Tuning of the Valence-Band Structure of GaAs Quantum Wells by Uniaxial Stress

R. Sooryakumar
Department of Physics, The Ohio State University, Columbus, Ohio 43210

A. Pinczuk and A. C. Gossard
AT&T Bell Laboratories, Murray Hill, New Jersey 07974

D. S. Chemla
AT&T Bell Laboratories, Holmdel, New Jersey 07733

and

L. J. Sham
Department of Physics, University of California, San Diego, La Jolla, California 92093
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Uniaxial stress induces striking effects on the polarized emission from the 2D Fermi sea in modulation-doped GaAs quantum-well structures. These are interpreted within the effective-mass theory in terms of changes in valence-band mixing caused by modifications to the subband spacing and departure from tetragonal symmetry. Calculation of the electron-hole recombination together with a phenomenological approximation for the Fermi-sea shakeup processes successfully accounts for the luminescence spectra and their stress dependence.

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In semiconductor quantum layers, confinement of electron motion along the normal to the plane and the two-dimensional (2D) subband dispersion for in-plane motion determine their novel electronic properties.[1] In GaAs quantum wells the upper valence subbands have total angular momentum $J=\frac{3}{2}$ and are composed of two series of doubly degenerate levels which at $k=0$ have angular momentum components $M_j=\pm\frac{3}{2}$ (heavy series) and $M_j=\pm\frac{1}{2}$ (light series). Calculations show that at finite wave vectors the heavy and light states are strongly coupled, leading to valence subbands with mixed $M_j=\pm\frac{3}{2}$ and $M_j=\pm\frac{1}{2}$ character.[2–4] Optical-emission experiments have given direct evidence of this mixing in the top valence subband.[5,6] The observation of parity-forbidden exciton transitions has been explained by mixing in the higher valence subbands.[7] This complex character of the valence subbands is a consequence of the degeneracy present in states of the bulk semiconductor and leads to a set of separate, but coupled, nonparabolic subbands. Evidence of these complexities is also found in magnetotransport,[8,9] light-scattering,[10] and cyclotron-resonance[11] experiments.

In this paper we present a quantitative determination of the valence-band mixing in GaAs quantum wells. To make these determinations we have taken advantage of the tunability of the subband structure that is achieved by application of uniaxial stress in various directions.[12] In the experiments we measure optical emission by 2D electron gases across the energy gap of modulation-doped GaAs-(AlGa)As quantum-well heterostructures. Mixing between heavy and light states in the ground valence subband is obtained from emission intensities with optical polarization normal to the layers.[5] The method is unique in allowing quantitative determinations as a function of wave vector in the part of the 2D Brillouin zone in which valence-band mixing has a significant impact on the electronic structure of the quantum wells. Compressive stress along the superlattice axis while preserving axial symmetry reduces the spacing between light and heavy valence levels. This configuration has thus allowed the critical dependence of band mixing at finite wave vector on the subband spacing to be measured. Uniaxial stress in the plane of the layers, however, destroys the tetragonal symmetry and moves heavy and light subbands such that their band-edge separation increases. The effects of reduced symmetry on band mixing of the highest subband are thus evaluated from the emission under an in-plane stress. The effect of many-body interactions on optical emission from doped quantum layers[5,13,14] complicates the determination of the simple valence-band mixing present in the electron-hole recombination. Stress provides a means to modify the contributions of these two processes to the emission. This hence allows an estimate of their separate contributions to the measured spectra. A crude approximation for the Fermi-sea shakeup processes added to the calculation of the simple electron-hole recombination reproduces the observed spectra and their stress dependence.

Figure 1 illustrates the effects of compressive uniaxial stress on the valence-subband structure of GaAs-(AlGa)As quantum wells. The three subbands shown correspond to the heavy ground state h_0, the light hole l_0, and the first excited heavy state h_1. The effective-mass calculations are based on a $\mathbf{k}\cdot\mathbf{p}$ Luttinger Hamiltonian[15] appropriate to bulk GaAs.[16] Warping in the

