A semiclassical approach to Coulomb scattering of conduction electrons on ionized impurities in nondegenerate semiconductors

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In the proposed model of mobility, the time of electron–ion interaction equals the time taken by the conduction electron to pass a spherical region, corresponding to one impurity ion in crystal, and the minimum scattering angle is determined after Conwell–Weisskopf. We consider the acts of electron scattering on ions as independent and incompatible events. It is shown in the approximation of quasimomentum relaxation time, that for nondegenerate semiconductors, the mobility μ_i , limited by the elastic scattering by impurity ions with the concentration N_i , is proportional to $T/N_i^{2/3}$; the Hall factor equals 1.4. The calculated dependences of the mobility of the majority charge carriers upon their concentration for different temperatures T agree well with known experimental data. It is shown, that the Brooks–Herring formula $\mu_{BH} \propto T^{3/2}/N_i$ gives overestimated values of mobility. Comparison of the calculations of mobility in degenerate semiconductors with experimental data also yields $\mu_i < \mu_{BH}$. © 2003 American Institute of Physics. [DOI: 10.1063/1.1573735]

I. INTRODUCTION

The concentration of ionized impurities in crystal is usually evaluated from the comparison of experimental charge carrier mobility μ_i , limited by the elastic scattering by ions, with the calculated μ_{BH} by the Brooks–Herring (BH) formula (see, for example, Refs. 1–6). But, as noted in Ref. 7, the concentration of donors, found using μ_{BH} from the Hall mobility of electrons in the n part of the InSb ingot with a p - n junction measured at $T=77$ K, is several times greater than those found from the distribution curve of donors along the ingot. The conclusion that $\mu_i < \mu_{BH}$ is confirmed by the comparison of experimental data for different semiconductors with the calculations using the BH formula (see Ref. 8). The fact that $\mu_i < \mu_{BH}$ is also confirmed by the simulation of the dependence of the drift mobility on the doping impurity concentration using the Monte Carlo method.⁹

In the BH model, the interaction time of the conduction electron with one impurity ion is nominally taken to be infinite. In the Conwell–Weisskopf (CW) model^{2–6,10} the minimum scattering angle (maximum impact parameter) is introduced. It is known, that in numerical simulation of the dependence of the drift velocity of the electrons on the electric-field strength in n GaAs¹¹ the CW model gives better agreement with experiment than the BH model. When simulating the scattering by impurity ions in semiconductors by the Monte Carlo method,¹² the Ridley approximation⁴ is used, which reconciles the BH and CW models by introducing the geometrical probability that the ion is the nearest scattering center for the conduction electron. Moreover, as pointed out in Ref. 6: “...it is difficult to observe experimentally a $\mu_i \propto T^{3/2}$ behavior over a wide temperature range.”

The purpose of this work is to calculate the electron (hole) mobility in relaxation time approximation under the condition, that the act of elastic pure Coulomb scattering by an ion continues only during the time taken by the conduction electron to pass a spherical region of the crystal, corresponding to one impurity ion, and the minimum scattering angle is defined in accordance with CW.

Let us consider the crystalline semiconductor of volume V , which contains impurity ions with concentration N_i . Thus, the number of ions in the crystal is $N_i V$. We will describe the electron in the effective-mass approximation by the wave function in the plane wave form $\psi_{\mathbf{k}} = V^{-1/2} \exp(i\mathbf{k}\mathbf{r})$, where $\mathbf{k}$ is the quasiwave vector, $\mathbf{r}$ is the coordinate of the electron. In such a description, the electron plane wave interacts with all impurity ions of the crystal.

