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ELECTRONIC PROPERTIES OF SEMICONDUCTORS

Quasi-Classical Model of the Static Electrical Conductivity of Heavily Doped Degenerate Semiconductors at Low Temperatures

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Abstract—Germanium, silicon, gallium arsenide, and indium antimonide *n*-type crystals on the metal side of the insulator–metal transition (Mott transition) are considered. In the quasi-classical approximation, the static (direct current) electrical conductivity and the drift mobility of electrons of the *c* band, and electrostatic fluctuations of their potential energy and the mobility edge are calculated. It is considered that a single event of the elastic Coulomb scattering of a mobile electron occurs only in a spherical region of the crystal matrix with an impurity ion at the center. The results of calculations using the proposed formulas without using fitting parameters are numerically consistent with experimental data in a wide range of concentrations of hydrogenlike donors at their weak and moderate compensation by acceptors.

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1. INTRODUCTION

The problem of the quantitative description of electron and hole migration in three-dimensional crystalline semiconductors as the impurity atom concentration in them increases and a quasi-metal state is reached remains important for applications (see, e.g., [1–3]). Heavily doped degenerate *n*- and *p*-type semiconductor materials are radiation-resistant elements of devices of cryogenic micro- and optoelectronics [4–6]. Their electrical and optical parameters weakly depend on the radiation fluence even at low temperatures, which is important for device operation in space (the temperature of the cosmic microwave background is ≈2.7 K). For power-electronics purposes, it is pertinent to analytically describe the conductivity of semiconductor elements in current breakers [7, 8]. One of the practically important problems is the development of three-dimensional electrodes to a two-dimensional conductor (e.g., to graphene) with matched resistances in the electrical circuit.

We note that, although the first experiments for measuring the electrical resistance in controllably heavily doped degenerate semiconductors at liquid helium and nitrogen temperatures were performed half a century ago (see, e.g., [9–12]), so far there is no theory which would quantitatively explain the collected experimental data. For example, a method of analytical approximation of the majority carrier mobility in crystalline semiconductors was proposed in [1].

The electrical conductivity is controlled by the degree of electrical activity of impurity atoms immobile in a crystal matrix (see, e.g., [13]). In general, in the case of the heavy doping of monatomic semiconductors (e.g., Ge, Si), the electrical activity of the major (doping) impurity slightly decreases due to the transition of a part of it from sites to interstices or the formation of energetically inactive associates from the impurity. In binary crystalline semiconductor compounds (e.g., GaAs and InSb), dopant atoms can be in part arranged in two sublattices, which results in a decrease in its electrical activity. For the most part, electrons and holes in heavily doped semiconductors at cryogenic temperatures are scattered at impurity ions.

The objective of the study is calculation of the dc conductivity of heavily doped degenerate crystalline *n*-type semiconductors, taking into account the elastic Coulomb scattering of mobile electrons at hydrogenlike impurity ions at low temperatures. For definiteness, an *n*-type crystalline semiconductor was considered, since the drift mobility of electrons is higher than that of holes. Therefore, the relative contribution of scattering at impurity ions to a decrease in the electron mobility is larger than to a decrease in the hole mobility.

In a heavily doped *n*-type semiconductor, all donors with the average concentration N are in the charge state (+1); all acceptors with the average concentration KN (where $0 < K < 1$ is the degree of compensation) are in the charge state (−1). From the electrical neutrality condition, it follows that the average concentration of all electrons in the *c* band $n = (1 - K)N$ is lower than the ion concentration $N_{\text{ion}} = (1 + K)N$.

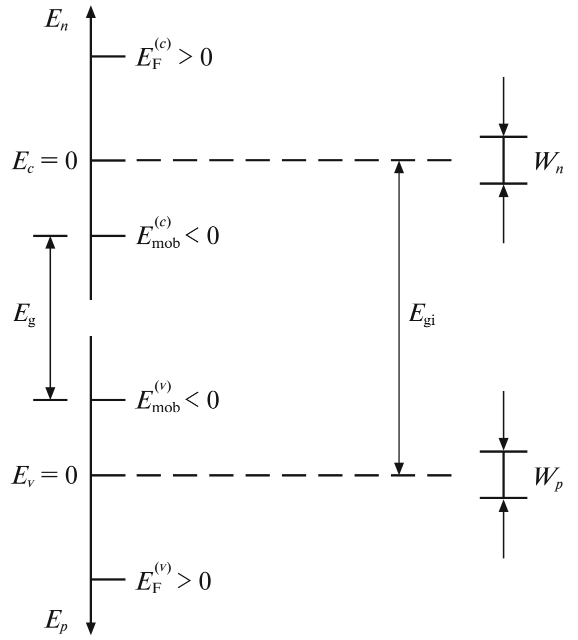

Fig. 1. Schematic diagram of counting the electron and hole energy levels in heavily doped degenerate *n*-type (upper scale) and *p*-type (lower scale) crystalline semiconductors: $E_c - E_v = E_{gi}$ is the band-gap width of an undoped (intrinsic) crystal, $E_g = E_{gi} - |E_{mob}^{(c)}| - |E_{mob}^{(v)}|$ is the band gap of the doped crystal, E_n is the *c*-band electron energy, $E_F^{(c)} > 0$ is the Fermi level for electrons in an *n*-type semiconductor, $E_{mob}^{(c)} < 0$ is the mobility edge for electrons; E_p is the *v*-band hole energy, $E_F^{(v)} > 0$ is the Fermi level for holes in a *p*-type semiconductor, $E_{mob}^{(v)} < 0$ is the mobility edge for holes; W_n, W_p are the root-mean-square fluctuations of the potential energy of electrons (*n*) and holes (*p*).

At low temperatures, the electron transitions from the *v* band to the *c* band are insignificant for maintaining ionization equilibrium.

