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Γ and X bandgap hydrostatic deformation potentials for epitaxial $In_{0.52}Al_{0.48}As$ on InP(001)

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Abstract. The pressure dependence of the direct and indirect bandgap of epitaxial $In_{0.52}Al_{0.48}As$ on InP(001) substrate has been measured using photoluminescence up to 92 kbar hydrostatic pressure. The bandgap changes from Γ to X at an applied pressure of ~ 43 kbar. Hydrostatic deformation potentials for both the Γ and X bandgaps are deduced, after correcting for the elastic constant (bulk modulus) mismatch between the epilayer and the substrate. For the epilayer we obtain $(\Xi_d + \frac{1}{3}\Xi_u - \mathbf{a})$ as $-(6.92 \pm 0.3)$ eV and $+(2.81 \pm 0.15)$ eV for the Γ and X bandgaps respectively. From the pressure dependence of the normalized Γ-bandgap photoluminescence intensity a Γ-X lifetime ratio, (τ_Γ/τ_X), of 4.1×10^{-3} is deduced.

Keywords. Hydrostatic deformation potentials; bandgap; pressure dependence.

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$In_{0.52}Al_{0.48}As$ is a wide bandgap (1.46 eV at 300 K) semiconductor which is lattice-matched to InP at an ambient pressure. $In_{0.52}Al_{0.48}As$ serves as the barrier material for lattice-matched $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ heterostructures. The latter have found numerous optoelectronic applications in the 1.3–1.55 μm spectral range due to the narrow bandgap of the $In_{0.53}Ga_{0.47}As$ (0.76 eV at 300 K) and the large value for the conduction band discontinuity, ΔE_c in this system (People *et al* 1983; Weiner *et al* 1985; Reddy *et al* 1986). In many applications it is desirable to have an even larger value for ΔE_c (Capasso 1983). One way of achieving this goal is the use of lattice mismatch-induced coherency strains. It is now well-known that coherent layer strains can dramatically alter the optical and electronic properties of semiconductors, as well as heterojunction band-offsets (Osbourn 1983; Van de Walle and Martin 1985). The use of deformation potential theory has pròved widely successful in providing estimates of strained layer bandgaps and transport masses. In this connection a parameter of particular importance is the hydrostatic deformation potential. In this paper, we present measurements of the Γ and X bandgap hydrostatic deformation potentials for $In_{0.52}Al_{0.48}As$. These results, we believe, would be useful in modelling the optoelectronic properties of pseudomorphic $In_{0.53}Ga_{0.47}As/In_{(0.52+\delta)}Al_{(0.48-\delta)}As$ heterostructures on InP(001).

High pressure photoluminescence measurements were made using a diamond anvil cell operated at room temperature (Jayaraman 1986). Samples were grown by molecular beam epitaxy and consisted of a (001) InP substrate onto which was deposited 2.7 μm thick unintentionally doped $In_{0.52}Al_{0.48}As$ layer and a 200 Å thick cap-layer of $In_{0.53}Ga_{0.47}As$ to avoid surface recombination effects (Nelson and Sobers

1978). Samples were lapped down to a thickness of 40 μm before being broken into pieces of approximately 100 μm square. A sample piece along with a ruby chip were placed inside the 250 μm hole of the pressure cell gasket fabricated out of 301 tempered stainless steel ribbon. For the pressure medium a 4:1 mixture of methanol and ethanol was employed. The latter remains hydrostatic up to 100 kbars. The pressure was measured by the ruby fluorescence technique (Barnett *et al* 1973). For exciting the luminescence a frequency-doubled and Q-switched Nd: YAG laser (peak power of 2 W at 532 nm and 2×10^{-4} duty) was used. The photoluminescence spectrum was analysed using a 0·5 m grating spectrometer, equipped with a photomultiplier, having either S1 or GaAs photocathode.

