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The variation of the pressure coefficient of resistivity in gallium arsenide with carrier concentration

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Abstract. The dependence of the resistivity of GaAs on pressure was investigated over a range of carrier concentrations. The change in effective mass of the electrons in the Γ_{1c} conduction band was found from measurements on samples with 10^{13} carriers cm^{-3}. In heavily doped material, where impurity scattering determines the electron mobility, the pressure coefficient of resistivity becomes strongly dependent on carrier concentration. The transition from polar to impurity dominated scattering occurs at about 10^{17} cm^{-3}.

Introduction

The variation in resistivity of GaAs single crystals with pressures of up to 10 kbar is examined as a function of carrier concentration. The results are presented in two parts. At low carrier concentrations, the pressure coefficient of resistivity is caused by the change in effective mass of the electrons in the Γ_{1c} conduction band, and this is related to the pressure coefficient of the direct gap through $k \cdot p$ perturbation theory. In heavily doped material, however, where the Fermi level has risen above the bottom of the conduction band, the pressure coefficient of resistivity becomes strongly dependent on the carrier concentration.

Experimental techniques

Full details of the preparation and characteristics of the n-type GaAs are shown in Table 1. The carrier concentrations range from 10^{13} cm^{-3} in undoped material to 10^{19} cm^{-3} in Se-doped material, while the Hall mobilities decrease from 8500 to 2000 cm^2 V^{-1} s^{-1} over the same region.

Four-probe resistivity measurements were made on a van der Pauw clover leaf at pressures of up to 10 kbar. A piston and cylinder device which contained a 1 : 1 mixture of paraffin and diala-C oil was used. Contacts to the crystal were passed through one piston using sheathed Chromel-Alumel thermocouples, brazed to the piston and sealed with epoxy resin. The pressures were recorded directly with a manganin gauge. A considerable increment in temperature accompanied each increase in pressure, but an equilibrium at 296°K was regained within a few minutes.

Table 1. The carrier concentrations and Hall mobilities at 300°K.

crystal	carrier concentration n (cm^{-3})	Hall mobility (cm^2 V^{-1} s^{-1})	dopant	method of growth
LE 39	$3{\cdot}9 \times 10^{13}$	8300	none	liquid epitaxy
A*	$7{\cdot}0 \times 10^{14}$	7700	unknown	unknown
LE 19A	$5{\cdot}0 \times 10^{15}$	6850	none	liquid epitaxy
LE 43A	$2{\cdot}6 \times 10^{16}$	5840	Se	liquid epitaxy
D 303A	$1{\cdot}1 \times 10^{17}$	4320	Se	vapour epitaxy
LE 152	$7{\cdot}3 \times 10^{17}$	3160	Se	liquid epitaxy
LE 168	$3{\cdot}0 \times 10^{18}$	2180	Se	liquid epitaxy

* The origin of sample A, which was used in preliminary measurements, was unknown.

Results and discussion

The variation with carrier concentration of the resistivity at 10 kbar, normalised to zero pressure, is presented in Figure 1. For comparison, the data of Sagar (1958), Hutson et al. (1967), and Pitt and Lees (to be published) have also been included.

Ehrenreich (1960) has shown that the resistivity normalised to zero pressure is

$$\frac{\rho(10)}{\rho(0)} = \frac{\mu(0)}{\mu(10)}\left[1+\left(\frac{m^*(0)}{m^*(10)}\right)^{3/2}\frac{N_2}{N}\exp\left(-\frac{\Delta E(10)}{kT}\right)\right], \quad (1)$$

where $m^*(p)$ and $\mu(p)$ are respectively the effective mass and mobility in the Γ_{1c} conduction band, N_2/N is the pressure-independent ratio of the densities of states in the X_{1c} and Γ_{1c} conduction bands and, for non-degenerate material, $\Delta E(p)$ is the energy separation between the X_{1c} conduction band minima and the Γ_{1c} minimum, while in degenerate material, it is the separation of the X_{1c} minima from the Fermi energy in the Γ_{1c} band. The band structure (Pollak et al., 1966), with single-group labels for band edges, is shown in an inset to Figure 1. The results may now be divided into two regions.

