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Mobility of Electrons in Compensated Semiconductors. II. Theory*

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A theory of the electron mobility in compensated semiconductors for ionized-impurity scattering is developed. It differs from the existing theory due to Brooks and Herring in that it avoids the expansion of Fermi functions in powers of the electrical potential over the temperature. The mobility depends essentially on the pair correlation function between acceptors and donors. A simple model for this correlation is presented as an example, and an attempt is made to extract the pair-correlation function from the experimentally measured values of the mobility. Strong screening and antiscreening effects are obtained from an analysis of the experiment.

1. INTRODUCTION

THE electron mobility in doped semiconductors, mostly Ge and Si, has been the center of attention of many investigations,[1] both experimental[2] as well as theoretical,[3–5] in the last twenty years. In particular, the influence of ionized impurity scattering on the motion of the electrons has been the subject of the now classical papers by Conwell and Weisskopf,[3] Brooks,[1,4] and Herring.[1,5] In all cases mentioned above, the scattering potential due to all the ionized impurities is approximated by the superposition of Coulomb potentials of point charges in a dielectric, continuous medium. However, since the total scattering cross section of a Coulomb charge diverges due to the long-range character of the potential, proper care should be taken in screening the "bare" charge or introducing otherwise suitable cutoffs. In the first paper on the subject[3], the differential cross section was cut off at a given angle corresponding to an impact parameter equal to half the average distance between neighboring scattering centers.

The approach of Brooks[4] and Herring[5] is more accurate and consists of letting the carriers and ionized impurities redistribute themselves in such a way so as to produce mutual screening. Since our theory is essentially an extension of that of Brooks and Herring, which can be applied to compensated semiconductors at low temperatures where the original treatment fails, it is important for our purposes to review the salient features of their calculations and to show explicitly where their approximations break down.

Let us consider a compensated semiconductor with N_D donors and N_A acceptors per unit volume, such that

$$N_D > N_A .$$

The following notation is used throughout this paper: $N_D^+[N_A^-]$ average density of ionized donors [acceptors], $\mathcal{N}_D(\mathbf{r})[\mathcal{N}_A(\mathbf{r})]$ local density of donors [acceptors], $\mathcal{N}_D^+(\mathbf{r})[\mathcal{N}_A^-(\mathbf{r})]$ local density of ionized donors acceptors], n_e average density of electron carriers in the crystal, $\mathcal{N}_e(\mathbf{r})$ local density of electron carriers, e (negative) charge of the electron, $\varphi(\mathbf{r})$ self-consistent electric potential in the crystal, ζ Fermi level measured from the bottom of the conduction band, $\epsilon_D(\epsilon_A)$ energy of the donor (acceptor) level measured from the bottom of the conduction band, κ macroscopic dielectric constant of the crystal, m^* effective mass of the electron carriers, Ω volume of the sample. The electron carriers are scattered by the potential $\varphi(\mathbf{r})$ which satisfies Poisson's equation

$$\nabla^2\varphi = (4\pi e/\kappa)[\mathcal{N}_e(\mathbf{r}) + \mathcal{N}_A^-(\mathbf{r}) - \mathcal{N}_D^+(\mathbf{r})] , \qquad (1.1)$$

where, according to the well-known statistical formulas,[6]

$$\mathcal{N}_e(\mathbf{r}) = \frac{n_e}{1+\exp\{[e\varphi(\mathbf{r})-\zeta]/k_BT\}} , \qquad (1.2)$$

$$\mathcal{N}_A^-(\mathbf{r}) = \mathcal{N}_A(\mathbf{r}) - \frac{\mathcal{N}_A(\mathbf{r})}{1+\frac{1}{2}\exp\{[\zeta-\epsilon_A+e\varphi(\mathbf{r})]/k_BT\}} , \qquad (1.3)$$

$$\mathcal{N}_D^+(\mathbf{r}) = \mathcal{N}_D(\mathbf{r}) - \frac{\mathcal{N}_D(\mathbf{r})}{1+\frac{1}{2}\exp\{[\epsilon_D+e\varphi(\mathbf{r})-\zeta]/k_BT\}} . \qquad (1.4)$$

If Eq. (1.1) is solved for $\varphi(\mathbf{r})$, the matrix element for electron scattering is then given by

$$M(\mathbf{k},\mathbf{k}') = (e/\Omega)\Phi(\mathbf{k}-\mathbf{k}') , \qquad (1.5)$$

where $\Phi(\mathbf{k})$ is the Fourier transform of $\varphi(\mathbf{r})$. If the electron carriers are assumed to have a parabolic isotropic dispersion law

$$\epsilon(\mathbf{k}) = \hbar^2k^2/2m^* , \qquad (1.6)$$

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[1] For a review of the field, which includes many important contributions see e.g., F. G. Blatt, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1957). Vol. 4, p. 200; E. G. S. Paige, in *Progress in Semiconductors*, edited by A. F. Gibson and R. E. Burgess (John Wiley & Sons, Inc., New York, 1964), Vol. 8; H. Brooks, Advan. Electron. Electron Phys. **7**, 85 (1955).

[2] M. Cuevas, preceding paper, Phys. Rev. **164**, 1021 (1967), referred to as I; many other references are quoted there.

[3] E. M. Conwell and V. F. Weisskopf, Phys. Rev. **77**, 388 (1950).

[4] H. Brooks, Phys. Rev. **83**, 879 (1951).

[5] C. Herring (unpublished results).

