Effect of coherent strain on hydrogenic acceptor levels in $In_yGa_{1-y}As$/ $Al_xGa_{1-x}As$ quantum well structures

J. P. Loehr, Y. C. Chen, D. Biswas, P. Bhattacharya, and J. Singh
Center for High Frequency Microelectronics, Department of Electrical Engineering and Computer Science, The University of Michigan, Ann Arbor, Michigan 48109-2122

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The biaxial strain produced in lattice-mismatched epitaxy can have a substantial effect on the valence band structure. Theoretical results are presented for a hydrogenic acceptor in a quantum well under tensile and compressive strain. The acceptor level energy is a strong function of strain and could be used as a signature for the effect of strain on the valence band structure. Experimental studies are carried out on compressively strained $In_yGa_{1-y}As$/ $Al_xGa_{1-x}As$ quantum well structures and the acceptor level energy is determined by photoluminescence measurements. Good agreement is found with the experiments.

In a number of electronic and optical devices, performance can be improved by using coherent strain to tailor the valence band structure. Lifting the degeneracy between light and heavy holes at the top of the valence band can lead to reduced hole masses and result in superior hole transport and improved laser thresholds. Although quantum confinement will lift the degeneracy, the separation (~ 10 meV) is too small for any useful device implications. Biaxial compressive strain produced from growing a thin layer on a lattice-mismatched substrate, however, can produce an order of magnitude larger degeneracy lifting as compared to quantum confinement. In some optical devices, it is advantageous to maximize the valence band edge density of states by using tensile strain to restore the degeneracy between light and heavy holes. If part of the strain is released by dislocation formation, however, the benefits are lost and device performance can degrade. Hence, it is important to identify a simple characterization technique to study the effects of strain on the valence band structure. While it is possible to study these effects by Shubnikov–de Haas and magneto-optical techniques, we show in this letter that the acceptor level energy can be a simple and effective signature. Work has been reported on acceptors in strained quantum wells, although a detailed comparison between theory and experiment is not present.[1-3] Here we present both theoretical and experimental results for the $In_yGa_{1-y}As/Al_xGa_{1-x}As$ system; they show the strong sensitivity of the acceptor level energies in strained quantum wells to the strain present.

To calculate the acceptor binding energies in a quantum well in the presence of strain we need to describe the effect of strain and quantum confinement on the valence band structure. We model these effects in via the Kohn–Luttinger formalism which takes into account the coupling between the $|3/2, \pm 3/2\rangle$ heavy hole (hh) and $|3/2, \pm 1/2\rangle$ light hole (lh) states.[4] The influence of biaxial strain is then described by the deformation potential theory for the valence band states. In this formalism, the hole wave function Ψ_h is given by

$$\Psi_h(\mathbf{r}) = \frac{e^{i\mathbf{k}\cdot\rho}}{2\pi} \sum_{\nu} g_m^{\nu}(\mathbf{k},z) U_0^{\nu}(\mathbf{r}), \qquad (1)$$

where $\mathbf{k}$ is the in-plane two-dimensional wave vector, z is the coordinate in the growth direction, the U_0^{ν} are the zone center Bloch functions having spin symmetry ν, and m is a subband index. The envelope functions $g_m^{\nu}(\mathbf{k},z)$ satisfy the Kohn–Luttinger equation in a quantum well.[5] The effect of strain is incorporated via a splitting δ between the light and heavy hole diagonal elements. For the $In_yGa_{1-y}As$ system it is given (in eV) by $\delta = -5.966\epsilon$, where ϵ is the lattice mismatch between the well and the $Al_xGa_{1-x}As$ barrier.[6] We assume that the compressive strain produced by sandwiching an $In_yGa_{1-y}As$ well between $Al_xGa_{1-x}As$ barriers is completely absorbed within the well region; in this case, the lattice mismatch ϵ is related to the indium mole fraction y by $\epsilon = -(0.07)y$. For quantum wells placed under tensile strain by adding indium to the barrier region, the relation is less clear and we present our theoretical results in terms of the positive lattice mismatch ϵ.

We solve for the hole dispersion relations by writing the Kohn–Luttinger equation in finite difference form and diagonalizing the resulting matrix to obtain the in-plane band structure.[5] Figure 1 shows the [100] band structure for a 100 Å quantum well confined by $Al_{0.3}Ga_{0.7}As$. The well region is lattice-matched GaAs for Fig. 1(a) and $In_{0.2}Ga_{0.8}As$ for Fig. 1(b). The resulting lattice mismatch of $\epsilon = -1.4\%$ in Fig. 1(b) places the quantum well under compressive strain. As a result, the first three subbands in Fig. 1(b) are of heavy hole character and the band-edge states have much sharper curvature. In Fig. 1(c) we place the quantum well under tensile strain by assuming a lattice mismatch of $\epsilon = 1.4\%$. In this case the most significant effect is that the first subband is now of light hole character. We remark that a lattice mismatch of $\epsilon = 0.26\%$ (tensile strain) is required to merge the first light and heavy hole subbands for this quantum well.