Let the criterion of a degenerate *n*-type semiconductor at the absolute temperature $T \to 0$ be an electron concentration corresponding to the metal side of the Mott transition [14, 15]. The insulator–metal transition at $T \to 0$ (Mott transition) [16, 17] occurs when $n > n_M$, where n_M is the critical concentration of mobile electrons of the *c* band, corresponding to the Mott transition. The value $n_M = (1 - K)N_M$ (at the zero temperature $T \to 0$ limit) is defined, according to [15], by the relation

$$\frac{N_M^{1/3} a_B}{\nu^{2/3}} = \frac{0.1}{(1-K)^{2/3}}, \qquad (1)$$

where $a_B = 4\pi\varepsilon_r\varepsilon_0\hbar^2/m_{nd}^{(1)}e^2$ is the Bohr radius for a *c*-band electron in one of the ν equivalent valleys (ν = 6 for *n*-Si, ν = 4 for *n*-Ge, ν = 1 for *n*-GaAs and *n*-InSb) with the effective mass $m_{nd}^{(1)}$; $\varepsilon = \varepsilon_r\varepsilon_0$ is the absolute static permittivity of the semiconductor, ε_r is the relative permittivity caused by *v*-band electrons against a background of positively charged cores of the crystal matrix, neutralizing them, ε_0 is the permittivity of free space, *e* is the elementary charge, and $N_M^{1/3}a_B$ is the Mott parameter. Formula (1) shows that the smaller the number of valleys *v* in the *c* band and the smaller the degree of semiconductor compensation *K*, the lower the concentration of major impurities $N_M = n_M/(1 - K)$, required to implement the Mott transition.

In this study, the quasi-classical theory of the elastic scattering of *c*-band electrons at hydrogenlike impurity ions, proposed in [18, 19] for lightly doped semiconductors, applies to heavily doped degenerate *n*-type semiconductors. Hereafter, it is believed that the spherical region of the crystal matrix in which one electron scattering event occurs in the Coulomb field of one impurity ion has the volume $4\pi R_{ion}^3/3 = N_{ion}^{-1/3}$, where $N_{ion} = (1 + K)N$ is the average impurity ion concentration. The diameter of this region

$$2R_{ion} = 1.24N_{ion}^{-1/3} \qquad (2)$$

is approximately equal to the average distance between ions ($\approx 1.28N_{ion}^{-1/3}$) determined in [20] by the Voronoi–Dirichlet polyhedra method. The duration of one event of electron–ion interaction (scattering) is equal to the electron time of flight through the *c* band of the spherical region per impurity ion in the crystal. In this case the Born approximation and the electron wave function in the form of a plane wave (effective-mass approximation) are used.

Then two types of heavily doped degenerate crystalline *n*-type semiconductors are considered: conditionally ideally doped [symbol (id)] and really doped [symbol (re)] semicondusctors, which differ only by the dependence of the one-electron energy of the band edges of allowed energies E_c and E_v on the spatial coordinates *x*, *y*, *z*. For id-crystals, E_c and E_v are independent of *x*, *y*, *z*, i.e., the bottom of the *c* band and the top of the *v* band are flat. For re-crystals, $E_c(x, y, z)$ and $E_v(x, y, z)$ are antisymmetric functions with respect to the band-gap center [16, 21] due to electrostatic fluctuations of the potential energy and electrons of the *c* band W_n and holes of the *v* band W_p (see Fig. 1). The average concentrations of electrons $n^{(id)} = n^{(re)} = n$, donors *N*, and acceptors *KN* for id- and re-semiconductors are considered to be equal.

2. STATISTICS OF ELECTRONS IN IDEAL AND REAL CRYSTALLINE SEMICONDUCTORS AT LOW TEMPERATURES

In *n*-type id-semiconductors (with flat band edges of allowed one-electron energies E_n, i.e., when $W_n =$

$W_p = 0$ and $E_{\rm mob}^{(c)} = E_c = 0$; see Fig. 1), the electron concentration in the c band $n^{\rm (id)}$ under the condition of the complete ionization of donors with the concentration N and acceptors with the concentration KN are given by (see, e.g., [16, 22])

$$n^{\rm (id)} = \frac{1}{V}\int_{E_c=0}^{\infty} g_n^{\rm (id)}(\varepsilon_{\rm kin}) f_n(\varepsilon_{\rm kin})\, d\varepsilon_{\rm kin} = (1-K)N, \qquad (3)$$

where V is the volume of a bulk crystalline sample, $g_n^{\rm (id)}(\varepsilon_{\rm kin}) = V[(2m_{nd})^{3/2}/2\pi^2\hbar^3]\varepsilon_{\rm kin}^{1/2}$ is the one-electron density of states in the c band of crystal, $f_n(\varepsilon_{\rm kin}) = \{1 + \exp[(\varepsilon_{\rm kin} - \varepsilon_{\rm F}^{(c)}/k_{\rm B}T]\}^{-1}$ is the Fermi–Dirac function, $\varepsilon_{\rm kin}$ is the kinetic energy of a c-band electron, $\varepsilon_{\rm F}^{(c)}$ is the chemical potential, $k_{\rm B}$ is the Boltzmann constant, T is the absolute temperature; $m_{nd} = \nu^{2/3} m_{nd}^{(1)}$ is the effective mass of the c-band electron density of states, ν is the number of valleys (equivalent energy minima of c-band electrons), $m_{nd}^{(1)}$ is the effective mass of the electron density of states in one valley, and $\hbar = h/2\pi$ is Planck's constant.

From (3), when the chemical potential $\varepsilon_{\rm F}^{(c)}$ is more than three times higher than the thermal energy $k_{\rm B}T$ and the electron Fermi gas in the id-semiconductor c band can be considered as degenerate, we obtain (see, e.g., [16, 17, 22])

$$\varepsilon_{\rm F}^{(c)} = \zeta_{\rm F}^{(c)}[1 - (\pi^2/12)(k_{\rm B}T/\zeta_{\rm F}^{(c)})^2] > 3k_{\rm B}T, \qquad (4)$$

where $\zeta_{\rm F}^{(c)} = (\hbar^2/2m_{nd})[3\pi^2 n^{\rm (id)}]^{2/3}$ is the Fermi energy, i.e., the chemical potential $\varepsilon_{\rm F}^{(c)}$ at the limit of the zero absolute temperature ($T \to 0$).

In the three-dimensional crystalline n-type re-semiconductor ($W_n \neq 0$ and $E_{\rm mob}^{(c)} \neq E_c = 0$; see Fig. 1), the one-electron density of states in the c band is given by [23, 24]

$$g_n^{\rm (re)}(E_n) = V\frac{(2m_{nd})^{3/2}}{2\pi^2\hbar^3}\int_{-\infty}^{E_n}(E_n - U_n)^{1/2}\mathcal{P}(U_n)dU_n, \qquad (5)$$

where E_n is the total electron energy, U_n is the potential electron energy, $E_n - U_n = E_{\rm kin}$ is the kinetic energy of a c-band electron, $\mathcal{P}(U_n)$ is the probability distribution density of potential electron energy fluctuations. Then the electron concentration in the c band, averaged over the crystalline sample volume V (at the complete ionization of hydrogenlike impurity atoms) is given by

$$n^{\rm (re)} = \frac{1}{V}\int_{-\infty}^{+\infty} g_n^{\rm (re)}(E_n) f_n(E_n)dE_n = (1-K)N, \qquad (6)$$

where $f_n(E_n) = \{1 + \exp[(E_n - E_{\rm F}^{(c)})/k_{\rm B}T]\}^{-1}$ is the Fermi–Dirac function and $E_{\rm F}^{(c)}$ is the Fermi level.