[6] See, for instance, J. P. McKelvey, *Solid-State and Semiconductor Physics* (Harper & Row, New York, 1966), p. 271.

the relaxation time τ then is given by[7]

$$\frac{1}{\tau}=\frac{m^*k\Omega}{2\pi\hbar^3}\int_{-1}^{1}|M(\mathbf{k},\mathbf{k}')|^2(1-\cos\Theta)d(\cos\Theta)\,, \quad (1.7)$$

where Θ is the angle between $\mathbf{k}$ and $\mathbf{k}'$. Finally, the mobiltiy is obtained by the usual formula.[8]

$$\mu_e=(2|e|/3m^*k_BT)\langle\epsilon\tau(\epsilon)\rangle\,, \quad (1.8)$$

where the angular brackets symbolize an average over the electron distribution in energy

$$\langle f(\epsilon)\rangle\equiv\int_0^\infty f(\epsilon)\rho(\epsilon)\exp(-\epsilon/k_BT)d\epsilon\Big/\int_0^\infty\rho(\epsilon)\exp(-\epsilon/k_BT)d\epsilon\,. \quad (1.9)$$

Consequently, the object of any theory is the calculation of the self-consistent potential $\varphi(\mathbf{r})$, as given by the Eqs. (1.1)–(1.4).

The approximation used by Brooks and Herring consists of expanding the right-hand side of (1.1) in powers of $[e\varphi(\mathbf{r})/k_BT]$ as well as in powers of the departure of the local densities from their average values

$$[\mathfrak{N}_A(\mathbf{r})-N_A]\,,$$
$$[\mathfrak{N}_D(\mathbf{r})-N_D]\,,$$

and keeping only terms linear in these three quantities. When this procedure is followed and charge neutrality is invoked,

$$n_e+N_A^- - N_D^+=0\,, \quad (1.10)$$

a straightforward calculation yields for the matrix elements

$$|M(\mathbf{k}-\mathbf{k}')|^2=|M(\boldsymbol{\sigma})|^2=\frac{1}{\Omega^2}\left(\frac{4\pi e^2}{\kappa}\right)^2$$
$$\times\left[\sigma^2+\frac{4\pi e^2}{\kappa k_BT}n_s\right]^{-2}\langle\langle|F_A^-(\boldsymbol{\sigma})-F_D^+(\boldsymbol{\sigma})|^2\rangle\rangle\,. \quad (1.11)$$

where $\boldsymbol{\sigma}=\mathbf{k}-\mathbf{k}'$ is the Fourier conjugate variable of $\mathbf{r}$,

$$n_s=n_e+(n_e+N_A)[1-(n_e+N_A)/N_D]\,, \quad (1.12)$$

F_A^- and F_D^+ are the Fourier transforms of the functions $[\mathfrak{N}_A(\mathbf{r})-N_A]N_A^-/N_A$ and $[\mathfrak{N}_D(\mathbf{r})-N_D]N_D^+/N_D$ respectively, and the double angular brackets indicate the ensemble average over the distribution of impurities.

In addition, if complete randomness is assumed,

$$F_A^-(\boldsymbol{\sigma})=\sum_{l=1}^{N_A^-\Omega}\exp(-i\boldsymbol{\sigma}\cdot\mathbf{r}_l)\,, \quad (1.13)$$

$$F_D^+(\boldsymbol{\sigma})=\sum_{i=1}^{N_D^+\Omega}\exp(-i\boldsymbol{\sigma}\cdot\mathbf{r}_i)\,, \quad (1.14)$$

$$\langle\langle|F_A^-(\boldsymbol{\sigma})|^2\rangle\rangle=N_A^-\Omega\,, \quad (1.15)$$

$$\langle\langle|F_D^+(\boldsymbol{\sigma})|^2\rangle\rangle=N_D^+\Omega\,, \quad (1.16)$$

$$\langle\langle F_D^+(\boldsymbol{\sigma})F_A^{-*}(\boldsymbol{\sigma})\rangle\rangle=0\,, \quad (1.17)$$

and, since at ordinary temperatures for an n-type semiconductor $N_A^+=N_A$, a final result is obtained

$$|M(\boldsymbol{\sigma})|^2=\frac{1}{\Omega}\left(\frac{4\pi e^2}{\kappa}\right)^2\left[\sigma^2+\frac{4\pi e^2}{\kappa k_BT}n_s\right]^{-2}(2N_A+n_e)\,, \quad (1.18)$$

which yields for the mobility

$$\mu_I=\frac{2^{7/2}\pi^{-3/2}(k_BT)^{3/2}\kappa^2|e|^{-3}m^{*-1/2}[2N_A+n_e]^{-1}}{\ln(1+b)-b(1+b)^{-1}}\,, \quad (1.19)$$

where

$$b=[6\kappa(k_BT)^2m^*/\pi e^2\hbar^2n_s]\,. \quad (1.20)$$

Formulas (1.1) to (1.20) constitute in essence the theory as originally developed for only one kind of impurities[4] (donors) and extended to include both majority (donors) and minority (acceptors) impurities.[1] The most drastic approximation made in this approach is the linearization of Eqs. (1.2)–(1.4) coupled to the assumption of random distribution in the calculation of the ensemble averages.

The linearization of the source term in Poisson's equation is equivalent to an expansion in $e\varphi(\mathbf{r})/k_BT$. It is thus evident that this approximation is valid if the electric potential resulting from the ionized impurities is small compared with the thermal energy. This condition is satisfied in two cases:

(a) at high enough temperatures for any kind of impurity content;

(b) at all temperatures for semiconductors doped with only one kind (donors) of impurities.

