

Transition temperature from band to hopping direct current conduction in crystalline semiconductors with hydrogen-like impurities: Heat versus Coulomb attraction

N. A. Poklonski,^{1,a)} S. A. Vyrko,¹ O. N. Poklonskaya,¹ and A. G. Zabrodskii²

¹Belarusian State University, pr. Nezavisimosti 4, Minsk 220030, Belarus

²Ioffe Physicotechnical Institute RAS, Politekhnikeskaya ul. 26, St. Petersburg 194021, Russia

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For nondegenerate bulk semiconductors, we have used the virial theorem to derive an expression for the temperature T_j of the transition from the regime of “free” motion of electrons in the c -band (or holes in the v -band) to their hopping motion between donors (or acceptors). Distribution of impurities over the crystal was assumed to be of the Poisson type, while distribution of their energy levels was assumed to be of the Gaussian type. Our conception of the virial theorem implementation is that the transition from the band-like conduction to hopping conduction occurs when the average kinetic energy of an electron in the c -band (hole in the v -band) is equal to the half of the absolute value of the average energy of the Coulomb interaction of an electron (hole) with the nearest neighbor ionized donor (acceptor). Calculations of T_j according to our model agree with experimental data for crystals of Ge, Si, diamond, etc. up to the concentrations of a hydrogen-like impurity, at which the phase insulator-metal transition (Mott transition) occurs. Under the temperature $T_h \approx T_j/3$, when the nearest neighbor hopping conduction via impurity atoms dominates, we obtained expressions for the electrostatic field screening length Λ_h in the Debye-Hückel approximation, taking into account a nonzero width of the impurity energy band. It is shown that the measurements of quasistatic capacitance of the semiconductor in a metal-insulator-semiconductor structure in the regime of the flat bands at the temperature T_h allow to determine the concentration of doping impurity or its compensation ratio by knowing Λ_h . © 2011 American Institute of Physics. [doi:10.1063/1.3667287]

I. INTRODUCTION

In order to form highly sensitive photodetectors (from infrared to terahertz wavelengths) based on crystalline semiconductors, the hopping conduction via hydrogen-like impurities should be inhibited (see, e.g., Refs. 1 and 2). It is necessary to block (minimize the value of) hopping conduction by epitaxially growing the layer of semiconductor with a low content of impurities at the surface of the heavily doped semiconductor; this technique provides the energetic barrier for electron (hole) transport over the impurity band states. For this purpose, it is useful to know the characteristic temperature T_j (see Fig. 1), when the band-like electrical conduction (of electrons in the c -band or holes in the v -band) is superseded by the hopping conduction via impurities. Our work aims to present a quasiclassical model of the temperature T_j dependence on the concentration of hydrogen-like impurities in crystalline semiconductors.

In homogeneous-doped and nondegenerate semiconductors, drift and diffusion of electrons and/or holes are commonly described in the terms of their transitions between single-electron states (see, e.g., Refs. 3–8). The direct current electrical conduction is tentatively subdivided into three regimes (mechanisms) (see Fig. 1): the *propagating (or band) conduction* (BC), the *hopping conduction* (HC), and the hybrid regime (BC + HC), which is sometimes called the *jumping conduction*.⁴ It should be noted that, at the characteristic temperature

T_j , the electrical conductivity $\sigma_p = 1/\rho_p$ with thermal activation energy ε_1 in the BC regime is equal to the electrical conductivity $\sigma_h = 1/\rho_h$ with thermal activation energy ε_3 in the nearest neighbor hopping (NNH) regime of the dc conduction. Here, resistivity in the BC regime is $\rho_p = \rho_1 \exp(\varepsilon_1/k_B T)$ and resistivity in the NNH regime is $\rho_h = \rho_3 \exp(\varepsilon_3/k_B T)$, where $k_B T$ is the thermal energy and ρ_1 , ε_1 , ρ_3 , and ε_3 are the parameters which weakly depend on temperature T . Some partial expressions for T_j obtained by fitting experimental data for germanium crystals of p -type are reported in Refs. 9 and 10. However, for applications, it is necessary to have an analytical dependence of T_j on concentration N of the majority (doping) impurity and the ratio $0 < K < 1$ of its compensation by the minority impurity with the concentration KN .

The BC regime is realized in crystalline semiconductors at temperatures $T > T_j$. Here, the states of electrons in the c -band and the states of holes in the v -band are characterized by eigenvalues of a quasimomentum operator and average values of lifetime in delocalized states of the c - or v -bands, which are determined by phonons and atomic defects of a lattice (as well as by a capture of electrons and holes on traps and an electron-hole recombination). In the BC regime, electrons and holes are “free” to move by tunneling in the crystalline matrix between successive acts of scattering on structure defects and phonons. In the HC regime, an ordinary mobile electron (or hole) is localized near a single impurity atom the majority of the time. Electrons (or holes) can migrate between immovable impurities only due to phonons (or other quasiparticles); thus, the conductivity is exponentially decreased under the temperature

^{a)}Electronic mail: poklonski@bsu.by.

