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Theory of the Electronic and Optical Properties of Semiconductor Heterostructures

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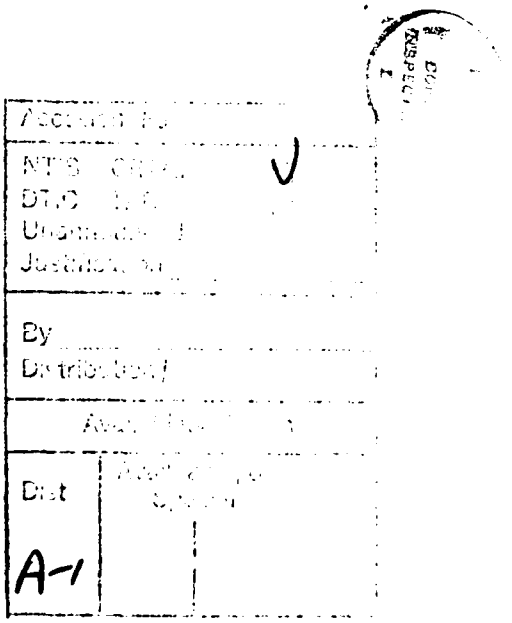

Statement "A" per telecon Dr. Larry Cooper. ONR/Code 1114SS

I. Summary of Research Accomplished

The research performed during the period of funding can be categorized into two areas. First, a theoretical investigation of the optical properties of strained layer quantum wells grown along the [111] crystallographic direction, and second, an examination of the far infrared response of quantum dot systems.

A. Optical Properties of Strained Piezoelectric Quantum Wells

Excitonic Spectrum:

The initial portion of this research involved the study of the excitonic properties of strained layer superlattices (SLS) composed of III-V compounds and grown along the [111] crystallographic direction. It has been proposed that such systems should exhibit large electric fields in each layer as a consequence of the piezoelectric effect.[1,2] It is well known that the strain shifts the conduction and valence band energies, and that large electric fields modify substantially the band structure through the quantum confined stark effect.[3] Because of the strong mixing of the heavy and light hole valence band in the III-V compounds, both the strain and electric field can alter dramatically the exciton binding energies and oscillator strengths, by modifying the mixing between different hole subbands. A systematic study of the resulting quantum well exciton mixing has been conducted in GaAs-AlGaAs quantum wells through the application of uniaxial stress.[4,5] Calculations by Broido and Yang[5] of the absorption spectrum as a function of uniaxial stress were in excellent agreement with the measured excitation spectra,[4] and were able to identify the origin of previously unexplained features in the spectrum as being due to the mixing of different quantum well excitons. The mixing of quantum well excitons was studied in strained [111] piezoelectric $Ga_{.47}In_{.53}As$-$Al_{1-y}In_yAs$ and GaSb-AlSb multi-quantum wells, with layer thickness of 100Å. For the GaInAs system with sufficiently

large y (e.g. y=0.64) and for the GaSb system a tensile strain is generated in the quantum well, which causes the first light hole subband (1L) to lie above the first heavy hole subband (1H). For y≈0.58 the first light hole subband lies very close in energy to the second heavy hole subband (2H). These two subbands are strongly mixed and are responsible for the observed mixing of the corresponding quantum well excitons.[4,5] It was shown in this work that the mixing can cause substantial (~30%) changes in the binding energies and oscillator strengths of the first light hole and second heavy hole excitons.[6] It is noted, however, that since the quality of the [111] samples is not as high as the [100] grown material, it is difficult to observe the sharp exciton lines required to resolve the exciton mixing. This problem is compounded by the fact that the light hole transitions are, in general, weaker than the heavy hole transitons, and that the binding energies in many of the strained layer systems are smaller than in GaAs because the bandgaps are smaller leading to smaller effective masses for electrons and holes.

Optically Induced Screening:

The latter portion of this research concerned a problem that is of particular interest for optoelectronics; namely, the possibility of screening the piezoelectric field throught the optical generation of electron-hole pairs.[2] Evidence for this optically induced screening has been obtained from recent resonant Raman scattering measurements.[7,8] Spin density excitations (SDE) and charge density excitations (CDE) of the lowest electronic intersubband transition in strained [111] and [100] GaSb/AlSb multi-quantum well samples with identical layer thicknesses (250Å of GaSb; 230Å of AlSb) have been measured as a function of the incident laser excitation density. For the lowest power densities, the CDE and SDE in a given sample occur at the same energy, namely the intersubband energy. Yet, this energy is considerably smaller (37 meV) in the [100] sample than in the [111] sample (58 meV).