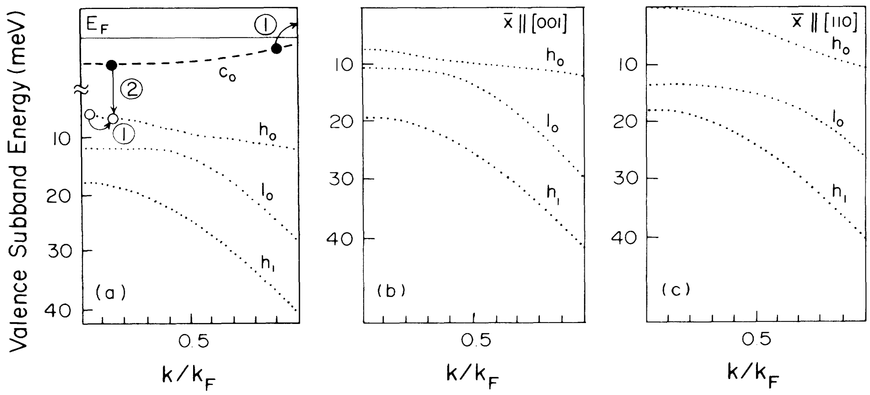

FIG. 1. Calculated subband dispersion of h_0, l_0, h_1 for n-type GaAs-(Al_xGa_{1-x})As quantum layers. (a) Unstressed layers. Shown schematically is the shakeup many-body process in the Fermi sea. (b) Compressive uniaxial stress $X=0.5$ kbar is along [001]; (c) $X=3$ kbar along [110]. The sample had the following parameters: $n=9\times10^{11}/\mathrm{cm}^2$, $x=0.29$, $d_1=166$ Å, $d_2=228$ Å, $d_3=177$ Å, where n=carrier density, d_1, d_2, and d_3 are thicknesses of GaAs, doped AlGaAs, and undoped AlGaAs spacer layer.

layer plane is neglected for simplicity and a self-consistent symmetric n-type quantum-well potential is added to account for the superlattice. The effects of uniaxial stress are introduced by the strain-orbit Hamiltonian H_x.[12] It is seen from Fig. 1 that compressive stress normal to the layers yields significant changes to the subband dispersion. They are associated with increased admixture of $M_j=\pm\frac{3}{2}$ and $M_j=\pm\frac{1}{2}$ basis states in each level. Compression along [110], shown in Fig. 1(c), reduces the tetragonal symmetry and, thus, increases mixing of $\pm\frac{3}{2}$ and $\pm\frac{1}{2}$ components of h_0 and l_0 even at the zone center. These calculations show that for appropriate choice of orientations, uniaxial stress is an excellent means to tune the quantum-well subband structure. It follows that the determination of changes in valence-band mixing under uniaxial stress provide a crucial test of theories of the electronic structure of quantum wells.

We studied several modulation-doped samples grown by molecular beam epitaxy on (001)GaAs substrates. We present data from one sample with parameters given in the caption of Fig. 1, which has the lowest two conduction subbands c_0 and c_1 occupied. The layers were grown between thick ($Ga_{0.71}Al_{0.29}$)As claddings that form a waveguide for the optical emission along the layers. Emission near the fundamental gap E_G was stimulated by weak photoexcitation and the emitted intensity was selectively analyzed for polarization components along the normal to (I_z) and in the plane of (I_x) the layers. In order to maintain a photoexcited carrier density significantly below that in the conduction Fermi sea, incident power densities were kept well below 0.1 W/cm^2. Uniaxial stress at 2 K was applied either parallel to [110] or along [001], in an apparatus similar to that described in Sooryakumar and Simmonds.[17]

In Fig. 2(a) we show emission spectra from the quantum layers when unstressed and with uniaxial stress applied separately along two directions. The main optical transitions are between the lowest conduction subband c_0 and h_0. Emission above $E_G (E-E_G>0)$ is interpreted as a scan through the Brillouin zone.[6] The lowest wave vector is $k_{\min}\approx3\times10^5\ \mathrm{cm}^{-1}$, at $E=E_G$, and the highest corresponds to the Fermi wave vector $k_F\simeq2\times10^6\ \mathrm{cm}^{-1}$. If the states of h_0 had only $M_j=\pm\frac{3}{2}$ character, I_z should vanish. Effects of c_1 are seen well separated from the fundamental recombination. Weak emission to about 10 meV below E_G is understood in terms of inhomogeneous broadening.[18] Extrinsic contributions such as impurities and waveguide effects provide negligible influence on the spectral features. In the unstressed spectra of Fig. 2(a) the increasing I_z for $E>E_G$ is qualitatively in agreement with single-particle processes of the effective-mass theory.[5] However, the surprisingly large amount of polarization mixing at smallest k ($E-E_G=0$) cannot be quantitatively explained only by elementary recombination processes and require consideration of shakeup of the 2D Fermi sea.[5]