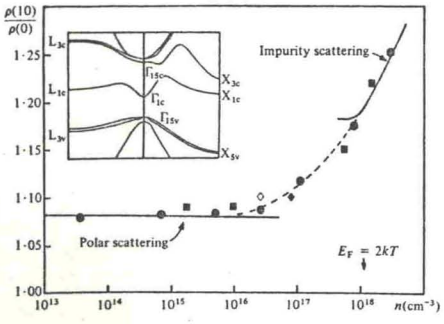

Figure 1. The resistivity of n-type GaAs at 10 kbar, normalised to zero pressure, as a function of carrier concentration.

● This work; ■ Pitt and Lees (to be published); ♦ Sagar (1958); ◇ Hutson et al. (1967).

Low carrier concentration (polar scattering)

When polar scattering is the dominant scattering process, Equation (1) becomes

$$\frac{\rho(10)}{\rho(0)} = \left(\frac{m^*(10)}{m^*(0)}\right)^{3/2} + \frac{N_2}{N}\exp\left(-\frac{\Delta E(10)}{kT}\right).$$

Moreover, the effective mass of the electrons in the Γ_{1c} band of GaAs may be calculated from $\mathbf{k}\cdot\mathbf{p}$ theory, in the manner described by Kane (1957) for InSb. Since the spin-orbit splitting Δ of the valence band is small compared to the direct forbidden gap E_g, the effective mass is adequately described by

$$\frac{1}{m^*} = \frac{1}{m_0^*}\left[1-\frac{5kT}{E_g}\left(\frac{F_{3/2}}{F_{1/2}}\right)\right], \quad (2)$$

where $F_{3/2}$ and $F_{1/2}$ are the Fermi integrals (Madelung, 1957) and m_0^* is the effective

mass at the bottom of the Γ_{1c} conduction band; this may be written as

$$\frac{1}{m_0^*} = \frac{1}{m}\left[1+\frac{2m\mathscr{M}}{3\hbar^2}\left(\frac{2}{E_g}+\frac{1}{E_g+\Delta}\right)\right], \quad (3)$$

where $\mathscr{M}$ is the momentum matrix element between Γ_{1c} and Γ_{15v} states. Since lattice vibrations are ignored in the derivation of Equations (2) and (3), only the dilational change in the energy gap E_g should be introduced in calculating the temperature dependence of m^*/m_0^* (DeMeis and Paul, 1965). Finally, the Fermi energy E_F, as determined by the doping level, is found from the expression

$$n = \frac{\sqrt{2}(kT)^{3/2}m_0^{*3/2}}{\pi^2\hbar^3}\left(F_{1/2}+\frac{5kT}{2E_g}F_{3/2}\right).$$

The change in effective mass with pressure may therefore be found, assuming that $\mathscr{M}$ and Δ are essentially constant.

The calculation of $\rho(10)/\rho(0)$ in the polar scattering region, namely $n \leqslant 10^{16}$ cm^{-3}, is included in Figure 1. The following values, for the parameters used in the calculation, were taken from the literature:

T =	296°K
$m_0^*(0)$ =	0·065 m (DeMeis and Paul, 1965)
Δ =	0·35 eV
$E_g(0)$ =	1·52 eV
$\Delta E(0)$ =	0·38 eV (Ehrenreich, 1960)
$\partial E_g/\partial p$ =	$10{\cdot}7\times10^{-6}$ eV bar^{-1} (Feinleib et al., 1963)
$\partial\Delta E/\partial p$ =	$-11{\cdot}0\times10^{-6}$ eV bar^{-1} (Pitt and Lees, to be published)
N_2/N =	45 (Pitt and Lees, to be published)

The agreement with experiment is very good. A larger value of $\partial E_g/\partial p$ (DeMeis, 1965), however, produces a much less satisfactory fit, but the calculation is rather insensitive to changes in the other parameters.

High carrier concentration (impurity scattering)

Figure 1 shows that the experimental values of $\rho(10)/\rho(0)$ deviate from the polar scattering curve at a carrier concentration of about 10^{16} cm^{-3} and thereafter are increasingly affected by scattering from screened impurity ions. Owing to the small effective mass in the Γ_{1c} conduction band, the carriers become degenerate at relatively low concentrations (4×10^{17} cm^{-3}). The consequences have been discussed in great detail by Moore (1967), but when polar scattering is negligible, the mobility (Mansfield, 1956) is approximately

$$\mu = \frac{3h^3\epsilon^2}{16\pi^2e^3m^{*2}f(x)} \qquad \text{for } E_F \gg kT,$$

where

$$f(x) = \ln(1+x)-\frac{x}{1+x},$$

$$x = \left(\frac{h}{e}\right)^3\frac{\epsilon}{m^*}\left(\frac{3n}{8\pi}\right)^{1/3},$$

and ϵ is the dielectric constant at the impurity energy.