The hydrogenic acceptor problem for an impurity placed at (x_i, y_i, z_i) in a crystal of relative permittivity ϵ_r is addressed by including the Coulomb potential

$$-e^2/\epsilon_r[(x-x_i)^2 + (y-y_i)^2 + (z-z_i)^2]^{1/2} \qquad (2)$$

in the quantum well Kohn–Luttinger equation. The equation is then solved by rewriting the potential in $\mathbf{k}$ space along the plane of growth and solving for the acceptor levels by a discretization method;[7] note that the acceptor energy de-

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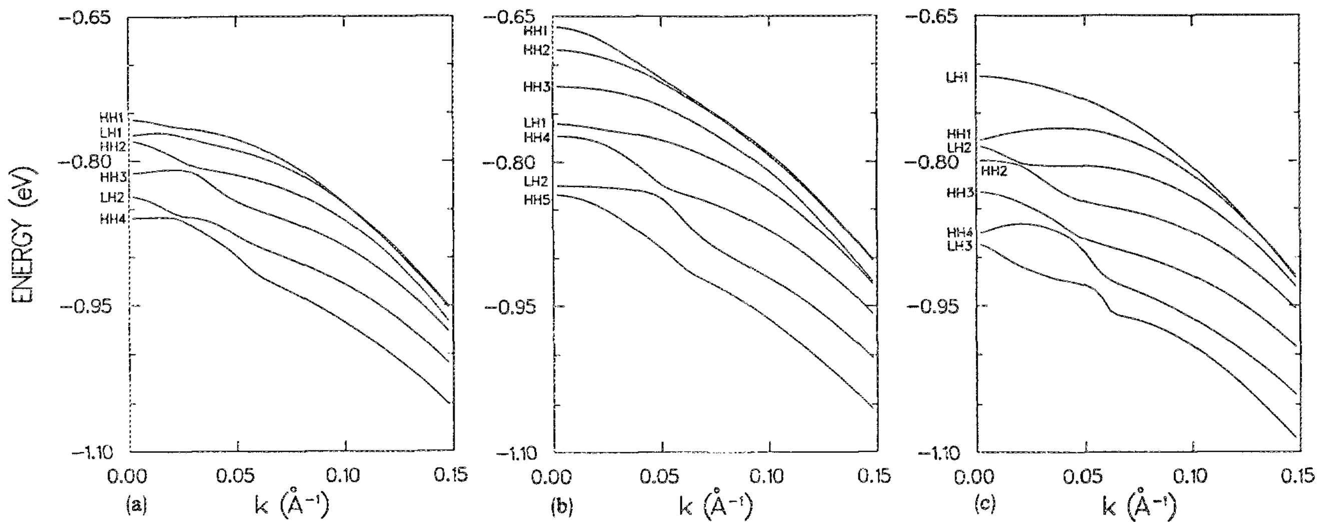

FIG. 1. Valence band structure in a 100 Å (a) lattice-matched $GaAs/Al_{0.3}Ga_{0.7}As$, (b) compressively strained ($\epsilon = -1.4\%$) $In_{0.2}Ga_{0.8}As/Al_{0.3}Ga_{0.7}As$, and (c) tensiley strained ($\epsilon = 1.4\%$) $GaAs/Al_{0.3}Ga_{0.7}As$ quantum well.

pends upon the position of the impurity in the quantum well. In Fig. 2 we show the calculated lowest energy acceptor level as a function of impurity position in the well in a 100 Å GaAs and $In_{0.2}Ga_{0.8}As$ quantum well bounded by $Al_{0.3}Ga_{0.7}As$. In both the strained and unstrained quantum wells we see that moving the impurity off center reduces the acceptor level energies as described in Ref. 7. In addition, we see a dramatic change in the acceptor energy due to the strain in the system. In Fig. 3 we show the effect of strain on the lowest energy acceptor in a 100 Å $In_yGa_{1-y}As$ well with the impurity in the center; the well is bounded by $Al_{0.3}Ga_{0.7}As$. The compressive strain curve was calculated by letting the indium mole fraction y in the well vary; for the tensile strain curve we used a GaAs well and imposed varying degrees of lattice mismatch. Note that the acceptor level energy is significantly affected by the strain and can be used as an important signature to characterize the valence band structure in a strained well. In particular, the binding energy is especially sensitive to tensile strain and peaks sharply at the strain value which merges the light and heavy hole bands. At this value ($\epsilon = 0.26\%$) the coupling between the hh and lh states in the Kohn–Luttinger equation is strongest, consequently the hole subband masses are greatest. For values of ϵ increasing past this value, the lowest energy subband takes on a light hole character and its mass begins to decrease.