In the latter case, as the temperature goes down the thermal energy decreases linearly with T while the number of ionized impurities (equal in this case to the number of carriers) decreases exponentially with T, so that the ratio $e\varphi(\mathbf{r})/k_BT$ remains always small.

In the cases which are of interest to us, as T approaches zero the average density of ionized minority impurities N_A^- remains finite and equal to N_A; the number of carriers n_e decreases exponentially to zero and, due to requirements of charge neutrality, the density of ionized majority impurities N_D^+ approaches the same value, N_A,

$$\lim_{T\to 0}N_D^+=N_A\,. \quad (1.21)$$

Under such circumstances the electric potential $\varphi(\mathbf{r})$ remains finite and large at very low temperatures, and the linearization of Poisson's equation to first-order terms in $e\varphi(\mathbf{r})/k_BT$ becomes meaningless.

In Sec. 2 we propose a modification of the existing theory which is valid in the limit of low temperatures

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[7] See e.g., Ref. 6, p. 315.

[8] See e.g., J. M. Ziman, *Electrons and Phonons* (Clarendon Press, London, 1960), p. 424.

in the compensated case. This theory is compared with experiment in Sec. 3, where general conclusions are also drawn.

2. MODIFIED THEORY AND SIMPLE MODEL

In this section we propose to solve Poisson's Eq. (1.1) without resorting to an expansion in a series of $e\varphi(\mathbf{r})/k_BT$. We rather consider the distribution of carriers $\mathfrak{N}_e(\mathbf{r})$, ionized acceptors $\mathfrak{N}_A{}^-(\mathbf{r})$, and ionized donors $\mathfrak{N}_D{}^+(\mathbf{r})$, as actually "frozen" in the configuration of minimum electrostatic energy, but, on the other hand, we take fully into account the statistical correlations between charges. This correlation provides the necessary "static" screening of the individual charges and eliminates the unwanted divergences of the Coulomb interaction. In this respect our theory resembles the classical Debye-Hückel theory of electrolytic solutions.

We think of our system as composed of three species in a continuous dielectric medium:

(1) electrons, whose coordinates are given by $\mathbf{x}_i$,

$$i=1,2,3,\cdots n_e\Omega\,;$$

(2) ionized acceptors, with coordinates $\mathbf{y}_l$;

$$l=1,2,3,\cdots N_A\Omega\,;$$

and

(3) ionized donors, with coordinates $\mathbf{z}_s$,

$$s=1,2,3,\cdots N_D{}^+\Omega.$$

In general, charge neutrality requires

$$N_D{}^+=N_A+n_e\,, \tag{2.1}$$

and the existing concentration of impurities is such that

$$N_A<N_D{}^+<N_D\,. \tag{2.2}$$

At low temperatures and for compensations

$$K=N_A/N_D \tag{2.3}$$

not too small, the number of carriers is much smaller than the number of acceptors, and consequently it is a good approximation to assume that only two species are present, and that

$$n_e=0\,,\quad N_D{}^+=N_A\,. \tag{2.4}$$

The solution of Poisson's equation proceeds now as follows. We write

$$\mathfrak{N}_A{}^-(\mathbf{r})=\sum_l \delta(\mathbf{r}-\mathbf{y}_l)=\sum_{\sigma,l}\exp[i\boldsymbol{\sigma}\cdot(\mathbf{r}-\mathbf{y}_l)] \tag{2.5}$$

and similarly for the donors and electrons. If we now take the Fourier transform of (1.1), we obtain

$$\sigma^2\Phi(\boldsymbol{\sigma})=\frac{4\pi e}{\kappa}{}^{\frac{1}{2}}\{\sum_i \exp[i\boldsymbol{\sigma}\cdot\mathbf{x}_i]+\sum_l \exp[i\boldsymbol{\sigma}\cdot\mathbf{y}_l]$$
$$-\sum_s \exp[i\boldsymbol{\sigma}\cdot\mathbf{z}_s]\}\,, \tag{2.6}$$

and with the use of (1.5) and the ensemble averages, the square of the matrix element is given by

$$|M(\mathbf{k},\mathbf{k}')|^2=\left(\frac{4\pi e^2}{\kappa}\right)^2\frac{1}{\Omega^2\sigma^4}\{\langle\langle\sum_{ij}\exp[i\boldsymbol{\sigma}\cdot(\mathbf{x}_i-\mathbf{x}_j)]\rangle\rangle$$
$$+\langle\langle\sum_{lm}\exp[i\boldsymbol{\sigma}\cdot(\mathbf{y}_l-\mathbf{y}_m)]\rangle\rangle+\langle\langle\sum_{st}\exp[i\boldsymbol{\sigma}\cdot(\mathbf{z}_s-\mathbf{z}_t)]\rangle\rangle$$
$$+\langle\langle\sum_{il}2\cos[\boldsymbol{\sigma}\cdot(\mathbf{x}_i-\mathbf{y}_l)]\rangle\rangle-\langle\langle\sum_{is}2\cos[\boldsymbol{\sigma}\cdot(\mathbf{x}_i-\mathbf{z}_s)]\rangle\rangle$$
$$-\langle\langle\sum_{ls}2\cos[\boldsymbol{\sigma}\cdot(\mathbf{y}_l-\mathbf{z}_s)]\rangle\rangle\}\,. \tag{2.7}$$

