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Piezo-Photoreflectance of the Direct Gaps of GaAs and $Ga_{0.78}Al_{0.22}As$

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We have investigated the effects of compressive uniaxial stress (T) on the photoreflectance spectra at 300K of the fundamental direct band gap (E_o) and its spin-orbit split component ($E_o + \Delta_o$) of GaAs and $Ga_{0.78}Al_{0.22}As$ for $\vec{T}$ along [001] and [110]. From the stress-induced shifts and splittings we have deduced the hydrostatic (a) and shear (b and d) deformation potentials of these materials.

The application of a uniaxial stress to a semiconductor produces changes in the lattice parameter and symmetry of the solid. These, in turn, cause significant changes in the electronic band structure that manifest themselves in the optical properties.[1-4] The hydrostatic and shear components of the strain produce shifts and splittings of the energy bands, respectively. Modulation spectroscopy has proven to be a very useful method for investigating the effects of uniaxial stress on the optical properties of semiconductors.[2,3] From such studies it has been possible to evaluate hydrostatic and shear deformation potentials as well as other valuable information concerning symmetry characteristics, excitons, etc. Deformation potentials are significant from both fundamental and applied points of view.[4] For example, they are crucial parameters for evaluating the quantum levels of strained layer heterostructures such as InGaAs/GaAs.[5]

In this work we have investigated the effects of compressive uniaxial stress (T) on the photoreflectance (PR) spectra of the fundamental direct band gap (E_o) and its spin-orbit split component ($E_o+\Delta_o$) of GaAs and $Ga_{0.78}Al_{0.22}As$. The transitions were studied at 300K for $\vec{T}$ parallel to [001] and [110], including polarization effects. From the stress-induced shifts and splittings, we have been able to deduce the hydrostatic (a) and shear (b and d) deformation potentials of these materials. Although GaAs has been studied extensively, this is the first investigation of $Ga_{1-x}Al_xAs$ under large, variable external stress.

The semi-insulating GaAs samples were cut from a [100] commercial wafer of thickness 0.5mm fabricated by the liquid-encapsulated Czochralski method. Such material is frequently employed as a substrate for the fabrication of various thin-film GaAs-related structures. No special treatment was given to the surface. The $Ga_{0.78}Al_{0.22}As$ sample was an epitaxial layer of thickness 0.25 μm grown by molecular beam epitaxy on a [100] GaAs buffer and substrate. The substrate was similar to the material described above. The growth temperature was 650°C. The samples for uniaxial stress were typically 2mm wide and 15mm long and oriented along either [001] or [110] by x-ray backscattering to better than 1°. The uniaxial stress rig[3] and PR apparatus[6] have been described in the literature.

In zincblende-type semiconductors, the top of the valence band at $\vec{k} = 0$ is a fourfold degenerate $P_{3/2}$ multiplet ($J = 3/2$; $M_J = \pm 3/2, \pm 1/2$) and a spin-orbit split $P_{1/2}$ doublet ($J = 1/2$, $M_J = \pm 1/2$). The $P_{3/2}$ bands have been designated v_1 and v_2 while the $P_{1/2}$ bands are v_3.[3,4] Transitions from the $P_{3/2}$ and $P_{1/2}$ multiplets to the S-like conduction band are labeled E_o and $E_o + \Delta_o$, respectively. The application of a uniaxial stress along [001] or [111] (i) splits the degeneracy of v_1 and v_2, resulting in the transitions $E_o(1)$ and $E_o(2)$, respectively, and (ii) causes a coupling between v_1 and v_3. The hydrostatic pressure component of the strain results in a uniform shift of $E_o(1)$, $E_o(2)$ and $E_o(3)$. For

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consistency we label the spin-orbit split transition as $E_o(3)$.

