Electron Mobility in High-Purity GaAs*

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The combination of polar optical phonon, piezoelectric acoustic photon, deformation potential acoustic phonon, ionized impurity, and neutral impurity scattering in the relaxation time approximation is shown to give results which are in good agreement with the temperature and concentration dependence of the electron mobility in high-purity GaAs. For polar optical phonon scattering a relaxation time is defined at each temperature from Ehrenreich's variational calculation. Since most of the parameters are well known, the only adjustable parameter in the calculation is the conduction band deformation potential with the best agreement with experiment given by $|E_1|=7.0$ eV. Using this value a 77°K lattice scattering limited mobility of 240 000 cm²/V sec is obtained.

I. INTRODUCTION

The scattering mechanisms which determine the transport properties of GaAs were originally examined by Ehrenreich[1] who showed that a combination of polar optical phonon and ionized impurity scattering yielded qualitative agreement with the temperature and impurity concentration dependence of the electron mobility for the purest bulk GaAs. Since then vapor- and liquid-phase epitaxial techniques have been used to improve the quality of GaAs. Also, there are now sufficiently accurate additional experimental data (such as piezoelectric measurements) to examine the effects of other scattering mechanisms. In this paper we combine the relevant scattering mechanisms to obtain calculated mobilities which are in good agreement with the temperature and impurity concentration dependence of the purest vapor-phase epitaxial samples.

II. CALCULATION

A. Assumptions

In the analysis we have made the following simplifying assumptions:

(1) Each scattering process is described by a relaxation time $\tau_i(x)$ which may depend on the electron energy x. Although this assumption is not completely valid for most of the scattering mechanisms considered here,[2] it introduces considerable simplification in the analysis.

(2) The scattering mechanisms are independent of each other. An effective relaxation time $\tau(x)$ can thus be determined from

$$1/\tau(x)=\sum_i [1/\tau_i(x)],$$

where $\tau_i(x)$ are the relaxation times for the individual scattering processes. This assumption is not strictly valid since, for example, an electron can be scattered by a phonon while traversing the potential of an ionized impurity.

(3) The electrons are scattered in a parabolic band. This allows us to use simpler formulations for the various scattering processes.

Although these assumptions are not *a priori* strictly valid, calculations based on these assumptions are in good agreement with experiment.

For high-purity GaAs, classical statistics are applicable, and with the above simplifying assumptions an average relaxation time $\langle\tau\rangle$ can be calculated from the equation

$$\langle\tau\rangle=\frac{4}{3(\pi)^{1/2}}\int_0^\infty \tau(x)x^{3/2}\exp(-x)dx,$$

where x is the electron energy in kT. The electron mobility is then determined from $\mu=e\langle\tau\rangle/m^*$, where e is the electronic charge and m^* is the electron effective mass.

B. Scattering Processes

We first consider the scattering of electrons by optical phonons through the polar interaction. In these collisions, the energy change of the electrons can be large compared with their initial energy, and a universal relaxation time cannot be defined except at low and high temperatures. It is thus necessary to use a variational method to solve the Boltzmann equation[3] to determine the mobility of the electrons. However, following Ehrenreich[4] we use a relaxation time which gives the correct solutions to the Boltzmann equation at low and high temperatures. This is given by

$$1/\tau_{PO}(x)=1.0404\times10^{14}$$

$$\times\left(\frac{\epsilon_0-\epsilon_\infty}{\epsilon_0\epsilon_\infty}\right)\left(\frac{m^*}{m}\right)^{1/2}\theta_l^{1/2}\frac{(\theta_l/T)^r}{[\exp(\theta_l/T)-1]}x^{-r}\ \text{sec}^{-1},$$

where r is a temperature-dependent parameter determined from

$$\tfrac{1}{2}\theta_l^{1/2-r}\Gamma(\tfrac{5}{2}+r)=G^{(1)}e^{-\xi}$$

and Ehrenreich's[5] variational calculations for $G^{(1)}e^{-\xi}$. Here ϵ_0 and ϵ_∞ are the low- and high-frequency dielectric constants and θ_l is the longitudinal optical phonon temperature. For GaAs this method of analysis fails completely from about 120° to 330°K (see Fig. 5 of Ref. 4) and this places an upper temperature limit of 115°K on our calculation.

