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Pressure studies of impurity levels in $Al_xGa_{1-x}As$†

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Abstract. We present a study of the deep and shallow donor levels under hydrostatic pressure. The shallow levels follow the conduction bands, while the deep levels are strongly sublinear with pressure. The temperature dependence of the intensities and energies is used to obtain an energy level diagram of the deep levels at high pressures.

1. Introduction

It is well known that the application of hydrostatic pressure moves the conduction bands (CB) in GaAs in a manner similar to alloying with AlAs: the initial Γ–L–X ordering changes to X–L–Γ both with higher Al composition and with hydrostatic pressure. We present a study of $Al_xGa_{1-x}As$ (with $\sim 10^{15}\,cm^{-3}$ Si) up to a pressure of 60 kbar at temperatures between 15 and 125 K using photoluminescence (PL) spectroscopy. Shallow donor levels that manifest themselves both via bound exciton (BE) and donor–acceptor (DA) recombination are observed at low pressures, where the lowest CB is still at Γ. BE and deep-donor-to-acceptor recombination are seen at higher pressures where the lowest CB is at X. At a few pressures chosen to be typical of Γ and X, we study the temperature evolution of the PL spectrum and its dependence on excitation intensity. We obtain activation energies and thereby an energy level scheme for the sample as the lower CB changes from Γ to X.

2. Results and discussion

Our experiments were carried out on MBE-grown samples 1 μm thick on a GaAs substrate. The samples were undoped but contain some silicon impurities [2]. A diamond anvil cell was used with Ar as the pressure transmitting medium, and the 5145 Å laser line was used to excite the PL.

Figure 1 is a plot of the peak energies of various transitions observed under pressure. Data from two samples with $x=0.29$ [1] and $x=0.30$ are included in this plot. The energy axes are shifted so that the BE at zero pressure coincide. At 1 bar, a strong BE (Γ) and a weaker DA peak are seen. The BE (Γ) shifts at the rate

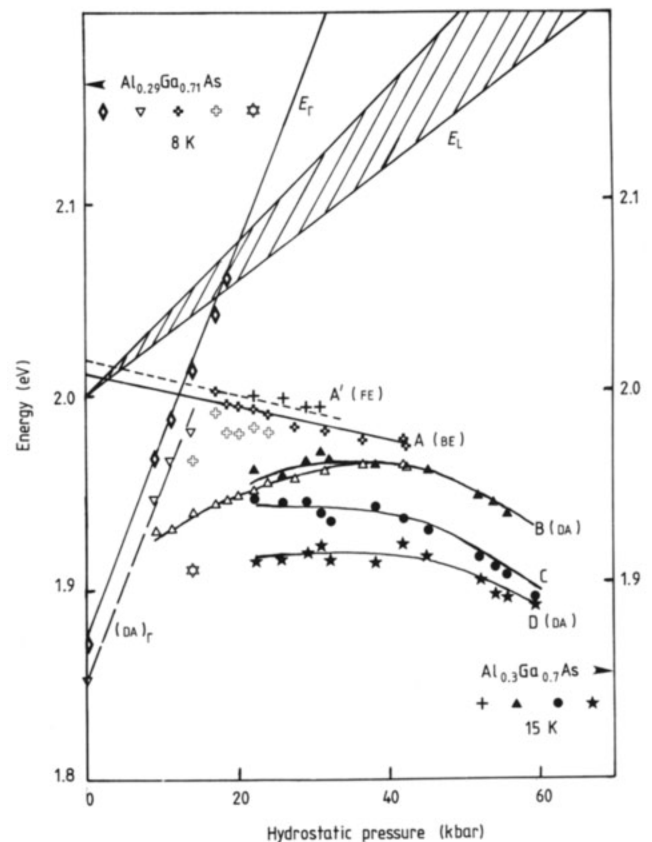

Figure 1. Energies of the peaks in the PL spectra of $Al_{0.29}Ga_{0.71}As$ and $Al_{0.3}Ga_{0.7}As$ as a function of pressure. The data from both samples have been plotted so that the BE (Γ) peaks coincide at zero pressure. Note the appearance of transitions from deep donor levels beyond 9 kbar.

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of 9.9±0.1 meV kbar^{-1}. Around 9 kbar, new peaks from the deep-donor levels are observed. The strongest, labelled B, has a non-linear pressure behaviour: it increases in energy between 9 and 30 kbar, flattens and then decreases in energy after 40 kbar. This is typical of deep donor levels that do not follow any particular band. A weak shoulder, C, and second deeper level, D, are also observed to have a similar pressure dependence.

