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Electron scattering in heavily doped compensated polar semiconductors

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A calculation of electron mobility in heavily doped compensated polar semiconductors is presented including lattice scattering as well as scattering from point-impurity charges and from the hitherto neglected dipoles formed by the donor-acceptor pairs. Comparison with experimental data for GaAs doped heavily with Si gives evidence that the consideration of dipoles is essential in accounting for the electron transport.

In a compensated semiconductor, Coulomb attraction between donor and acceptor ions leads to the formation of dipoles. The presence of dipoles has, however, received little attention so far in mobility analyses for compensated semiconductors. In the present Communication we report a calculation of electron mobility in a compensated polar semiconductor including the formation of dipoles. Our calculated results show that the dipoles must be incorporated in accounting for the measured mobility values in GaAs highly doped with Si.

In addition to dipoles, we consider scattering from point-impurity charges together with lattice scattering due to polar optic and deformation-potential acoustic phonons. In the presence of an electric field $\vec{\mathscr{E}}$, the carrier distribution function may be written as

$$f(\vec{k}) = f_0(E) - \left(\frac{e\hbar\mathscr{E}}{m^*}\right) k\phi(E)\cos\theta \ , \tag{1}$$

where $\vec{k}$ is the Bloch vector of an electron with energy E, e is the charge on the electron, $\hbar$ is Planck's constant divided by 2π, m^* is the electron effective mass, and θ is the angle between $\vec{\mathscr{E}}$ and $\vec{k}$. The perturbation function $\phi(E)$ has to be determined from the Boltzmann equation, which reads[1]

$$\begin{aligned}&[S_o(E) + \tau_d^{-1} + \tau_i^{-1} + \tau_{\mathrm{ac}}^{-1}]\phi(E)\\ &\quad = 1 + S_+(E)\phi(E+\hbar\omega_0) + S_-(E)\phi(E-\hbar\omega_0) \ ,\end{aligned} \tag{2}$$

where τ_d, τ_i, and τ_{ac} are the relaxation times for scattering by dipoles, point-charge impurities, and acoustic phonons, respectively. $S_o(E)$ is the scattering-out rate and $S_\pm(E)$ correspond to the scattering-in rates due to the emission and absorption of polar optic phonons of energy $\hbar\omega_0$.

The expressions for τ_{ac}, $S_o(E)$, and $S_\pm(E)$ are well known.[1] For dipole scattering, the Born approximation is found to be good enough for polar semiconductors.[2] The corresponding relaxation time for the scattering is given by[2]

$$\frac{1}{\tau_d} = \frac{m^{*1/2}e^4N_d a_1^2}{6\sqrt{2}\pi\hbar^2\epsilon^2\epsilon_0^2} E^{-1/2}\left(\frac{2+b}{1+b} - \frac{2}{b}\ln(1+b)\right) \ , \tag{3}$$

where N_d is the concentration of dipoles, a_1 is the dipole length, ϵ is the dielectric constant of the material, ϵ_0 is the permittivity of free space, $b = 8m^* \times E(\hbar^2\beta^2)^{-1}$, β is the inverse screening length:

$$\beta^2 = \frac{\sqrt{2}e^2m^{*3/2}}{\pi^2\hbar^3\epsilon\epsilon_0} \int_0^\infty E^{-1/2}\left(-\frac{\partial f_0}{\partial E}\right) dE \ , \tag{4}$$

and f_0 is the Fermi-Dirac distribution.

If N_A and N_D are the concentrations of ionized acceptors and donors, respectively, the concentration of the point-charge impurities is $N_i = N_A + N_D - 2N_d$. The relaxation time for scattering by such point charges has been worked out by Brooks and Herring using the Born approximation and the dielectric function independent of the wave vector.[3] Meyer and Bartoli have recently compared the Born-approximation results with those obtained on the basis of phase-shift calculations.[4] They have shown that for a polar semiconductor like GaAs the use of the Born approximation at room temperature does not overestimate the mobility by more than 10% for carrier concentrations less than 10^{19} cm^{-3}. The exact contribution of the wave-vector dependence of the dielectric function is currently being debated; but it appears that the effect would not be significant for practical concentration ranges.[5] We may thus use, for point-charge scattering at room temperature, the Brooks-Herring formula which greatly simplifies the calculations. This formula is[3]

$$\frac{1}{\tau_i} = \frac{e^4N_i}{16\sqrt{2}\pi\epsilon^2\epsilon_0^2m^{*1/2}} E^{-3/2}\left(\ln(1+b) - \frac{b}{1+b}\right) \ . \tag{5}$$