In the Appendix we introduce pair-distribution functions and pair correlation functions, and, by assuming that charge distributions of the same species are uncorrelated, we arrive at the following result, valid for $\boldsymbol{\sigma}\neq 0$

$$|M(\mathbf{k},\mathbf{k}')|^2=\left(\frac{4\pi e^2}{\kappa}\right)^2\frac{1}{\Omega\sigma^4}$$
$$\times\{n_e+N_A+N_D{}^++2n_eN_AD_{eA}(\sigma,T)$$
$$-2n_eN_D{}^+D_{eD}(\sigma,T)-2N_AN_D{}^+D_{AD}(\sigma,T)\}\,, \tag{2.8}$$

where the three functions $D(\sigma,T)$ are directly connected with the Fourier transform of the pair correlation functions. At this point it is important to point out that if correlations are neglected, i.e., if we take $D(\sigma,T)\equiv 0$, (2.8) yields a divergent cross section for scattering due to the σ^{-4} factor in the matrix element. The limiting behavior of the D functions as σ approaches zero guarantees, for any type of distribution, convergence in all integrals involved in the calculation of the mobility. Physically this means that in the long-wave limit $\sigma\rightarrow 0$, the carriers and the impurities as well as the impurities among themselves screen each other so as to look like a neutral system. This is reflected in the vanishing of the bracket in the right-hand side of (2.8) in that limit.

If the number of electrons is small and can be neglected, the use of (2.4) yields for the bracket in (2.8)

$$2N_A[1-N_AD_{AD}(\sigma,T)] \tag{2.9}$$

which, by taking, for example, the temperature independent exponential distribution discussed in the Appendix [formula (A29)], reduces to

$$2N_A[\sigma^2(2a^2+\sigma^2)/(a^2+\sigma^2)^2]\,, \tag{2.10}$$

where a, a function of N_A and N_D, is given by

$$a^3=8\pi(N_D-N_A)\,. \tag{2.11}$$

In general, we could express that bracket by an expression of the form

$$2N_AF(\sigma,N_A,N_D,T]\,, \tag{2.12}$$

where F is a dimensionless function of σ which vanishes a σ approaches zero. If F is known, the rest of the calculation proceeds as before, i.e., it is necessary to calculate the relaxation time by integrating, as in (1.7), over the angle Θ and calculate the mobility, as in (1.8), by computing the average over the electron energy distribution (1.9).

As an example of the kind of effects involved here, we work out in detail the exponential distribution and calculate the resulting mobilities. By making the substitutions

$$2x=1-\cos\Theta\,, \tag{2.13}$$

$$\sigma^2=4k^2x\,, \tag{2.14}$$

$$\eta=4k^2a^{-2}\,, \tag{2.15}$$

and replacing (2.10) and (2.8) in (1.7), we obtain fo the relaxation time

$$\frac{1}{\tau}=\frac{m^*N_A}{4\pi\hbar^3}\left(\frac{4\pi e^2}{\kappa}\right)^2\frac{1}{k^3}\left\{\ln(1+\eta)+\frac{\eta}{1+\eta}\right\}. \tag{2.16}$$

The factor k^3 constitutes the most important energy dependence of τ; the factor $[\ln(1+\eta)+\eta(1+\eta)^{-1}]^{-1}$ is also energy-dependent but very weakly so. Following the usual practice of taking the latter outside the integral over the energies and replacing for k in η the value where the remaining integrand takes its maximum value,[9] we obtain for the mobility

$$\mu_I\cong\frac{2^{7/2}\pi^{-3/2}(k_BT)^{3/2}\kappa^2|e|^{-3}m^{*-1/2}(2N_A)^{-1}}{\ln(1+\eta_0)+\eta_0(1+\eta_0)^{-1}}\,, \tag{2.17}$$

where

$$\eta_0=\frac{6(k_BT)m^*}{\pi^{2/3}\hbar^2(N_D-N_A)^{2/3}}\,. \tag{2.18}$$

which differs from the Brooks and Herring formulas (1.19)–(1.20) in the sign of one of the terms in (2.17) and the fact that the inverse screening radius R^{-1} of their formula

$$R^{-1}=\left[\frac{4\pi e^2}{\kappa k_BT}n_s\right]^{\frac{1}{2}}\,, \tag{2.19}$$

which diverges as T approaches zero, is replaced by the static inverse correlation length a, which is essentially temperature-independent in the range of temperatures of interest. In Fig. 1 we plot for comparison the screening radius R of formula (2.19) as a function of temperature together with the value a^{-1}. The values correspond to sample $C3$ of I. Figure 2 shows for $T=20°$ the dependence of R and a^{-1} on the concentration of majority impurities.

It should be emphasized that the exponential assumption for the correlation function is only introduced here as an example, but it shows the important features of the theory and demonstrates how the correlation between charges has to be necessarily taken into account and how it gives a "static" screening which explains why, at higher concentrations of majority impurities, it is possible to obtain larger mobilities. In other words, the presence of extra impurities improves the screening but alters only slightly the number of ionized scattering centers. The number of neutral impurities is, however, increased.

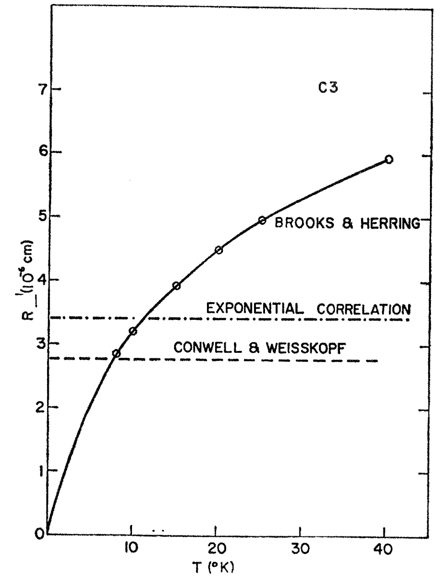

FIG. 1. A comparison between the screening radius R as a function of the temperature in the theory of Refs. 4 and 5 with the present theory (simple model). The curves correspond to a sample with $N_A=2.9\times10^{15}$ cm^{-3} and $N_D=3.9\times10^{15}$ cm^{-3}.