As the power density (or, equivalently, the optically-generated carrier density) is increased in the [100] sample, the energy of the SDE remains relatively unchanged because the Hartree fields generated by the photo-excited electrons and holes virtually cancel, while that of the CDE increases as a consequence of the so-called depolarization effect.[9] In constrast, in the [111] sample the SDE shifts rapidly to lower energy with increasing laser power density, approaching the energy of the [100] sample (37 meV) at the highest densities, while the CDE exhibits a much slower downward shift.

This behavior can be explained qualitatively in terms of the following model. For low power densities the large piezoelectric field in the [111] sample causes a large downward shift of the first electron subband but only a much smaller shift of the second subband, thus creating the larger intersubband spacing in the [111] sample. As the power density increases, the optically-generated electrons and holes are polarized to opposite sides of the layer in which they are confined. The resulting polarization field screens the piezoelectric field thereby causing a reduction in the intersubband spacing. For the highest densities the piezoelectric field is almost completely screened so that the intersubband spacing approaches that of the [100] sample.

Self-consistent calculations were performed[7,8,10] of the intersubband spacing, and of the CDE and SDE energies as a function of the photo-excited density of electron-hole pairs in the [111] GaSb/AlSb system. The calculations included the effects of 1) effective mass mismatch between the GaSb and AlSb; 2) strain and electric field on the electron and hole subband structure; 3) exchange and correlation; and 4) finite temperature. The strain in the layers was determined by x-ray diffraction measurements. Employing the piezoelectric coefficient of GaSb[11] lead to a resulting electric field of about 60 kV/cm, in good agreement with that needed to produce the 58 meV intersubband separation for the 250Å GaSb layer.

The piezoelectric field pushes the first heavy hole subband upward relative to the first light hole subband, while the tensile strain in the GaSb layer produces the opposite

effect. For low electron-hole density these effects almost cancel and the heavy hole subband lies slightly above the light hole subband. Thus in this regime only the heavy hole states are occupied and, because their wave functions are sharply localized, these carriers are very effective at screening the internal field. However, for moderate and high densities the decreased net field causes the light holes to become the dominant carrier type. Importantly, it was found that the large overlap of the light hole and electron wave functions decreased substantially the screening efficiency. This mechanism is reflected in the data, where a much weaker shift of the SDE with power density was observed than would be obtained if only heavy hole states were occupied.

The energies of the CDE and SDE for the electron gas were calculated using a one-component model in the Random Phase approximation.[12] Calculations were also performed including exchange-correlation effects are included in the Local Density approximation and the Time-Dependent Local Density approximation.[13-15] In order to translate the laser power density into a corresponding photo-excited carrier density in the sample the calculated energy differences between the CDE and SDE are matched with those obtained in experiment.[16] The agreement between theoretically and experimentally determined CDE and SDE was quite good.

B. Electromagnetic Response of Quantum Dot Structures

With recent advances in nanofabrication technology it has become possible to confine electrons in all three spatial dimensions in semiconductor structures called quantum dots.[17-20] Such structures are analogous to atoms but, in place of an atomic potential electrons see the artificially constructed dot potential. Typically, the lateral electron confinement is produced either from periodic etching[17,19] or periodic gating[18,20] of a quasi-two dimensional (2D) electron gas. In the first case, the electrons in each dot are confined by layers of positively charged impurities and possibly surface states.[17] In the

second, a gate voltage can effectively be viewed as producing positively charged disks that confine electrons to the dots.

A recent experimental study[18] of the far infrared (FIR) electromagnetic properties of quantum dots revealed that for zero magnetic field, the (FIR) absorption spectrum is governed by a single peak whose corresponding frequency is roughly independent of the number of electrons, N, occupying each dot. For nonzero magnetic field, applied perpendicular to the dots, a splitting of the resonance occurs producing two peaks that are also relatively insensitive to changes in N. In the current work, it has been shown that this behaviour can be explained[21] when the potential that confines electrons in a single dot is parabolic and the dots are well-separated. Then, the FIR resonance frequency, is independent of electron-electron interactions, and the number of electrons in the system (See also Refs. 22-24).