The scattering of electrons by optical phonons through the deformation potential interaction is not important for the [000] conduction band[6] in GaAs and is thus not considered further.

Because of the lack of inversion symmetry in GaAs there is another source of polar scattering due to the piezoelectrically active acoustic phonons. A relaxation time for piezoelectric scattering was first formulated by Meijer and Polder.[7] With spherical averaging of the piezoelectric and elastic constants over the zinc-blende structure[8] this is given by

$$1/\tau_{PE}(x)=1.0524\times10^{7}$$
$$\times h_{14}^2[(4/c_l)+(3/c_t)](m^*/m)^{1/2}T^{1/2}x^{-1/2}\ \text{sec}^{-1},$$

where h_{14} is the one independent piezoelectric constant in V/cm and the average longitudinal and transverse elastic constants are

$$c_l=\tfrac{1}{5}(3c_{11}+2c_{12}+4c_{44}),$$
$$c_t=\tfrac{1}{5}(c_{11}-c_{12}+3c_{44})$$

in dyn/cm^2.

Since there is a 90° phase difference between the matrix elements for piezoelectric and deformation potential scattering of electrons by acoustic phonons,[9] these mechanisms can be considered separately. The relaxation time for acoustic phonon deformation potential scattering was first calculated by Bardeen and Shockley[10] as

$$1/\tau_{DP}(x)=4.1667\times10^{19}(E_1^2/c_l)(m^*/m)^{3/2}T^{3/2}x^{1/2}\ \text{sec}^{-1},$$

where E_1 is the deformation potential in eV and we use the spherically averaged longitudinal elastic constant c_l given above.

TABLE I. Parameters from Hall constant analyses.

Sample No.	N_D (cm^{-3})	N_A (cm^{-3})	E_D (eV)	N_A/N_D
1	4.80×10^{15}	2.13×10^{13}	5.52×10^{-3}	0.444
2	4.61×10^{15}	2.97×10^{13}	5.57×10^{-3}	0.644
3	7.15×10^{13}	3.66×10^{13}	5.31×10^{-3}	0.512
4	1.91×10^{14}	2.61×10^{13}	5.30×10^{-3}	0.137

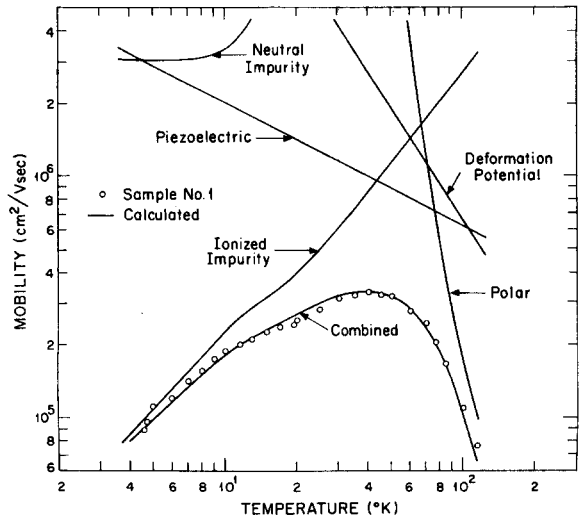

FIG. 1. Temperature dependence of the mobility for the highest purity sample showing the mobility curves calculated for each scattering process, the calculated combined mobility curve, and the experimental points.

The scattering of electrons by singly ionized impurities is described by the Brooks–Herring equation[11] which takes into account screening of the scattering potential. The relaxation time is

$$1/\tau_{II}(x)=2.4149[(2N_A+n)/\epsilon_0^2]$$
$$\times(m^*/m)^{1/2}T^{-3/2}g(n^*,\ T,\ x)x^{-3/2}\ \text{sec}^{-1},$$

where the screening term

$$g(n^*,\ T,\ x)=\ln(1+b)-[b/(1+b)]$$

and

$$b=4.3085\times10^{13}(\epsilon_0/n^*)(m^*/m)T^2x.$$

The effective screening concentration is given by

$$n^*=n+[(n+N_A)(N_D-N_A-n)/N_D]\ \text{cm}^{-3},$$

where n is the electron concentration, N_D is the shallow donor concentration, and N_A is the total compensating acceptor concentration.

