Electron mobility limited by ionized impurity scattering with nonlinear screening in semiconductors

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(Received 19 May 1980; revised manuscript received 28 July 1980)

Electron mobility in GaAs due to ionized impurity scattering is calculated by considering nonlinear screening charge. The calculated values are larger than those obtained with the conventional linearized screening charge. The discrepancy is most important at intermediate carrier densities and may be as large as a factor of 1.8 at 77 K for a carrier concentration of a few times 10^{16} cm^{-3}. The Hall-to-drift mobility ratios are, however, not much altered when nonlinear screening is included. Incorporation of nonlinear screening is shown to enhance the disparity between the theoretical and the experimental mobilities at 77 K.

I. INTRODUCTION

Ionized impurity scattering strongly affects electron mobility in semiconductors at low temperatures and also figures importantly near room temperature for large doping levels. Usually this type of scattering is described in the Born approximation with a simple screened Coulomb potential[1] resulting from two simplifying assumptions. First, the medium is characterized by the static dielectric constant of the undoped semiconductor. Second, the screening charge is linearized by keeping only the first-order term in potential over thermal energy. A number of researchers have sought to remove the first approximation by allowing for the dispersive valence screening in the calculation of mobility.[2] These calculations were criticized since they did not consider the correct impurity potential.[3,4] If the correct potential is used, the effect of the valence electron dispersive screening turns out to be quite small.[3] A recent numerical calculation[4] shows that the second approximation, i.e., linear screening, is usually more severe than the first so far as electron scattering is considered. The present paper aims at evaluating the effect of nonlinear screening on electron mobility by numerically solving the Poisson's equation. Calculations are presented for the technologically important material GaAs. The formulas are contained in Sec. II. The numerical results are given and discussed in Sec. III. The conclusions are presented in Sec. IV.

II. THEORY

The electrostatic potential $\phi(r)$ surrounding an impurity ion at $\vec{r}=0$ satisfies the Poisson's equation

$$\nabla^2\phi = \frac{e[n(r)-n]}{\epsilon_0 K_0}\,, \tag{1}$$

where e is the electron charge, ϵ_0 is the permittivity of free space, K_0 is the static dielectric constant of the material, n is the uniform carrier concentration, and $n(r)$ is the carrier concentration at a distance r from the ion. The boundary conditions are $\phi(r\to 0)=e(4\pi\epsilon_0 K_0 r)^{-1}$ and $\phi(r\to\infty)=0$.

For parabolic band structures,[5]

$$n(r)=\frac{Z}{\sqrt{2}\hbar^3}\left(\frac{m^* k_B T}{\pi}\right)^{3/2}\mathfrak{F}_{1/2}\left(\eta+\frac{e\phi}{k_B T}\right), \tag{2}$$

where Z is the number of degenerate conduction band valleys, $\hbar$ is Planck's constant divided by 2π, m^* is the carrier effective mass, k_B is Boltzmann's constant, T is the lattice temperature, $\mathfrak{F}_j$ is the Fermi-Dirac integral[6] of order j, and $\eta=E_F(k_B T)^{-1}$, E_F being the Fermi energy. The quantity n is given by Eq. (2) with $\phi=0$.

In the usual theory of ionized impurity scattering, $\mathfrak{F}_{1/2}$ in Eq. (2) is expanded in a Taylor series to the first order in $e\phi/k_B T$. Equation (1) is thus linearized and yields the screened Coulomb potential[5]

$$\phi_0(r)=\frac{e}{4\pi\epsilon_0 K_0 r}\exp(-\beta r)\,, \tag{3}$$

where β is the inverse screening length:

$$\beta^2=\left(\frac{ne^2}{\epsilon_0 K_0 k_B T}\right)\frac{\mathfrak{F}_{-1/2}(\eta)}{\mathfrak{F}_{1/2}(\eta)}\,. \tag{4}$$

When terms higher than the first order in $e\phi/k_B T$ are retained in the Taylor series expansion of $\mathfrak{F}_{1/2}$ in Eq. (2), Eq. (1) becomes nonlinear. Keeping terms up to the second order in $e\phi/k_B T$ in Eq. (2), Csavinszky[7] and Adawi[8] have solved Eq. (1) and have obtained an analytic expression for the impurity potential. This is

$$\phi(r)=\phi_0(r)\{1+\alpha[\exp(2r\beta)\,\mathrm{Ei}(-3r\beta) - \mathrm{Ei}(-r\beta)-\ln 3]\}\,, \tag{5}$$

where $\phi_0(r)$ is given by Eq. (3),

$$\alpha = \frac{e^2\beta}{16\pi\epsilon_0 K_0 k_B T} \frac{\mathfrak{F}_{-3/2}(\eta)}{\mathfrak{F}_{-1/2}(\eta)} , \tag{6}$$

