Effect of valence dielectric screening on ionized-impurity scattering in semiconductors

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The effect of valence dielectric screening on ionized-impurity scattering is considered for n-type silicon, germanium, and gallium arsenide. The validity of the two ionized impurity potentials developed by Csavinszky and Resta, incorporating the spatial dependence of the dielectric function, is critically examined. The relevance of Friedel sum rule is briefly discussed using quantum statistics. The relaxation time for electrons is evaluated using Born phase shifts. The results are compared with earlier published work.

I. INTRODUCTION

The scattering of charge carriers by ionized impurities in a doped semiconductor has been widely studied in terms of the Brooks-Herring[1] (BH) theory which uses the Born approximation. Several attempts[2] have been made to improve the BH treatment by removing one or more of its simplifying assumptions or by allowing for the effects neglected in that theory.

In the BH theory, the dielectric response of the valence electrons to the field of the ionized impurity is taken to be described by the static dielectric constant of the semiconductor. Csavinszky[3,4] introduced impurity-ion potentials which included the dispersive screening of the dielectric medium. The impurity-ion potentials derived by him were also used by others[5-8] to calculate the ionized-impurity-scattering-limited mobilities. Unfortunately, these impurity-ion potentials were shown to be incorrect and were subsequently corrected[9-11] Following an approach that is different from Csavinszky's, Resta[12] developed a screening theory in a doped semiconductor at nonzero temperature. The theory was applied by Resta and Resca[13] (RR) to calculate the ionized-impurity-scattering-limited mobility in Si. The departure from the BH result was found to be negligible at both high and low concentration limits. At intermediate concentrations also the departure was not more than 5% at 300 K. It should be mentioned that RR used classical statistics in their analysis and thus the Friedel[14] sum rule which is a quantum-mechanical result did not enter in their work. Using Fermi-Dirac statistics, Scarfone and Richardson[15] found that increasing doping above 10^{18} cm^{-3} in Si at 300 K the mobility decreases monotonically from the BH value. The change from the BH value is less than 10% for concentrations as high as 10^{21} cm^{-3}. The boundary conditions used by them have, however, been criticized.[16]

In the present work, we examine the effect of spatial variation of the dielectric function on the ionized-impurity-limited mobility of n-type, Si, Ge, and GaAs at 300 K by computing the relaxation time for the Fermi wave vector K_F from the Born phase shifts that satisfy the Friedel sum rule for a concentration of 10^{21} cm^{-3}.

The method of partial wave was first applied by Blatt[17] to calculate the scattering due to the screened Coulomb potential. While Blatt's results apply mostly to nondegenerate semiconductors, Csavinszky[18] employed a variational technique to obtain analytic approximations for the zero-order phase shifts in the limit of extreme degeneracy. Neither of these authors attempted to satisfy the Friedel[14] sum rule. This shortcoming was corrected by Krieger and Strauss[19] who provided a phase-shift treatment for the scattering of degenerate electrons by a screened Coulomb potential. In a more recent paper Brownstein[20] corrected some errors in Ref. 18. Boardman and Henry[21] have performed the phase-shift analysis for the nondegenerate scattering problem, using the generalized Friedel sum rule.[22] Meyer and Bartoli[23] have done a full partial-wave analysis of the ionized-impurity scattering for Si, Ge, and GaAs over a wide range of temperatures and concentrations. Their calculations show a more than 10% reduction in mobility from the BH value for Ge with an impurity concentration of 10^{20} cm^{-3} at 300 K. None of them have taken into account the spatial variation of dielectric function in the impurity-ion potential.

In Sec. II we examine critically the validity of the two theories developed by Csavinszky and Resta to incorporate the dispersive screening of the dielectric medium in the impurity-ion potential. In Sec. III the details of the relaxation-time calculations based on the Born phase shifts are presented. Care was taken to satisfy the Friedel sum rule while incorporating the spatial variation of dielectric function.