Equation (2) is solved for the $\phi(E)$ by the numerical iterative method detailed in Ref. 1. In the ith step of iteration, $\phi(E)$ is evaluated from the values of $\phi(E \pm \hbar\omega_0)$ obtained in the $(i-1)$th step through the relation

$$\phi^{(i)}(E) = [S_o(E) + \tau_d^{-1} + \tau_i^{-1} + \tau_{\mathrm{ac}}^{-1}]^{-1} \times [1 + S_+(E)\phi^{(i-1)}(E+\hbar\omega_0) + S_-(E)\phi^{(i-1)}(E-\hbar\omega_0)] \ . \tag{6}$$

The quantities $\phi^{(0)}(E \pm \hbar\omega_0)$ are put to zero. A few iterations are needed to yield a convergent value of the mobility given by

$$\mu = \int_0^\infty E^{3/2}\phi(E)\left(-\frac{\partial f_0}{\partial E}\right) dE \left[\int_0^\infty E^{3/2}\left(-\frac{\partial f_0}{\partial E}\right) dE\right]^{-1} \ . \tag{7}$$

The method given above may be applied to samples which are so strongly compensated that a sizable number of dipoles are present. In the data reported in the literature, usually the compensation ratio is not large enough to reveal the importance of dipole scattering. Often the impurity and carrier concentrations are not separately measured; the nature of the impurities and the crystal growth temperature are also not mentioned. It is thus difficult to calculate the number of dipoles present. Recently, Druminski *et al.*[6] have made a systematic measurement of electron mobility at room temperature in GaAs doped highly with Si. The samples are very strongly compensated: the impurity and the carrier concentrations, measured by secondary ion mass spectrometry (SIMS) and Hall effect, being in the region 10^{20} and 10^{18} cm^{-3}, respectively. They provide all the information needed for an estimate of the number of dipoles. Therefore, we consider their data here for a meaningful application of the mobility calculation given above.

Si is known to be a substitutional impurity in GaAs, being present in both Ga and As sites.[7] Si acts as a donor, if substitutional on the Ga site and as an acceptor, if substitutional on the As site. In addition to isolated donor and acceptor ions, there are dipoles formed by the nearest-neighbor pairs ($\mathrm{Si_{Ga}}$-$\mathrm{Si_{As}}$).

In order to evaluate dipole scattering, one must estimate the concentration N_d. The theory of donor-acceptor pairing when at least one type of impurity is interstitial has been developed by Reiss *et al.*[8] When the impurities are substitutional, as in the case of Si-doped GaAs, the treatment of Wiley[9] is more appropriate. He considers the Coulomb energy of the paired ions and also the Debye-Hückel interaction of the unpaired charges. Using the principle that the interacting charges distribute themselves during crystal growth in a way to minimize the free energy, it can be shown that

$$\frac{N_d}{N_I} = \frac{1}{2}\left(1 + \frac{1}{N_I\Omega}\right) - \frac{1}{2}\left[\left(1 + \frac{1}{N_I\Omega}\right)^2 - \frac{4N_AN_D}{N_I^2}\right]^{1/2} , \tag{8}$$

where $N_I = N_A + N_D$ is the total concentration of impurities, and

$$\Omega = \frac{Z}{N}\exp\left[\frac{e^2}{4\pi\epsilon\epsilon_0 k_B T}\left(\frac{1}{a_1} - \frac{K}{1+Ka_2}\right)\right] \ . \tag{9}$$