The transport relaxation time τ_k of the quasiwave vector $\mathbf{k}$ of the electron with the kinetic energy $E = (\hbar\mathbf{k})^2/2m$ for elastic, independent, and incompatible scattering on $N_i V$ impurity ions of the same type in the crystal is given by:^{2,3,13}

$$\begin{aligned} \frac{1}{\tau_k} &= N_i V \sum_{\mathbf{k}'} W_{\mathbf{k}'\mathbf{k}} (1 - \cos \theta) \delta_{\mathbf{k}'\mathbf{k}} \\ &= \frac{N_i V^2}{(2\pi)^3} \int W_{\mathbf{k}'\mathbf{k}} (1 - \cos \theta) \delta\left(\frac{\mathbf{k}' - \mathbf{k}}{k}\right) d^3\mathbf{k}', \end{aligned} \quad (1)$$

where N_i is the concentration of impurity ions, $W_{\mathbf{k}'\mathbf{k}}$ is the electron scattering probability per unit time into the angle $\theta = (\widehat{\mathbf{k}, \mathbf{k}'})$ induced by the spherically symmetric Coulomb potential of an ion, $\delta_{\mathbf{k}'\mathbf{k}}$ is the Kronecker delta, $\delta((\mathbf{k}' - \mathbf{k})/k)$ is the dimensionless Dirac delta function introduced to take into account the conservation law of quasiwave vector absolute value ($k' = k$) in elastic scattering, $\hbar = h/2\pi$ is Planck's constant, and m is the electron effective mass.

In the first order of perturbation theory, the ratio of the probability of electron transition between $\mathbf{k}$ and $\mathbf{k}'$ states

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with E and E' energies to the “duration” t_c of an impurity ion influence $U_{k'k}$ upon the electron is equal:¹⁴

$$W_{k'k} = \frac{2}{t_c} \left| \frac{U_{k'k}}{E' - E} \right|^2 \left\{ 1 - \cos \left[\frac{t_c}{\hbar} (E' - E) \right] \right\}, \quad (2)$$

when the probability of elastic scattering of electron by an ion $t_c W_{k'k} \ll 1$.

II. MAIN IDEA OF THE PROPOSED MODEL

Let us consider a doped semiconductor with impurity ions of one type in the charge state $Z \neq 0$. The first assumption is that the impurity ion with the charge Ze does not possess internal degrees of freedom and scatters the electron with quasimomentum $\hbar \mathbf{k}$ elastically. The second assumption is that the conduction electron (regarded as a reasonably well-localized wave packet) interacts with one impurity ion only during the time $t_c \approx 2R/v = 2Rm/\hbar k$, where v is the electron velocity, $R = (4\pi N_i/3)^{-1/3}$ is the radius of the spherical region of the crystal associated with an ion.¹⁵ After interaction with an ion during the time t_c , the electron scatters on the next ion over the same period of time and so on, i.e., scattering occurs permanently.¹⁶ Then, the minimum scattering angle θ_i of the electron on the Coulomb potential $Ze/4\pi\epsilon r$, where $\epsilon = \epsilon_r \epsilon_0$ is the static permittivity of a non-doped crystal, ϵ_0 is the electric constant, and the duration $t_c = R(2m/E)^{1/2}$ of the scattering act are bound up by a relation from classical mechanics:¹⁷

$$\cot \frac{\theta_i}{2} = \frac{4\pi\epsilon b m v^2}{|Z|e^2} = t_c \frac{4\pi\epsilon}{|Z|e^2} \left(\frac{2}{m} \right)^{1/2} E^{3/2}, \quad (3)$$

where the maximum impact parameter $b = R$ is determined from the relation $4\pi R^3/3 = 1/N_i$.

Note, that introduction of the finite interaction time t_c of the electron with an impurity ion and minimum scattering angle θ_i makes the problem classical.

So, when determining the action sphere of an impurity ion upon the conduction electron, we follow the CW model,^{2-6,10} but additionally take into account the finiteness of time t_c of the Coulomb interaction of the electron with an ion. The lower bound on the angle θ_i and upper on the time t_c make consecutive scattering acts of the conduction electron by different impurity ions independent and incompatible events.¹⁸ According to Ref. 19, the condition of validity of classical mechanics while obtaining formula (3) is the minuteness of the electron de Broglie wavelength in comparison to the size of the scatterer: $2\pi/k \ll 2R$. It should be noted that at scattering, the form of the wave function does not change, only the direction of the electron quasiwave vector changes.