II. GENERALIZATION OF THE DINGLE POTENTIAL

The first attempt at generalizing Dingle's model[24] of the screening of impurity ion in doped semiconductors at nonzero temperature by incorporating valence screening effect is due to Csavinszky[3,4] who has used the relation

$$\vec{E}(\vec{r})=K^{-1}(\vec{r})\vec{D}(\vec{r}) , \tag{1}$$

which should be treated as an approximation to the usual nonlocal relation in the linear-response theory,

$$\vec{E}(\vec{r})=\int \epsilon^{-1}(\vec{r},\vec{r}\,')\vec{D}(\vec{r}\,')d^3r' . \tag{2}$$

It can be seen that Eq. (2) results in Eq. (1) if $\epsilon^{-1}(\vec{r},\vec{r}\,')=K^{-1}(\vec{r})\delta(\vec{r}-\vec{r}\,')$. $K^{-1}(\vec{r})$ in Eq. (1) is the reciprocal of the "spatially variable dielectric function" $K(\vec{r})$,[11] while $\epsilon(\vec{r})$ is the spatial dielectric function.[11] In

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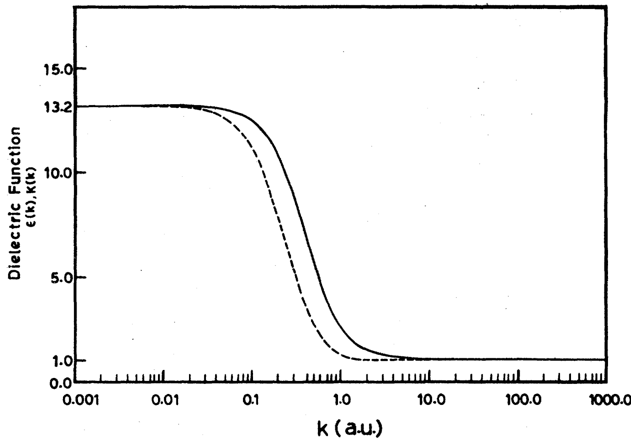

FIG. 1. k-dependent dielectric functions $\epsilon(k)$, solid line, and $K(k)$, dashed line.

what follows, both $K(r)$ and $\epsilon(r)$ are taken to be spherically symmetric.

Using the nonlocal relation, Eq. (2), Resta[12] obtained an integro-differential equation for the screened point-charge potential. It is easy to establish the relation between $K(r)$ and $\epsilon(r)$,[16]

$$\frac{1}{K(r)} = \frac{1}{\epsilon(r)} - r\frac{d}{dr}\left[\frac{1}{\epsilon(r)}\right] . \tag{3}$$

The dielectric function $\epsilon(r)$ is obtained on the basis of a model due to Cornolti and Resta,[25] solved variationally by Csavinszky and Brownstein.[26] Knowing $\epsilon(r)$, one can obtain $K(r)$ from Eq. (3). We have plotted for comparison $\epsilon(k)$ and $K(k)$ for GaAs with $Z=1$ in Fig. 1. $\epsilon(k)$ is related to $\epsilon(r)$ by

$$\frac{1}{r\epsilon(r)} = \frac{1}{2\pi^2}\int \frac{e^{i\vec{k}\cdot\vec{r}}}{k^2\epsilon(k)} d^3k . \tag{4}$$

Similarly one can obtain $K(k)$ from $K(r)$. $\epsilon(r)$ and $K(r)$ are also plotted for GaAs in Fig. 2. It is easy to see that $K(r)$ approaches $\epsilon(r)$ for $r \geq R$, the screening radius. The