Figure 2(a) shows that increasing stresses to a few kilobars have drastic effects on the I_z line shapes and intensities, while I_x retain their line shape under stress. For symmetry-preserving [001] axial stress of 1 kbar the overall I_z emission intensity rises by a factor of 2 at zone center with more rapid increases for wave vectors approaching k_F. For larger stresses in this geometry, I_z and I_x become comparable even at lower k. This is a remarkable result that shows there is about equal mixing of light- and heavy-hole character in h_0 at zone center. It demonstrates that light- and heavy-hole states can be reversed by application of uniaxial stress with profound effects on the optical properties of quantum wells. In-plane stress $X_\parallel[110]$ induces a modest increase to the band-edge I_z emission while dramatically reducing the

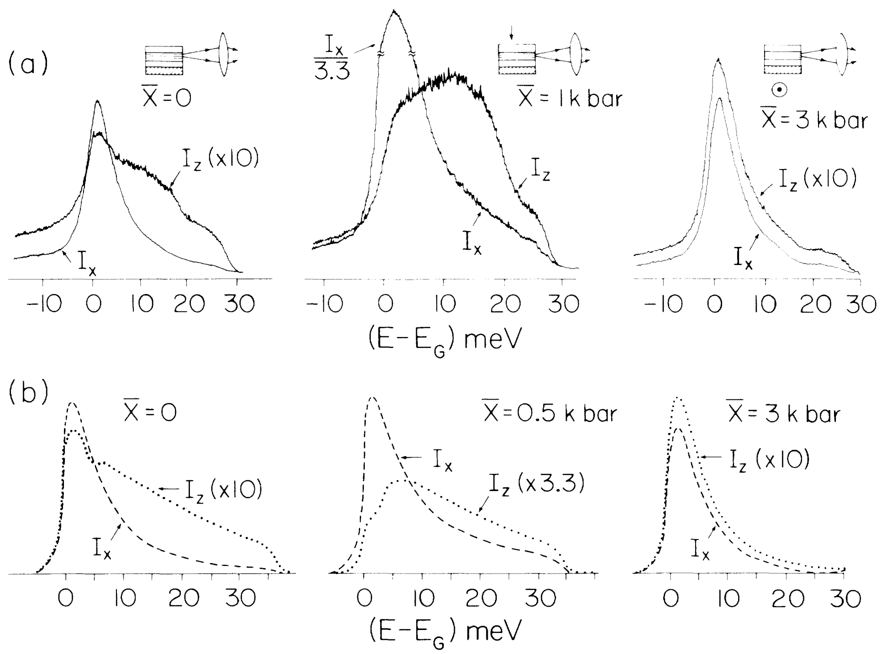

FIG. 2. (a) Emission spectra from the modulation-doped sample. I_z,I_x respectively refer to the emission with polarizations along [001] (the normal to the layers) and in the [110] direction. The spectra in each column correspond to stress geometries and magnitudes shown in the insets. (b) Calculated I_z,I_x emission spectra from Eq. (1). Each panel corresponds to the geometries directly above in (a).

finite-k transition of this polarization. In this case I_z steadily approaches the I_x line shapes with increasing stress. The data in Fig. 2 reveal that mixing of light- and heavy-hole character of h_0 can be changed by uniaxial stress, and from Fig. 1 it is seen that, while at zero stress the polarization mixing is dominated by the shakeup, band-mixing effects become evident by narrowing the space between light and heavy subbands.

In the following we provide a quantitative determination of the mixing. Calculation of I_z and I_x requires consideration of many-body processes in the Fermi sea, which are important in describing optical properties of doped semiconductor quantum layers.[5,13,14] In our measurements, the emission spectra and their modifications with uniaxial stress provide an excellent means to separate the contributions of single-particle from many-body processes. We show that the anomalously large I_z intensity in the unstressed case are due to many-body effects and do not reflect valence-band mixing at $k=0$.