The resistivity, normalised to zero pressure, now becomes

$$\frac{\rho(10)}{\rho(0)} = \left(\frac{m^*(10)\epsilon(0)}{m^*(0)\epsilon(10)}\right)^2\left[1+\left(\frac{m^*(0)}{m^*(10)}\right)^{3/2}\frac{N_2}{N}\exp\left(-\frac{\Delta E(10)}{kT}\right)\right].$$

The contribution of interband scattering, between the Γ_{1c} minimum and the X_{1c} minima, has been neglected. This seems justified (Nathan et al., 1961) for the range of carrier concentration and pressures studied here.

The calculation of $\rho(10)/\rho(0)$ for $n \geqslant 8 \times 10^{17}$ cm^{-3} ($E_F \geqslant 2kT$) is shown in Figure 1. The pressure variation of ϵ, taken from DeMeis (1965) for an energy 1·3 eV above the Γ_{15v} valence band, is

$$\frac{\epsilon(10)}{\epsilon(0)} = \frac{n(10)^2 - k(10)^2}{n(0)^2 - k(0)^2} = \frac{n(10)^2}{n(0)^2} = 0{\cdot}97$$

since below 2·5 eV, the absorption constant k is negligible in comparison with the refractive index n. The dotted line represents the transition from polar scattering through Brooks–Herring scattering to degenerate scattering.

The close agreement with experiment is somewhat fortuitous, since $\rho(10)/\rho(0)$ varies rapidly near the energy gap. In addition, the mobility in the degenerate region was calculated by assuming that each scattering event is random and independent of all others. Certainly the charged centres are sufficiently screened that they behave as independent scattering centres. On the other hand, the de Broglie wavelength of the electrons covers several impurity spacings, so that the carriers do not fully resolve the impurity structure. This leads to correlation in the scattering events. However, the result may not be greatly different from the scattering by the same number of widely separated ions, because the impurities are randomly distributed and should therefore produce mostly incoherent scattering. The preceding arguments then cannot be quantitatively applied, but the qualitative description should still hold. The quantum transport theory of Moore (1967) attempts to overcome this problem but the results are not easily re-evaluated at high pressures.

Conclusion

It was found that the variation with pressure in effective mass of the electrons in the Γ_{1c} conduction band could be described by $\mathbf{k} \cdot \mathbf{p}$ perturbation theory, provided

$$\frac{\partial E_g}{\partial p} = (10{\cdot}7 \pm 0{\cdot}5) \times 10^{-6} \text{ eV bar}^{-1}.$$

We then find that

$$\frac{\partial m_0^*}{\partial p} = (6{\cdot}0 \pm 0{\cdot}2) \times 10^{-6}\, m_0^* \text{ bar}^{-1}.$$

In the heavily doped samples the initial deviation from the polar scattering curve is caused by the onset of screened impurity scattering, but we note that when $n > 3 \times 10^{18}$ cm^{-3}, electron transfer rapidly dominates the value of $\rho(10)/\rho(0)$. This may be seen at greater pressures in the experiments of Pitt and Lees (to be published) on Te-doped GaAs, in which the carrier concentration was $1{\cdot}5 \times 10^{18}$ cm^{-3}. The reduction in mobility to 10 kbar is accompanied by a constant carrier concentration but at about 20 kbar, when transfer becomes important, the mobility rapidly falls towards its value in the X_{1c} minima.

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Experimental techniques

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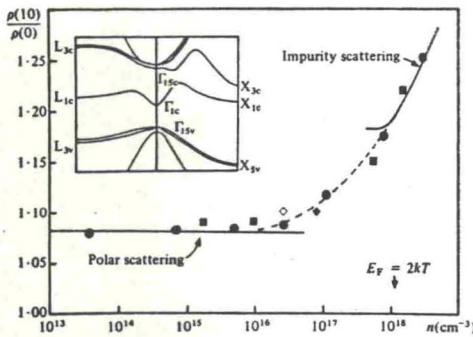

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