Significance of Hall measurements in Ga_{1-x} Al_xAs alloys at 300 K

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Abstract. The Hall mobility, electron concentration and resistivity have been measured as a function of alloy composition for Ga_{1-x} Al_x As alloys at 300 K. The data have been explained on the multiconduction band structure of the alloys. The alloy composition for the direct-indirect conduction band minima cross-over, the electron mobility in the X minima and the activation energy of the deep level below these minima have been determined.

Keywords. Ga_{1-x} Al_x As; Hall measurement; cross-over composition; mobility; deep levels.

1. Introduction

It is well known that Ga_{1-x} Al_x As is a very potential semi-conductor material among the series of 3-5 group ternary compounds because of the minimal lattice mismatch (Neuberger 1968) between the end compounds GaAs and AlAs and the consequent minimal defect density for heterostructure devices (Lang and Logan 1977). From the point of view of practical applications these ternary compounds have great advantages in various optical (Craford and Groves 1973), microwave (Sitch *et al* 1975), current limiting (Immorlica and Pearson 1974, Sugeta *et al* 1977), switching (Immorlica and Pearson 1975) and pressure sensing (Saxena 1982a) devices. Hence there is considerable interest in the electrical transport properties of these alloys. Deep energy levels have been found to dominate the transport properties of Ga_{1-x} Al_x As alloys intentionally doped with various impurities. The presence of such levels has either been determined indirectly from the temperature dependence ($T < 300K$) of the Hall carrier concentration (Springthorpe *et al* 1975; Kaneko *et al* 1977; Nelson 1977; Dzhafarov *et al* 1977; Saxena 1981) or in order to explain the photoluminescence spectra in the alloys (Gonda *et al* 1976; Dingle *et al* 1977). Capacitance techniques on the Schottky barrier diodes have also been used to detect and characterize such levels in Ga_{1-x} Al_x As (Bhattacharya *et al* 1979).

For optical devices of Ga_{1-x} Al_x As material, it is important to know the critical alloy composition at which the direct and indirect conduction band minima are equal in energy. For alloy compositions at which the material has an indirect energy band gap, the efficiency of optical recombinations will be reduced due to the involvement of phonons. Various techniques have been used to obtain the value of this critical composition and the quoted values in the literature vary from 0·36 to 0·46 (Monemar *et al* 1976). Recently Saxena (1980) has shown that the value of this composition is

0·43 as obtained from the pressure dependence of the Hall electron concentration for the alloys. For high field devices of $Ga_{1-x} Al_xAs$, the electron mobility in the X conduction band minima is an important parameter. There have been some doubts, as the measured value of the electron mobility in the X minima of the alloys with indirect energy band gap has been found to be very different from the electron mobility in the X minima of GaAs (Pitt and Lees 1970, Saxena and Gurumurthy 1982).

In this paper, we report the direct evidence of deep energy levels in the alloys with high Al content and also estimate their activation energy. The alloy composition for the direct-indirect cross-over is also determined and the electron mobility in the X minima estimated from a simple interpretation of the Hall data for $Ga_{1-x} Al_xAs$ alloys at 300 K.

2. Experimental

Single crystal layers of $Ga_{1-x} Al_xAs$ were grown on semi-insulating GaAs substrates by liquid phase epitaxial technique (Saxena 1982 b). The layer thickness measured by angle lapping and staining was between 10 and 15 μm for various crystals. The alloy compositions were determined by measuring the cathodoluminescence band-gap energy and converted to compositions using the data given by Panish (1973). The compositions were also cross-checked by electron beam microprobe analysis and were consistent with the previous measurements to within $\pm 0.5\%$.

The Van-der Pauw (1958/59) pattern was delineated on the epitaxial layers using photolithographic techniques. Sn metal was used to make the ohmic contacts to the samples which were subsequently annealed in H_2 atmosphere at about 600°C for 2 min. The Hall measurements were made in a magnetic field of 5 gauss and with a reasonable current through the epitaxial layers to avoid the ohmic heating. The current varied from 10 μa to 1 ma to give a measurable signal from the sample. It is because the resistivity rises with composition by almost two orders of magnitude at $x \simeq 0.45$ (figure 1). Also the direction of the current was reversed for each measurement and an average of the measured values used to eliminate the contact effects. A small correction factor ($\sim 5\%$) was applied to calculate the actual sample resistivity and the Hall mobility to account for the finite size of the ohmic contacts relative to the samples. Van-der Pauw has given the formulae for such corrections.

