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Neutral Impurity Scattering in Semiconductors

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The scattering of free charge carriers by neutral impurities in semiconductors has been calculated using the partial wave technique by considering the source of scattering to be an attractive potential caused by a negative-energy state associated with the neutral impurity. This calculation has been compared with that due to Erginsoy and with a calculation in Born approximation where the neutral impurity is represented by a hydrogen atom in the dielectric medium of the semiconductor. The present treatment gives a mobility that differs from the Erginsoy treatment by only a few percent but predicts a slight temperature dependence. The calculation in Born approximation gives a result similar to that obtained for ionized impurity scattering calculated to the same approximation. The nature of the energy state giving rise to the scattering in this treatment and the possibility of distinguishing experimentally between the different calculations is discussed.

NEUTRAL impurity scattering in semiconductors has been treated by Erginsoy[1] who assumed that the neutral impurity may be represented by a hydrogen atom immersed in the dielectric medium of the semiconductor. He analyzed the curves obtained by numerical calculations[2] of the scattering of slow electrons from hydrogen atoms (including polarization and exchange effects), to obtain an approximate analytic expression for the cross section for scattering. The partial-wave technique, using only the zero-order phase shift, was then employed to calculate a relaxation time for this scattering. This yielded

$$\tau = 8\pi^3 m^{*2} q^2 / 20 D N_N h^3 \text{ sec}, \qquad (1)$$

where m^* and q are the effective mass and charge of the charge carriers, D is the dielectric constant, N_N is the concentration of neutral impurities, and h is Planck's constant. If one assumes spherical energy surfaces, the applicability of the Boltzmann transport equation, classical statistics, and small magnetic fields, then the mobility, μ, and Hall coefficient, R, are given with $\mathcal{E}$ the carrier energy, and k_0, Boltzmann's constant, by

$$\mu = \frac{4q}{3\pi^{1/2} m^* (k_0 T)^{5/2}} \int_0^\infty \tau \mathcal{E}^{3/2} \exp(-\mathcal{E}/k_0 T) d\mathcal{E}, \qquad (2)$$

$$R = \frac{1}{nqc} \times \frac{3\pi}{8} \left(\frac{2(k_0 T)^{5/2}}{\pi^{1/2}} \right) \int_0^\infty \tau^2 \mathcal{E}^{3/2} \exp(-\mathcal{E}/k_0 T) d\mathcal{E} \times \left[\int_0^\infty \tau \mathcal{E}^{3/2} \exp(-\mathcal{E}/k_0 T) d\mathcal{E} \right]^{-2}. \qquad (3)$$

Using Eq. (1), we compute for the mobility and Hall coefficient

$$\mu = \frac{8\pi^3 m^* q^3}{20 D N_N h^3} \times \frac{1}{300} = \frac{1.43 \times 10^{22} \beta}{D N_N} \text{ cm}^2/\text{volt sec} \qquad (4)$$

$$R = (1/nqc) \text{ cm}^3/\text{coul}, \qquad (5)$$

which is Erginsoy's result, where β is the ratio of the effective to the free mass of the charge carrier. The technique used in computing τ sets up the condition for the validity of this treatment, i.e., $ka \ll 1$. Here k is equal to $2\pi mv/h$, with v equal to the velocity of the charge carrier, and a is the range of the neutral scattering potential. Erginsoy selects $a = a_h$, where a_h is the Bohr radius in the semiconductor medium:

$$a_h = (Dh^2 / m^* q^2) \text{ cm}. \qquad (6)$$

As neutral imputities are expected to be an important scattering source only at low temperatures in most materials, the condition $ka \ll 1$ may be taken to be satisfied since $\langle ka \rangle_{\text{Av}} \ll 1$, where $\langle ka \rangle_{\text{Av}}$ is the average value of ka. We list, however, for completeness the corresponding expressions obtained for neutral impurity scattering by a Born approximation calculation using the same model as Erginsoy but with the neglect of polarization and exchange effects. These expressions will be valid only at higher temperatures when the condition $ka_h \gg 1$ may be appropriate.

