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Experimental determination of the X_6 shear tetragonal deformation potential of AlAs

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The X_6 shear tetragonal deformation potential of AlAs, E_2, is estimated by studying the effect of uniaxial stress on the time-resolved photoluminescence spectra from two type-II AlAs/$\mathrm{Al_{0.15}Ga_{0.85}As}$ superlattices at 5 K. The time-resolved technique provides a direct measure of the energy separation of excitons associated with the in-plane and out-of-plane X valleys in the AlAs, thus removing complications due to the stress dependence of the valence-band energy. The value of E_2 obtained from two samples with different layer thicknesses is 5.8±0.1 eV.

Compared to other III-V semiconductors, relatively few material parameters have been measured accurately for AlAs due largely to the difficulty in obtaining good-quality single crystals in the bulk form. As AlAs is playing an increasingly important role as a barrier to vertical tunneling in AlAs/$\mathrm{Al_xGa_{1-x}As}$ heterostructures, there are now simultaneously (i) an increased demand for reliable material constants and (ii) a source of good-quality material with which to make the appropriate measurements.[1] Since the conduction-band minima in AlAs lie at the X points of the Brillouin zone, the X_6 shear tetragonal deformation potential E_2 is a particularly important parameter to measure accurately since it determines many of the ground-state electronic properties of heterostructures containing AlAs.[2-4] This is particularly true of so-called type-II AlAs/$\mathrm{Al_xGa_{1-x}As}$ superlattices grown on GaAs substrates, because the residual biaxial strain in the AlAs layers due to a small (~0.14%) lattice mismatch has been shown to play an important role in determining the energy alignment of the six nondegenerate X minima.[5-11] Indeed, when the first measurements of the strain-induced shift of the X valley energies in AlAs quantum wells were reported, the deformation potential of GaP was used to compare the experimentally observed shift with the lattice mismatch.[11] The present measurements indicate that the deformation potential of AlAs is actually ~12% less than that of GaP.[12]

Lefebvre *et al.*[13] recently estimated E_2 in AlAs to be 5.1±0.7 eV by studying the shift of X-valley-related photoluminescence (PL) features with uniaxial stress in two different AlAs/GaAs type-II superlattices. In their technique, the total shift of an excitonic PL feature reflected contributions from both the X-valley electron and the Γ-valley hole that condense to form the exciton. Thus to deduce the X-valley deformation potential it was necessary to subtract from the absolute transition energy an estimate of the valence-band contribution, resulting in a rather large uncertainty in E_2. The technique described below relies on monitoring *differences* in the shifts of two type-II excitonic PL features under uniaxial stress, so the contribution of the valence band to both transitions is automatically subtracted off. Using this technique the values of E_2 deduced from two different samples agree to within 2%.

For clarity of presentation, the growth axis of the epitaxial AlAs and $\mathrm{Al_{0.15}Ga_{0.85}As}$ layers discussed here is chosen as the z axis. The technique makes use of the fact that for AlAs layers thicker than ~6 nm on GaAs substrates, the biaxial compressive strain in the AlAs has been shown experimentally to raise the energy of the two X_z valleys (i.e., the minima with K vector along the growth direction) above that of the four $X_{x,y}$ valleys.[5,6,10,11] When the alloy layers are sufficiently thin, confinement effects raise the energy of the Γ levels and make the system type II, so that the lowest conduction-band states of the entire sample are those of $X_{x,y}$ symmetry in the AlAs. If electrons are photoinjected in the alloy layer they scatter quickly into the AlAs, rapidly thermalize into the low-energy $X_{x,y}$ valleys and form excitons with holes at the Γ point of the Brillouin zone in the alloy layers.[14,15] The steady-state PL from such type-II samples has been described in detail elsewhere,[2,5,6,8,10] and it is the stress dependence of this PL which Lefebvre *et al.*[13] used to deduce E_2. By using pulsed laser excitation and time-resolving the PL emission from such samples, we recently showed that it was possible to simultaneously observe PL from excitons associated with both the $X_{x,y}$ and X_z valley electrons.[5] The $X_{x,y}$-type excitons totally dominate the steady-state spectra but, for a short time after excitation, excitons formed from electrons temporarily trapped in the X_z valley can dominate because the oscillator strength associated with these transitions is enhanced with respect to the $X_{x,y}$ transitions because of superlattice mixing effects. This type of measurement therefore provides a direct measure of the X_z-$X_{x,y}$ valley energy separation δE to within the difference in binding energy of the two different excitons. We have now extended this work by quantitatively measuring the effect of applying uniaxial stress along the [110] direction. Since both types of excitons are associated with holes from the same valence band in the same alloy layer, any stress dependence of the valence-band energy cancels when the difference in PL transition energies is used to isolate the effect of stress on the different symmetry X valley energies. The *differential* effect of stress on the binding energies of the two type of excitons is neglected since this would be a higher-order correction than the stress-induced change of the *absolute* exciton binding energies, which itself is expected to be negligible at the stresses used here.[16]