3. Results and interpretation of data

The measured values of the sample resistivity ρ and the Hall electron mobility μ_h for various alloys compositions are shown in figure 1. The average variation of ρ and μ_h is also shown in figure 1. These curves have been designated as average variations since they represent the best fit to the experimental data scattered around these lines. Using these variations, the Hall electron concentration n_h is calculated from the simple relation: $n_h = 1/e \, \mu_h \cdot \rho$, where e is the electronic charge and the Hall scattering factor has been assumed to be unity for all the alloy compositions. The variation of n_h with the alloy composition x, thus obtained is shown in figure 2.

For simplicity, these variations can be qualitatively explained on a two- conduction band model involving the Γ minimum at the Brillouin zone centre and a subsidiary
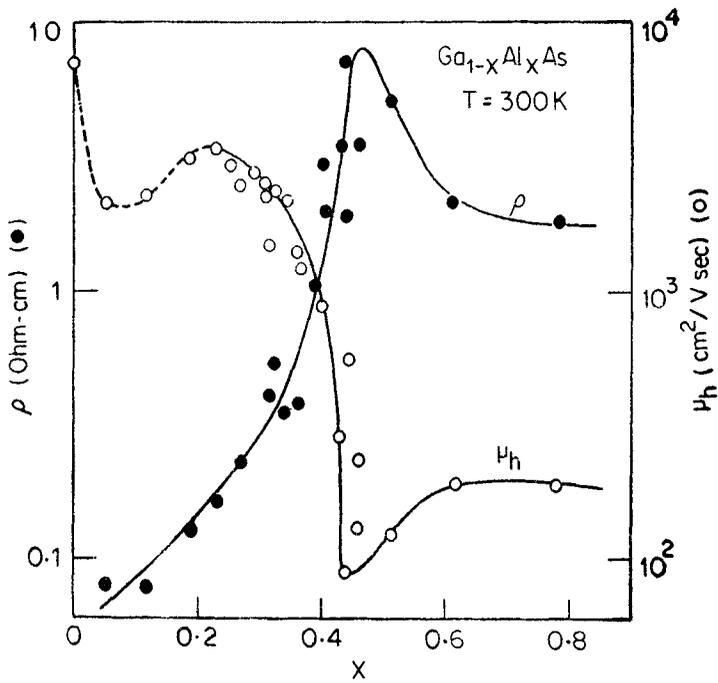
Figure 1. Composition dependence of the resistivity and Hall mobility for
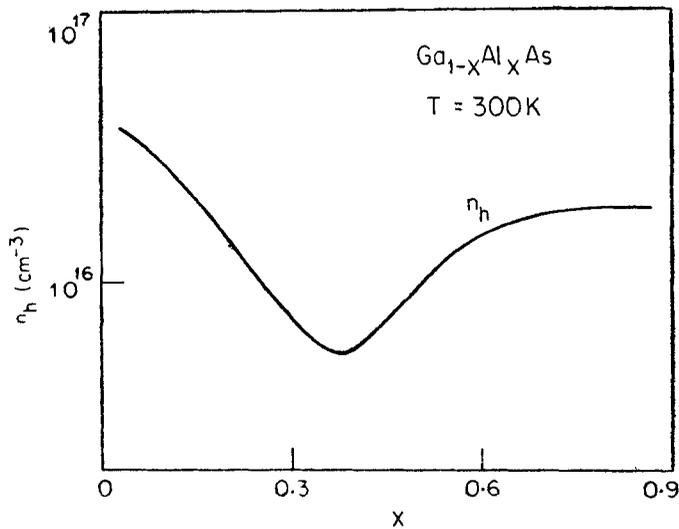$Ga_{1-x} Al_x As$ alloys at 300 K.