Then, according to [24, 25], we suppose that

$$\mathcal{P}(U_n) = \frac{1}{\sqrt{2\pi}W_n}\exp\left(-\frac{U_n^2}{2W_n^2}\right), \qquad (7)$$

where W_n is the root-mean-square fluctuation of the c-band electron energy (Fig. 1). At $n^{\rm (re)} = (1-K)N$, W_n is related to the root-mean-square fluctuation of the electrostatic energy of an immobile impurity ion W_d as [25, 26]

$$W_n \approx 0.21(1-K)^{1/2}W_d. \qquad (8)$$

If the Coulomb interaction of only the nearest point charged particles (impurity ions and electrons) is taken into account, W_d can be written as [17, 25]

$$W_d \approx 2.64\frac{e^2}{4\pi\varepsilon}N_{\rm ch}^{1/3}, \qquad (9)$$

where $N_{\rm ch} = N_{+1} + KN + n^{\rm (re)} = 2N$ is the concentration of all point particles (with the charge $\pm e$), satisfying the conditions of semiconductor electrical neutrality (6).

We note that at $W_n \to 0$, the distribution density of the probabilities of electrostatic fluctuations of c-band electron energies $\mathcal{P}(U_n) \to \delta(U_n)$, where $\delta(U_n)$ is the Dirac δ-function, and formula (6) transforms into (3).

From formula (6), we determine the concentration of mobile c-band electrons $n_{\rm mob}$ with energies $E_n = E_{\rm kin} + U_n$ higher than the energy $E_{\rm mob}^{(c)}$ necessary for their migration within the entire three-dimensional crystalline re-semiconductor,

$$n_{\rm mob} = \frac{(2m_{nd})^{3/2}}{2\pi^2\hbar^3}\int_{E_{\rm mob}^{(c)}}^{\infty} f_n \int_{-\infty}^{E_n}\sqrt{E_n - U_n}\,\mathcal{P}(U_n)\,dU_n dE_n = n^{\rm (re)} - n_{\rm loc}, \qquad (10)$$

where $n_{\rm loc}$ is the concentration of electrons which can move only in limited sample regions.

The quantity $E_{\rm mob}^{(c)} < 0$ entering expression (10) is the migration edge (or "percolation threshold") of c-band electrons [17, 26]; $E_{\rm mob}^{(c)}$ is also denoted by $E_{\rm per}^{(c)}$, i.e., as the electron-liquid percolation energy. According to [23, 27, 28], we suppose that the critical fraction of the three-dimensional semiconductor sample, inaccessible for c-band electron migration through the whole sample and corresponding to the electron percolation energy ($E_n \leq E_{\rm mob}^{(c)}$), is 0.17. Then, if Eq. (7) is taken into account, we have

$$\int_{-\infty}^{E_{\rm mob}^{(c)}}\mathcal{P}(U_n)dU_n = \frac{1}{\sqrt{2\pi}W_n}\int_{-\infty}^{E_{\rm mob}^{(c)}}\exp\left(-\frac{U_n^2}{2W_n^2}\right)dU_n = 0.17,$$

from which we obtain

$$E_{\rm mob}^{(c)} \approx -0.955W_n < 0, \qquad (11)$$

where W_n is given by formula (8) if (9) is taken into account.

3. CALCULATION OF THE CONDUCTIVITY AND DRIFT MOBILITY IN THE CASE OF ELASTIC ELECTRON SCATTERING AT IMPURITY IONS IN REAL SEMICONDUCTORS

According to [16, 22, 29, 30], the static (dc) conductivity of an ideally (id) doped n-type semiconductor, taking into account formula (3), is given by

$$\sigma_n^{(\mathrm{id})} = \frac{2e^2}{2m_{n\sigma}Vk_\mathrm{B}T} \times \int\limits_{E_c=0}^{\infty} \tau_n^{(\mathrm{id})}(\varepsilon_\mathrm{kin}) g_n^{(\mathrm{id})}(\varepsilon_\mathrm{kin}) f_n(1-f_n)\varepsilon_\mathrm{kin} d\varepsilon_\mathrm{kin} \equiv en^{(\mathrm{id})}\mu_n^{(\mathrm{id})}, \tag{12}$$

where $m_{n\sigma}$ is the effective mass of a conduction electron, $\tau_n^{(\mathrm{id})}(\varepsilon_\mathrm{kin})$ is the relaxation time of the electron quasimomentum (with the kinetic energy ε_kin), and $\mu_n^{(\mathrm{id})}$ is the drift mobility;

$$f_n(1-f_n) = \{4\cosh^2[(\varepsilon_\mathrm{kin} - \varepsilon_\mathrm{F}^{(c)})/2k_\mathrm{B}T]\}^{-1}.$$

Based on formula (12), let us determine the re-semiconductor conductivity $\sigma_n^{(\mathrm{re})} = \sigma_n$. To this end, we replace the electron density of states in Eq. (12) $g_n^{(\mathrm{id})}(\varepsilon_\mathrm{kin})$ from (3) by $g_n^{(\mathrm{re})}(E_n)$ from (5), the bottom of the c band $E_c = 0$ by $E_\mathrm{mob}^{(c)} < 0$, and the relaxation time $\tau_n^{(\mathrm{id})}(\varepsilon_\mathrm{kin})$ by $\tau_\mathrm{ion}^{(\mathrm{re})}(E_n - U_n) = \tau_\mathrm{ion}^{(\mathrm{re})}(E_\mathrm{kin})$. As a result, the static conductivity of the really (re) doped n-type semiconductor, taking into account Eqs. (5)–(11), can be written as

$$\sigma_n = \sigma_n^{(\mathrm{re})} = \frac{e^2}{m_{n\sigma}} \frac{(2m_{nd})^{3/2}}{3\pi^2\hbar^3} \int\limits_{E_\mathrm{mob}^{(c)}}^{\infty} \frac{f_n(1-f_n)}{k_\mathrm{B}T} \times \int\limits_{-\infty}^{E_n} \tau_\mathrm{ion}^{(\mathrm{re})}(E_n - U_n)(E_n - U_n)^{3/2}\mathcal{P}(U_n)\,dU_n dE_n, \tag{13}$$

where $f_n(1 - f_n) = \{4\cosh^2[(E_n - E_\mathrm{F}^{(c)})/2k_\mathrm{B}T]\}^{-1}$.

