Si**, G. D. Sanders and Y. C. Chang, Phys. Rev. **B45**, 9202 (1992).

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13. **Theory of electron resonant tunneling of Si-based double-barrier tunneling structures**, J. C. Chiang and Y. C. Chang, J. Appl. Phys. 73, 2402 (1993).

14. **Interference effects in the resonant tunneling spectrum**, J. C. Chiang and Y. C. Chang, Phys. Rev. B 47, 7140 (1993).

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16. **Theory of Electronic structures of porous Si**, J. B. Xia and Y. C. Chang, Phys. Rev. B 48, 5179 (1993).

17. **Giant Magnetoresistance in Magnetic Granular Solids**, L. Xing and Y. C. Chang, Phys. Rev. B 48, 4156 (1993).

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19. **Planar-basis Pseudopotential Calculations of Si (001) 2X1 Surface with and without Hydrogen Passivation**, G. Li and Y. C. Chang, Phys. Rev. B48, 12032 (1993).

Papers submitted to refereed journals:

1. **Complex-band Method for Claculating Ruderman-Kittel-Kasuya-Yosida Interaction in Magnetic Superlattcies**, B. Lee and Y. C. Chang, Phys. Rev. B (in press).