$$\tau = \frac{(2m^*)^{\frac{1}{2}} \mathcal{E}^{\frac{3}{2}}}{\pi N_N q^4} \times \left\{ \ln[1 + (ka_h)^2] - \frac{1}{1 + 1/(ka_h)^2} \right\}^{-1} \text{ sec}, \qquad (7)$$

$$\mu = \frac{8\sqrt{2} (k_0 T)^{\frac{3}{2}}}{300 \pi^{\frac{3}{2}} q^3 m^{*\frac{1}{2}} N_N} \times \left\{ \ln[1 + \langle ka_h \rangle_{\text{Av}}^2] - \frac{1}{1 + 1/\langle ka_h \rangle_{\text{Av}}^2} \right\}^{-1} \text{ cm}^2/\text{volt sec}, \qquad (8)$$

$$R = (1.93/nqc) \text{ cm}^3/\text{coul}. \qquad (9)$$

Comparison of these expressions with the Conwell-Weisskopf or Brooks-Herring[3] formulas for ionized impurity scattering indicates a very close similarity. The difference is the omission of the multiplicative dielectric constant factor in the numerator (although

[1] C. Erginsoy, Phys. Rev. **79**, 1013 (1950).
[2] H. S. W. Massey and B. L. Moiseiwitsch, Phys. Rev. **78**, 180 (1950).
[3] P. P. Debye and E. M. Conwell, Phys. Rev. **93**, 693 (1954).

this factor occurs in the brackets in the denominator), the replacement of the concentration of ionized centers by neutral centers and the replacement of the logarithmic term by another.

Another treatment for the scattering by neutral impurities has been suggested by Ansel'm.[4] In this treatment, cognizance is taken of the tendency of neutral atoms to acquire an electron and become negative ions. Such neutral atoms must therefore exhibit a short-range attractive influence[5] for free carriers which will give rise to an additional mechanism for scattering. Under this circumstance, the equations formulated for ionized impurity scattering using the partial wave technique become applicable[6] and we obtain Eq. (34) to describe the relaxation time and Eq. (37) of this reference to give the corresponding mobilities and Hall coefficients. We list here the limiting mobilities in cm²/volt sec calculated for the different cases possible:

$$\mu_A=\frac{q}{3\sqrt{2}\pi^{\frac{3}{2}}N_N a_N^2(m^*k_0T)^{\frac{1}{2}}}\times\frac{1}{300}\left[\frac{\tan\alpha a_N}{\alpha a_N}-1\right]^{-2},$$
$$\mu_R=\frac{q}{3\sqrt{2}\pi^{\frac{3}{2}}N_N a_N^2(m^*k_0T)^{\frac{1}{2}}}\times\frac{1}{300}\left[\frac{\tanh\alpha a_N}{\alpha a_N}-1\right]^{-2}. \quad (10)$$

Case 1:—

$$\mu_{1A}=\frac{4q(m^*k_0T)^{\frac{1}{2}}}{3\sqrt{2}\pi^{\frac{3}{2}}N_N\hbar^2}\times\frac{1}{300}. \quad (11)$$

Case 2:—

$$\mu_{2A}\rightarrow\infty, \quad (12)$$

Case 3:—

$$\mu_{3A}=\mu_{1A}(1+\epsilon_N/2k_0T), \quad (13)$$

with

$$\alpha a_N=\left[(ka_N)^2+\frac{2m^*q^2}{\hbar^2 D}a_N\right]^{\frac{1}{2}}. \quad (14)$$

In Eq. (10), μ_A and μ_R are the mobilities resulting from scattering by attractive and repulsive centers. Case 1 is obtained as $\alpha a_N\rightarrow(2n+1)\pi/2$; case 2 when $(\tan\alpha a_N)/\alpha a_N\rightarrow 1$, and case 3 when $\epsilon_N\simeq k_0T$. The quantity $|-\epsilon_N|$ is the binding energy associated with the attractive influence of the neutral impurities, and a_N refers to the radial extent of this force. Ansel'm in his calculation considers only "resonance" scattering (case 3) and appears to have made the additional assumption that $k_0T\ll\epsilon_N$ which corresponds to $\langle\mathcal{E}\rangle_{\text{Av}}\ll|-\epsilon_N|$, where $\langle\mathcal{E}\rangle_{\text{Av}}$ is the average energy of the charge carriers. He obtains for the mobility

$$\mu_N=\frac{2q|\epsilon_N|}{3\sqrt{2}\pi^{\frac{3}{2}}N_N\hbar^2}\left(\frac{m^*}{k_0T}\right)^{\frac{1}{2}}\text{ esu.} \quad (15)$$

[4] A. I. Ansel'm, J. Exptl. Theoret. Phys. (U.S.S.R.) 24, 85 (1953).