The relaxation time (entering Eq. (13)) of the electron quasimomentum with the kinetic energy $E_\mathrm{kin} = E_n - U_n > 0$ (at $E_n > E_\mathrm{mob}^{(c)}$) during elastic scattering at hydrogenlike impurity ions in the crystalline matrix with the permittivity $\varepsilon = \varepsilon_r\varepsilon_0$, according to [18, 19], is given by

$$\tau_\mathrm{ion}^{(\mathrm{re})}(E_n - U_n) = \left(\frac{4\pi}{3}\right)^{1/3}\left(\frac{4\pi\varepsilon}{e^2}\right)^2 \frac{\hbar(E_n - U_n)}{N_\mathrm{ion}^{2/3}} \times \ln^{-1}\left[1 + \left(\frac{8\pi\varepsilon R_\mathrm{ion}(E_n - U_n)}{e^2}\right)^2\right], \tag{14}$$

where $N_\mathrm{ion} = (1 + K)N$, the value of R_ion is determined from formula (2). We note that only the Coulomb interaction of the electron with an ion placed at the center of a sphere of volume $1/N_\mathrm{ion}$ was taken into account in deriving formula (14). It was considered that the local static permittivity ε_r in the vicinity of each impurity ion is controlled by v-band electrons.

The drift mobility of c-band electrons, limited by their elastic scattering at impurity ions, is defined in n-type re-semiconductors by analogy with Eq. (12) as

$$\mu_n = \mu_\mathrm{ion}^{(\mathrm{re})} = \frac{\sigma_n^{(\mathrm{re})}}{en_\mathrm{mob}} = \frac{\sigma_n}{en_\mathrm{mob}}, \tag{15}$$

where $\sigma_n = \sigma_n^{(\mathrm{re})}$ is determined by Eq. (13) taking into account (14), and n_mob is determined by Eq. (10).

Let us compare formulas (13) and (15) for re-semiconductor with a degenerate electron gas in the c band. On the one hand, according to formula (13), electrons whose energy E_n exceeds the mobility threshold $E_\mathrm{mob}^{(c)}$ are involved in the dc conductivity of the re-semiconductor. In this case, only c-band electrons whose total energy E_n is close to the Fermi level $E_\mathrm{F}^{(c)}$ are efficiently involved in scattering events at impurity ions. (This is formally caused by the fact that the function $f_n(1 - f_n)$ under the integral sign in Eq. (13) has a sharp maximum at $E_n = E_\mathrm{F}^{(c)}$). On the other hand, in writing formula (15), it is supposed that the value of $\sigma_n = en_\mathrm{mob}\mu_n$ is controlled by all mobile electrons with the concentration n_mob, but as though they all have identical mobilities μ_n (and drift velocities). Thus, in writing formulas (13) and (15), it was supposed that the static conductivity of the re-semiconductor with a degenerate electron gas in the c band is equal to the product of the elementary charge, the concentration of all mobile electrons, and the drift mobility of electrons with a total energy in the vicinity of the Fermi level. This is consistent with the conventional theory of semiconductor conductivity [16, 22, 30, 31], but is inconsistent with the concepts developed in [32].

We note that, disregarding electrostatic fluctuations of the electron potential energy ($W_n \ll k_\mathrm{B}T$), i.e., setting $\mathcal{P}(U_n) \to \delta(U_n)$ and $|E_\mathrm{mob}^{(c)}| \ll k_\mathrm{B}T$, according to (10), we have $n_\mathrm{loc} \to 0$ and $n_\mathrm{mob} \approx n^{(\mathrm{re})} \approx n^{(\mathrm{id})}$. In this case, formulas (13) and (15) transform to standard formulas (12) and $\mu_n^{(\mathrm{id})} = \mu_\mathrm{ion}^{(\mathrm{id})} = \sigma_n^{(\mathrm{id})}/en^{(\mathrm{id})}$ for the id-semiconductor [16, 22, 30, 31].

Let us describe the calculation algorithm in accordance with formulas (6)–(15) by the example of an n-type semiconductor (see also [25, 26]).

(i) The initial parameters of the n-type semiconductor are set: ε_r, m_{nd}, $m_{n\sigma}$, temperature T, the variation range of the hydrogenlike donor concentration N, the degree of compensation of donors by hydrogenlike acceptors K, and the relative calculation error $\varepsilon_{\text{goal}} = 10^{-5}$.

(ii) Using formulas (8) and (9), where $N_{\text{ch}} = 2N$, the root-mean-square fluctuations of the electrostatic potential energy of electrons and ions W_n and W_d are calculated.

(iii) The nonlinear equation of electrical neutrality (6) is solved by numerical methods with respect to the unknown Fermi level $E_{\text{F}}^{(c)}$ taking into account the obtained values of W_n and W_d.

(iv) Using formula (11), based on the obtained W_n, $E_{\text{mob}}^{(c)}$ is calculated. Then, using formula (10), n_{mob} is calculated.

(v) Using Eq. (13), taking into account (14) and (2), the conductivity $\sigma_n = \sigma_n^{(\text{re})}$ is calculated.

(vi) Finally, using Eq. (15), the mobility $\mu_n = \mu_{\text{ion}}^{(\text{re})}$ is calculated.

4. CONWELL–WEISSKOPF (CW) MODEL FOR THE ELECTRON DRIFT MOBILITY IN IDEAL SEMICONDUCTORS

For comparison with formulas (13) and (15), we present here the necessary formulas of the CW model for an ideal degenerate electron gas of the id-semiconductor c band (see also formulas (3) and (12)). According to this model, the relaxation time of the c-band electron quasimomentum with the kinetic energy ε_{kin} upon elastic scattering at hydrogenlike impurity ions (see, e.g., [33–35]) is given by

$$\tau_n^{(\text{id})}(\varepsilon_{\text{kin}}) = \tau_{\text{CW}}(\varepsilon_{\text{kin}}) = \left(\frac{4\pi\varepsilon}{e^2}\right)^2 \frac{(2m_{nd}^{(1)})^{1/2}\varepsilon_{\text{kin}}^{3/2}}{\pi N_{\text{ion}}} \times \ln^{-1}\left[1 + \left(\frac{4\pi\varepsilon\varepsilon_{\text{kin}}}{e^2 N_{\text{ion}}^{1/3}}\right)^2\right], \tag{16}$$

where ε_{kin} is the electron kinetic energy ($\varepsilon_{\text{kin}} = E_n$ at $W_n = E_{\text{mob}}^{(c)} = 0$; see also Fig. 1), $N_{\text{ion}} = (1 + K)N$ is the impurity-ion concentration. (We note that the interaction time of an electron with one impurity ion was formally taken as infinitely large in writing formula (16).)