Figure 2. Composition dependence of the average Hall electron concentration for
$Ga_{1-x} Al_x$ As alloys at 300 K.

minima (X) at a higher energy. For a full understanding, the complete schematic
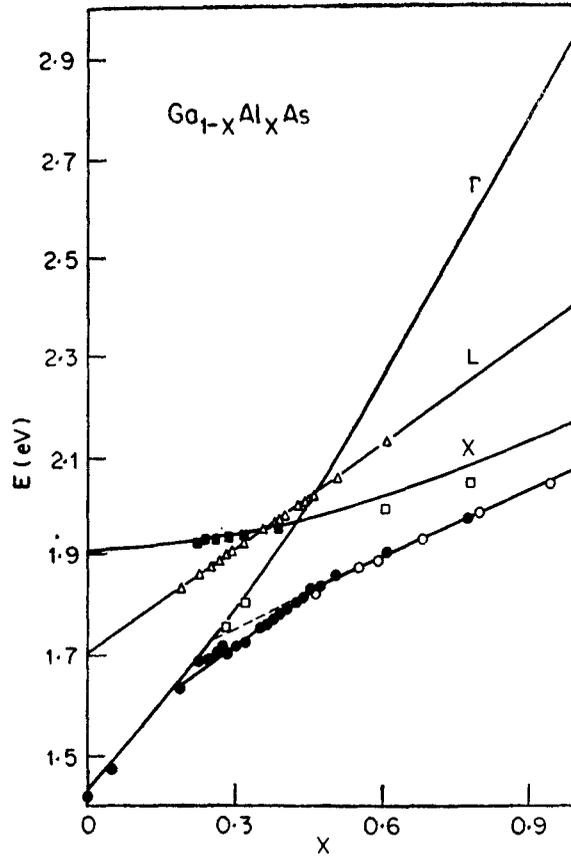diagram of the conduction band structure of $Ga_{1-x} Al_x$ As alloys is given in figure 3
(Saxena 1980, 1981, 1982b).

Figure 3. Conduction band structure of $Ga_{1-x}Al_xAs$ alloys and the energy levels (Saxena 1980, 1981, 1982b).

Since the electron effective mass in the X minima is much higher than in the Γ minimum, the density of states in the X minima is also higher (Pitt and Lees 1970). For the same reason, the electron mobility in the X minima is much lower than in the Γ minimum. With increasing alloy composition ($0<x<0.4$), the sub-band energy separation between the Γ and X minima decreases (Panish 1973) and, therefore, an increasing number of electrons are transferred to the X minima from the Γ minimum. This causes a decrease in μ_h and an increase in ρ as shown. For compositions $x>0.6$, the electron transfer to the X minima is almost complete and ρ and μ_h saturate with x. The minimum in μ_h at $x \simeq 0.45$ occurs due to the intense intervally scatterings among the various minima which lie close in energy at this composition (Saxena and Guru-murthy 1982). The maximum in ρ at $x \simeq 0.45$ can only be explained if the electrons are lost to the deep energy states at this composition. For $x>0.45$, the energy of these states decreases, thus decreasing the resistivity.

At $x \simeq 0.4$, the resistivity and mobility curves cross each other, hence the Hall electron concentration n_h shows a minimum at this composition as shown in figure 2. For compositions on either side of this value, n_h rises. Again the decrease in n_h for $0<x<0.4$ is due to electron transfer from the Γ to the X minima. For $x>0.6$, this

transfer is almost complete and n_h saturates with x. For $x<0.6$, the sub-band energy separation between the two minima again decreases, thus decreasing n_h. The reason for the anomalous behaviour of electron mobility for low alloy compositions (shown by broken curve in figure 1) is not yet understood and is, therefore, left without any explanation.

4. Analysis

In GaAs ($x=0$), mot of the electrons stay in the Γ minimum and, therefore, $n_h \simeq n_\Gamma$ $\simeq n_t$ since there are no deep energy levels in GaAs as found from the temperature dependence ($T<300K$) of n_h (Saxena 1981). Here n_Γ and n_t are the electron densities in the Γ minimum and the total density of conduction electrons, respectively. As the composition is increased (figure 2), the electrons redistribute among the various minima. For $x>0.8$, the X states are considerably lower in energy than the Γ and, therefore, $n_h \simeq n_X$ where n_X is the number of electrons in the X minima. The experimental observation that $n_X<n_\Gamma$ clearly shows that there is a 'freeze out' of electrons to the deep energy levels lying below the X states. From figure 2, it is obvious that $n_\Gamma=N_D \simeq 4 \times 10^{16}$ cm^{-3} since there is no 'freeze out' at $x=0$. Here N_D is the net donor concentration. Further $n_X \simeq 2 \times 10^{16}$ cm^{-3} because an equal number of electrons are lost to the deep levels below the X minima ($x>0.8$), assuming N_D to be constant. Thus, we obtain $n_\Gamma \simeq 2n_X$.