[5] This attractive influence is partially due to polarization effects. Although the numerical calculation[2] upon which Erginsoy's result depends includes such effects, they influence the scattering in a different way and are based on a variety of approximations.

[6] N. Sclar, Phys. Rev. 104, 1548 (1956), preceding paper.

The choice of $k_0T\ll\epsilon_N$ is unfortunate since it seems that the condition for the validity of resonance scattering is that $\langle\mathcal{E}\rangle_{\text{Av}}\simeq|-\epsilon_N|$ [see Eq. (35) in reference 6]. A further objection to this choice is that ϵ_N must of necessity be smaller than the energy required to ionize the neutral impurity and give rise to a free charge carrier. The condition then that $k_0T\ll\epsilon_N$ thus practically ensures that all free charge carriers will already have been bound at the deeper levels giving rise to the neutral impurities.

If we consider the resonance scattering with what seems to be the more reasonable choice, i.e., $k_0T\simeq\epsilon_N$, we obtain

$$\mu_N=\frac{2qm^{*\frac{1}{2}}|\epsilon_N|^{\frac{1}{2}}}{\sqrt{2}\pi^{\frac{3}{2}}N_N\hbar^2}\times\frac{1}{300}\text{ cm}^2/\text{volt sec.} \quad (16)$$

The binding energy for the hydrogen negative ion is 0.71 ev. If we assume that the neutral impurity may be represented as a hydrogen atom in the medium of the semiconductor, we obtain

$$\epsilon_N=(0.71\beta/D^2)\text{ ev.} \quad (17)$$

For n-type germanium and silicon, this is approximately 5×10^{-4} ev and 2×10^{-3} ev, respectively, corresponding to temperatures of about 6°K and 20°K. Inserting (17) in (16) gives

$$\mu_N=\frac{1.17\times10^{22}\beta}{DN_N}\text{ cm}^2/\text{volt sec,} \quad (18)$$

which upon comparison with (4) indicates that we have a result which is essentially equivalent to Erginsoy's mobility, differing only by about 15% from it. It is to be noted, however, that our result is obtained by substituting ϵ_N for k_0T. When this condition is not exactly satisfied, then the more general result of Eq. (13) holds, which may be expressed as

$$\mu_N=\frac{1.17\times10^{22}\beta}{DN_N}\left[\frac{2}{3}\left(\frac{k_0T}{\epsilon_N}\right)^{\frac{1}{2}}+\frac{1}{3}\left(\frac{\epsilon_N}{k_0T}\right)^{\frac{1}{2}}\right]\text{ cm}^2/\text{volt sec.} \quad (19)$$

This expression involves a binding energy associated with the neutral impurity but is otherwise independent of the detailed description of the center. If we may assume the binding energy to be independent of temperature, then by fitting the appropriate experimental data to the theory, it should be possible to deduce ϵ_N and to compare it with the predictions based on possible models for the imputity. To compare this mobility with Erginsoy's result, we take the impurity to be hydrogen-like and, using Eq. (17), obtain

$$\mu_N=\frac{1.17\times10^{22}\beta}{DN_N}\left[0.734\times10^{-2}\frac{DT^{\frac{1}{2}}}{\beta^{\frac{1}{2}}}+30.2\frac{\beta^{\frac{1}{2}}}{DT^{\frac{1}{2}}}\right]\text{ cm}^2/\text{volt sec.} \quad (20)$$

As may be seen, there will be a slight temperature dependence for the mobility in contrast with the calculation of Erginsoy. This is illustrated in Fig. 1. In the range of the validity of this treatment, the maximum deviation between the two results is 22%. Careful measurements at low temperature may thus distinguish between these two calculations for neutral impurity scattering.