According to [30, 34, 36], the electron drift mobility in the CW model is determined from the formula (12) as

$$\mu_{\text{CW}} = \mu_{\text{ion}}^{(\text{id})} = \frac{\sigma_n^{(\text{id})}}{en^{(\text{id})}} = \frac{e\langle\tau_{\text{CW}}\rangle}{m_{n\sigma}}, \tag{17}$$

where the average relaxation time of the c-band electron quasimomentum (at $W_n = E_{\text{mob}}^{(c)} = 0$, Fig. 1) is given by

$$\langle\tau_{\text{CW}}\rangle = \int\limits_{E_c=0}^{\infty} \tau_{\text{CW}}(\varepsilon_{\text{kin}})\varepsilon_{\text{kin}}^{3/2} f_n(1 - f_n)\,d\varepsilon_{\text{kin}} \times \left[\int\limits_{E_c=0}^{\infty} \varepsilon_{\text{kin}}^{3/2} f_n(1 - f_n)\,d\varepsilon_{\text{kin}}\right]^{-1}. \tag{18}$$

The conductivity σ_{CW} is given by formula (12) at $\tau_n^{(\text{id})}(\varepsilon_{\text{kin}}) = \tau_{\text{CW}}(\varepsilon_{\text{kin}})$ and is related to the electron drift mobility μ_{CW} by the standard expression [33, 34, 36]

$$\sigma_{\text{CW}} = \sigma_n^{(\text{id})} = en^{(\text{id})}\mu_{\text{CW}}, \tag{19}$$

where $n^{(\text{id})} = (1 - K)N$ is the electron concentration in the id-semiconductor c band according to formula (3), which defines the Fermi level $\varepsilon_{\text{F}}^{(c)}$ in the formula (18).

We note that all formulas written in Sections 3 and 4 are also valid for a p-type semiconductor containing hydrogenlike acceptor and donor ions if the effective mass of the density of states in them m_{nd} is replaced with m_{pd}, the effective mass of the conductivity $m_{n\sigma}$ is replaced with $m_{p\sigma}$, and the average c-band electron concentration n is replaced the average v-band hole concentration p.

5. COMPARISON OF THE CALCUATED RESULTS WITH EXPERIMENTAL DATA

For comparison the dc conductivity σ_n and drift mobility μ_n calculations with experimental data, heavily doped n-type germanium, silicon, gallium arsenide, and indium antimonide crystals were chosen. The electron concentration for these semiconductors $n = n^{(\text{id})} = (1 - K)N$ according to Eq. (3) satisfied inequality (4), and the donor concentration N was higher than the Mott concentration N_{M} determined from relation (1). We note that numerical calculation according to Eq. (10) yields for degenerate n-type crystals the ratio $n_{\text{loc}}/n^{(\text{re})} < 0.2$ (for Si, Ge), $n_{\text{loc}}/n^{(\text{re})} < 0.02$ (for GaAs, InSb) at $n^{(\text{re})} > n_{\text{M}}$, where the Mott electron concentration is $n_{\text{M}} = (1 - K)N_{\text{M}}$.

This circumstance allows the conclusion that the concentration $n_{\text{mob}} = n^{(\text{re})} - n_{\text{loc}}$ of free (within the entire crystalline sample) c-band electrons is almost equal to their average concentration in the sample. This conclusion is consistent with analytical estimates [37, 38] identifying the dc-measured Hall concentration of majority carriers in a strong magnetic field with their average concentration in three-dimensional partially disordered crystalline semiconductors. Electrons of c band with the concentration n_{loc} are not directly involved in the dc conductivity and Hall effect, but contribute to the macroscopic static permittivity of the semiconductor.

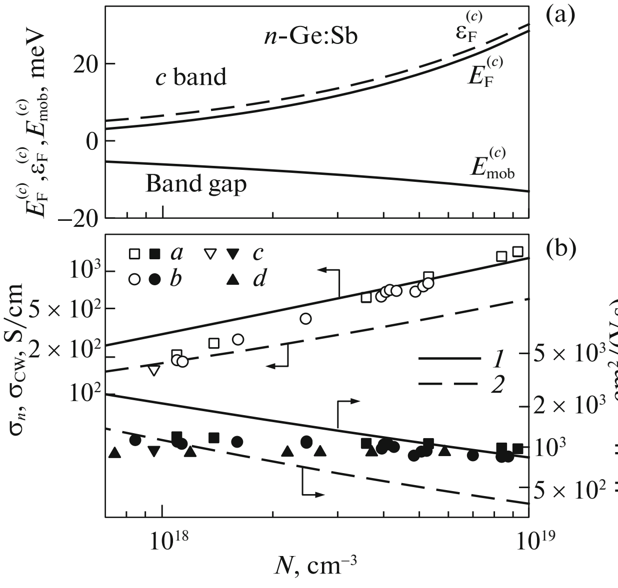

Fig. 2. (a) Calculated dependences of the Fermi level $E_F^{(c)}$ and the electron migration threshold $E_{mob}^{(c)}$ (according to formulas (6) and (11)) on the antimony-atom concentration (as hydrogenlike donors) N in n-Ge:Sb crystals at the degree of compensation $K = 0.01$, temperature $T = 3$ K, and c-band electron concentration $n = (1 - K)N$. The dashed curve is the $\varepsilon_F^{(c)}$ calculation by formula (3) for an ideal Fermi gas. (b) Dependences of the static conductivity σ_n and the electron Hall mobility μ_n on the antimony-atom concentration. The measurement temperatures T are (a) 4.2 [40], (b) 1.3 [9, 10], (c) 2.5 [41], (d) 4.2 K [42]. Lines are the calculations for $K = 0.01$, $T = 3$ K, and $n = (1 - K)N$: (*1*) σ_n according to Eq. (13), the drift mobility μ_n according to Eq. (15); (*2*) σ_{CW} according to Eq. (19) and μ_{CW} according to Eq. (17).