For neutral impurity scattering we use Erginsoy's result[12]

$$1/\tau_{NI}=1.225\times10^{-7}\epsilon_0N_N(m^*/m)^{-2}\ \text{sec}^{-1},$$

where the concentration of neutral impurities N_N is taken as

$$N_N=N_D-N_A-n\ \text{cm}^{-3}.$$

This scattering process has an appreciable effect on the resultant mobility only for relatively uncompensated samples at low temperatures.

C. Parameters

In these equations there are a number of parameters, most of which have or can be determined from other measurements.

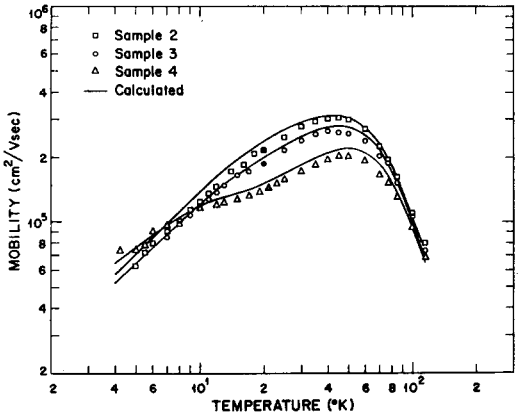

FIG. 2. Temperature dependence of the mobility for three samples showing the calculated combined mobility curves and the experimental points.

The shallow donor concentration N_D and the total acceptor concentration N_A can be determined by fitting the experimental temperature variation of the carrier concentration for each sample to the single donor statistics given by

$$n(n+N_A)/(N_D-N_A-n)=2.415\times10^{15}$$
$$\times(m^*/m)^{3/2}T^{3/2}\exp[(-1.1605\times10^4E_D)/T]\ \text{cm}^{-3},$$

where E_D, the donor thermal ionization energy in eV, is also determined from this analysis.

Other workers have obtained fits to this equation with electron effective masses from $m^*/m=0.070$ to $m^*/m=0.072$.[13–15] We use the value of $m^*/m=0.072$ in the mobility calculations which is consistent with the value most commonly used in the literature. The use of $m^*/m=0.070$ results in an increase in the calculated combined mobility of from 2.0% to 4.8% in the temperature range from 4° to 115°K.

For the dielectric constants there are sizeable variations in the values reported in the literature. We use the values $\epsilon_0=12.53\pm0.10$ and $\epsilon_\infty=10.90\pm0.04$ of Hambleton *et al.*,[16] whose ϵ_0 is in reasonable agreement with the $\epsilon_0=12.35\pm0.07$ of Rogers *et al.*[17]

The reported longitudinal optical phonon temperatures are in good agreement and we use 423°K which is the 77°K value of Iwasa *et al.*[18]

The piezoelectric constant for GaAs has been measured by several independent techniques with the results in generally good agreement. Hambleton's[19] 77°K measurement of $h_{14}=1.41\times10^7$ V/cm is used in the calculation.

The elastic constants are well known and we use the 77°K values of Garland and Park[20]: $c_{11}=1.221\times10^{12}$, $c_{12}=0.566\times10^{12}$, and $c_{44}=0.599\times10^{12}$ dyn/cm².

The only remaining parameter is the conduction band deformation potential. To our knowledge the only reported experimental value is due to Haga and Kimura.[21] Their value of $|E_1|=6.3$ eV is based on an analysis of free-carrier absorption data for heavily doped GaAs in terms of acoustic phonon, optical phonon, and ionized impurity absorption. Since this is probably the least well-known parameter, it is adjusted in the calculation to obtain agreement with the experimental mobility of the highest purity sample.