For the energy of Coulomb interaction of a conduction electron with an ion $U(r) = -Ze^2/4\pi\epsilon r$ we have:¹⁴

$$U_{k'k} = \int_V \psi_{k'}^* U(r) \psi_k d^3r \rightarrow U(k, \theta) = -\frac{Ze^2}{V\epsilon q^2}, \quad (4)$$

where $\hbar q = \hbar|\mathbf{k}' - \mathbf{k}| = 2\hbar k \sin(\theta/2)$ is the absolute value of electron quasimomentum transfer at elastic scattering ($|\mathbf{k}'| = |\mathbf{k}|$) on the angle θ ; $\psi_{k'}^* = V^{-1/2} \exp(-ik'\mathbf{r})$.

According to Ref. 14, the sufficient condition for the validity of formula (4) is $kR \gg 1$. The same condition, in Ref. 19, denotes the range of validity for formula (3).

For $t_c \ll \hbar/|E' - E|$, when in the scattering act on an impurity ion, the electron changes only the direction of motion,²⁰ formula (2) is transformed according to Ref. 14 in the following way:²¹

$$W_{k'k} \rightarrow \frac{t_c}{\hbar^2} |U(k, \theta)|^2 = \frac{2Rm}{\hbar^3 k} |U(k, \theta)|^2, \quad (5)$$

where $U(k, \theta)$ is found from Eq. (4).

Substitution of Eq. (5) into Eq. (1) taking into account Eqs. (4) and (3) gives

$$\frac{1}{\tau_k} = \left(\frac{3}{4\pi} \right)^{1/3} \left(\frac{Ze^2}{4\pi\epsilon} \right)^2 \frac{N_i^{2/3}}{\hbar E} \ln \left[1 + \left(\frac{8\pi\epsilon R E}{|Z|e^2} \right)^2 \right]. \quad (6)$$

Note, that from Eqs. (2)–(5), the averaged by angles frequency ν_i of elastic collisions of the electron having the kinetic energy E with ionized impurities can be written in the form:

$$\begin{aligned} \nu_i &= \frac{N_i V^2}{(2\pi)^3} \int_0^\infty \int_{\theta_i}^\pi W_{k'k} \delta\left(\frac{k' - k}{k}\right) 2\pi \sin \theta d\theta k'^2 dk' \\ &= \frac{N_i R}{2\hbar E} \left(\frac{Ze^2}{4\pi\epsilon} \right)^2 \cot^2 \frac{\theta_i}{2} = \frac{3}{2\pi\hbar} E. \end{aligned}$$

The impurity scattering limited mobility of a conduction electron $\mu_i = e\langle\tau\rangle/m$ is determined by the average relaxation time^{4-6,22}

$$\langle\tau\rangle = \int_0^\infty \tau_k E^{3/2} \frac{\partial f}{\partial E} dE \left(\int_0^\infty E^{3/2} \frac{\partial f}{\partial E} dE \right)^{-1}, \quad (7)$$

where $f = \{1 + \exp[(E - E_F)/k_B T]\}^{-1}$ is the Fermi–Dirac function, E_F is the Fermi energy, and $k_B T$ is the thermal energy.