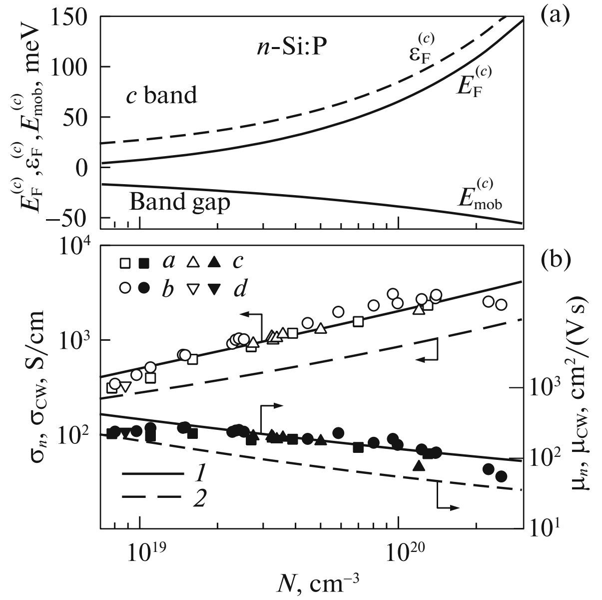

Fig. 3. (a) Calculated dependences of the Fermi level $E_F^{(c)}$ and the electron migration threshold $E_{mob}^{(c)}$ (according to formulas (6) and (11)) on the phosphorus-atom concentration (as hydrogenlike donors) N in n-Si:P crystals at the degree of compensation $K = 0.01$, temperature $T = 3$ K, and c-band electron concentration $n = (1 - K)N$. The dashed curve is the $\varepsilon_F^{(c)}$ calculation by formula (3) for an ideal Fermi gas. (b) Dependences of the static conductivity σ_n and the electron Hall mobility on the phosphorus-atom concentration. The measurement temperatures T are (a) 4.2 [11], (b) 4.2 [12], (c) 78 [12], (d) 4.2K [45]. Lines are the calculations for $K = 0.01$, $T = 3$ K, and $n = (1 - K)N$: (*1*) σ_n according to Eq. (13), the drift mobility μ_n according to Eq. (15); (*2*) σ_{CW} according to Eq. (19) and μ_{CW} according to Eq. (17).

Figures 2–5 show the experimental and calculated dependences of the dc conductivity, the Hall (experiment) and drift (calculation by the proposed algorithm) mobilities of c-band electrons, as well as the Fermi level and migration threshold $E_{mob}^{(c)}$ on the dopant N and electron $n = (1 - K)N$ concentrations. Weakly compensated ($K \ll 1$) n-Ge (Fig. 2) and n-Si (Fig. 3) crystals were considered, as well as moderately compensated ($K \approx 0.1$) n-GaAs and n-InSb crystals at cryogenic temperatures (Figs. 4 and 5). The solid curves in Figs. 2–5 were calculated by formulas (6), (10), (13), and (15) according to the quasi-classical model of equilibrium states and electron scattering, developed in this study; dashed curves are μ_{CW} and σ_{CW} calculations by formulas (19) and (17) according to the CW model [33, 39]. The points correspond to the experimental data for n-Ge:Sb from [9, 10, 40–42] (see also [39, 43, 44]) for n-Si:P [11, 12, 45] (see also [39, 43, 46]), for n-GaAs:Sn [47, 48], n-GaAs:Te [49, 50], and n-GaAs [51], as well as for n-InSb:Se [52], n-InSb:Sn [53, 54], and n-InSb:Te [55].

Here we note that the electron Hall mobility in extremely pure crystals of Ge, Si, GaAs, and InSb at a temperature of $T \approx 78$ K, when scattering at phonons dominates (the mobility μ_{lat}) according to [56, 57] is $\mu_{lat} \approx 4 \times 10^4$ cm^2/(V s) for n-Ge, $\mu_{lat} \approx 2 \times 10^4$ cm^2/(V s) for n-Si, $\mu_{lat} \approx 2 \times 10^5$ cm^2/(V s) for n-GaAs, and $\mu_{lat} \approx 10^6$ cm^2/(V s) for n-InSb. Due to the fact that $\mu_{lat} \gg \mu_n$ (see Figs. 2b, 3b, 4b, and 5b), scattering at phonons at cryogenic temperatures was disregarded.

In calculating the conductivity and drift mobility of electrons in germanium and silicon, the following physical quantities [56, 57] were used: for n-Ge (the number of valleys in the c band $\nu = 4$): $\varepsilon_r = 15.4$, $m_{nd} = 0.554m_0$, $m_{n\sigma} = 0.119m_0$; for n-Si ($\nu = 6$): $\varepsilon_r = 11.47$, $m_{nd} = 1.062m_0$, $m_{n\sigma} = 0.259m_0$, where m_0 is the electron mass in free space. (The dependence of the electron effective mass on the electron concentration for

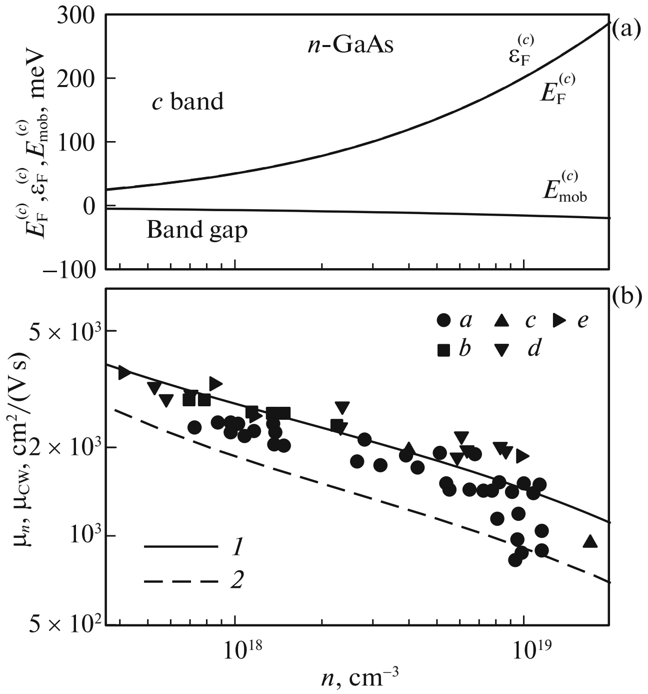

Fig. 4. (a) Calculated dependences of the Fermi level $E_F^{(c)}$ and the electron migration threshold $E_{mob}^{(c)}$ in *n*-GaAs crystals according to formulas (6) and (11) on the electron concentration $n = (1 - K)N$ for the degree of compensation $K = 0.1$, temperature $T = 78$ K, and hydrogenlike donor concentration *N*. The dashed curve is the $\varepsilon_F^{(c)}$ calculation by formula (3) for an ideal Fermi gas if the dependence $m_{nd} = m_{n\sigma}$ on *n* according to Eq. (20) is taken into account. (b) Dependence of the electron Hall mobility μ_n on the electron concentration in *n*-GaAs at temperature $T = 78$ K. The measurement data: (a) *n*-GaAs:Sn [47], (b) *n*-GaAs:Sn [48], (c) *n*-GaAs:Te [49]; (d) *n*-GaAs:Te [50]; (e) *n*-GaAs [51]. Curves are calculations for $K = 0.1$, $T = 78$ K, and $n = (1 - K)N$ according to Eq. (20) of (*1*) the drift mobility μ_n according to Eq. (15) and (*2*) μ_{CW} according to Eq. (17).