The exponential example gives for the screening radius a function which is independent of temperature (in the range $n_e\ll N_A$) and depends on concentration as $(N_D-N_A)^{-1/3}$. In contraposition to this, the Conwell-Weisskopf theory yields a cutoff radius which varies approximately like $N_A^{-1/3}$ (i.e., is essentially constant for all samples and temperatures of I), and the Brooks-

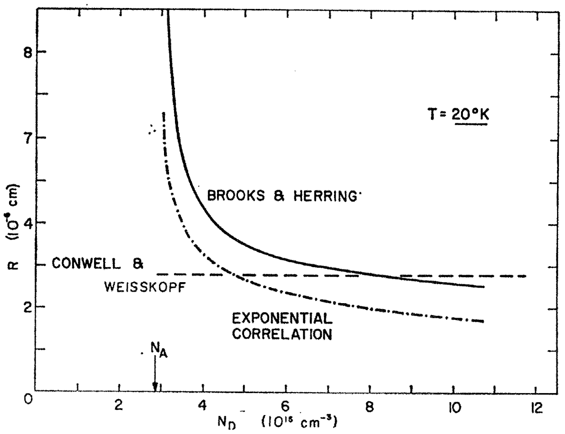

FIG. 2. A comparison between the screening radius R as a function of majority impurity concentration N_D for samples at $T=20$°K.

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[9] P. P. Debye and E. M. Conwell, Phys. Rev. 93, 693 (1954).

Herring theory gives a screening radius which varies like $T^{1/2}N_A^{-1/2}N_D^{1/2}(N_A-N_A)^{-1/2}$.

It is seen in the next section that an analysis of the experimental data presented in I proves that the actual correlation functions encountered in the experiments cannot be approximated by any of these models, and that it is possible to invert the procedure described in this section and obtain the pair correlation function from the experimental values.

3. CONCLUSIONS AND COMPARISON WITH EXPERIMENT

We have seen that the values of the mobility depend essentially on the function $F(\sigma,N_A,N_D,T)$ introduced in (2.12) and related, in the case $n_e \ll N_A$, only to the Fourier transform $D_{AD}(\sigma,T)$ of the acceptor-donor pair correlation function by

$$F(\sigma,N_A,N_D,T)=1-N_A D_{AD}(\sigma,T). \tag{3.1}$$

We attempt in this section to obtain from the experimental values of μ_I some information about the function $D_{AD}(\sigma,T)$.

Substitution of (2.8) in (1.7) and use of (2.13) and (2.14) yields for the relaxation time

$$\frac{1}{\tau}=\frac{m^* N_A}{4\pi\hbar^3}\left(\frac{4\pi e^2}{\kappa}\right)^2\frac{1}{k^3}Q(k,N_A,N_D,T), \tag{3.2}$$

where

$$Q(k,N_A,N_D,T)=2\int_0^{2k}\frac{F(\sigma,N_A,N_D,T)}{\sigma}d\sigma. \tag{3.3}$$

If, as in the previous treatments, we assume that the dependence of Q on k is very weak compared with the k^3 dependence in τ, the integral over energies in (1.8) yields for the mobility

$$\mu_I \cong \frac{2^{7/2}\pi^{-3/2}(k_B T)^{3/2}\kappa^2|e|^{-3}m^{*-1/2}(2N_A)^{-1}}{Q(k_0,N_A,N_D,T)}, \tag{3.4}$$

where

$$k_0=\hbar^{-1}(6k_B T m^*)^{1/2}. \tag{3.5}$$

The use of (3.4)–(3.5) permits the calculation of $Q(\sigma,N_A,N_D,T)$ from the measured values of μ_I [10]; from Q the acceptor-donor pair correlation function D can then be determined:

$$D_{AD}(2k_0,T)=N_A^{-1}\left(1-\frac{k_0}{2}\frac{\partial Q}{\delta k_0}\right). \tag{3.6}$$

TABLE I. Experimental values of the function $Q(k_0,N_A,N_D)$; $N_A=2.9\times10^{15}$ cm^{-3}.

		$Q(k_0,N_A,N_D,T)$[a]					
$N_D(10^{15}$ cm$^{-3})$		3.04	3.54	3.89	4.16	6.07	10.76
T °K	k_0 10^6 cm^{-1}						
10	1.22		11.0	6.5	5.3	4.1	
15	1.49		7.4	5.8	4.8	3.7	2.6
20	1.73	17.7	7.2	5.8	4.8	3.8	2.45
25	1.93	15.8	7.2	5.9	5.1	3.7	2.3
40	2.44		7.7	6.6			

[a] All values from I.