We now consider the scattering of holes expected from neutral impurities in *p*-type material. We recall that a neutral acceptor in the diamond-type lattice consists of an element from the third periodic column with an extra electron and hole. It is commonly believed that the situation is essentially hydrogen-like with the hole (speaking classically) revolving about the combination of a neutral atom plus one electron. A hole scattering from this system will find an attractive field of the same nature as that encountered by the electrons in *n*-type impurities. The mobility would be given by Eqs. (10)–(12) and for resonance by Eq. (13). On the other hand, if the neutral impurity is the neutral atom, the hole and extra electron having annihilated each other,[7] then the scattering from this neutral imputity may be entirely different, being repulsive rather than attractive. In this case an equation of the type of Eq. (10) with $\mu=\mu_R$ may be more appropriate, with no resonances possible. A comparison between neutral impurity scattering in *p* and *n* material may elucidate this point.

The extra level ϵ_N to be associated with the neutral impurity differs from the usual impurity level in that it does not give rise to any free charges in the manner of donor or acceptor impurities. It can, however, at sufficiently low temperatures, compete with the deeper level of the impurities in capturing free electrons and cause a flattening of a curve of log (resistivity) *vs* $1/T$, which would suggest a smaller ionization energy. For every electron captured in the shallow level ϵ_N, an ion will be formed from the neutral impurity. These are expected to play only a negligible role, however, in controlling the mobility because of the much smaller concentration of these centers compared to the neutral centers. It does not seem possible at this time to give a reliable estimate for the distance parameter a_N appearing in Eqs. (10)–(14). The estimates available for ionized impurities[6] do not appear to be applicable here.

[7] Ionization of this neutral impurity will involve generating a hole and electron (pair production) in the vicinity of the impurity and the freeing of the hole.

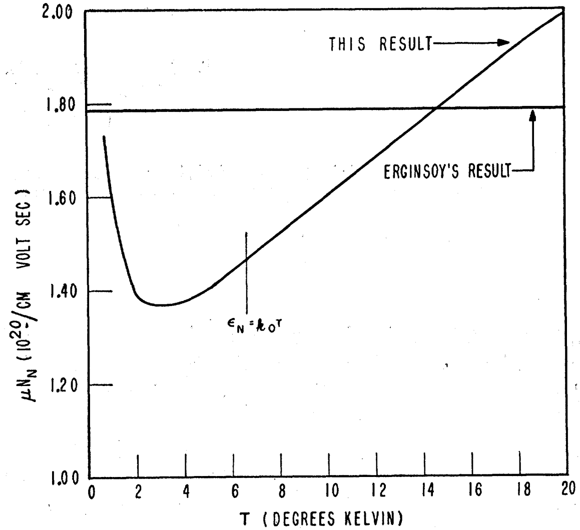

FIG. 1. Comparison with Erginsoy's calculation for the mobility multiplied by the concentration of neutral impurities for *n*-type germanium. The temperature at which $\epsilon_N=k_0T$ is indicated.

It is clear, however, that this distance must be exceedingly small because of the essentially neutral character of the impurity. For small a_N and small αa_N, inspection of Eq. (10) with

$$\left\{\left[\left(\begin{matrix}\tan\\ \tanh\end{matrix}\,\alpha a_N\right)\Big/\alpha a_N\right]-1\right\}^2\simeq\frac{(\alpha a_N)^4}{9}$$

indicates that a high mobility results, which implies a small cross section for this scattering. Thus only the resonance scattering described above is likely to be of importance for the mechanism considered here.

The mobility for neutral impurities calculated in the Born approximation [Eq. (8)] is not expected to apply to semiconductors with low impurity activation energies such as the usual impurity levels in germanium and silicon. The reason is that neutral impurities become dominant only at the low temperatures when the criteria for the validity of the Born approximation cannot be satisfied. For the deeper levels, where neutral impurities can occur at higher temperatures, a range of validity may be found, but the approximation of describing the impurity as hydrogen-like may need reexamination since the deeper levels in germanium and silicon show appreciable deviations from hydrogen-like states.