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Final Technical Report

for ONR Contract #N00014-88-K-0268

entitled

Theory of the Electronic and Optical Properties of Semiconductor Heterostructures

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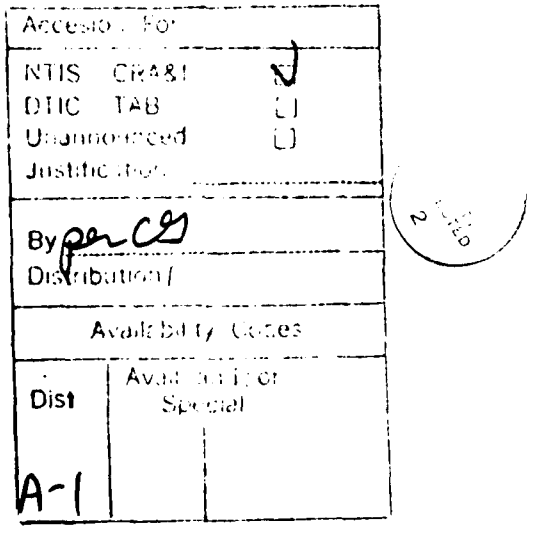

I. Summary of Research Accomplished

Introduction

The optical spectrum of quantum wells is characterized by a series of excitonic peaks corresponding roughly to transitions between valence and conduction subband pairs subject to appropriate selection rules. In a simple model where these subbands are taken to be parabolic, the exciton spectrum for each subband pair follows a hydrogen-like series, with each exciton characterized by a two dimensional (2D) angular momentum symmetry e.g. 1s, 2s, 2p, 3d, etc. Accounting for the two types of valence subbands (heavy hole and light hole) and for the fact that only excitons with s symmetry are optically active (i.e. contribute to the oscillator strength), the excitonic transitions can then be labeled 11H(1s), 11L (1s), etc. Here, the first two indices designate the conduction and heavy (H) or light (L) hole valence subbands, respectively.

For zincblende structures such as GaAs the conduction subbands can in fact be approximated accurately by parabolas. The valence subbands are, however, much more complicated because of the four-fold degeneracy of the bulk heavy and light hole valence bands at the valence band edge. This degeneracy causes the heavy and light hole subbands to be coupled resulting in the so-called valence band mixing (VBM) effects, such as 1) Strong nonparabolicities and anisotropy in the valence subband structure;[1-3] 2) Magnetic field-dependent cyclotron masses;[1,2] 3) Mixing of Excitons and resulting effects on the optical absorption.[4-6]

The aim of this work has been to examine the theoretical basis for these latter effects. The theory developed employs the multi-band effective mass approximation for quantum well excitons. First, the subband structure for

electrons and holes is calculated. The coupled, nonparabolic heavy and light hole subbands are obtained from a 4x4 effective mass equation following the method of Broido and Sham.[3] The four-component subband wave functions reflect the mixing between the heavy and light hole states. The exciton wave function is then expanded in terms of products of the electron and hole subband functions with different in-plane wave vectors, **k**, and different electron and hole subband indices, n and m, respectively (n=1,2,3..., m=1H, 1L, 2H, ...). From this expansion, a set of coupled integral eigenvalue equations is derived whose solution gives the excitonic spectrum of the quantum well. A quadrature method is used here, which has the advantage of providing not only the bound exciton states but also a discrete set of continuum states. Excitons lying in a set of continuum states become resonances which are broadened and shifted in energy.[7] It is, therefore, important to include these effects in order to produce more accurate values for the exciton binding energies which can be compared to experiment.

As a result of the VBM the exciton wave function consists of four components each of which possesses a different angular momentum symmetry .e.g. 1s, 2p, 3d, etc. Thus, the exciton states which mix are only those with different symmetries. For example, the 11H(1s) exciton does not mix with the 11L(1s) exciton, but rather the 11L(3d) exciton. Similarly, the 11L(1s) exciton mixes with the 12H(2p) exciton. This result is an important ingredient in determining the allowed optical transitions for the quantum well. Specifically, the optical selection rules for quantum wells can be stated as:[5] 1) Only exciton components with s symmetry are optically active; 2) For these components, the corresponding electron and hole subband functions cannot have opposite parity.