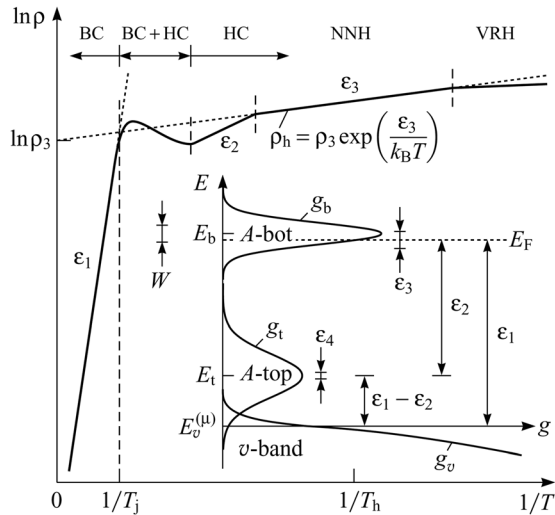


FIG. 1. Schematic inverse temperature ($1/T$) dependence of the logarithm of the electrical resistance ($\ln \rho$) of p -type crystalline semiconductor in different regimes of hole transport: BC is the band conduction, BC + HC is the mixture of the band and hopping conduction, HC is the hopping conduction, NNH is the hopping conduction $\sigma_h = 1/\rho_h$ via the nearest neighbor acceptors, and VRH is the hopping conduction via nearest acceptors by energy. In the inset: g_v is the density of states near the top of the valence band (E is the single-electron energy, $E_v^{(\mu)}$ is the mobility edge of holes in the v -band), g_b and g_t are the density of states of the A -bot and the A -top bands (centered on E_b and E_t) of a hydrogen-like acceptor impurity, which can be in three charge states ($-1, 0, +1$) (see also Ref. 3). (In compensated semiconductors ($K > 0.1$) the A -top band is not pronounced and acceptors can be only in the charge states (0) and (-1) of the A -bot band. D -bot and D -top bands of hydrogen-like donors are below the mobility edge of electrons in the c -band and are not shown.)

decrease. In the BC + HC regime,⁴ electrons (or holes) are almost delocalized, but the phase coherence is destroyed for their thermally activated tunneling motion from atom to atom (it can be an atom of a crystalline matrix as well as an impurity atom). It should be noted that, in the band scheme (see the inset in Fig. 1), the BC + HC regime corresponds to merged-into-each-other conduction mechanisms: the thermally activated tunneling of holes in the A -top band (activation energy ϵ_4) and hole transitions from the A -top band to the v -band (activation energy $\epsilon_1 - \epsilon_2$). On the one hand, in contrast to the BC regime, alternating paths of hole tunneling have accidental phases and do not interfere with each other. On the other hand, in contrast to the HC regime with thermal activation energies ϵ_2 and ϵ_3 (in the temperature range close to $T_h \approx T_j/3$), thermally activated tunneling in the BC + HC regime slightly depends on temperature comparing to the hopping conduction (activation energy $\epsilon_4 < \epsilon_3 < \epsilon_2$). [Note that the temperature $T_h \approx T_j/3$ was chosen as an average value from analysis of dependences $\ln(\rho)$ on $1/T$ in the NNH temperature range of whole experimental data from Refs. 9, 11–31.] The activation energy ϵ_1 corresponds to the transition of a typical acceptor from the charge state (0) to the charge state (-1) and appearance of a hole in the v -band. The activation energy ϵ_2 corresponds to the transition of two electrically neutral acceptors into negative- and positive-charged ions; this transition is contributed to the ϵ_2 -conduction. The activation energy $\epsilon_1 - \epsilon_2 < \epsilon_2$ corresponds to the transition of a typical acceptor from the charge state ($+1$) to the charge state (0) and appearance of a hole in the v -band. As a rule, in

the BC + HC regime, it is quite difficult to measure thermal activation energies ϵ_4 and $\epsilon_1 - \epsilon_2$, which are not pronounced in the galvanomagnetic measurements and require the low-temperature photoconduction measurements.³²