Table I shows the function $Q(k_0,N_A,N_D,T)$ obtained from the experimental values reported in I. In the range of temperatures and impurity concentrations of interest, it is possible to approximate Q by a formula of the form

$$Q(k_0,N_A,N_D,T)\simeq A(T)(4k_0/a), \tag{3.7}$$

where a is defined by (2.11) and the function $A(T)$ is given in Table II. When (3.7) is replaced in (3.6), the pair correlation function is approximately expressed by

$$D_{AD}(\sigma,T)\simeq N_A^{-1}\{1-A(T)(\sigma/a)\}. \tag{3.8}$$

It can now be seen that the acceptor and donors in compensated Ge are very strongly correlated. As clearly shown by (3.8), there is a strong screening effect in the long-wavelength limit ($\sigma \lesssim 4a$) and a surprising antiscreening effect at shorter wavelengths. It is worth remarking that (3.8) is only approximate and not to be taken as even approximately valid beyond a given maximum value of σ; it is important also to point out that the derivation of (3.8) depends on the accuracy of the experiment as well as the way in which other scattering effects were subtracted. However, we are confident that the screening-antiscreening effect is a real one and that the very strong correlation between ionized impurities has been proved beyond any doubt.

A more complete and satisfactory theory should be developed in which, in addition to the acceptor-donor correlation, donor-donor as well as electron-donor and electron-acceptor correlations are taken into account. We feel that all these effects, although smaller than the one considered here, are important enough to make significant contributions.

In conclusion, we would like to point out that the problem under consideration shows the inadequacy of the approximation of linear screening, which yields an infinite mobility as T approaches zero, while experiment clearly indicates that in that limit μ tends to zero. The

TABLE II. Values of the coefficient $A(T)$.

T °K	$A(T)$
10	0.37
15	0.28
20	0.23
25	0.21
40	0.20

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[10] In obtaining Q from the experimental values of the mobility, it should be remembered that m^* appearing in (3.4) corresponds to the ratio of the square of the conductivity average effective mass to the density-of-states effective mass; m^* appearing in (3.5), on the other hand, is simply the density-of-states effective mass. In the actual calculations, the better approximation of taking $(2N_A+n_e)$ instead of $(2N_A)$ was made; the correction is in the worst case considered only 10%.

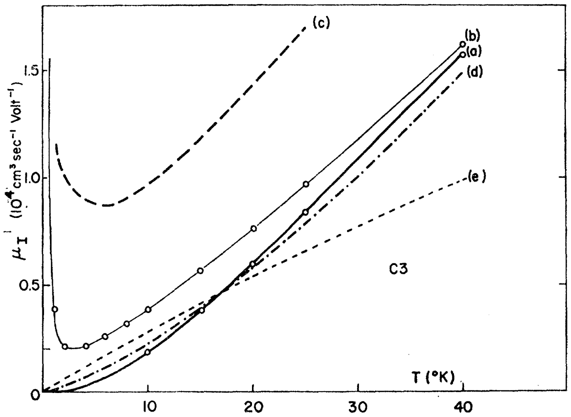

FIG. 3. A comparison of the various mobilities as a function of temperature for the sample $C3$ of Fig. 1. (a) Experimental values. (b) Brooks and Herring (Refs. 4 and 5) (c) Conwell and Weisskopf (Ref. 3). (d) Simple exponential correlation. (e) From formulas (3.4)–(3.7)with a temperature-independent coefficient $A(T)=0.27$.

breakdown of the linearized approach to the solution of Eqs. (1.1)–(1.4) is the fundamental reason which led us to use statistical methods which look at the distribution of ionized impurities in a "frozen" state rather than consider them as distributed in a "smooth" state obtained by perturbation from a completely homogeneous distribution. In the limit of high temperatures, when the $e\varphi/k_BT$ expansion is valid, the theory of Brooks and Herring becomes valid and can be interpreted as if it corresponded to an acceptor-donor pair correlation function given by

$$D_{AD}(\sigma,N_A,N_D,T)\simeq[(1+2\sigma^2R^2)/N_A(1+\sigma^2R^2)^2], \quad (3.9)$$

where R is the screening radius given by (2.19).

Finally, in Figs. 3 and 4 we plot the mobility μ_I as a function of temperature for the parameters of sample $C3$ of I and the mobility μ_I as a function of donor concentration for $T=20$°K. The various curves correspond to

(a) Experimental values,
(b) Brooks and Herring theory,
(c) Conwell and Weisskopf theory,
(d) Exponential simple model (2.17),
(e) Empirical correlation function (3.8) for a temperature-independent coefficient $A(T)=0.27$.

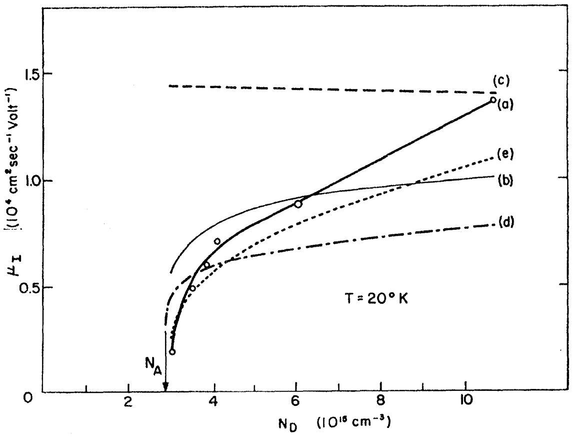

FIG. 4. A comparison of the various mobilities as a function of majority impurity concentration for $T=20$°K. (a) Experimental values. (b) Brooks and Herring (Refs. 4 and 5). (c) Conwell and Weisskopf (Ref. 3). (d) Simple exponential correlation. (e) From formulas (3.4)–(3.7) with a temperature-independent coefficient $A(T)=0.27$.

It can be seen from them that although satisfactory in given regions, all the theoretical curves are far from representing accurately the experimental mobility in the whole range of temperatures and concentrations. It is evident that the pair correlation function $D_{AD}(\sigma,N_A,N_D,T)$ is more complicated than any of the simple forms proposed here.