and $\mathrm{Ei}(-x)$ is the exponential integral

$$-\mathrm{Ei}(-x) = \int_x^\infty t^{-1}\exp(-t)dt . \tag{7}$$

Equation (5) has been used by Adawi[8] to derive the momentum transfer cross section in the Born approximation. This equation is adequate when[8] $\alpha \ll 1$. In the general case, however, one has to solve the complete nonlinear Poisson's equation by numerical methods[4,8] to obtain the scattering potential. Alternatively, since the theory of ionized impurity scattering has been developed on the basis of a single screened Coulomb potential,[1] one may choose as a solution to the nonlinear Poisson's equation a linear combination of screened Coulomb potentials with coefficients to be determined by the variational principle.[9] We have obtained here numerical solutions to the complete nonlinear Poisson's equation by a combination of Runge-Kutta and predictor-corrector methods.[10] The solution is started by the Runge-Kutta method and taken over subsequently by the predictor-corrector method. The starting value of r is taken to be $0.001\beta^{-1}$, and the values of ϕ and ϕ' at this point were supplied from the boundary conditions. This choice of the starting point is somewhat arbitrary, but is seen to be adequate from previously reported results.[4]

The numerical solutions of the potential are used to calculate electron mobility through the Born approximation. The use of the Born approximation is along the lines of the previous calculations[1,3,8] and it also makes the calculations tractable. Although some question has been raised[11] about the applicability of this approximation when the scattering potential deviates from that given by Eq. (3), the general features of the results are expected to remain valid.

The drift and Hall mobilities μ_D and μ_H are obtained by means of the relations

$$\mu_D = e\langle\tau\rangle/m^* , \tag{8}$$

and

$$\mu_H = (e/m^*)(\langle\tau^2\rangle/\langle\tau\rangle) , \tag{9}$$

where

$$\langle Q\rangle = \tfrac{2}{3}\int_0^\infty E^{3/2}Q(E)\left(-\frac{\partial f_0}{\partial E}\right)dE \Big/ \int_0^\infty E^{1/2}f_0 dE . \tag{10}$$

E is the energy of a conduction electron with Bloch wave vector $\vec{k}$ and f_0 is the Fermi-Dirac distribution function. The momentum relaxation time $\tau(E)$ is given by[12]

$$1/\tau(E) = 2\pi N_I (2E/m^*)^{1/2} \times \int_0^\pi (1-\cos\theta)|f(\theta)|^2 \sin\theta\, d\theta , \tag{11}$$

where N_I is the concentration of the ionized impurities and $|f(\theta)|^2$ is the cross section for scattering into the angle θ. In the Born approximation we have

$$|f(\theta)| = \frac{2m^*e}{\hbar^2}\int_0^\infty \phi(r)\frac{\sin[2kr\sin(\theta/2)]}{2kr\sin(\theta/2)} r^2 dr . \tag{12}$$

III. CALCULATED RESULTS

Electron drift and Hall mobilities in GaAs, computed on the basis of the formulas given above, will be presented in this section. We have assumed $K_0 = 12.91$ and have allowed for the temperature variation of the effective mass by the formula[13] $m^*(T)/m_0 = 0.0681 - 9.33\times10^{-6}T$, m_0 being the free electron mass.

To appreciate the effect of the nonlinear screening on mobility we have depicted in Fig. 1 the behavior of the quantity $\phi(r)/\phi_0(r)$ in the neighborhood of the screening length. The nonlinear potential is found to be lower than the linear one. This reflects the fact that in the nonlinear theory the screening charge is enhanced in the neighborhood of the impurity atom, but is weakened at large distances.[4] It is also observed that in the region concerned, the exact nonlinear potential is lower than that obtained from the approximate expression of Adawi[8] [Eq. (5)].

As the scattering potential is weaker in the nonlinear treatment, one would expect a corresponding increase in mobility. This is indeed found to be the case in Fig. 2. The difference between the

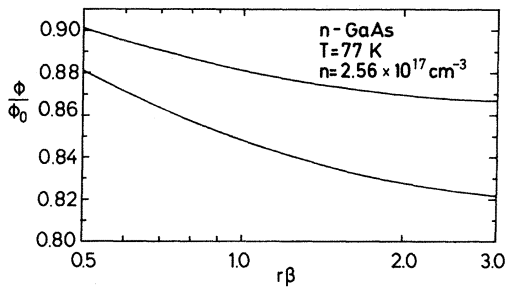

FIG. 1. Ratio of the impurity potential ϕ obtained with the nonlinear screening charge to the potential ϕ_0 obtained with the linear screening charge vs $r\beta$. The lower curve represents the solution of the complete nonlinear Poisson's equation. The upper curve represents the results with ϕ given by Eq. (5).