For a p -type semiconductor at very low temperatures (less than $T_h/2$), conduction is realized by hops of holes (electron vacancies) between acceptors which are not necessarily neighbored to each other, but which have a minimal difference in their energy levels. [We estimate that the variable range hopping (VRH) regime starts dominating over the NNH regime at a temperature less than $T_h/2$, which was chosen as an average value from analysis of dependences $\ln(\rho_h)$ on $1/T$ (see Fig. 1) of experimental data from Refs. 9, 11–31. In the temperature range $T < T_h/2$, the hopping activation energy ϵ_3 behaves as $\epsilon_3 \propto T^{3/4}$ (Mott model)³³ or $\epsilon_3 \propto T^{1/2}$ (Efros-Shklovskii model).³⁴] This regime is usually called variable range hopping (VRH). When the temperature increases, this mechanism of conduction is superseded by hops of holes between the nearest neighbor acceptors (NNH) with activation energy ϵ_3 , which is equal within an order of magnitude to the root-mean-square fluctuation W of their energy levels (the width of the acceptor A -bot band). [In Ref. 35, a relation of proportionality for boundary temperature between NNH and VRH regimes is obtained based on statistics of pair donors, between which an electron jump takes place, taking into account the D -bot and D -top donor bands in crystalline n -type semiconductors.] Further increase of temperature leads to the emission of the holes from the A -bot and A -top bands to the v -band; ϵ_2 -conduction takes place. In the temperature region intermediate between ϵ_2 -conduction and ϵ_1 -conduction, the BC + HC regime can be observed. For temperatures $T > T_j$, the emission of holes from the A -bot and A -top bands to the v -band occurs as well as the capture of holes from the v -band on the A -bot and A -top bands. These processes correspond to the band conduction (BC) with activation energy ϵ_1 , which is equal within an order of magnitude to the thermal ionization energy of the acceptor. According to the common experimental observations, the conduction with activation energy ϵ_2 rarely happens in crystalline semiconductors with hydrogen-like impurities for compensation ratios $K > 0.1$.³⁶ Note that ϵ_2 energy can be considered as a difference between energies of the ground and excited states of a neutral acceptor, e.g., a boron atom in the diamond crystalline matrix site.³⁷ In the BC + HC regime ($T < T_j$), the decrease of resistivity $\rho = 1/\sigma$ with decreasing in T is caused by capturing holes from the v -band on acceptors in the charge state (-1) and by the consequent decrease of scattering on ions for the holes left in the v -band. It is clear that, for all three regimes of hole transport (BC, BC + HC, and HC), the charge states (0) and (-1) of immobile acceptors can migrate over a crystal and all donors, which are in the charge state ($+1$), are also immobile. Charge state migration occurs due to the capture of holes from the v -band on acceptors and emission of holes from acceptors into the v -band and also due to hops of holes from acceptors in the charge state (0) to acceptors in the charge state (-1). Figure 1 shows (not in the scale) a typical picture in moderately doped and moderately compensated semiconductors, when only the BC and HC regimes are well approximated by straight lines in the dependence of $\ln \rho$ on $1/T$.

II. CALCULATIONS OF TRANSITION TEMPERATURE FROM THE BAND TO HOPPING CONDUCTION

Let us consider a nondegenerate semiconductor of p -type, in which only the A -bot acceptor band is pronounced. We have adopted that p is the concentration of holes in the v -band (valence band), $N = N_0 + N_{-1}$ is the total concentration of acceptors in the charge states (0) and (-1), and KN is the concentration of donors, which are all in the charge state (+1). Thus, an electroneutrality condition of semiconductor has the form: $p = N_{-1} - KN$. The band mechanism of the conduction is determined by the motion of gas of holes, and it is characterized by the average value of kinetic energy of a hole, which is equal to $3k_B T/2$, where k_B is the Boltzmann constant and T is the absolute temperature. Let us note that, at $T \approx T_j$ (Fig. 1), the concentration of holes in the v -band $p \ll K(1 - K)N$, so we yield $N_{-1} = N_{+1} = KN$, where N_{-1} and N_{+1} are concentrations of ionized acceptors and donors (see, e.g., Ref. 38). In accordance with models (Refs. 39 and 40), the effective concentration of holes hopping between acceptors is $N_h = N_0 N_{-1} / N$; thus, from the condition $\sigma_p = \sigma_h$, i.e., $ep\mu_p = eN_h M_h$, at temperature T_j , it follows that $p \ll N_h$ and the drift mobility of holes in the v -band μ_p is much larger than the drift hopping mobility of holes M_h via acceptors.

If particles in an equilibrium system interact obeying the Coulomb's law, then according to the virial theorem (see, e.g., Ref. 41 and 42),

$$E_{\text{kin}} = -\frac{1}{2}U_{\text{tot}}, \quad (1)$$

where E_{kin} is the average kinetic energy of all particles and U_{tot} is the average potential energy of the Coulomb interaction between all particles. In a first order approximation, the virial theorem can be applied separately to two subsystems (see, e.g., Ref. 42): i) holes and migrating over a crystal the charge states (-1) of immobile acceptors and ii) immobile donors in the charge state (+1), electrically neutral acceptors (bound states of holes and negatively charged acceptors), and bounded electrons and nuclei of the crystalline matrix. Further, for calculations of T_j , we apply the virial theorem to the first subsystem.