The experimental samples were grown by molecular beam epitaxy in a Varian Gen II system. To estimate the acceptor level binding energies, photoluminescence (PL) studies were performed on GaAs and $In_yGa_{1-y}As$ (compressive strain) single quantum wells with $Al_{0.3}Ga_{0.7}As$ barriers. The samples were pulse doped with Be at the center of the quantum well. Photoluminescence measurements were made at 6 K with the sample in a liquid-He cryostat. Excita-

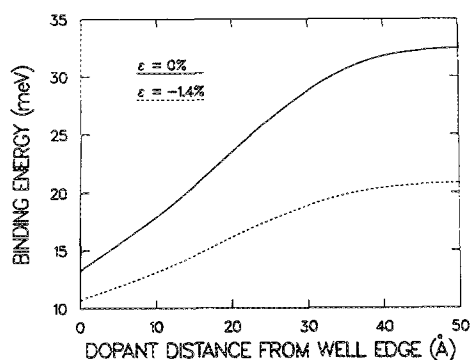

FIG. 2. Lowest energy acceptor level as a function of impurity position in a 100 Å lattice-matched $GaAs/Al_{0.3}Ga_{0.7}As$ and compressively strained ($\epsilon = -1.4\%$) $In_{0.2}Ga_{0.8}As/Al_{0.3}Ga_{0.7}As$ quantum well.

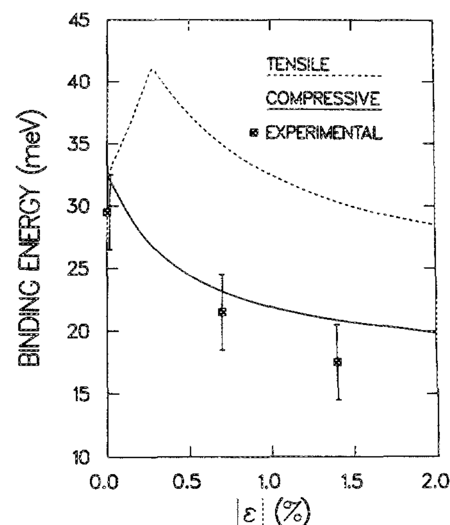

FIG. 3. Lowest energy acceptor level as a function of lattice mismatch ϵ in a 100 Å $In_yGa_{1-y}As/Al_{0.3}Ga_{0.7}As$ quantum well.

tion was provided with the 5145 Å line of an Ar^+ laser and the luminescence was analyzed with a 1 m Jarell–Ash spectra and detected with a liquid-N_2-cooled photomultiplier tube. In the undoped samples the dominant peak results from recombination of free excitons, but in the doped samples the dominant peak results from recombination of acceptor–bound excitons. In the doped samples a weaker extrinsic peak, possibly resulting from band to acceptor transitions involving the Be centers, is also seen. We estimate the acceptor binding energy (E_a) from the PL spectra by using the relation:

$$E_a = E_{\mathrm{EP}} - E_{\mathrm{AP}} + E_b. \quad (3)$$

Here E_{EP} is the energy of the free-exciton peak, E_{AP} is the energy of the acceptor level peak, and E_b is the binding energy of the free exciton which we calculate at 8.5 meV. We include an error bar of 3 meV on these estimated values. This error could be due to the Stokes shift (i.e., the undoped sample peak could be from a donor-bound exciton instead of from a free exciton as we have assumed). The estimated energies are shown alongside the calculated ones in Fig. 3 and the agreement is remarkably good. It therefore appears that low-temperature PL measurements on doped quantum wells may be a good technique to study variations in the band structure with strain.

In summary, we have addressed the problem of acceptor level binding energies in pseudomorphically strained $In_yGa_{1-y}As/Al_xGa_{1-x}As$ quantum wells. The acceptor level energies change dramatically as the strain in the system increases. We note that the change is due to the biaxial strain and not due to the addition of indium. Experimental studies confirm the theoretical results. The effect of strain on the acceptor binding energies is quite large and could be used quite effectively to probe the valence band structure in these strained wells.

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