The calculation of $\langle\tau\rangle$ for nondegenerate conduction electrons, when $f \approx \exp[(E_F - E)/k_B T]$, will be performed using the standard method.^{4-6,10} Namely, the function $\ln\{1 + [8\pi\epsilon R E/(|Z|e^2)]^2\}$ at energy $E = (\hbar k)^2/2m$ can be taken outside the integral in the numerator (7), when according to Eqs. (7) and (6), the expression $E^{5/2} \exp[(E_F - E)/k_B T]$ under the integral sign as a function of E reaches its maximum value. This procedure corresponds to $E = 5k_B T/2$. Then, as follows from formulas (6) and (7), the Hall factor $\langle\tau^2\rangle/\langle\tau\rangle^2 = 1.4$, and the mobility

$$\mu_i = \frac{5}{2} \left(\frac{4\pi}{3} \right)^{1/3} \frac{\hbar (4\pi\epsilon)^2 k_B T}{e^3 m Z^2 N_i^{2/3}} \frac{1}{\ln(1 + \gamma)}, \quad (8)$$

where $\gamma = 25[3/(4\pi N_i)]^{2/3} (4\pi\epsilon k_B T)^2 / (Z^2 e^4)$.

Formula (8) is applicable to conduction electrons with the mean thermal energy $(\hbar k)^2/2m = 3k_B T/2$ and wavelength $2\pi/k_i$, when $k_i R > 1$.

It should be noted here, that the value of the Hall factor $\langle\tau^2\rangle/\langle\tau\rangle^2 = 1.4$ obtained from Eq. (6) agrees more closely with experimental data for nondegenerate crystalline p type semiconductors with prevailing scattering of holes by impurity ions,^{23,24} than $\langle\tau^2\rangle/\langle\tau\rangle^2 = 1.93$, which is obtained from BH and CW models.^{2,6}

Let us consider the case, when in n -type crystal, the impurity ions of different types are presented, so that the electroneutrality equation takes the form: $n = \sum_j \sum_z Z N_{jz}$, where n is the concentration of conduction electrons, and N_{jz} is the concentration of ions of type j in the charge state $Z(j)$. We are assuming that the minimum scattering angles θ_i for the impurities of type j in the charge states $|Z(j)| > 1$ and $|Z| = 1$ are the same, i.e., $\theta_i(Z(j)) = \theta_i(|Z| = 1)$. Then, according to Eq. (3), for the maximum impact parameter $b_{jz} = R_{jz}$ of electron scattering on the ion with the charge $Z(j)e$, we have $b_{jz} = R_{jz} = |Z(j)|R_1$, where $b_1 = R_1$ is the maximum impact parameter for the ion in the charge state $|Z| = 1$. The concentration of all impurity ions in the crystal $\sum_j \sum_z N_{jz}$ satisfies the condition: $4\pi/3 \sum_j \sum_z R_{jz}^3 N_{jz} = 1$, so that $\sum_j \sum_z |Z|^3 N_{jz} = 3/(4\pi R_1^3)$. The time of interaction of the electron with an impurity ion (charge Ze) is $t_c \approx 2R_{jz}/v = 2R_{jz}m/\hbar k$, where $R_{jz} = |Z|R_1$ for all j and $Z \neq 0$. In formulas (6) and (8), the presence of a different sort of ions may be considered by substituting:

$$Z^2 N_i^{2/3} \rightarrow \left(\sum_j \sum_z N_{jz} |Z|^3 \right)^{2/3}.$$

It should be noted, that if the anisotropy of quasimomentum relaxation time in a multivalley semiconductor at elastic scattering on the ionized impurities can be neglected, then the mobility of electrons, say, in n Si is $\mu_i^* = e\langle\tau\rangle/m_c = (m/m_c)\mu_i$, where $m = m_d/6^{2/3} = 0.36m_0$ and $m_c = 0.28m_0$ are the density of states and electric conductivity effective masses for one of the six equivalent valleys, respectively; m_0 is the mass of a free electron.

The electron mobility in a nondegenerate semiconductor, limited by the elastic scattering on impurity ions (concentration N_i and charge Ze) according to BH model¹⁻⁶ is

$$\mu_{\text{BH}} = \frac{2^{7/2} (4\pi\epsilon)^2 (k_B T)^{3/2}}{\pi^{3/2} e^3 m^{1/2} Z^2 N_i [\ln(1+\beta) - \beta/(1+\beta)]}, \quad (9)$$

where $\beta = (24m\epsilon/n)(k_B T/e\hbar)^2$.