The shifts and splittings can be described by deformation potentials related to hydrostatic ($\underline{a}$) and shear effects due to tetragonal ($\underline{b}$) and rhombohedral ($\underline{d}$) symmetries, respectively. It has been shown that $E_o(1)$ and $E_o(3)$ are allowed for the electric-field ($\vec{E}$) of the incident photon polarized both parallel ($||$) and perpendicular ($\perp$) to $\vec{T}$ while $E_o(2)$ is allowed only for $\vec{E} \perp \vec{T}$.[3,4] For $\vec{T}||$ [011] the situation is somewhat more complex since for this low symmetry direction v_1 is coupled to both v_2 and v_3.[3,4]

For $\vec{T}$ ||[001] the stress-induced splittings and shifts[3,4] of $E_o(1)$, $E_o(2)$ and $E_o(3)$ can be written as:

$$E_0(2) = E_0 + \delta E_h + \delta E_S^{(001)} \tag{1a}$$

$$E_0(1) = E_0 + \delta E_h - \delta E_S^{(001)} - 2[\delta E_S^{(001)}]^2/\Delta_0 + \cdots \tag{1b}$$

$$E_0(3) = E_0 + \Delta_0 + \delta E_h + 2[\delta E_S^{(001)}]^2/\Delta_0 + \cdots \tag{1c}$$

where E_o and Δ_o are the zero-stress direct gap and spin-orbit splitting, respectively.[3,4] The quantities δE_h amd $\delta E_s^{(001)}$ are given by

$$\delta E_h = \underline{a}T/(C_{11} + 2C_{12}) \tag{2a}$$

$$\delta E_S^{(001)} = \underline{b}T/(C_{11} - C_{12}) \tag{2b}$$

where C_{ij} are elastic stiffness constants.

For $\vec{T}$ ||[110] the stress-dependence of the various transitions, to terms quadratic in T, can be expressed as:[3,4]

$$E_0(1) = E_0 + \delta E_h + \delta E_S^{(110)} + (3/32)[(\delta\varepsilon_S)^2/\delta E_S^{(110)}] - (27/32)(\delta\varepsilon_S)^2/\Delta_0 + \cdots \tag{3a}$$

$$E_0(2) = E_0 + \delta E_h - \delta E_S^{(110)} - (3/32)[(\delta\varepsilon_S)^2/\delta E_S^{(110)}] - 2[\delta E_S^{(110)}]^2/\Delta_0 + \cdots \tag{3b}$$

$$E_0(3) = E_0 + \Delta_0 + \delta E_h + 2[\delta E_S^{(110)}]^2/\Delta_0 + (27/32)(\delta\varepsilon_S)^2/\Delta_0 + \cdots \tag{3c}$$

where

$$\delta E_S^{(110)} = (1/4)[\delta E_S^{(001)} + 3\,\delta E_S^{(111)}] \tag{4a}$$

$$\delta\varepsilon_S = \delta E_S^{(001)} - \delta E_S^{(111)} \tag{4b}$$

$$\delta E_S^{(111)} = \underline{d}T/(2\sqrt{3})C_{44} \tag{4c}$$

Shown in Fig. 1a are the stress-dependent energies of $E_o(1)$, $E_o(2)$ and $E_o(3)$ for GaAs for $\vec{T}||$[001]. In the region of $E_o(1)$ and $E_o(2)$ measurements were made for $\vec{E}||\vec{T}$ and $\vec{E} \perp \vec{T}$. However, since $E_o(3)$ is weaker than E_o no polarization dependent studies were made for this feature. Representative error bars are shown. The transition $E_o(2)$ is linear in the stress. The solid lines are least-squares fits to Eqs. (1) which enabled us to determine the deformation potentials $\underline{a}$ and $\underline{b}$. These are listed in Table I. In Fig. 1b is displayed similar data for $\vec{T}||$[110]. The solid lines are least-squares fits to Eqs. (3) which produce $\underline{a}$ and $\underline{d}$ since $\underline{b}$ is known from the [001] data. The non-linear terms for $E_o(2)$ are very small and hence we did not detect any quadratic dependence on T. These results also are listed in Table I.