Here Z is the number of nearest-neighbor sites, N is the concentration of host atoms of either sublattice, k_B is the Boltzmann constant, T is the growth temperature, a_2 is the distance of closest approach for the unpaired ions, and K is the inverse Debye-Hückel length:

$$K^2 = \frac{2(N_D - N_d)e^2}{\epsilon\epsilon_0 k_B T} \ . \tag{10}$$

It should be noted that we consider here only nearest-neighbor pairing. For GaP at similar temperatures, however, the first three to six shells of neighbors should probably be included before the ions can be considered "unpaired."[9] For example, at 1000 K in GaP, about 20% of the pairing is at sites further away than nearest neighbors. This small contribution from higher-order pairing is neglected here for the sake of simplicity. Furthermore, in Eq. (9) we take the dielectric constant appropriate for the bulk material. This assumption is justified since Srinivasan has shown that the dielectric function attains its bulk value at the nearest-neighbor distance.[10]

For numerical calculations, we note that the nearest-neighbor distance in pure GaAs is 2.44 Å. When Si atoms occupy the nearest-neighbor sites, the distance is likely to be somewhat smaller since the sum of the covalent radii of two Si atoms is 2.22 Å. An intermediate value of 2.33 Å is thus reasonably chosen for the nearest-neighbor separation a_1 for Si ions substituted in GaAs. Using $a_2 = 4.67$ Å, $\epsilon = 12.91$, $Z = 4$, and $N = 2.23 \times 10^{22}$ cm^{-3}, the quantity N_d/N_I is calculated for the doping levels and the growth temperature of 923 K of the samples in question. The values of N_A and N_D required in the computations are obtained from the values of the impurity and the carrier concentrations, quoted by the experimenters.[6] Since K depends on N_d, we first calculate Ω and N_d/N_I from Eqs. (9) and (8), respectively, by setting $K = 0$. The calculated values of N_d are then used in Eq. (10) to determine K; the quantities Ω and N_d/N_I are then recalculated with the K term included. Ordinarily, two iterations are sufficient since the convergence is very rapid. The computed values of N_d/N_I are displayed in Fig. 1. A sizable fraction of the silicon ions is found to form dipoles for the doping levels of concern here.

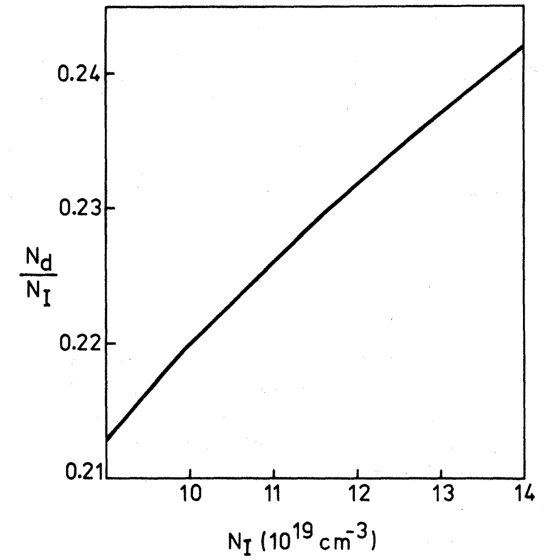

FIG. 1. Variation of the relative concentration of dipoles as a function of the concentration of the silicon impurity atoms for a growth temperature of 923 K.