The present experiment was carried out on two $Al_{0.15}Ga_{0.85}As/AlAs$ multiple quantum-well structures grown by molecular-beam epitaxy on GaAs substrates. Each sample consisted of 30 periods of alternating $Al_xGa_{1-x}As$ and AlAs layers. The $Al_xGa_{1-x}As$ layers were 4.2 nm thick and the AlAs layer thicknesses were 7.2 nm in sample I and 7.8 nm in sample II. Both samples have the $X_{x,y}$ valleys as their lowest conduction-band states so the steady-state spectra are characterized by a relatively weak, no-phonon peak with three relatively strong phonon replicas. As reported previously,[5] when 0.1-nJ, 4-ps, 640-nm dye laser pulses at 2 MHz are used to excite such samples, time-resolved PL spectra reveal a short lived (~ 1.5 ns) peak towards the high-energy end of the steady-state features. This peak was identified as recombination radiation from excitons made up of X_z electrons in the AlAs and Γ symmetry holes from the alloy layer. The steady state and time-windowed (a 1.5-ns-wide window coincident with the laser pulse) spectra in the vicinity of the no-phonon transitions of an unstressed piece of sample I are shown in Fig. 1 as curves (*a*) and (*b*), respectively. The entire spectral range shown in Fig. 1 was recorded without scanning, using an imaging photomultiplier tube in a correlated-photon-counting mode.[17] The $X_{x,y}$ and X_z transitions dominate the steady-state and time-windowed spectra, respectively. As discussed above, the two types of excitons that give rise to these two peaks are associated with the same type of hole states in the alloy layer so δE, the energy separation of the two X valleys, can be obtained directly from the energy separation of the two peaks. Application of stress causes an increase of δE which can be used to deduce the shear tetragonal deformation potential E_2.

Traces (*c*) and (*d*) in Fig. 1 show the cw and time-windowed spectra from sample I with a uniaxial stress of 1.45 kbar applied along the [110] direction. The stress was applied to the 5×0.5 mm^2 cleaved surfaces of the sample by a pneumatically driven piston, and was calibrated by using PL excitation (PLE) to determine the stress-induced splitting of the free excitons of the GaAs buffer material. The calibration was done on exactly the same spot from which the time-resolved PL was collected, so any nonuniformity of stress inside the sample was not important. This splitting deduced from PLE was converted to stress using a calibration factor derived from Gil *et al.*[18] A summary of the stress-induced increase of δE for samples I and II, up to ~ 1.7 kbar, is given in Fig. 2.

For stress applied along the [110] direction, the rate of change of δE with stress, R, is related to the AlAs elastic compliance coefficients S_{11} and S_{12} and E_2 by

$$R = E_2(S_{11} - S_{12})/2 \ .$$

From the slopes of the lines in Fig. 2, both samples give the same value of R, within experimental error. Using $S_{11} = 1.20 \times 10^{-12}$ cm^2/dyn and $S_{12} = -0.39 \times 10^{-12}$ cm^2/dyn (from Ref. 1), we therefore deduce $E_2 = 5.8 \pm 0.1$ eV.[19,20]

This value is approximately 12% less than that of GaP, and approximately 12% larger than that estimated by Lefebvre *et al.*[13] from the stress dependence of the entire interband exciton recombination energy. With no *externally* applied stress there is still an energy shift δE caused by the compressive biaxial stress in the AlAs which has a different equilibrium lattice constant than the GaAs substrate. This is estimated by van Kesteren *et al.*[11] and ourselves[5] to be about 23 meV. Using the value of E_2 deduced above, this 23-meV splitting implies a lattice mismatch of 0.20% between AlAs and GaAs at 4.5 K.