n-Ge (to 3×10^{19} cm^{-3}) and *n*-Si (to 3×10^{20} cm^{-3}) can be neglected [56, 57].)

For heavily doped degenerate *n*-GaAs crystals ($\nu = 1$; $\varepsilon_r = 12.4$) and *n*-InSb ($\nu = 1$; $\varepsilon_r = 16.8$), the dependence of the effective masses $m_{nd} = m_{n\sigma}$ of electrons on their concentration in the *c* band [56, 57] should be considered:

$$n\text{-GaAs: } m_{nd}(n) = m_{nd}[1 + 6.4 \times 10^{-4}(n/n^*)^{0.645}], \quad (20)$$

where $m_{nd} = m_{n\sigma} = 0.067m_0$, $n^* = 1 \times 10^{15}$ cm^{-3};

$$n\text{-InSb: } m_{nd}(n) = m_{nd}[1 + 2.6 \times 10^{-2}(n/n^*)^{0.3}], \quad (21)$$

where $m_{nd} = m_{n\sigma} = 0.013m_0$, $n^* = 3.1 \times 10^{12}$ cm^{-3}.

We can see in Figs. 2b, 3b, 4b, and 5b that the calculations by formulas (13) and (15) are in general agreement with the experimental data for *n*-Ge:Sb, *n*-Si:P, *n*-GaAs, and *n*-InSb crystals.

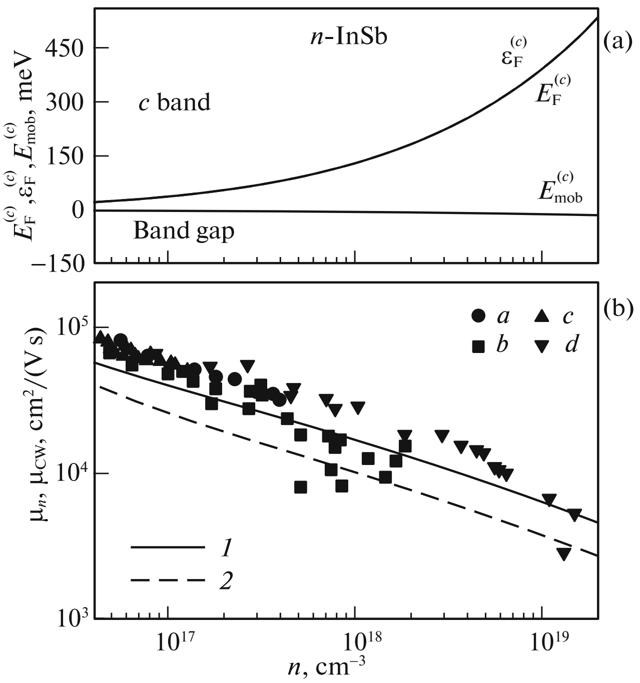

Fig. 5. (a) Calculated dependences of the Fermi level $E_F^{(c)}$ and the electron migration threshold $E_{mob}^{(c)}$ in *n*-InSb crystals according to formulas (6) and (11) on the electron concentration $n = (1 - K)N$ for the degree of compensation $K = 0.1$, temperatures $T = 78$ K, and hydrogenlike donor concentration *N*. The dashed curve is the $\varepsilon_F^{(c)}$ calculation by formula (3) for an ideal Fermi gas taking into account the dependences $m_{nd} = m_{n\sigma}$ on *n* according to Eq. (21). (b) Dependence of the Hall mobility μ_n of electrons on their concentration in *n*-InSb at the temperature $T = 78$ K. The measurement data: (a) *n*-InSb:Se [52], (b) *n*-InSb:Sn [53], (c) *n*-InSb:Sn [54], (d) *n*-InSb:Te [55]. Curve are calculations at $K = 0.1$, $T = 78$ K, and $n = (1 - K)N$ taking into account Eq. (21): (*1*) the drift mobility μ_n according to Eq. (15), (*2*) μ_{CW} according to Eq. (17).

For weakly compensated *n*-Ge:Sb crystals at the antimony concentration $N < 10^{18}$ cm^{-3}, a certain disagreement of the results calculated according to Eqs. (13) and (15) with experiments is observed. This is probably associated with elastic strains of the lattice in the vicinity of Sb atoms, which are smoothed at high concentrations of this dopant [58–60].

As for the electron mobility in *n*-GaAs (Fig. 4), we note that a decrease in μ_n at $n \approx 10^{19}$ cm^{-3} is probably caused by a small increase in the degree of compensation with increasing dopant concentration for both *n*-GaAs:Sb and *n*-GaAs:Te (see, e.g., [13, 61]).

As for the electron mobility in *n*-InSb (Fig. 5), we note that an electron can be scattered not at one (as in the relaxation-time calculation model proposed in this study), but simultaneously at two impurity ions in this semiconductor with a small effective electron mass

[62]. Therefore, the electron mobility will be slightly higher than for scattering at one center (ion).

We can see in Figs. 2a, 3a, 4a, and 5a that an increase in the concentration of major impurities (and electrons) shifts the Fermi level $E_{\mathrm{F}}^{(c)}$ (solid curve) for re-semiconductors deeper into the c band in comparison with the Fermi level $\varepsilon_{\mathrm{F}}^{(c)}$ (dashed curve) for id-semiconductors. Other conditions being equal, the less the value of the effective electron mass m_{nd} the less the difference between $\varepsilon_{\mathrm{F}}^{(c)}$ and $E_{\mathrm{F}}^{(c)}$.