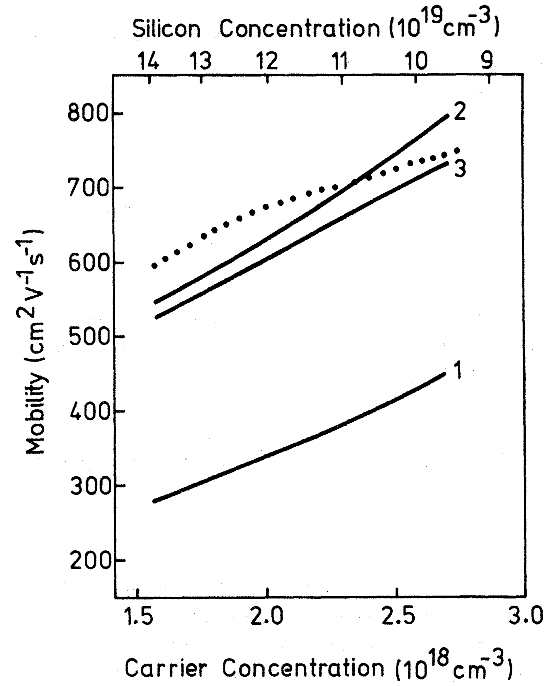

FIG. 2. Electron mobility against carrier and impurity concentrations in heavily Si-doped GaAs at 300 K. Lattice scattering is excluded in curves 1 and 2. Curve 1 considers scattering from impurity point charges; curve 2 considers scattering from point charges as well as from dipoles. Curve 3 includes lattice, point charge, and dipole scattering. The dotted line represents experimental data (Ref. 6).

The mobility is calculated considering the shift of the Fermi-level characteristic of the heavy doping regime,[11] and using the scattering parameters given in Ref. 1. Figure 2 shows the computed values of mobility at room temperature. In curves 1 and 2 lattice scattering is not incorporated. Curve 1 represents the results obtained by completely neglecting the formation of dipoles and assuming that all the silicon ions act as point-charge scatterers; these mobility values are much lower than the experimental ones. Curve 2 gives the results when the presence of dipoles is considered and scattering by both point charges and dipoles are included. Curve 2 lies above curve 1, since scattering due to dipoles is nearly two orders of magnitude weaker than that because of an equal number of point charges.[2] Consideration of dipoles thus removes a corresponding number of impurities from effectively scattering the carriers, giving a higher value of mobility. Finally, we calculate the mobility incorporating lattice scattering in addition to scattering by point charges and dipoles. The results, displayed by curve 3, are close to the experimental data. The small discrepancy between theory and experiment may arise from higher-order pairing and from the complications associated with the point-ion scattering which have been ignored in the analysis. A noteworthy complication is the occurrence of multiple scattering.[5] A general theory including multiple scattering is not available, but some insight has recently been provided.[12]

In conclusion, we have included dipole scattering, among others, in the calculation of electron mobility in a compenstated polar semiconductor, and have applied the method to GaAs doped heavily with Si. The reasonable agreement obtained between calculated and measured mobilities in this case shows that the electron transport is strongly influenced by dipoles formed between nearest-neighbor donor-acceptor pairs. Evidences of such pair formation have already been obtained in infrared absorption measurements.[7]

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[1] B. R. Nag, *Electron Transport in Compound Semiconductors* (Springer-Verlag, Berlin, Heidelberg, New York, 1980).

[2] R. Stratton, J. Phys. Chem. Solids 23, 1011 (1962).

[3] H. Brooks, in *Advances in Electronics and Electron Physics,* edited by L. Marton (Academic, New York, 1955), Vol. 7, p. 85

[4] J. R. Meyer and F. J. Bartoli, Phys. Rev. B 23, 5413 (1981).

[5] For a recent review, see D. Chattopadhyay and H. J. Queisser, Rev. Mod. Phys. 53, 745 (1981).

[6] M. Druminski, H. D. Wolf, K. H. Zschauer, and K. Wittmaack, J. Cryst. Growth (in press).

[7] W. G. Spitzer and M. B. Panish, J. Appl. Phys. 40, 4200 (1969).

[8] H. Reiss, C. S. Fuller, and F. J. Morin, Bell Syst. Tech. J. 35, 535 (1956).

[9] J. D. Wiley, J. Phys. Chem. Solids 32, 2053 (1971).

[10] G. Srinivasan, Phys. Rev. 178, 1244 (1969).

[11] V. L. Bonch-Bruevich, Fiz. Tverd. Tela 4, 2660 (1962) [Sov. Phys. Solid State 4, 1953 (1963)]; I. P. Zvyagain, *ibid.* 5, 581 (1963) [5, 422 (1963)].

[12] J. R. Meyer and F. J. Bartoli (unpublished).