The virial theorem is applicable to the semiconductor at any temperature. At temperatures $T > T_j$, the v -band conduction dominates and holes freely move over the crystal. Then, the average kinetic energy of a typical hole in the v -band is equal to $3k_B T/2$; however, the average potential energy of the hole is not known. At temperatures $T < T_j$, the hopping conduction dominates and holes in the A -bot band are quasi-localized on acceptors. Then, the hole potential energy is equal to the Coulomb energy of interaction between a hole and the nearest acceptor, whereas the average kinetic energy of a typical hole moving by means of hops is not known. Thus, only at the edge between hopping and band conduction, we can assess both the average kinetic energy and the average potential energy of a hole in the field of the negatively charged acceptor. Since they are connected to each other according to the virial theorem, the temperature in the kinetic energy gives the temperature of equality between the hopping and band conduction. To this end, the transition

from the band conduction to the hopping conduction at $T = T_j$ is determined by equality of the average kinetic energy of motion of a free (delocalized) hole in the v -band $E_{\text{kin}} \rightarrow 3k_B T_j/2$ to the half of the average potential energy of a hole in the Coulomb field of the nearest ionized acceptor $U_{\text{tot}} \rightarrow U_j$, i.e., from Eq. (1), we yield

$$\frac{3k_B T_j}{2} = -\frac{U_j}{2}. \quad (2)$$

We take into account that all the other holes of the v -band, acceptors in the charge states (-1) and (0), and donors in the charge state (+1) by virtue of the electrical neutrality of a crystal form an electrically neutral background. It is clear that, at temperature T_j , due to low concentration of holes, the interhole interaction can be neglected as well as the possibility of capturing holes on acceptors in the charge state (0). These assumptions allow to approximately describe the many-particle closed system with the pair Coulomb interaction between charged particles as a set of two-particle systems containing a hole and the closest to it acceptor in the charge state (-1). Note that the proposed procedure of the virial theorem application in description of the interaction of charge carriers and impurity ions in nondegenerate semiconductor resembles a scheme of substantiation of the Boltzmann kinetic equation in Ref. 43.

In order to determine U_j , we assume that acceptors in the charge states (-1) and (0) and donors in the charge state (+1) are randomly distributed in a crystal, i.e., according to the Poisson distribution. Then, the probability that, at the distance r from hole in the interval $(r, r + dr)$, the nearest negatively charged acceptor occurs and there are no negatively charged acceptors in the volume $4\pi r^3/3$ is (see, e.g., Refs. 44 and 45)

$$\mathcal{P}(r)dr = 4\pi r^2 KN \exp\left(-\frac{4\pi}{3}r^3 KN\right)dr, \quad (3)$$

where KN is the concentration of ionized acceptors, i.e., acceptors in the charge state (-1).

The average Coulomb energy of the hole interaction with the nearest negatively charged acceptor, taking into account Eq. (3), is

$$\begin{aligned} U_j &= \int_0^\infty U(r)\mathcal{P}(r)dr = -\Gamma\left(\frac{2}{3}\right)\frac{e^2}{4\pi\epsilon_r\epsilon_0}\left(\frac{4\pi}{3}KN\right)^{1/3} \\ &\approx -1.354\frac{e^2}{4\pi\epsilon_r\epsilon_0}\left(\frac{4\pi}{3}KN\right)^{1/3}, \end{aligned} \quad (4)$$

where $U(r) = -e^2/(4\pi\epsilon_r\epsilon_0 r)$ is the potential energy of a v -band hole interacting by the Coulomb's law with the nearest neighbor acceptor in the charge state (-1), e is the elementary charge, ϵ_r is the relative permittivity of the crystalline matrix, ϵ_0 is the electric constant, $\Gamma(z) = \int_0^\infty t^{z-1} \exp(-t) dt$ is the Euler's gamma-function, and $N_{-1} = KN$ is the concentration of negatively charged acceptors.

Thus, substitution of expression (4) into Eq. (2) yields

$$k_B T_j \approx 0.73 \frac{e^2}{4\pi\epsilon_r\epsilon_0} (KN)^{1/3}, \quad (5)$$

where T_j is the temperature of equality of hopping and band conductions (Fig. 1). [For description of kinetic phenomena in gas plasma, the Landau length $d_L = e^2/(4\pi\epsilon_r\epsilon_0k_B T)$ is used.^{46,47} At the temperature $T = T_j$ for a nondegenerate gas of v -band holes against a background of neutralizing their charge negatively charged acceptors from Eq. (5), we obtain $d_L \approx 1.37(KN)^{-1/3}$.]

Let us now relate the temperature T_j with the ionization energy of a single hydrogen-like impurity I_{im} and its concentration N_M , which corresponds to the phase insulator-metal transition (the Mott transition)⁴⁸.