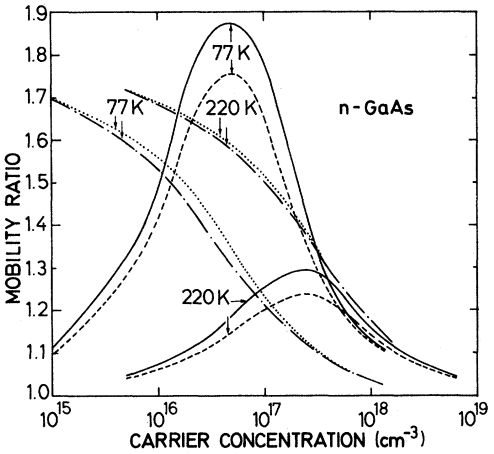

FIG. 2. Mobility ratio versus carrier concentration at two different temperatures. The solid lines give the ratio of the drift mobility in the exact nonlinear screening model to that in the linear screening model; the dashed lines give the same ratio when the approximate nonlinear screening model [Eq. (5)] is used. The dash-dotted curves represent the Hall-to-drift mobility ratio in the nonlinear screening model; the dotted lines give the corresponding quantity in the linear screening model.

exact numerical results and those based on the approximate expression of Adawi[8] [Eq. (5)] is more at intermediate carrier concentrations than at low and high carrier concentrations. This is understandable from the result[7] that the parameter α, which is a measure of the convergence of the expansion of $\mathfrak{F}_{1/2}$, is a maximum at intermediate carrier concentrations. At high carrier concentrations, the electron system is almost degenerate, and here α is independent[7] of T. Consequently, in Fig. 2 the ratio of the drift mobility in the nonlinear theory to that in the linear theory is insensitive to changes in T for large values of n. It is striking that the ratio of the nonlinear theory to the linear-theory mobility is about 1.9 at 77 K for a carrier concentration of 5×10^{16} cm^{-3}.

The Hall-to-drift mobility ratio, also plotted in Fig. 2, decreases and approaches unity as n rises. This is because in the degenerate limit only the carriers at the Fermi energy contribute to transport. At low values of n, the Hall-to-drift mobility ratio is found to be lower than the usually accepted value of 1.93 which is obtained in the non-degenerate limit, taking $\tau(E)$ to be proportional to $E^{3/2}$. It is observed that the Hall-to-drift mobility ratios in the nonlinear theory are not much different from those in the linear one.

Figure 3 shows electron Hall mobility in uncompensated GaAs ($N_I = n$) limited by ionized impurity scattering in the nonlinear theory at 77 K (topmost solid curve). The dotted curve represents the mobility including phonon scattering and ionized impurity scattering in the linear theory.[1] As the nonlinear theory, impurity-scattering mobility is larger than the linear-theory value, it is obvious that the overall mobility incorporating phonon scattering would lie above the dotted curve. The discrepancy between the calculated and experimental results[14] (represented by the lowermost solid curve) is thus enhanced when nonlinear screening is accounted for in the ionized impurity scattering. To explain the experimental results, one must consider the compensation of the samples and some other scattering mechanisms like electron-electron[15] and space-charge scattering,[16] which are not included in the theory.[1]

IV. CONCLUSIONS

The scattering potential due to the ionized impurities is reduced when the nonlinear screening charge is taken into account. This reduction causes significant enhancement of electron mobility in GaAs at 77 K for carrier densities in the region of 10^{16} cm^{-3}. The effect is found to increase the discrepancy between the theoretical and experimental mobilities. The ratio between the Hall and drift mobilities is, however, practically unaffected when nonlinear screening is incorporated.

ACKNOWLEDGMENTS

The author is indebted to Professor H. J. Queisser for his continued interest and valuable advice and to Professor Frank Stern for helpful discussions. Thanks are due to the Max-Planck-Gesellschaft for support.

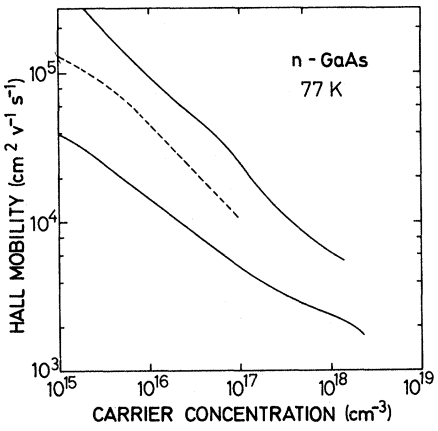

FIG. 3. Hall mobility versus carrier concentration at 77 K. The upper solid curve gives the ionized impurity scattering limited values in the nonlinear treatment. The lower solid line is the empirical curve introduced in Ref. 14. The dashed lines represent the theoretical curve of Rode (Ref. 1).

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