In this work the exciton mixing has been revealed through an investigation of the changes in the optical spectrum of semiconductor heterostructures brought about by; a) reorienting the growth axis to lie along the [111] crystallographic direction, and b) the application of uniaxial stress in the plane of the quantum well layer.

a) Excitonic Spectrum of [111]-oriented quantum wells

Photoluminecense excitation spectroscopy and electronic Raman scattering measurements on [111]-oriented quantum wells have shown[8] recently that the heavy hole mass along the [111] direction is more than twice as large as it is along the [001] direction. In addition, they have shown the binding energy of the lowest light-hole exciton (11L) is enhanced compared to its value in the [001] quantum wells. The first result is expected from a simple **k·p** calculation of the bulk valence band structure. The second result can only be understood by considering the exciton mixing. A calculation of the exciton binding energies for [111] quantum wells which neglects the VBM shows that the transition energies of the 11L(1s) and 12H(2p) excitons are nearly identical over a large range of well thicknesses, 50Å<L<200Å. It has been shown in this work[9] that these two excitons are coupled strongly because of the strong interaction between the 1L and 2H valence subbands. The resulting exciton anti-crossing has the effect of pushing the 11L exciton peak to lower energies thereby increasing the binding energy of this exciton. In contrast, in the [001]-oriented quantum wells the larger confinement energies for the heavy holes resulting from the smaller effective masses causes the 11L(1s) exciton and the 12H(2p) exciton to be much farther apart so that the symmetry mixing effect is much weaker, and a smaller 11L binding energy is obtained.

b) Excitonic Spectrum of Uniaxially-Stressed Quantum Wells

The application of uniaxial stress in the plane of the quantum well causes the light hole subbands to shift down in energy relative to the heavy hole subbands. As a result, the transition energies of the light hole excitons increase relative to that of the heavy hole excitons, and it becomes possible to pass light hole excitons through heavy hole excitons in a controlled way. This system is then ideal for studying the symmetry mixing effects. In particular, PLE measurements[4] of quantum wells subjected to in-plane uniaxial stress reveal a prominent exchange of oscillator strength between two exciton peaks suggesting that a strong exciton mixing is taking place. This observation was interpreted[4] as a mixing between the 11L and 13H excitons. However, the theoretical model developed in this work shows[10] instead that the 11L(1s) exciton is mixing strongly with the 12H (2p) state and with the 11H continuum. In addition, the exciton peak identified as 12H in the data has been shown to be forbidden because of the opposite parity of the electron and hole subband functions. It is instead identified as the (2s) state of the 11H exciton. The agreement obtained between the calculated excitonic transition energies and those from experiment is excellent. In addition, the exchange of oscillator strength between the 11L(1s) and 12H(2p) excitons and the enhanced continuum contribution to the absorption are reproduced accurately by the theory. It is worth noting that other theories which calculate exciton binding energies and oscillator strengths without including the interaction of the bound exciton states with the continuum could not reproduce these results.

c) Electromagnetic Response of Semiconductor Heterostructures

An additional problem which was addressed in this research was that of a realistic formulation of the optical response of a semiconductor

heterostructure to electromagnetic radiation. This problem was motivated by the fact that previous theories[11] focussed primarily on a calculation of the energy locations of the single particle and collective excitations in the response spectra . The model developed here[12] is based on the Feibelman d-function approach,[13] which has been employed successfully to treat the electromagnetic response of metal surfaces. The advantage of this method is that it provides not only the mode locations but produces realistic reflectivity and transmittivity spectra which can be compared directly to experimental data. The model has been applied to the calculation of the differential transmittivity of a GaAs heterojunction. Very good agreement has been achieved between the calculated intrasubband and intersubband plasma modes, and between the differential transmission line shapes observed in experiment.[14]

d) References

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II. Publications and Presentations stemming from Research

Publications

1. Theory of Excitons in [111]-Oriented Quantum Wells, D. A. Broido, in Proceedings of the 4th International conference on Superlattices, Microstructures, and Microdevices, Trieste, 1988, pg. 471.

2. Exciton States in Undoped Quantum Wells Under Uniaxial Stress, D. A. Broido and S.-R. Eric Yang, in Proceedings of the 19th International Conference on the Physics of Semiconductors, Warsaw, 1988, pg. 419.

3. Symmetry Mixing of Excitons in Quantum Wells, D. A. Broido and S.-R. Eric Yang, (to be submitted to Physical Review Letters).

4. Effects of the Continuum on the Excitonic Spectrum of Quantum Wells, D. A. Broido, (to be submitted to Physical Review B).

5. D-Function Approach to the Electromagnetic Response of Semiconductor Heterostructures, K. Kempa, D. A. Broido, C. Beckwith and J. Cen, Phys. Rev. B (to appear in the Oct. 15, 1989 issue).

Presentations

1. Theory of Excitons in [111]-Oriented Quantum Wells, 4th International conference on Superlattices, Microstructures, and Microdevices, Trieste, August, 1988.

2. Exciton States in Undoped Quantum Wells Under Uniaxial Stress, 19th International Conference on the Physics of Semiconductors, Warsaw, August, 1988.

3. Symmetry Mixing of Exciton States in Quantum Wells, University Dortmund, Dortmund, West Germany, May, 1989.

4. Theory of Exciton States in Quantum Wells, University of Regensburg, Regensburg, West Germany, May, 1989.

5. Symmetry Mixing of Exciton States in Quantum Wells, University Dortmund, Dortmund, West Germany, May, 1989.