The concentration of majority (doping) hydrogen-like impurity $N = N_M$, which corresponds to the Mott transition, and the Bohr radius a_{im} of a single (insulated) doping impurity in a crystal are satisfied by the relation⁴⁹

$$N_M^{1/3} a_{im} \approx \frac{0.542}{\left[(1-K)(\epsilon_r + 2)\right]^{1/3}}. \quad (6)$$

Let us divide the left and right parts of the relation (5) by ionization energy of the hydrogen-like impurity $I_{im} = e^2/(8\pi\epsilon_r\epsilon_0 a_{im})$ and then multiply and divide the right part of the obtained expression by $N_M^{1/3}$; thus, from Eq. (5), taking into account Eq. (6), we obtain

$$\frac{k_B T_j}{I_{im}} \approx 0.79 \left[\frac{K}{(1-K)(\epsilon_r + 2)} \right]^{1/3} \left(\frac{N}{N_M} \right)^{1/3}. \quad (7)$$

Calculations by using Eq. (7) were compared with experimental data for p -Ge crystals doped with gallium (and compensated with arsenic and partially with selenium) by transmutation reactions under the influence of thermal neutrons of a nuclear reactor.^{50,51} Figure 2 shows T_j values (points *a-f*), which we obtain according to Fig. 1 from the experimental dependences of $\ln\rho$ on $1/T$ of germanium samples (Refs. 9 and 12–17). Experimental values of T_j were

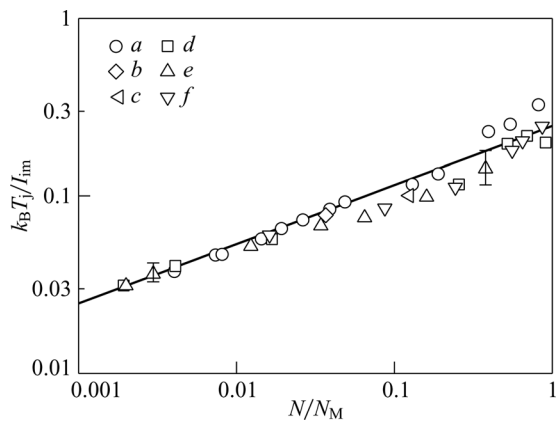


FIG. 2. Dependence on concentration N of gallium atoms of the transition temperature T_j from hopping to the band conduction in neutron-transmutation doped p -Ge:Ga crystals. The line is the calculations by using Eq. (7) for $K = 0.35$. The points *a-f* are experimental data from the works: (a) Refs. 12 and 13, (b) Ref. 14, (c) Ref. 15, (d) Ref. 9, (e) Ref. 16, and (f) Ref. 17. The typical deviation of T_j for two values of N (at the beginning and at the end of doping degree range) is indicated by vertical bars.

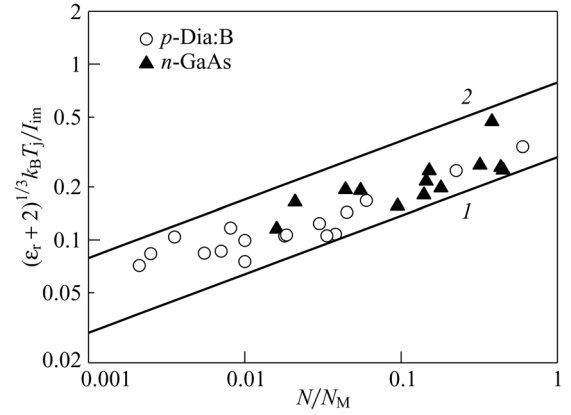


FIG. 3. Dependence on concentration of the doping impurity N of the transition temperature T_j from hopping to the band conduction in p -Dia:B and n -GaAs. The lines are calculations by using Eq. (7) for $K = 0.05$ (1) and $K = 0.5$ (2). The points are experimental data from the works: Refs. 18–24 (p -Dia:B) and Refs. 25–27 (n -GaAs).

obtained as an intersection between the straight lines, representing the asymptotic behaviors of the band and hopping conductions $\ln\rho_p = \ln\rho_1 + \epsilon_1/k_B T$ and $\ln\rho_h = \ln\rho_3 + \epsilon_3/k_B T$, respectively, assuming ρ_1 , ρ_3 , ϵ_1 , and ϵ_3 to be constants (Fig. 1). The deviations of the experimental data from the fitting straight lines were within 3%.

The line in Fig. 2 shows the calculations of T_j using Eq. (7) for the compensation ratio $K = 0.35$. Parameters of p -Ge:Ga are presented in Table I.^{17,23,52–59} It is seen that the temperature T_j is described in the wide range of doping impurity concentration by relation (7). The small deviations of T_j from the calculations are due to the fact that the neutron-transmutation doping of germanium crystals allows accurately, within percents, to control the concentration of the doping impurity (Ga) and the compensation ratio of samples (see, e.g., Refs. 50, 51, 60, and 61).

Figure 3 shows the dependence of the transition temperature T_j from hopping to the band conduction in boron-doped

TABLE I. Semiconductor crystal parameters.