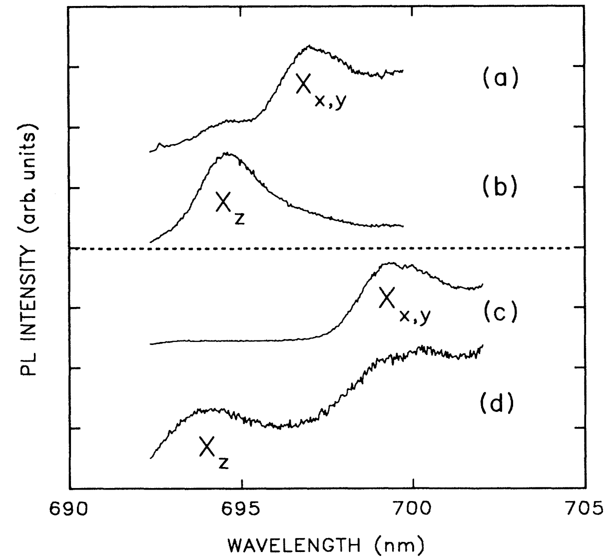

FIG. 1. (*a*) and (*c*), the steady state, and (*b*) and (*d*), time-windowed, PL spectra from sample I at applied stresses of (*a*) and (*b*), 0 kbar, and (*c*) and (*d*) 1.45 kbar.

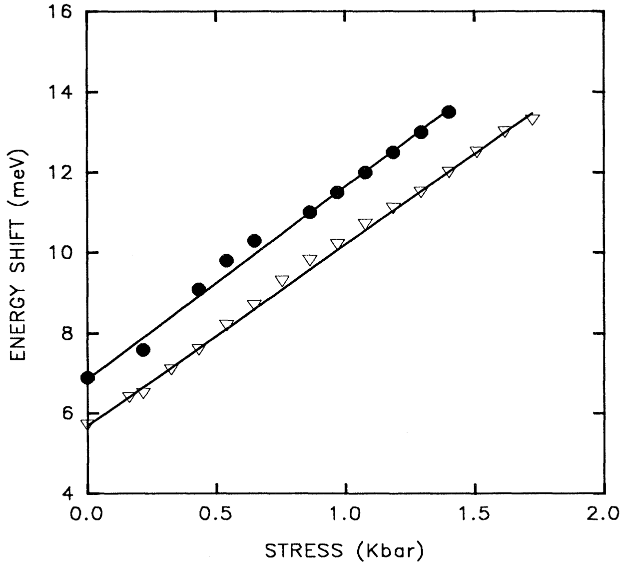

FIG. 2. The energy separation between the X_z and $X_{x,y}$ exciton PL transitions as a function of applied stress along the [110] direction for sample I (▽) and sample II (●).

This is significantly larger than the room-temperature value (0.14%), but is close to the value of 0.18% obtained by extrapolating from the room-temperature value using the temperature-dependent coefficient of linear expansion.[11]

In summary we have determined a value for the shear tetragonal deformation potential of AlAs by using a time-resolved PL technique to measure of the stress-induced shift of the X_z-$X_{x,y}$ valley energies without needing to apply corrections for the shifts of the valence band. The value we deduce, $E_2=5.8\pm0.1$ eV, is consistent with other III-V materials, and using it we also deduce that the lattice mismatch between AlAs and GaAs is 0.20% at 4.5 K.

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[19] We note that due to Γ-X_z mixing, the level shifts we observe are in principle due to stress-induced shifts of both the X_z and the Γ components of the (predominantly) X_z states. However, the weighting factor for the Γ contribution goes as the *squared* ratio of the $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$/AlAs mixing potential V_m to the energy difference between the lowest type-I and type-II transition energies in the sample E. In the present samples $E\sim120$ meV, and a conservatively large estimate for V_m is ~12 meV (Ref. 20), so that the weighting factor for the Γ contribution should be less than $\sim1\%$, and the value we deduce for E_2 is therefore representative of the AlAs X point as claimed.

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