The lowest-order many-body shakeup process that we consider is shown schematically in Fig. 1(a). Here, in step 1 the electron-hole Coulomb interaction scatters the hole to a new valence-subband state creating a pair excitation or a plasmon in the conduction band. In step 2, an electron in the conduction band recombines with the new hole having different combinations of $M_j=\pm\frac{1}{2}$ and $M_j=\pm\frac{3}{2}$, and emitting a photon. A summation of higher-order diagrams is necessary[19] since evaluation of the lowest-order term leads to an unphysical singularity at the energy gap.[20] A simple phenomenological formula, which includes these effects, for the emission intensity in the polarization direction α ($\alpha=x$ or z), is

$$I_\alpha(\omega)=\sum_{jk}[M_\alpha(jk)+\lambda\langle M_\alpha(j'k')\rangle_{j'k'}]e^{-E_{jk}/\Gamma}\times\delta(E_{ck}-E_{jk}-\hbar\omega). \quad (1)$$

Here, $M_\alpha(jk)$ is the square of the matrix element for the transition at polarization α from the electronic state at the lowest conduction subband, ck, to the three top valence-subband states jk spanning over h_0,l_0,h_1 (see Fig. 1). $\langle\rangle_{j'k'}$ denotes average over the Fermi sea and the valence subbands. This term simulates the shakeup which puts the hole in another state $j'k'$ within the Fermi circle, $k'<k_F$. Thus λ is a dimensionless measure of the electron-hole interaction. The exponential term gives the hole self-energy broadening due to interaction with the electron Fermi sea. E_k is the energy of the hole and Γ the constant energy width. A convolution with a Lorentzian of half-width 1 meV accounts for other causes of broadening.

Figure 2(b) shows calculated I_x and I_z spectra. There are only two adjustable parameters, λ and Γ. $\Gamma=1.75$ meV is used to fit the shape of the I_x spectrum at zero external stress. For the unstressed I_z spectrum, the elementary electron-hole recombination dominates for energy above the energy difference $E_{g1}(=E_G+E_{h0}-E_{l0})$ between the conduction and the light-hole band. The contribution to I_z from the electron–heavy-hole transition below E_{g1} is small. Between E_G and E_{g1} the shakeup term dominates the I_z spectrum. λ is 0.6 to fit the strength of the shakeup peak in this energy range. The calculated spectra for the unstressed layers shown in Fig. 2(b) are in good agreement with experiment. A test of this model is its ability to track the behavior under [110] and [001] uniaxial stress. λ and Γ are assumed to be weakly dependent on stress and the same values are used for finite stress.

Figure 2 shows that there is good agreement between calculated and measured spectra obtained with $X=0$ and $X \parallel [110]$. Small discrepancies can be attributed to emission introduced from c_1. For [110] stress, the first term on the right of Eq. (1) dominates, yielding I_x and I_z in good agreement with experiment. This analysis shows that the lack of tetragonal symmetry under this stress correctly accounts for the finite increase in I_z/I_x at zone edge while the large decrease on the high-energy side of I_z is due to the increase in $E_{h0}-E_{l0}$ yielding weaker band mixing. We consider these results as a strong indication that effective mass theory provides an excellent description of valence-band mixing in the ground state. The calculated I_z spectrum at 0.5 kbar of [001] stress, as shown in Fig. 1(b), shows the observed features of a low-energy shoulder due to the shakeup term of Eq. (1) and a broad peak due to the increase of band mixing because of the reduced spacing between h_0 and l_0 subbands. At 1 kbar or greater, the band-mixing peak of the calculated spectrum completely dominates the shakeup shoulder because of the h_0 and l_0 reversal. This reversal now results in the upper subband being mainly derived from l_0, thus yielding an enhanced I_z emission. The discrepancy in stress values with observation is partly due to the uncertainty in the estimate of the experimental stress. It reflects the very sensitive dependence of band mixing on the small subband spacing that is present at this stress. The good agreement on the significant spectral features between measured and calculated spectra and their evolution with uniaxial stress thus confirms our description of valence-band mixing in the quantum layers over an important wave-vector region.

In summary we have probed, through optical emission, valence mixing in doped-GaAs quantum wells. The measurements have made possible an analysis of the mixing of the valence-subband structure by the use of external uniaxial stress. We find that valence-band mixing is well described by the effective-mass theory. Our work demonstrates that stress tuning of the subband spacing and valence-band mixing provided a unique means to alter the optical properties of semiconductor quantum wells. Many-body effects in the Fermi sea, analogous to the shakeup in x-ray emission, are shown to be relevant to the interpretation of optical emission.

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