	ϵ_r^a	I_{im} , meV ^a	N_M , cm ⁻³
p -Ge:Ga	15.4	11.32	1.85×10^{17b}
p -Dia:B	5.7	370	2×10^{20c}
n -GaAs	12.4	6	2×10^{16d}
n -Si:Sb	11.5	42.7	3×10^{18e}
n -Si:P	11.5	45.6	$\approx 4 \times 10^{18f}$
n -Si:As	11.5	53.8	7.8×10^{18g}
p -Si:B	11.5	44.39	4×10^{18h}
p -Si:Al	11.5	69.03	1.6×10^{19i}
p -Si:Ga	11.5	72.73	1.8×10^{19i}
n -ZnSe:Al	8.6	23.6	4.7×10^{17i}

^aData on ϵ_r and I_{im} are taken from Ref. 52.

^bReference 17.

^cReference 23.

^dReferences 53 and 54.

^eReference 55.

^fReferences 56 and 57.

^gReference 58.

^hReference 59.

ⁱThe Mott concentration of impurity N_M is assessed by Eq. (6).

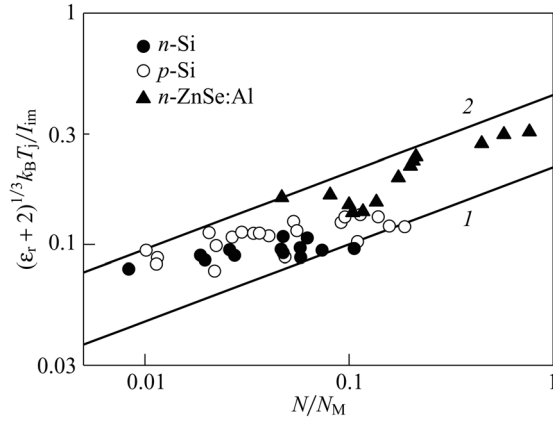


FIG. 4. Dependence on concentration of the doping impurity N of the transition temperature T_j from hopping to the band conduction in n -Si, p -Si, and n -ZnSe:Al. The lines are calculations by using Eq. (7) for $K=0.02$ (1) and $K=0.15$ (2). The points are experimental data from the works: Refs. 28–30 (n -Si, p -Si) and Ref. 31 (n -ZnSe).

diamond of p -type^{18–24} (p -Dia:B) and gallium arsenide of n -type^{25–27} (n -GaAs) on the concentration of majority (doping) impurity. In order to compare T_j for materials with different relative permittivity ϵ_r in the same plot, we, in accordance with relation (7), carried over the multiplier $(\epsilon_r + 2)^{1/3}$ into the left part. Parameters of semiconductors (ϵ_r , I_{im} , N_M) used for the construction of experimental data dependences are given in Table I. Figure 4 shows the concentration dependence of T_j for silicon crystals of n - and p -types^{28–30} (n -Si, p -Si) and for aluminum-doped zinc selenide crystals³¹ (n -ZnSe:Al). It is seen from Figs. 3 and 4 that the calculations of T_j agree with experimental data in the limits of typical deviations of compensation ratios K for these semiconductor materials. Note that, for n -type semiconductor samples shown in Figs. 3 and 4, only the D -bot donor band is pronounced, i.e., donors are in the charge states (0) and (+1).

III. SCREENING LENGTH OF ELECTROSTATIC FIELD IN THE DEBYE-HÜCKEL APPROXIMATION AT THE NEAREST NEIGHBOR HOPPING CONDUCTION

Let us consider implementation of characteristic temperatures T_j and $T_h \approx T_j/3$ for estimates of concentration of hydrogen-like impurities from measurements of capacitance in a metal-insulator-semiconductor (MIS) structure on the example of the crystalline semiconductor of p -type (Fig. 1).

When the band conduction dominates ($\sigma_p \gg \sigma_h$), the capacitance of a MIS structure in the regime of the flat c - and v -bands is (see, e.g., Refs. 2 and 62) $C_{fb} = C_{ox} C_{DH} / (C_{ox} + C_{DH})$, where $C_{ox} = \epsilon_{ox} / d_{ox}$ is the capacitance of an insulator with permittivity ϵ_{ox} and thickness d_{ox} between a metal electrode of the unit area and semiconductor, and $C_{DH} = \epsilon_r \epsilon_0 / \Lambda_p$ is the capacitance of the semiconductor with permittivity $\epsilon = \epsilon_r \epsilon_0$ and the screening length Λ_p . The capacitance of insulator C_{ox} can be quite easily and accurately measured.⁶³ Then, the screening length of an external electrostatic field (screened by holes of the v -band), after Debye-Hückel, $\Lambda_p = (\epsilon_r \epsilon_0 k_B T / e^2 p)^{1/2}$ is found from the

flatband quasistatic capacitance of a MIS structure C_{fb} . Thus, this procedure allows to find concentration of holes p from Λ_p (when acceptors are totally ionized $p = (1 - K)N$).

When the hopping conduction by holes via acceptors dominates ($\sigma_h \gg \sigma_p$), to the best of our knowledge, the possibility to determine the electrostatic field screening length Λ_h from measurements of quasistatic capacitance $C_{DH} = \epsilon_r \epsilon_0 / \Lambda_h$ is not realized yet.