In order to determine whether the peak D is a separate donor level or a phonon replica of B, we studied the PL intensity as a function of exciting laser intensity. We found that peak D scales with B up to an intensity of 1 W cm^{-2}, beyond which it saturates and only then other recombination mechanisms such as peak B and the BE (X) (peak A) and FE (X) (peak A′) become viable [2]. We therefore conclude that D may arise from a different donor level which is deeper than B.

The excitons associated with the X CB, labelled A (BE) and A′ (FE) are observed beyond 14 kbar, and shift at the rate of about −1 meV kbar^{-1}. It should be noted that at high pressure (>40 kbar), peak B is the most intense, and it shifts in that region at the rate of about −2 meV/kbar^{-1}. Care should be taken not to identify it as the exciton, especially in situations where staggered transitions in GaAs–AlGaAs quantum-well systems are used to determine the valence band offsets [3,4].

The temperature dependence of the energies and intensities of the PL spectra were used to determine activation energies and scattering mechanisms at a few chosen pressures that are typical of the Γ and the X CBs. The Γ CB region is well described by the zero pressure spectrum. PL spectra in the X CB region, at 26 kbar, are shown at several temperatures in figure 2. The individual energy axes for the spectra have been shifted (relative to the lowest axis) to compensate for the change in the X band gap with temperature [5] (GaAs values were used for the Varshni coefficients). All spectra were taken with an exciting intensity of 40 W cm^{-2}. At 15 K, the BE (peak A), and two DA recombination peaks (B and D) are seen. It is evident from figure 2 that the peaks change both in intensity and energy.

In figure 3 we plot the peak energy positions (circles) as a function of temperature. The triangles are the peak energy positions shifted by the change in the X band gap with temperature. We see that as the temperature is raised, the BE shifts to higher energies by about 25 meV between 15 and 125 K, suggesting an ionisation of the level. In the zero-pressure case a similar plot showed the BE(Γ) increasing *to* the energy of the FE. Here the energy increases *smoothly* with temperature. This smearing is reasonable since it requires a phonon in order to make the transition, and both phonon emission and absorption are possible at higher temperatures, as well as several different phonon processes.

The DA peaks B and D shift down slightly in energy up to about 75 K, beyond which they decrease in intensity and new peaks appear at higher energies (B′ and D′ in figures 2 and 3). At 125 K, B′ is strong and D disappears entirely. Peaks B′ and D′ are about 20±5 meV above the 15 K levels of B and D, after

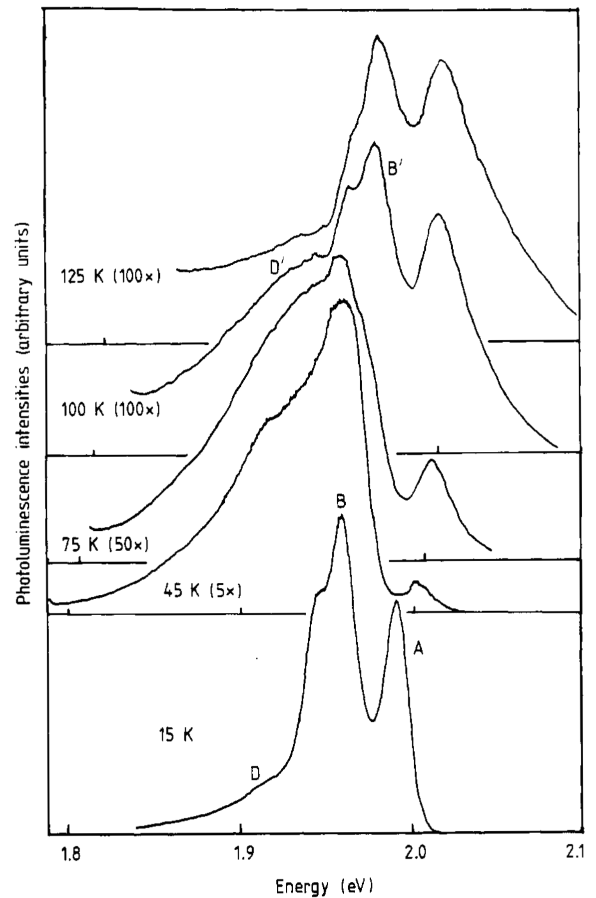

Figure 2. PL spectra for $Al_{0.3}Ga_{0.7}As$ at 26 kbar for several temperatures. The lowest energy axis corresponds to energies at $T=0$, and the other axes are shifted by an energy equal to the temperature shift of the X band gap.