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APPENDIX

We denote by

$$P(\mathbf{x},\mathbf{y},\mathbf{z})\equiv P(\mathbf{x}_1,\mathbf{x}_2,\cdots,\mathbf{y}_1,\mathbf{y}_2,\cdots,\mathbf{z}_1,\mathbf{z}_2,\cdots) \quad (A1)$$

the ensemble distribution function for the

$$(n_e+N_A+N_D{}^+)\Omega$$

particles, and abbreviate the differentials by

$$\begin{aligned} Dx&\equiv d^3x_1d^3x_2\cdots d^3x_i\cdots, 1\leqslant i\leqslant n_e\Omega,\\ Dy&\equiv d^3y_1d^3y_2\cdots d^3y_l\cdots, 1\leqslant l\leqslant N_A\Omega, \quad (A2)\\ Dz&\equiv d^3z_1d^3z_2\cdots d^3z_s\cdots, 1\leqslant s\leqslant N_D{}^+\Omega, \end{aligned}$$

where the x coordinates correspond to electrons, the y coordinates to ionized acceptors, and the z coordinates to ionized donors. The normalization is such that

$$\int P(\mathbf{x},\mathbf{y},\mathbf{z})DxDyDz=1. \quad (A3)$$

If we introduce generic indices I, J such that they can indicate e, A or D (corresponding to electrons, acceptors, and donors respectively), and redefine

$$n_A=N_A\,,\quad n_D=N_D{}^+,$$
$$\xi_e=\mathbf{x}\,,\quad \xi_A=\mathbf{y},\quad \xi_D=\mathbf{z}\,,\tag{A4}$$

and

$$D\xi=DxDyDz\,,$$
$$P(\xi)=P(\mathbf{x},\mathbf{y},\mathbf{z})\,,\tag{A5}$$

we can define pair distribution functions $C_{IJ}(\mathbf{r})$ such that

$$C_{IJ}(\mathbf{r})\equiv\sum_{ij}\int\delta(\mathbf{r}-\xi_{Ii}+\xi_{Jj})P(\xi)D\xi.\tag{A6}$$

These functions satisfy the normalization condition

$$\int C_{IJ}(\mathbf{r})d^3r=n_In_J\Omega^2.\tag{A7}$$

In a similar way we introduce pair correlation functions $g_{IJ}(\xi_{Ii},\xi_{Jj})$ by

$$g_{IJ}(\xi_{Ii},\xi_{Ji})=\int P(\xi)\left(\frac{D\xi}{d^3\xi_{Ii}d^3\xi_{Jj}}\right),\qquad (Ii)\neq(Jj).\tag{A8}$$

It can be seen that the formulas

$$C_{II}(\mathbf{r})=n_I\Omega\delta(\mathbf{r})+\sum_{\substack{lm\\ l\neq m}}{}'\int g_{II}(\xi_{Il},\xi_{Im}=\xi_{Il}-\mathbf{r})d^3\xi_{Il}\tag{A9}$$

$$C_{IJ}(\mathbf{r})=\sum_{ij}\int g_{IJ}(\xi_{Ii},\xi_{Jj}=\xi_{Ii}-\mathbf{r})d^3\xi_{Ii}\quad I\neq J\tag{A10}$$

relate pair distribution functions to pair correlation functions.

In our calculations and for the sake of simplicity we further assume that; (1) There is no correlation between particles of the same species, i.e.,

$$C_{II}(\mathbf{r})=n_I\Omega\delta(\mathbf{r})+n_I(n_I\Omega-1)\,;\tag{A11}$$

(2) The system is macroscopically uniform and isotropic:

$$\int g_{IJ}(\xi_{Ii},\xi_{Jj}=\xi_{Ii}-\mathbf{r})d^3\xi_{Ii}=\mathfrak{D}_{IJ}(r)\ \text{ for } I\neq J,\tag{A12}$$

where $\mathfrak{D}_{IJ}(r)$ is independent of the index j and is only a function of the scalar r. It is easily seen that

$$C_{IJ}(\mathbf{r})=n_In_J\Omega^2\mathfrak{D}_{IJ}(r)\quad I\neq J\tag{A13}$$

and

$$4\pi\int_0^\infty\mathfrak{D}_{IJ}(r)r^2dr=1.\tag{A14}$$

The most important of the $\mathfrak{D}(r)$ functions is $\mathfrak{D}_{AD}(\mathbf{r})$, since

$$n_e\ll N_A\cong N_D{}^+$$

in the temperature range of interest to us. In addition, since all acceptors are ionized, and only a fraction $N_D{}^+/N_D$ of the total number of donors is ionized, we would expect the donors to be preferentially ionized in those locations which are close to acceptor sites. This means that in the neighborhood of an acceptor the density of ionized donors should reach the value N_D, while at large distances it takes the average value $N_D{}^+$. Consequently

$$\mathfrak{D}_{DA}(r=0)=\frac{N_D}{N_D{}^+\Omega},\tag{A15}$$

$$\mathfrak{D}_{AD}(r\rightarrow\infty)=\frac{1}{\Omega}-\frac{1}{2\Omega^2}\left\{\frac{1}{N_A}+\frac{1}{N_D{}^+}\right\},\tag{A16}$$

where in (A16) we have kept terms up to order Ω^{-2}.