III. MOBILITY

A. Temperature Dependence

Figure 1 shows the experimental mobility measured at 5 kG for the purest sample (Sample No. 1), the mobility to be expected for the various scattering mechanisms, and the combined mobility which was calculated numerically using the equations in Sec. II.A. The values of N_D, N_A, and E_D for this sample as determined from the Hall constant analysis are listed in Table I. It can be seen that at low, intermediate, and higher temperatures the mobility is dominated by ionized impurity, piezoelectric, and polar optical scattering, respectively. For this sample, neutral impurity scattering is relatively unimportant. However, in the intermediate range, the combined mobility is fairly sensitive to deformation potential scattering because of its strong energy dependence. That is, from 45° to 85°K a variation in the deformation potential of 10% produces a variation in the combined mobility of from 5% to 6%. The deformation potential was thus adjusted to obtain agreement between the calculated and experimental mobility in this temperature range. The mobilities shown in Fig. 1 were calculated with a deformation potential of $|E_1|=7.0$ eV.

With this value the temperature dependence of the combined mobility for several other samples was calculated. These curves are shown in Fig. 2 with the values of N_D, N_A, and E_D for each sample as determined from the Hall constant analyses given in Table I. As can be seen there is good agreement between the cal-

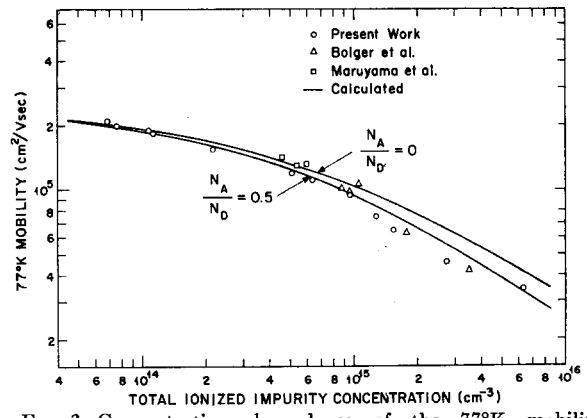

FIG. 3. Concentration dependence of the 77°K mobility showing curves calculated for two compensation ratios and the experimental values.

culated and experimental mobilities. It should be emphasized that these calculated curves are obtained with no adjustable parameters and that the agreement at low temperatures where ionized impurity scattering is dominant depends upon the accuracy of the values of N_D and N_A obtained from the Hall constant analyses.

It is interesting to note that the least pure sample in Fig. 2 (sample No. 4) has the highest experimental and calculated mobility at the lowest temperatures. As indicated in Table I this sample is the least compensated sample ($N_A/N_D=0.137$) and thus has fewer ionized impurities at low temperatures where the shallow donors are de-ionized. The contribution due to neutral impurity scattering is also more important for this sample.

B. Impurity Concentration Dependence

Since the 77°K mobility is a commonly used figure of merit for GaAs, we have plotted experimental values in Fig. 3 as a function of total ionized impurity concentration (N_D+N_A) over the donor concentration range where sufficient donor de-ionization is observed to allow meaningful analyses of the temperature variation of the Hall constant. Also shown are values determined in a similar manner by Bolger *et al.*[14] and Maruyama *et al.*,[15] where the low-field mobility values of Maruyama *et al.* were converted to the values that would be obtained at 5 kG. The curves shown were calculated using compensation ratios of $N_A/N_D=0$ and $N_A/N_D=0.5$, whereas our experimental values varied from 0.14 to 0.65. The points which lie above the calculated zero compensation curve may be caused by uncertainties in determining N_D and N_A. In any case, there is reasonably good agreement between experimental and calculated values over this concentration range.

It can also be seen in Fig. 3 that the 77°K mobility is becoming increasingly less sensitive to ionized impurity scattering in the low concentration range and is approaching a lattice scattering limit. The calculation presented here yields a lattice limited mobility of 240 000 cm²/V sec at 77°K. The less accurate value obtained by simply combining the individual mobilities is 258 000 cm²/V sec. Since the experimental value at $N_D+N_A=7\times10^{13}$ cm^{-3} is already 210 000 cm²/V sec, at lower concentrations the 77°K mobility is no longer very useful as a figure of merit for GaAs.

IV. CONCLUSION

Since the calculated mobility is in good agreement with experiment, we conclude that the combination of polar optical phonon, piezoelectric acoustic phonon, deformation potential acoustic phonon, ionized impurity, and neutral impurity scattering in the relaxation time approximation provides an adequate description of electron scattering in high-purity GaAs over the temperature range considered.

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