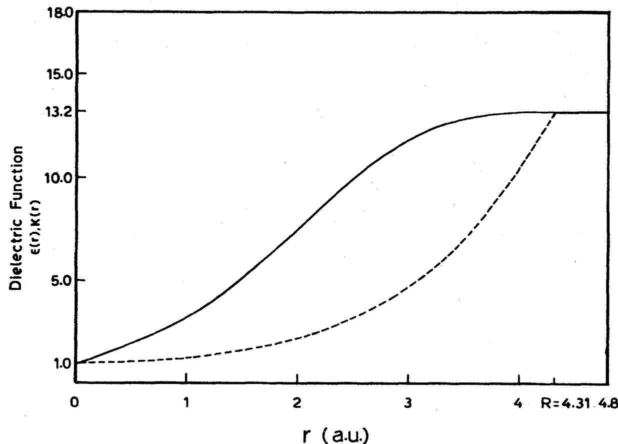

FIG. 2. Spatial variation of dielectric functions $\epsilon(r)$, solid line, and $K(r)$, dashed line.

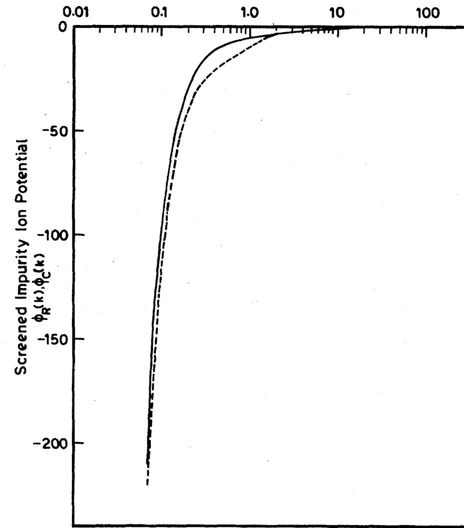

FIG. 3. Screened impurity-ion potentials in $\vec{k}$ space for the impurity concentration 10^{17} cm^{-3} for GaAs at 300 K. $\phi_R(k)$, solid line, and $\phi_C(K)$, dashed line.

discontinuity in the slope of $K(r)$ at $r=R$ is a consequence of the form of $\epsilon(r)$ obtained in Ref. 26.

Morrow[27] has shown the approximate equivalence of the impurity-ion potentials $\phi_R(r)$ and $\phi_C(r)$ obtained by Resta and Csavinszky, respectively. While these potentials can be nearly equal, a substantial difference exists between the Fourier components $\phi_R(k)$ of the potential $\phi_R(r)$ (Ref. 12) and those obtained with $\epsilon(k)$ replaced by $K(k)$ in $\phi_R(k)$. The latter is designated as $\phi_C(k)$. $\phi_R(k)$ and $\phi_C(k)$ are plotted in Figs. 3 and 4 for GaAs at 300 K for the concentrations 10^{17} and 10^{21} cm^{-3}. In view of the local approximation in Csavinszky's approach, we are using $\epsilon(k)$ instead of $K(k)$ in our calculations of Born phase shifts described in the next section. Geetha and Balasubramanian[28] have compared the various screened impurity

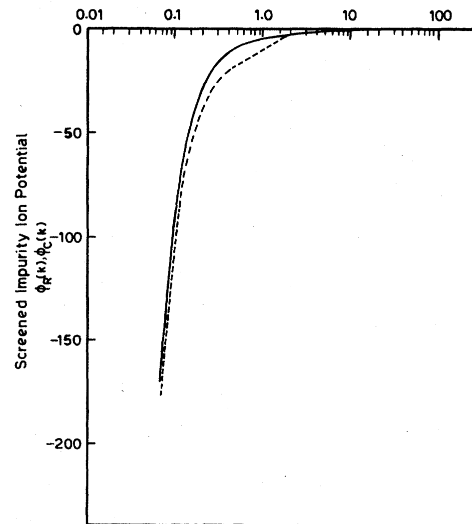

FIG. 4. Same as Fig. 3, but for an impurity concentration of 10^{21} cm^{-3}.