The electron mobility by the CW model^{4-6,10,25} is

$$\mu_{\text{CW}} = \mu_{\text{BH}} \frac{\ln(1+\beta) - \beta/(1+\beta)}{\ln(1+\alpha)}, \quad (10)$$

where $\alpha = (4\pi\epsilon/(Ze^2))^2 (3k_B T)^2 / N_i^{2/3}$ and μ_{BH} is defined by formula (9).

III. COMPARISON OF THE CALCULATIONS WITH EXPERIMENTAL DATA

The calculation of the electron mobility in nondegenerate gas of electrons μ will be carried out assuming, that $\mu^{-1} = \mu_1^{-1} + \mu_i^{-1}$, where μ_1 is the phonon scattering limited electron mobility in the crystal, and μ_i is the impurity ion scattering limited mobility.

Different experimental data²⁶⁻³⁰ on the dependence of the mobility of electrons on their concentration $n = (1-K)N$ at $T = 77-80$ K in n InSb crystals with average compensation ratio $K \approx 0.15$ is shown in Fig. 1. Here, K is the ratio of concentration of totally ionized hydrogenlike acceptors ($Z = -1$) to donors ($Z = +1$); $N_i = (1+K)N$ is the concentration of impurity ions and N is the concentration of

FIG. 1. The mobility μ of conduction electrons in n InSb vs their concentration n for $K \approx 0.15$ at $T = 78$ K. The results of calculation of μ : 1 using Eq. (8), when $|Z| = 1$ and $\mu_1 = 1.5 \times 10^6 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$; 2 using the BH formula (9); 3 using the CW formula (10). Experimental data on Hall mobility: [(a) see Ref. 26, (b) see Ref. 27, (c) see Ref. 28, and (d) see Ref. 29. Drift mobility (e) see Ref. 30]. The arrow shows effective density of states $N_c = 2(2\pi m k_B T)^{3/2} / (2\pi\hbar)^3$ in the c band of InSb; $n \leq N_c$ corresponds to nondegenerate case.

donors. The mobilities of electrons (when μ_1 was estimated by Refs. 7 and 26 as $1.5 \times 10^6 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) were calculated using formulas (9), (10), and (8) with the following parameters: $\epsilon_r = 17.8$ and $m = 0.013m_0$.³¹ The arrow in Fig. 1 indicates the concentration $n = N_c \equiv 2(2\pi m k_B T)^{3/2} / (2\pi\hbar)^3$ of conduction electrons, above which their degeneracy begins.

As seen in Fig. 1, formula (8) describes experimental data on mobility over a wide range of majority carrier concentrations. The condition $k_i R > 1$, where $\hbar k_i = (3mk_B T)^{1/2}$ is thermal quasimomentum of electrons, $R = (4\pi(1+K)N/3)^{-1/3}$, is satisfied. Note, that the BH (9) and CW (10) formulas give overestimated values of mobility. It should be noted, that for n InSb crystals in Fig. 1, the density-of-states effective mass of electrons does not depend on their concentration.³¹ Note, that our calculations for other nondegenerate semiconductors with isotropic effective masses of conduction electrons also confirm the conclusions of papers (Refs. 7-9 and 12).

Thus, the model of majority charge carrier mobility, limited by elastic scattering on randomly distributed in crystal ionized impurities, is presented. The finiteness of electron (hole) interaction time with an ion and impact parameter limitations are considered simultaneously. It is shown, that the mobility of charge carriers in a crystalline semiconductor, calculated using our model agrees more closely to experimental data over a wide range of concentrations of the doping impurities and temperatures, than BH (9) and CW (10) formulas.

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