Luminescence spectra obtained at four pressures are shown in figure 1. As expected, the direct bandgap luminescence exhibits a rapid shift towards higher energies with increasing pressure. A marked decrease in the direct gap luminescence occurs near 43 kbar, the pressure where Γ and X conduction band edges cross; a new lower energy peak observable at those pressures is denoted by X^c in the 46 kbar scan. The direct bandgap luminescence continues to decrease for $P \gtrsim 43$ kbar and we could not detect it beyond 60 kbars. With increasing pressure the lower energy feature moves down in energy, which indicates that it is associated with the X conduction band minimum (Yu and Welber 1978; Lee and Woolley 1979; Olego *et al* 1980; Wolford *et al* 1983; Leroux *et al* 1985). At 83·1 kbar only the weak X-bandgap emission from the epilayer is seen, as illustrated in figure 1. We have plotted the photoluminescence peak energies against applied pressure in figure 2. The filled circles denote the Γ-bandgap emissions and open circles denote X-bandgap emissions. The solid curve is a least squares fit to the Γ-bandgap data of the form

$$E_g^{(\Gamma)}(P) \equiv E_g^{\Gamma}(0) + \alpha^{\Gamma}P + \beta^{\Gamma}P^2, \tag{1}$$

from which we obtain: $E_g^{\Gamma}(0) = 1{\cdot}46$ eV, $\alpha^{\Gamma} = 10{\cdot}35$ meV/kbar, and $\beta^{\Gamma} = -3{\cdot}612 \times 10^{-2}$ meV/(kbar)^2. Similarly the X-bandgap data fit yields $E_g^X(0) = 1{\cdot}943$ eV; $\alpha^X = -2{\cdot}634$ meV/kbar and $\beta^X = 0$. We stress that the above fits are related to the applied pressure, which may actually be substantially different from the actual pressure

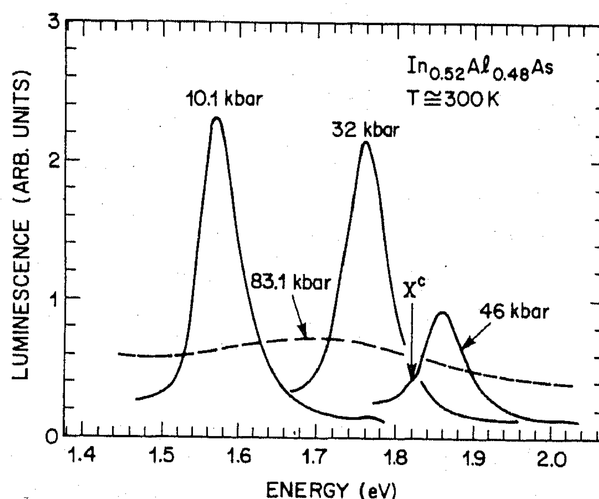

Figure 1. Luminescence spectra from epitaxial $In_{0{\cdot}52}Al_{0{\cdot}48}As$ on (001)InP at four different pressures.

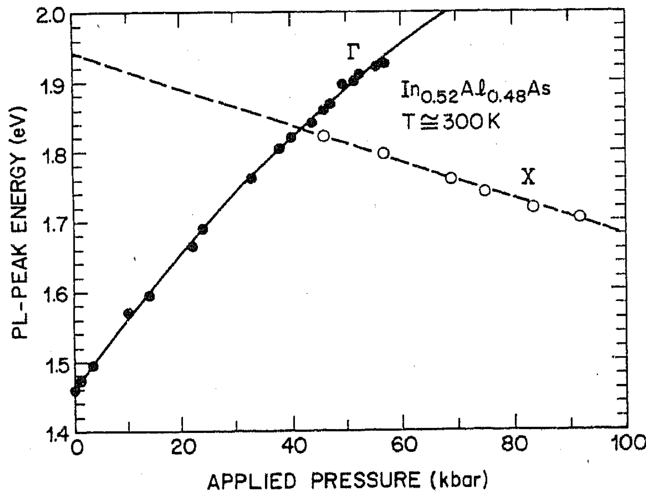

Figure 2. Photoluminescence peak energy variation against applied pressure plotted for epitaxial $In_{0\cdot52}Al_{0\cdot48}As$ on (001)InP substrate. The extrapolated X bandgap at zero pressure is different from that of a free standing film (see text).

experienced by the epilayer, since the bulk modulus of the epilayer and substrate are different. This effect is expected to increase with pressure and become significant at higher pressures (People *et al* 1988). Therefore the quantities $E_g^X(0)$ and α^X would deviate from the values for a free-standing film. In particular $E_g^X(0)$ will be affected most, because it has been obtained from an extrapolation of the data taken at high applied pressures. But the Γ bandgap parameters $E_g^\Gamma(0)$ and α^Γ are expected to be unchanged from those of a free standing film, since they were obtained from low pressure measurements. Hence the data in figure 2 cannot be used in its present form to extract hydrostatic deformation potentials.