Hopping conduction in the NNH regime dominates ($\sigma_h \gg \sigma_p$; Fig. 1) in the vicinity of temperature $T_h = T_j/3$, where T_j is defined by formula (5). The screening length determined by holes hopping between acceptors has, in the Debye-Hückel approximation, the form³⁹

$$\Lambda_h = \left(\frac{\epsilon_r \epsilon_0 \zeta_h k_B T_h}{e^2 N_h} \right)^{1/2}, \quad (8)$$

where $N_h = (1 - K)KN$ is the effective concentration of holes hopping between acceptors in the charge states (0) and (−1). The parameter $\zeta_h \geq 1$ characterizes the influence of fluctuations of the electrostatic potential in a crystal on the ratio of the hopping diffusion coefficient D_h to the drift hopping mobility M_h of holes, $D_h / M_h = \zeta_h k_B T / e$.^{39,40} When the acceptor A -bot bandwidth W (see Fig. 1) is less or about thermal energy $k_B T_h$, then $\zeta_h \approx 1$.^{39,40,64}

At hopping conduction the root-mean-square electrostatic fluctuation of acceptor energy levels (the width W of the acceptor A -bot band), at a random distribution of impurity ions over a crystalline semiconductor and taking into account the Coulomb interaction with the nearest neighbor ions only, has the form^{10,65}

$$W = \left(\sum_{i=1}^2 \int_0^\infty P_i U_i^2 dr \right)^{1/2} \approx 1.637 \frac{e^2}{4\pi\epsilon_r\epsilon_0} \left(\frac{8\pi}{3} KN \right)^{1/3}, \quad (9)$$

where $P_i dr = 4\pi r^2 C_i \exp[-2KN(4\pi r^3/3)] dr$ is the Poisson probability that the nearest to a given ion another ion of type i (acceptor ($i=1$) or donor ($i=2$)) is positioned at the distance from r to $r + dr$ (see Refs. 44 and 45) and there are no other impurity ions in a sphere of the volume $4\pi r^3/3$ centered at a given ion, $\sum_{i=1}^2 C_i = 2KN$ is the concentration of all ions in a crystal ($C_1 = C_2 = KN$), $U_i(r) = \pm e^2 / 4\pi\epsilon_r\epsilon_0 r$ is the Coulomb energy of interaction between the nearest neighbor ions having the same (sign +) or different (sign −) charge states, $\sum_{i=1}^2 \int_0^\infty P_i U_i dr = 0$ follows from the electrical neutrality of a crystal ($N_{-1} = N_{+1} = KN$), $\sum_{i=1}^2 P_i$ is the probability density of the nearest neighbor impurity ions, and $\int_0^\infty \sum_{i=1}^2 P_i dr = 1$. Further, we assume that, for moderately doped ($0.01 < N/N_M < 0.5$) and moderately compensated ($0.1 < K < 0.9$) semiconductors, the root-mean-square fluctuation of acceptor energy levels by Eq. (9) is much larger than the quantum-mechanical splitting of levels due to finiteness of localization time of hopping holes (see estimations in Ref. 64). Note that the quantum-mechanical splitting of levels is more noticeable for the A -top band than for the A -bot band (see Fig. 1).

Note that, at temperature T_j , the concentration of holes is $p \ll K(1-K)N$, leading to the root-mean-square fluctuation of the potential energy of a hole in the valence band $W_p \ll W$ (see Ref. 66 and references therein). Due to the mobility edge ($|E_v^{(u)}| \approx W_p$) is close to the top of the v -band (see Fig. 1), the fluctuations of the top of the valence band can be neglected ($W_p \ll k_B T_j$) for T_j calculations. Thus, the formula (5) for T_j is quite correct. At temperature $T_h = T_j/3$, where the hopping conduction dominates ($\sigma_h \gg \sigma_p$), the ratio of the acceptor bandwidth W by Eq. (9) to the thermal energy $k_B T_h$ is $W/k_B T_h \approx 13.7$ and it does not depend on the acceptor concentration N and the compensation ratio K . Thus, it follows from Eqs. (5) and (9) that $W \gg k_B T_h$.