potentials in a doped semiconductor. Csavinszky's earlier and incorrect impurity-ion potentials[3,4] have been used for comparison. The screened-ion potentials with spatial variation of the dielectric function have been used in the literature for calculating the concentration-dependent donor binding energies.[29,30]

III. CALCULATION OF RELAXATION TIME

In the Born approximation, the phase shifts are much less than unity and are given[31] by

$$\delta_l^B=-\frac{2m^*K_F}{\hbar^2}\int_0^\infty j_l^2(K_Fr)V(r)r^2dr\ , \tag{5}$$

where the superscript B indicates that the Born approximation is used and $j_l(K_Fr)$ is a spherical Bessel function. If the Born approximation is valid, then the phase shifts for the conventional screened Coulomb potential (Dingle) obey the Friedel sum rule. This result was pointed out by Stern[22] and also by Krieger and Strauss.[19] If the scattering potential differs from the conventional screened Coulomb one, then the Dingle screening length R_D must be adjusted to satisfy the Friedel sum rule in the Born approximation. This approach was used by Chattopadhyay[32] and also by Boardman and Henry.[21]

With the scattering potential given by the Dingle[24] form,

$$V(r)=-\frac{Ze^2}{K_0r}e^{-r/R_D}\ , \tag{6}$$

one obtains from Eq. (5)

$$\delta_l^B=\frac{m^*Ze^2}{\hbar^2K_FK_0}Q_l\left[1+\frac{1}{2K_F^2R_D^2}\right]\ , \tag{7}$$

where $Q_l(x)$ are the Legendre functions of the second kind. From Ref. 12

$$\phi_R(r)=-\frac{2Ze}{\pi r}\int_0^\infty\frac{\sin(kr)}{k\epsilon_{\rm eff}(k)}dk\ , \tag{8}$$

where

$$\epsilon_{\rm eff}(k)=\epsilon(k)+K_0R_D^{-2}k^{-2}\ . \tag{9}$$

Substituting $e\phi_R(r)$ in Eq. (5) in the place of $V(r)$, we obtain

$$\delta_l^{\rm BE}=\frac{m^*Ze^2}{\hbar^2K_F}\int_0^{2K_F}\frac{P_l(1-k^2/2K_F^2)}{k\epsilon_{\rm eff}(k)}dk\ , \tag{10}$$

where the superscript BE indicates the use of the effective dielectric function $\epsilon_{\rm eff}(k)$ in the Born approximation. In Eq. (10), $P_l(x)$ are the Legendre functions of the first kind.

We have computed δ_l^B and $\delta_l^{\rm BE}$ in Si, Ge, and GaAs at 300 K for the Fermi wave vector corresponding to the concentration of 10^{21} cm^{-3}. For the latter case R_D is adjusted to satisfy the Friedel sum rule (degenerate case),

$$Z=\frac{2\nu}{\pi}\sum_{l=0}^{\infty}(2l+1)\delta_l\ , \tag{11}$$

where ν is the number of equivalent conduction-band minima and Z is the valence of the impurity atom minus the valence of the host atom in the crystal. The adjusted values of R_D come out as 4.037, 6.172, and 16.151 Å for Si, Ge, and GaAs, respectively. These may be compared with the unadjusted values 4.037, 6.171, and 16.137 Å, respectively. The total momentum cross section

$$\sigma_T=\frac{4\pi}{K_F^2}\sum_{l=0}^{\infty}(l+1)\sin^2(\delta_l-\delta_{l+1})\ . \tag{12}$$

The inverse relaxation time is given by

$$\tau^{-1}=n_i\left[\frac{\hbar K_F}{m^*}\right]\sigma_T\ , \tag{13}$$

where n_i is the impurity concentration. The results for Si, Ge, and GaAs are given in Table I. The results are compared with BH values. The scattering cross section in the BH theory is calculated from[23]

$$\sigma_T^{\rm BH}=\frac{\pi}{2K_F^2y}\left[\ln(1+b)-\frac{b}{1+b}\right]\ , \tag{14}$$

where $b=4K_F^2R_D^2$, $y=\frac{1}{2}k_Fa_0$, and $a_0=\hbar^2K_0/m^*e^2$, being the effective Bohr radius. The material parameters are given in Table II.