It was earlier shown that for lattice mismatched epilayers on thick substrates the volume dilation ($\Delta V/V_0$) of the epilayer is related to the sum of the volume dilation of the cubic substrate and the non-cubic (tetragonal) distortion of the epilayer (People *et al* 1988). In order to determine hydrostatic deformation potentials for the epilayer we need to know the volume change of the epilayer, as opposed to the actual pressure it experiences. Following our previous analysis and procedure for calculating the dilation of the epilayer, we have obtained a plot of the Γ and X bandgap data versus ($\Delta V/V_0$) for the epilayer and this is shown in figure 3. It is to be noted that the higher pressure nonlinear behaviour of the Γ-bandgap has been removed which indicates that the β^Γ term directly reflects the nonlinear part of the high pressure equation of state (Murnaghan 1944). Secondly we find that the value for $E_g^X(0)$ is now 1·984 eV, which is substantially different from the value of 1·943 eV, obtained from extrapolation of the high pressure data. The present value of 1·984 eV for the $E_g^X(0)$ of $In_{0\cdot52}Al_{0\cdot48}As$ is in excellent agreement with the 1·983 eV value anticipated by Lorenz and Onton (1970). The slope of the curves in figure 3 yield bandgap hydrostatic deformation potentials ($\Xi_d + \frac{1}{3}\Xi_u - a$) of $-(6{\cdot}92 \pm 0{\cdot}35)$ eV and $+(2{\cdot}81 \pm 0{\cdot}15)$ eV for the Γ and X bandgaps of $In_{0\cdot52}Al_{0\cdot48}As$ respectively.

The pressure dependence of the photoluminescence intensity $I(P)/I_0$ due to the direct gap emission is plotted in figure 4, for constant I_0. The solid curve is a fit to an equation

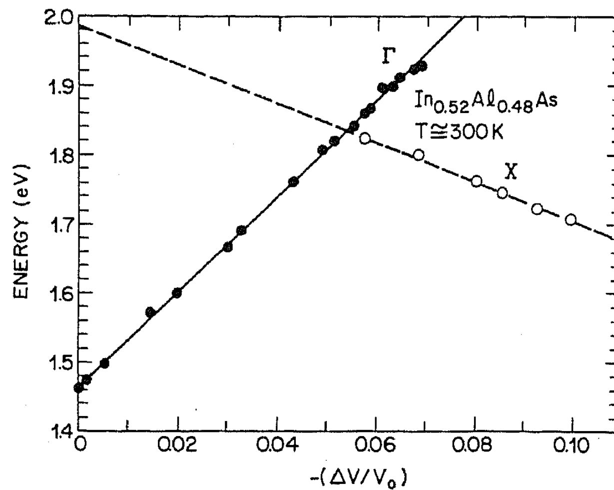

Figure 3. Photoluminescence peak energy versus actual volume dilation of the $In_{0\cdot52}Al_{0\cdot48}As$ epilayer. Corrections for the difference in bulk modulus of the epilayer and InP substrate have been made. For $In_{0\cdot52}Al_{0\cdot48}As$ we have assumed a bulk modulus of $B_0 = 653$ kbar (Ito 1985).

of the form (Olego *et al* 1980).