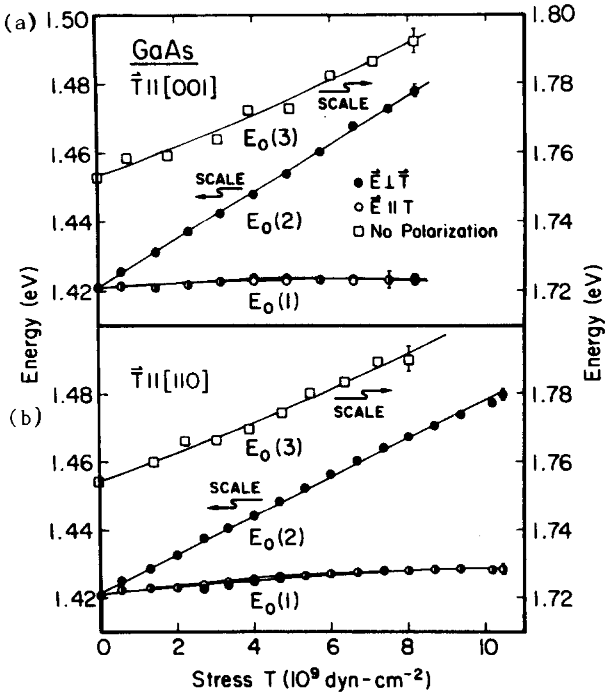

Fig. 1 Stress-dependence of $E_o(1)$, $E_o(2)$ and $E_o(3)$ of GaAs for (a) $\vec{T}||$[001] and (b) $\vec{T}||$[110].

Plotted in Figs. 2a and 2b are the results for $Ga_{0.78}Al_{0.22}As$ for $\vec{T}||$[001] and $\vec{T}||$[110], respectively. Representative error bars are shown. For this material $E_o(3)$ was very weak and hence no reliable results could be obtained. The solid lines in these figures are least-squares fits to Eqs. (1) and (3), respectively, yielding $\underline{a}$, $\underline{b}$ and $\underline{d}$ for this material. These values are listed in Table II.

In addition to the values of $\underline{a}$, $\underline{b}$ and $\underline{d}$ for GaAs and $Ga_{0.78}Al_{0.22}As$ obtained in this experiment we have also listed in Tables I and II, respectively, previous experimental as well as theoretical determinations.

Our numbers for GaAs are in very good agreement with prior evaluations. In particular, our result for $\underline{b}$ is probably more accurate than previous investigations since a detailed lineshape fit was used in our work to obtain the energies of the various transitions.

TABLE I Deformation Potentials for the E_o Transition in GaAs

	This Work	Previous Work	Theoretical Calculations
$\underline{a}$(eV)	-8.72 ± 0.2^a	-6.36^b	-7.2^c
	-8.81 ± 0.2^d	-6.70^b	-8.8^c
		-8.46^b	-12.0^e
		-9.43^b	-13.5^f
$\underline{b}$(eV)	-2.00 ± 0.2^a	-1.7^b	-2.2^f
		-2.9^b	-1.6^g
$\underline{d}$(eV)	-4.43 ± 0.6^h	-4.55^b	-4.2^f
		-5.4^b	-5.3^g
		-5.3^b	

a. $\vec{T}||[001]$.

b. Ref. 4.

c. Ref. 10.

d. $\vec{T}||[110]$.

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h. Deduced from the $\vec{T}||[110]$ results with $\underline{b}$ from the $\vec{T}||[001]$ data.

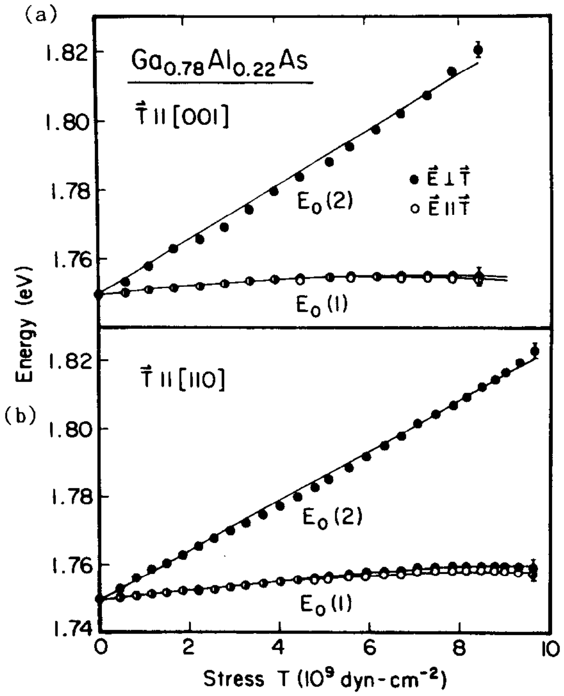

Fig. 2 Stress-dependence of $E_o(1)$ and $E_o(2)$ of $Ga_{0.78}Al_{0.22}As$ for (a) $\vec{T}||[001]$ and (b) $\vec{T}||[110]$.