Finally, the Fourier transform of the $\mathfrak{D}$ functions $D(\sigma)$ is defined by

$$D_{IJ}(\sigma)=\Omega\int\mathfrak{D}_{IJ}(r)\exp(i\boldsymbol{\sigma}\cdot\mathbf{r})d^3r,\tag{A17}$$

where

$$D_{IJ}(\sigma=0)=\Omega\,,\tag{A18}$$

$$\int D_{IJ}(\sigma)d^3\sigma=\frac{\mathfrak{D}(r=0)\Omega}{8\pi^3},\tag{A19}$$

and, from (A16) and (A18)

$$\lim_{\sigma\rightarrow0}D(\sigma)=\frac{1}{2}\left\{\frac{1}{N_A}+\frac{1}{N_D{}^+}\right\}\tag{A20}$$

up to terms of order unity.

It is necessary for our purposes to calculate expectation values of the form

$$G_{IJ}\equiv\langle\langle\sum_{ij}\exp[i\boldsymbol{\sigma}\cdot(\xi_{Ii}-\xi_{Jj})]\rangle\rangle$$
$$=\sum_{ij}\int\exp[i\boldsymbol{\sigma}\cdot(\xi_{Ii}-\xi_{Jj})]P(\xi)D\xi\tag{A21}$$

which after a few simple manipulations can be expressed in the form

$$G_{IJ}(\boldsymbol{\sigma})=\int d^3r\exp(i\boldsymbol{\sigma}\cdot\mathbf{r})C_{IJ}(\mathbf{r}),\tag{A22}$$

or equivalently from (A11)

$$G_{II}(\boldsymbol{\sigma})=n_I\Omega+n_I\Omega(n_I\Omega-1)\delta_{\sigma,0},\tag{A23}$$

and from (A13) and (A17)

$$G_{IJ}(\boldsymbol{\sigma})=n_In_J\Omega D_{IJ}(\sigma)\,,\quad I\neq J.\tag{A24}$$

It is worth emphasizing that the expectation values $G_{IJ}(\sigma)$ are *discontinuous* at $\sigma=0$. Values at $\sigma=0$ are of the order Ω^2, while values at $\sigma\neq0$ are of the order Ω. In particular, with our assumptions

$$\begin{cases} G_{II}(0)=n_I^2\Omega^2 \\ \lim\limits_{\sigma\to0} G_{II}(\sigma)=n_I\Omega \end{cases} \qquad \text{(A25)}$$

and for $I\neq J$

$$\begin{cases} G_{IJ}(0)=n_In_J\Omega^2 \\ \lim\limits_{\sigma\to0} G_{IJ}(\sigma)=\dfrac{n_In_J}{2}\Omega\left\{\dfrac{1}{n_I}+\dfrac{1}{n_J}\right\}. \end{cases} \qquad \text{(A26)}$$

As a final illustration of the statistical distributions involved in this paper, we include as an example an exponential correlation function:

$$\mathfrak{D}_{AD}(r)=\frac{1}{\Omega}-\frac{1}{2\Omega^2}\left\{\frac{1}{N_A}+\frac{1}{N_D{}^+}\right\} +\frac{N_D-N_D{}^+}{N_D{}^+\Omega}\exp(-ar)\,, \qquad \text{(A27)}$$

where the normalization condition requires

$$a^3=16\pi N_A(N_D-N_D{}^+)(N_A+N_D{}^+)^{-1}. \qquad \text{(A28)}$$

The Fourier transform, for $\sigma\neq0$, takes in this case the form

$$D_{AD}(\sigma)=\frac{1}{2}\left\{\frac{1}{N_A}+\frac{1}{N_D{}^+}\right\}\frac{a^4}{(a^2+\sigma^2)^2} \cong\frac{1}{N_A}\frac{a^4}{(a^2+\sigma^2)^2}. \qquad \text{(A29)}$$

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Strong-Coupled Piezoelectric Polaron

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A semiclassical, variational calculation for the strong-coupled piezoelectric polaron gives the following results for the ground-state energy and polaron radius, respectively:

$$U_0=-0.47\left(\frac{m^*}{m}\right)\left(\frac{\kappa^2}{\epsilon}\right)^2\text{eV},$$

and

$$R=3.5\left(\frac{\epsilon}{\kappa^2}\right)\left(\frac{m}{m^*}\right)\text{ Å},$$

where m^* is the band effective mass, κ is the electromechanical coupling constant, and ϵ is the strain-free dielectric constant. The theory is expected to be valid when $|U_0|$ is larger than thermal energies and R is considerably larger than unit-cell dimensions. A calculation of the polaron effective mass, having a more limited region of validity, gives

$$m_p\approx m^*\left[1+\frac{2|U_0|}{m^*v_s{}^2}\right],$$

where v_s is the velocity of sound.

I. INTRODUCTION

A GREAT deal of effort has been devoted to the polaron problem in recent years.[1] Most papers have been concerned with the case of electron coupling to the optical modes of ionic crystals. In both the weak- and strong-coupling limits this problem is now well understood and, in addition, some insight has been gained in the intermediate coupling region.[1] Much less attention has been devoted to the case of coupling to acoustic modes, either through a deformation potential,[1,2] or the piezoelectric constant.[2] In the latter case the weak-coupling limit has been, with only one exception,[3] the only region considered. The reason for this is evident: For most materials the weak-coupling theory is adequate except at extremely low temperatures, where impurity effects dominate.

However, a weak-coupling theory may not always

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[1] Several pertinent articles and an extensive bibliography are contained in *Polarons and Exitons*, edited by C. G. Kuper and G. D. Whitfield (Plenum Press, Inc., New York, 1962).

[2] G. D. Mahan, Phys. Rev. **142**, 366 (1966).

[3] George Whitfield, Bull. Am. Phys. Soc. **10**, 388 (1965).