$$I(P)/I_0 = \{[1 + A\exp\{(E_g^\Gamma - E_g^X)/kT\}]^{-1} + B\} \tag{2a}$$

where

$$A \equiv (m_{\text{d.s.}}^X/m_{\text{d.s.}}^\Gamma)^{3/2}(\tau_\Gamma/\tau_X) \tag{2b}$$

and

$$B \equiv \tau_{\Gamma-X}/\tau_{\text{rad}}. \tag{2c}$$

In the above $m_{\text{d.s.}}^{(j)}$ is the density of states electron effective mass for conduction band extremum "j", τ_Γ and τ_X are the total lifetime of conduction electrons at Γ and the non-radiative lifetime of electrons at X, respectively. The first term in (2a) reflects the fact that when the material becomes indirect (i.e. Γ and X cross) an increasingly large fraction of the Γ electrons relax to the lower X conduction minimum. The second term in (2a) reflects that part of the Γ electrons may recombine radiatively, even when the X conduction band edge is of lower energy, if τ_{rad} is sufficiently small. Here $\tau_{\Gamma-X}$ represents an average intervalley scattering time of the electrons from the conduction band at Γ to the X extremum, and τ_{rad} is the radiative recombination time for optical transitions across the direct gap. It is observed that the second term is significant only for heavily p-doped materials (Olego *et al* 1980; Leroux *et al* 1985). The best fit to the data in figure 4 is obtained when $A = 0{\cdot}2$ and $B = 0$. Assuming $m_{\text{d.s.}}^{(\Gamma)} = 0{\cdot}084\,m_0$ and $m_{\text{d.s.}}^X = 1{\cdot}126\,m_0$, we obtain $(\tau_\Gamma/\tau_X) = 4{\cdot}07 \times 10^{-3}$.

In summary, we have used photoluminescence measurements in a diamond anvil cell to determine the pressure dependence of the Γ and X bandgaps of an $In_{0\cdot52}Al_{0\cdot48}As$ epitaxial layer, for hydrostatic pressures up to 92 kbars. Taking account of the differences in the bulk modulus of the epilayer and the InP substrate, we have obtained the epilayer bandgap changes against epilayer volume dilation, from which we have extracted both the Γ and X bandgap hydrostatic deformation potentials. We find that $(\Xi_d + \frac{1}{3}\Xi_u - \mathbf{a}) = -(6{\cdot}92 \pm 0{\cdot}35)$ eV and $+(2{\cdot}81 \pm 0{\cdot}15)$ eV for the Γ and X bandgaps of $In_{0\cdot52}Al_{0\cdot48}As$ respectively. By fitting the pressure dependence of the relative intensity of the Γ-bandgap emission we have obtained the ratio of the Γ and X recombination

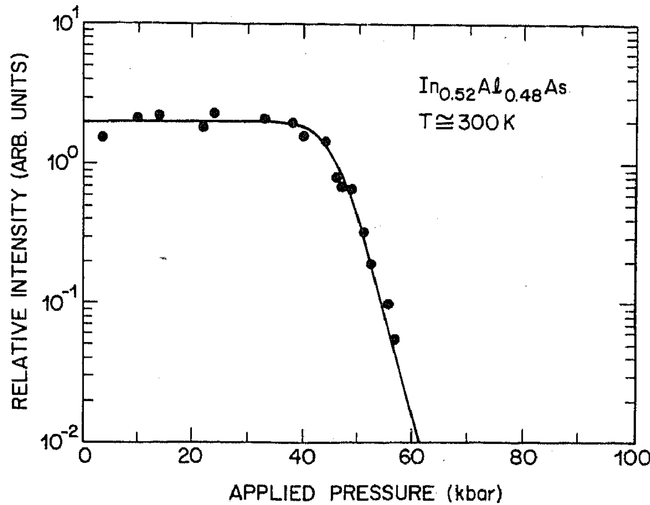

Figure 4. Relative photoluminescence intensity, $I(P)/I_0$, plotted against pressure. A fit of the data to equation (2a) in text is shown, from which we deduce the ratio of the Γ and X recombination lifetimes as $(\tau_\Gamma/\tau_X) \sim 4{\cdot}1 \times 10^{-3}$.

lifetimes (τ_Γ/τ_X) as $4{\cdot}1 \times 10^{-3}$. We believe that a knowledge of the hydrostatic deformation potentials for $In_{0.52}Al_{0.48}As$ would be useful in modelling the optoelectronic properties of pseudomorphic $In_{0.53}Ga_{0.47}As/In_{0.52+\delta}Al_{0.48-\delta}As$ heterostructures on InP(001).

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