For low alloy compositions $x=0.05$, the conduction band structure of the alloy is almost the same as for GaAs and the sample resistivity is thus: $\rho_\Gamma = 1/n_\Gamma e\mu_\Gamma$. Similarly for the alloy compositions $x>0.7$ $\rho_X=1/n_X e\mu_X$. From figure 2, we find that $\rho_\Gamma \simeq 0.08$ ohm-cm and $\rho_X \simeq 2$ ohm-cm. Therefore, we get $\mu_X \simeq 0.08 \mu_\Gamma$. The measured value of μ_Γ for $x=0.05$ is only 2200 cm^2/V-sec (figure 1), giving $\mu_X \simeq 176$ cm^2/ V-sec. This value is very close to the measured value of 190 cm^2/V-sec for the electron mobility in the X minima ($x>0.6$) as shown in figure 1.

The number of electrons n_d on the deep donor sites N_D below the X state is given by the expression

$$n_d/N_D = \frac{1}{1 + \frac{1}{2} \exp \ [(E_D - E_F)/KT]} \tag{1}$$

where E_D and E_F are the energies of the deep level and Fermi energy below the X minima, respectively. Since $n_d=N_D - n_X \simeq 2 \times 10^{16}$ cm^{-3}, equation (1) at $T=300$ K gives $(E_D - E_F) \simeq 20$ meV.

The Fermi energy is calculated from the relation

$$n_X = N_C^X \exp \ (- E_F/KT), \tag{2}$$

where N_C^X is the density of states in the X minima. Using an effective density of states mass m_X^{*d} of $0.73 \ m_0$ in all the equivalent X minima (Saxena and Gurumurthy 1982),

we find that $E_F \simeq 170$ meV at 300 K, thus giving $E_D \simeq 150$ meV for $x > 0.8$. The actual value will of course depend on the impurity compensation in the crystal, which has been neglected in the present calculations.

Since the minimum in n_h at $x \simeq 0.4$ occurs due to the cross-over of the Γ and X minima only (Saxena 1980), the expression for n_h can be written as:

$$n_h = \frac{n_\Gamma \left(1 + \dfrac{n_X}{n_\Gamma} \cdot \dfrac{\mu_X}{\mu_\Gamma}\right)^2}{\left(1 + \dfrac{n_X}{n_\Gamma} \cdot \dfrac{\mu_X^2}{\mu_\Gamma^2}\right)}, \tag{3}$$

where μ_Γ and μ_X are the electron mobilities in the Γ and X minima, respectively. Also

$$n_X/n_\Gamma = (m_X^{*d}/m_\Gamma^*)^{3/2} \exp\left(- \Delta E_{\Gamma X}/KT\right), \tag{4}$$

where m_Γ^* is the electron effective mass in the Γ minimum. Therefore, at the minimum in n_h, $en_X \mu_X \simeq en_\Gamma \mu_\Gamma$ from (3). This condition together with (4), therefore, leads to

$$\exp\left(- \Delta E_{\Gamma X}/KT\right) = \frac{\mu_\Gamma}{\mu_X} (m_\Gamma^*/m_X^{*d})^{3/2} \tag{5}$$

provided $\mu_X \ll \mu_\Gamma$, which holds true for $Ga_{1-x}Al_xAs$ alloys. Using $m_\Gamma^* = 0.088\, m_0$, $\mu_\Gamma = 1200$ cm²/V-sec and $\mu_X = 120$ cm²/V-sec for $x \simeq 0.4$ (Saxena and Gurumurthy 1982), we get $\Delta E_{\Gamma X} = 28.5$ meV. Since $\Delta E_{\Gamma X} = 0.485$ eV in GaAs ($x=0$) (Saxena 1980), this energy separation, therefore, decreases at the rate of 11.4 meV/%Al. This directly gives $x_c = 0.425$ as the alloy composition at which the Γ and X minima should be equal in energy. This value found from a simple interpretation of the present data is very close to the value of $x_c = 0.43$ obtained from a rigorous analysis of the pressure dependence of n_h for various alloy compositions (Saxena 1980).

5. Conclusions

The activation energy of the deep level has been determined below the X minima along with the critical composition for the Γ-X minima cross-over and the electron mobility in the X minima from a simple interpretation of data on composition dependence of the resistivity, Hall electron concentration and mobility in $Ga_{1-x}Al_xAs$ alloys at 300 K.

Acknowledgements

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