From Table I, it is clear that the inverse relaxation time is increased by about 10—30% which will result in the corresponding reduction of mobility in the degenerate case. The qualitative reduction in mobility due to the inclusion of the spatial dispersion of the dielectric function has been already pointed out in Ref. 15. However, as pointed out in the Introduction, the boundary conditions used in that reference have been questioned. The present work shows that the spatial variation of dielectric function must be included in the impurity-ion potential for the calculation of the ionized impurity-limited mobility for degenerate semiconductors.

To test the validity of the Born phase shifts used in our calculations we have done the calculations for Ge, as an example, by exactly solving for the partial-wave phase shifts as indicated below. The values of few phase shifts

TABLE I. Ratio of relaxation times. τ_B is the relaxation time using Dingle potential and Born phase shifts; $\tau_{\rm BE}$ is the relaxation time using the modified Dingle potential and the Born phase shifts; $\tau_{\rm BH}$ is the relaxation time in the BH theory.

Material	$\tau_B^{-1}/\tau_{\rm BH}^{-1}$	$\tau_{\rm Be}^{-1}/\tau_{\rm BH}^{-1}$
Si	0.9954	1.0873
Ge	0.9977	1.2113
GaAs	0.9998	1.3420

TABLE II. Material parameters. m^* is the effective mass; m_0 is the free-electron mass; K_0 is the static dielectric constant.

Material	m^*/m_0	K_0
Si	0.2981	11.94
Ge	0.2240	16.00
GaAs	0.0681	13.20

TABLE III. Phase shifts. δ_l^{BE} is the Born phase shift using modified Dingle potential; δ_l^{PE} is the full partial-wave phase shift using modified Dingle potential.

l	δ_l^{BE}	δ_l^{PE}
0	0.139 61	0.152 09
1	0.036 91	0.037 71
2	0.013 48	0.013 70
3	0.005 27	0.005 32
4	0.002 13	0.002 15

are given in Table III for Dingle screening radius R_D. The superscript PE indicates the use of effective dielectric function $\epsilon_{eff}(k)$ in the partial-wave method.

The radial part of the Schrödinger equation

$$-\frac{\partial^2 R_l}{\partial x^2}+\left[\frac{l(l+1)}{x^2}+U(x)-1\right]R_l=0\ , \tag{15}$$

where $U(x)=V(r)/E$, $x=kr$, and $E=\hbar^2k^2/2m^*$ is solved by the combined Runge-Kutta and predictor-corrector methods. Boardman and Henry[21] have pointed out that when Eq. (15) is solved numerically, one must often integrate to very large r value before the wave function obtains the form of a sine function, i.e.,

$$R_l \rightarrow \sin(x-\tfrac{1}{2}l\pi+\delta_l)\ , \tag{16}$$

where δ_l is the phase shift of the lth partial wave. We have therefore employed a technique discussed by those authors which allows one to find the phase shifts by locating the zeros of R_l and the corresponding j_l at sufficiently large distance from the origin. In Eq. (15), $U(x)=V(r)/E$ and $V(r)$ is replaced by $e\phi_R(r)$ and then solved: $\phi_R(r)$ at various r are computed by using a fast-Fourier-transform routine. From Table III it is clear that there is not much difference between δ_l^{BE} and δ_l^{PE} for the corresponding l values. The latter method takes longer computer time and thus we have done our calculations by computing Born phase shifts.

IV. CONCLUSIONS

In summary, we find that the valence dielectric screening is significant in computing ionized-impurity-limited relaxation times for high-impurity concentrations. The screened ionized-impurity potential may be better chosen by appropriate Fourier transformation of the potential in $\vec{k}$ space.

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