The inter-dot interaction of well separated dots was examined employing a point dipole approximation.[21,25] In this approximation, the dots were modeled as interacting point dipoles with given polarizablity, and the inter-dot correlation effects were treated exactly. It was shown that for such a system the inter-dot electrodynamic interaction produced a shift in absorption frequency that depended on an effective plasma frequency for the system, which scales as N/a^3 where a is the inter-dot spacing. For many samples investigated so far, this effective plasma frequency is very small, and therefore, in practice, the inter-dot interactions produce a negligible shift. However, it should be noted that it may be possible to enhance substantially the inter-dot effects by reducing a, thereby leading to potentially novel phenomena.

The electomagnetic response of a single dot was also investigated using the full many-electron Hamiltonian. Using a Hamiltonian approach[21] it was shown that if the potential that confines electrons in a given dot is parabolic then there is no shift of the FIR frequency due to electron-electron interactions in a given dot, irrespective of N. This result

is essentially a variation of Kohn's theorem.[22] It was also shown that the Hamiltonian approach can be extended to nearly parabolic confinement and to include inter-dot effects.

Finally, a complete theory of the electromagnetic response of a quantum dot that was developed that employed a realistic, self-consistently calculated confining potential.[26] In particular, the FIR electromagnetic response of a quantum dot containing between 1 and 30 electrons was calculated self-consistently, without and with an applied magnetic field. In this model, electrons were taken to be confined by a potential produced by a jellium disk of positive charge. It was shown that the parabolicity of the confining potential breaks down when the electron density extends to the edges of the dot. Such edge effects occur for large N or small dot radius. It was found that for small electron number the FIR absorption spectrum corresponds to that associated with parabolic confinement. For large electron number, an upward shift in the resonance frequencies occurs as the electron density probes increasingly the larger curvature of the dot potential. It was pointed out that additional effects of nonparabolic confinement such as multiple mode absorption and mode couplings can occur if the dot structures are designed with strongly reduced symmetry and electron occupancy that is sufficiently high to probe the edge asymmetries.

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II. Publications and Presentations stemming from Research

Publications

1. Excitonic Spectrum of Piezoelectric Heterostructures, D. A. Broido, Bull. Am. Phys. Soc. Vol. 35, p. 485 (1990).

2. Optically Induced Variability of the Strain-Induced Fields in [111] GaSb/AlSb Multi-Quantum Wells, B. V. Shanabrook, D. Gammon, R. Beresford, W. I. Wang R. P. Leavitt and D. A. Broido in Superlattices and Microstructures , Vol. 7, p. 363 (1990).

3. Modification of Piezoelectric Fields in Quantum Wells, B. V. Shanabrook, D. Gammon, R. Beresford, W. I. Wang, R. P. Leavitt and D. A. Broido in *Proceedings of 20th Int. Conf. on the Physics of Semiconductors, Thesseloniki, 1990* (to be published).

4. Theory of Optically-Induced Screening of Piezoelectric Fields in Strained [111] Quantum Wells, D. A. Broido, B. V. Shanabrook and D. Gammon, to be published in the Proceedings of the Fall, 1990 Meeting of the Materials Research Society, Boston.

5. Electromagnetic Response of quantum dots, P. Bakshi, D. A. Broido and K. Kempa, Phys. Rev. B **42**, 7416 (1990).

6. Electromagnetic Response of Lower-Dimensional Systems: Implications of Omitting the Ground State Potential, D. A. Broido, P. Bakshi and K. Kempa, Solid State Communications **76**, 613 (1990) .

7. Self-Consistent Far Infrared Response of Quantum Dot Structures, D. A. Broido, K. Kempa and P. Bakshi, Phys. Rev. B **42**, 11400 (1990).

Presentations

1. Excitonic Spectrum of Piezoelectric Heterostructures, D. A. Broido, American Physical Society March Meeting, Anaheim, March, 1990.

2. Theory of Optically-Induced Screening of Piezoelectric Fields in Strained [111] Quantum Wells, D. A. Broido, B. V. Shanabrook and D. Gammon, Fall, 1990 Meeting of the Materials Research Society, Boston.