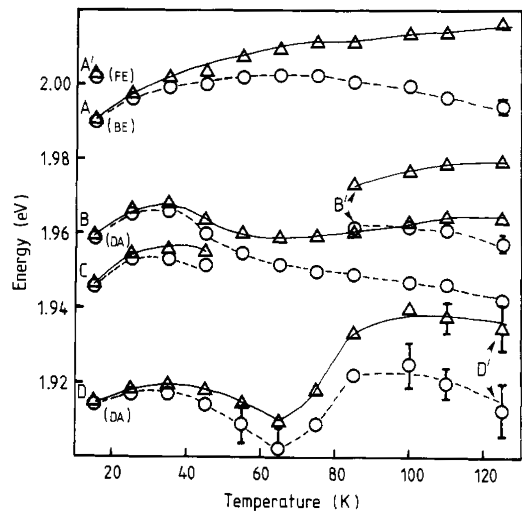

Figure 3. Peak energies of PL spectra of $Al_{0.3}Ga_{0.7}As$ at 26 kbar as a function of temperature. The circles correspond to actual peak energies, and the triangles are the energy positions corrected for the temperature shift of the X band gap.

Table 1. Activation energies at zero and 26 kbar.

Pressure	Transition	E_a (meV)	Temperature range (K)	Mechanism
Zero	FE	12±2	35 to 75	To Γ CB
	FE	80±10	75 to 125	Higher L CB
	DA	22±3	35 to 85	Ionisation of acceptor
26 kbar	BE (A)	7±1	15 to 55	BE to FE
	FE (A′)	38±4	55 to 125	To X CB
	DA (B)	52±5	65 to 125	To X CB

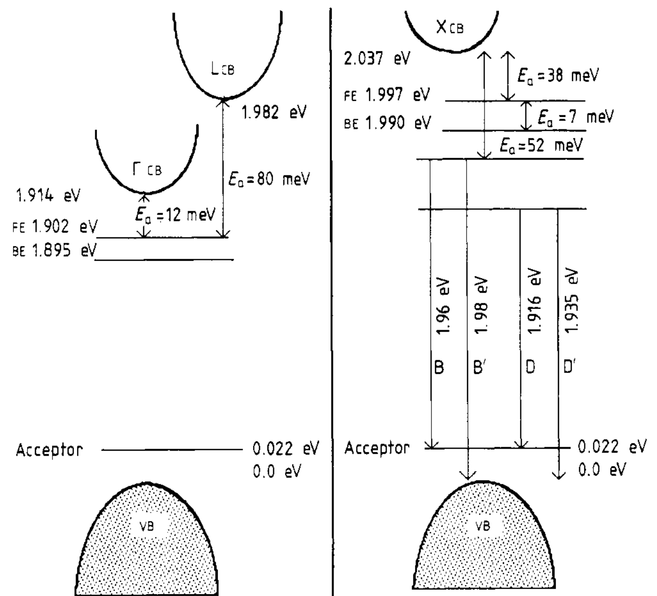

Figure 4. Energy level diagram of the levels observed for zero (left-hand side) and 26 kbar (right-hand side). The energy separations are deduced from activation energies and shifts in the energies of the peaks as a function of temperature (figure 3).

correcting for the temperature shift. This suggests an ionisation of the acceptor level.

The intensities of the peaks as a function of temperature were analysed via Arrhenius plots [4]. The linear parts of the curves give the activation energies shown in table 1.

From the activation energies E_a and peak energies as a function of temperature we draw an energy level diagram (figure 4). The energies for the Γ CB (at zero pressure) are in good agreement with the data of Dingle [6]. At high pressure, peaks B and D probably arise from DA recombination from *different* donor levels, since they have different excitation intensity dependences. They terminate on the same acceptor level, since the ionisation energy for both peaks is the same and occurs at the same temperature, (figure 3). The acceptor, from its ionisation energy and from zero pressure DA energy, is believed to be C_{As} [7]. The peak B is about 55 meV below the X CB (assuming the BE is 45 meV below X) and D is ~100 meV below X. The position of peak D agrees with the D^L–A transition seen by Henning [8], since it is 180 to 200 meV below the L CB (figure 1).

At this time the origin of these levels is not definitely known, though it is reasonably certain that they arise from Si donors. Further detailed temperature and excitation intensity studies over the entire pressure range are in progress.

Acknowledgments

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