By substituting temperature $T_h = T_j/3$ according to Eq. (5) into the expression (8) for the screening length Λ_h , we obtain

$$\Lambda_h \approx \frac{0.14}{(KN)^{1/3}} \left(\frac{\xi_h}{1-K} \right)^{1/2}, \quad (10)$$

where $\xi_h \approx K(1-K)(W/k_B T_h) \sqrt{2\pi} \exp(\chi^2)$ for $W \gg k_B T_h$, assuming the Gaussian distribution of acceptor energy levels (line g_b in Fig. 1), and χ is the parameter obtained from the electrical neutrality condition of a crystal: $2K = 1 - \text{erf}(\chi)$; $\xi_h = 1$ for $W \ll k_B T_h$. (Derivation of expressions for ξ_h and χ is presented in Refs. 39, 40, and 64.) Note that the screening length Λ_h given by Eq. (10) for $W \gg k_B T_h$ is larger than an average distance between neighbor impurity atoms⁴⁵ $d_{im} \approx 0.554/[(1+K)N]^{1/3}$ for all values of the compensation ratio K (see Fig. 5). As far as $\Lambda_h > d_{im}$, we can state that, according to Ref. 67, the Debye-Hückel approximation at temperature T_h for the wide impurity band ($W \gg k_B T_h$, $\xi_h > 1$) is valid. To the contrary, for the narrow impurity band ($W \ll k_B T_h$, $\xi_h = 1$), we get $d_{im} > \Lambda_h$ for $0.1 < K < 0.9$. Thus, the Debye-Hückel approximation for screening length calculation in the case of the narrow impurity band and intermediate compensation ratios is not valid.

From formula (10), for the wide impurity band ($W \gg k_B T_h$, $\xi_h > 1$), it follows that the quantity $\Lambda_h N^{1/3} \approx 0.81 K^{1/6} \exp(\chi^2/2)$, where $\text{erf}(\chi) = 1 - 2K$, depends only on the compensation ratio (see Fig. 5, curve 1). The dashed line

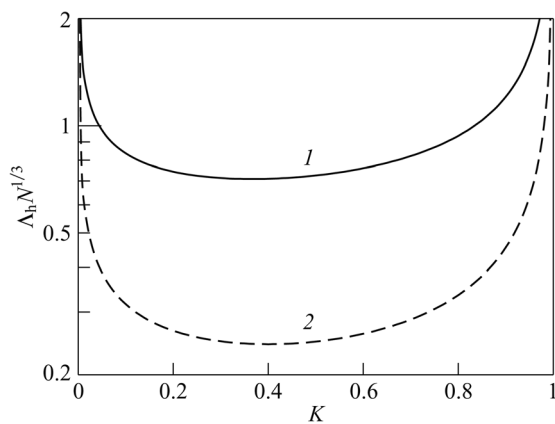


FIG. 5. Dependence of the screening length Λ_h at hopping electrical conduction via hydrogen-like impurities on the compensation ratio K calculated using Eq. (10) for temperature $T_h = T_j/3$: the curve 1—at $\xi_h > 1$ ($W \gg k_B T_h$) and the curve 2—at $\xi_h = 1$ ($W \ll k_B T_h$).

in Fig. 5 shows calculations of the screening length Λ_h by models^{68,69} for the case of the narrow impurity band ($W \ll k_B T_h$, $\xi_h = 1$) at temperature $T_h = T_j/3$. It is seen in Fig. 5 that the screening length $\Lambda_h \propto N^{-1/3}$ at temperature T_h weakly depends on the compensation ratio (for intermediate values of K) for both the wide (curve 1) and narrow (curve 2) impurity bands. Unlimited increase of the screening length at very low ($K \rightarrow 0$) and very high ($K \rightarrow 1$) compensation ratios is related to diminishing of the effective concentration of holes hopping between acceptors $N_h = (1-K)KN \rightarrow 0$.

Note that, at a large degree of compensation $1 - K \ll 1$, the long-range fluctuations of electrostatic potential energy of impurity ions arise (with characteristic size much larger than the average distance between impurity ions).^{6,70} Thus, for very high compensation ratios, the expression Eq. (10) becomes qualitative, due to Eq. (9) describes only short-range electrostatic fluctuations. To be more precise, Eq. (9) takes into account only Coulomb interactions between randomly distributed nearest neighbor impurity ions in a semiconductor.

IV. CONCLUSIONS

In the paper, we employ the virial theorem for a single typical pair “an electron in the c -band – a nearest to it donor in the charge state (+1)” for nondegenerate semiconductor of n -type or a pair “a hole in the v -band – a nearest to it acceptor in the charge state (–1)” for a nondegenerate semiconductor of p -type. As a result, an expression is obtained for the transition temperature T_j from the band electrical conduction (in the c - or v -band) to the electrical conduction by hops of electrons or holes between hydrogen-like impurities. Temperature T_j increases with the concentration of the doping impurity as well as with the compensation ratio. Calculated values of T_j agree well with known experimental data. For temperature $T_h = T_j/3$, we calculate the screening length Λ_h (after Debye-Hückel) when the hopping conduction dominates in approximations of the wide and narrow impurity bands. The value of Λ_h can be found from the measurements of quasistatic capacitance $C_{DH} = \epsilon_r \epsilon_0 / \Lambda_h$ (accounted for the unit area surface of semiconductor included in a MIS structure). Using the value of Λ_h , the concentration N (when K is known) or compensation K (when N is known) can be found within the framework of our model (for the wide impurity band, where the Debye-Hückel approximation is applicable).

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