In previous stress-dependent modulation experiments[2-4] only peak positions were employed for data analysis. The quantity $\underline{d}$ has large error bars since it was deduced from the [110] measurement which involves a linear combination of $\underline{b}$ and $\underline{d}$ rather than from a $\vec{T}||[111]$ experiment which depends only on $\underline{d}$.[2-4]

To date little work has been done concerning the effects of strain on the direct band gap of $Ga_{1-x}Al_xAs$. Lipshitz et al have reported the shift of the absorption edge of $Ga_{1-x}Al_xAs$ with hydrostatic pressure.[9] Our value of $\underline{a}$ is somewhat larger than that reported in the experimental work of Ref. 9 or the theoretical predictions of Ref. 10. Logothetides et al determined $\underline{b}$ for this alloy system from a study of the splittings of the direct gap exciton due to the lattice-mismatch in [100] $Ga_{1-x}Al_xAs$/GaAs grown by liquid phase epitaxy.[11] These authors find that $\underline{b}(Ga_{1-x}Al_xAs) = \underline{b}(GaAs) -0.5x$. Using $\underline{b}$(GaAs) = 2.00 we obtain, using their relationship, $\underline{b}(Ga_{0.78}Al_{0.22}As) = 2.10$, in good agreement with our experimentally obtained value listed in Table II.

Several workers have recently reported stress measurements for $\vec{T}$ along [001] and [110] on epitaxial layers of GaAs/GaAlAs quantum wells fabricated on thin (~0.5mm) GaAs substrates.[12,13] However, they attained stresses of only about 4 x 10^9 dyn/cm^2. Using

TABLE II Deformation Potentials for the E_o Transition in $Ga_{0.78}Al_{0.22}As$

	This Work	Previous Work	Theoretical Calculations
$\underline{a}$(eV)	-10.85 ± 0.2[a] -10.60 ± 0.2[d]	-9.11 ± 0.2[b]	-7.24[c]
$\underline{b}$(ev)	-2.08 ± 0.2[a]	-1.88[e] -1.86[f] -2.1[g]	
$\underline{d}$(ev)	-5.47 ± 0.6[h]		

a. $\vec{T}\|[001]$.

b. Evaluated from $\underline{a} = (1/3)(C_{11} + 2C_{12})(dE_o/dP)$ where (dE_o/dP) for $Ga_{0.78}Al_{0.22}As$ was taken from Ref. 9.

c. Linear interpolation of $\underline{a}$(GaAs) = -7.2 and $\underline{a}$(AlAs)= -7.4 from Ref. 10.

d. $\vec{T}\|[110]$.

e. From Ref. 11 with $\underline{b}(Ga_{1-x}Al_xAs) = -1.76 - 0.5x$.

f. From Ref. 11 with $\underline{b}(Ga_{1-x}Al_xAs) = -1.7 - 0.6x$.

g. From Ref. 11 with $\underline{b}(Ga_{1-x}Al_xAs) = -2.0 - 0.5x$.

h. Deduced from the $\vec{T}\|[110]$ results with $\underline{b}$ from the $\vec{T}\|[001]$ data.

the stress apparatus of Ref. 3 we have been able to achieve $T \approx 10 \times 10^9$ dyn/cm^2, a value comparable to that reported for samples cut from bulk material.[2-4]

In conclusion, we have measured the effects of an externally applied stress along [001] and [110] on the PR spectra of the direct gaps of GaAs and $Ga_{0.78}Al_{0.22}As$/GaAs. From the stress-induced splittings and shifts we have deduced the deformation potentials $\underline{a}$, $\underline{b}$ and $\underline{d}$. For GaAs our results agree very well with previous works. For $Ga_{0.78}Al_{0.22}As$ our value of $\underline{a}$ is somewhat larger than that obtained from hydrostatic pressure measurements and from a theoretical calculation. For $\underline{b}$ the value deduced in this experiment agrees with the Al composition dependence reported in Ref. 11. This is the first evaluation of $\underline{d}$ in this material. Our experiment also demonstrates that stresses can be applied to thin samples (~0.5mm x 2mm cross-section) fabricated from substrate material that are comparable to previous works on samples (~1.5mm x 1.5mm) cut from bulk semiconductors.

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