6. DISCUSSION

In deriving both formulas (14) in [18] and (16) in [33], the interaction of an electron during its scattering at an impurity ion was considered to be the purely Coulomb one. In the Brooks–Herring electron–ion scattering model [16, 22, 31, 39, 63], the Coulomb potential of the interaction of a c-band electron with an impurity ion is replaced with the screened Coulomb potential (in the Debye–Hückel or Thomas–Fermi approximation for a non-degenerate and degenerate electron gas, respectively). However, according to [64, 65], the screened Coulomb potential (i.e., the total potential of ion and a cloud of charges screening it) cannot be interpreted as the pair interaction potential of electron and ion.

We note that, according to the data shown in Figs. 2b, 3b, 4b, and 5b, the drift mobility limitation by c-band electron scattering at impurity ions at cryogenic temperatures dominates over scattering at phonons. Therefore, let us also briefly discuss the electron–electron and resonant scattering of electrons at donor ions within the id-semiconductor model (see formulas (3), (4), and (12)).

To estimate the mobility limited by electron scattering at electrons in the degenerate id-semiconductor c band, we proceed from the formula for the average relaxation time τ_{ee} after [66] (see also [67]),

$$\frac{1}{\tau_{ee}} = \frac{\pi}{8}\frac{(k_{\mathrm{B}}T)^2}{\hbar\varepsilon_{\mathrm{F}}^{(c)}} + \frac{\sqrt{3}}{2\hbar\sqrt{\varepsilon_{\mathrm{F}}^{(c)}}}\left(\frac{k_{\mathrm{B}}T}{k_{\mathrm{F}}l_{ee}}\right)^{3/2}, \tag{22}$$

where $l_{ee} = v_{\mathrm{F}}\tau_{\mathrm{CW}}(\varepsilon_{\mathrm{kin}})$ is the mean free path of an electron with the kinetic energy $\varepsilon_{\mathrm{kin}} \approx \varepsilon_{\mathrm{F}}^{(c)} \pm k_{\mathrm{B}}T$ and the Fermi velocity $v_{\mathrm{F}} \approx [2\varepsilon_{\mathrm{F}}^{(c)}/m_{nd}^{(1)}]^{1/2}$ for scattering at electron; $k_{\mathrm{F}} \approx [2\pi^2 n^{(\mathrm{id})}]^{1/3}$ is the wave vector of an electron with the kinetic energy $\varepsilon_{\mathrm{F}}^{(c)} \approx \zeta_{\mathrm{F}}^{(c)}$ according to formula (4). Then the electron mobility limited by electron–electron scattering is written as $\mu_{ee} = e\tau_{ee}/m_{n\sigma}$, where τ_{ee} is given by formula (22).

Let us estimate the minimum average relaxation time τ_{res} of the c-band electron quasi-momentum in the case of resonance scattering at donor ions in a degenerate id-semiconductor (see, e.g., [68, 69]). Conventionally considering that donor energy levels are uniformly distributed in the c band in the vicinity of $\varepsilon_{\mathrm{F}}^{(c)}$, we can estimate $1/\tau_{\mathrm{res}}$ as

$$1/\tau_{\mathrm{res}} \approx \frac{k_{\mathrm{B}}T}{\varepsilon_{\mathrm{F}}^{(c)}} N_{\mathrm{res}} v_{\mathrm{F}} \sigma_{\mathrm{res}}, \tag{23}$$

where $k_{\mathrm{B}}T/\varepsilon_{\mathrm{F}}^{(c)}$ is the fraction of resonantly scattered electrons with the kinetic energy $\varepsilon_{\mathrm{kin}} \approx \varepsilon_{\mathrm{F}}^{(c)} \pm k_{\mathrm{B}}T$ and velocity v_{F}; $N_{\mathrm{res}} \approx (k_{\mathrm{B}}T/\varepsilon_{\mathrm{F}}^{(c)})N$ is the fraction of donors in the (+1) charge state, resonantly scattering electrons; $\sigma_{\mathrm{res}} \approx \pi R_{\mathrm{ion}}^2$ is the resonant scattering cross section of an electron at a donor (estimate by the solid sphere model [70]); $R_{\mathrm{ion}} \approx 0.62\,[(1 + K)N]^{-1/3}$. Then the drift mobility of electrons, limited by resonant scattering is given by $\mu_{\mathrm{res}} = e\tau_{\mathrm{res}}/m_{n\sigma}$, where τ_{res} is given by formula (23).

The total electron drift mobility $\mu_n^{(\mathrm{id})}$ is determined by Matthiessen's rule (see, e.g., [16, 22, 30])

$$1/\mu_n^{(\mathrm{id})} = 1/\mu_{\mathrm{ion}}^{(\mathrm{id})} + 1/\mu_{ee} + 1/\mu_{\mathrm{res}} \approx 1/\mu_{\mathrm{ion}}^{(\mathrm{id})},$$

where the contribution of μ_{ee} and μ_{res} according to Eqs. (22) and (23) to the total mobility $\mu_n^{(\mathrm{id})}$ is no more than 3% of the contribution $\mu_{\mathrm{ion}}^{(\mathrm{id})} = \mu_{\mathrm{CW}}$ according to Eq. (17).

7. CONCLUSIONS

The quasi-classical model of the elastic scattering of majority carriers (c-band electrons) at immobile ions of hydrogenlike impurities in heavily doped degenerate n-type semiconductors. It was thought that a single event of elastic Coulomb electron scattering at an ion in the crystalline matrix occurs during its transit time through the spherical region (radius of $R_{\mathrm{ion}} \approx 0.62[(1 + K)N]^{-1/3}$) whose center contains one impurity ion at their total concentration $(1 + K)N$, where N is the donor concentration and KN is the concentration of acceptors compensating donors. Electrostatic fluctuations of the potential energy of c-band electrons and the shift of their migration threshold to the band-gap depth were taken into account. Based on the algorithm proposed in this study, the static (dc) conductivity and the electron drift mobility upon elastic scattering at impurity ions were calculated at low (cryogenic) temperatures. It was shown that the contribution of mobile electron scattering at phonons and electrons, as well as resonant electron scattering at donor ions to total electron scattering in degenerate n-type semiconductors at low temperatures is not determining.

The results of calculations by the formulas obtained in the quasi-classical approximation without using fitting parameters are in numerical agreement with the known experimental data for n-type germanium, silicon, gallium-arsenide, and indium-antimonide crystals at rather high donor concentrations for low and moderate degrees of their compensation. In general, the conductivities and electron drift mobilities calculated by the model developed in this study are higher than those obtained within the Conwell–Weisskopf model.

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