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Quasiclassical description of the nearest-neighbor hopping dc conduction via hydrogen-like donors in intermediately compensated GaAs crystals

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Abstract

Expressions for the pre-exponential factor σ_3 and the thermal activation energy ε_3 of hopping electric conductivity of electrons via hydrogen-like donors in n-type gallium arsenide are obtained in the quasiclassical approximation. Crystals with the donor concentration N and the acceptor concentration KN at the intermediate compensation ratio K (approximately from 0.25 to 0.75) are considered. We assume that the donors in the charge states (0) and (+1) and the acceptors in the charge state (−1) form a joint nonstoichiometric simple cubic 'sublattice' within the crystalline matrix. In such sublattice the distance between nearest impurity atoms is $R_\mathrm{h} = [(1 + K)N]^{-1/3}$ which is also the length of an electron hop between donors. To take into account orientational disorder of hops we assume that the impurity sublattice randomly and smoothly changes orientation inside a macroscopic sample. Values of $\sigma_3(N)$ and $\varepsilon_3(N)$ calculated for the temperature of 2.5 K agree with known experimental data at the insulator side of the insulator–metal phase transition.

1. Introduction

The isotropic effective mass of electrons and weak nonparabolicity of the dispersion law for the c-band represent gallium arsenide as a test system suitable for calibration of theoretical models of n-type crystalline semiconductors [1].

In GaAs crystals (and the other binary semiconductors), amphoteric behavior is typical even for hydrogen-like impurities [2]. For instance, a Si atom is a donor if it substitutes a Ga atom, and it is an acceptor if it substitutes an As atom in the crystalline matrix of GaAs. This special case of the impurity self-compensation mechanism in semiconductors [3] leads to the compensation ratio in obtained n-GaAs crystals usually ranging in the rather wide limits. Note that, according to [4], in crystalline n-GaAs an antistructural defect (an As atom in the Ga position or a Ga vacancy and an As atom bound to it at a tetrahedral or hexagonal interstitial site) is a metastable double donor. Consequently, it is hard to obtain a family of n-type gallium arsenide crystals with different concentrations of hydrogen-like donors and the fixed compensation ratio.

In n-GaAs, dc hopping conductivity via hydrogen-like donors is observed in the dark at liquid helium temperature and below[3]. Experimental data on the hopping conductivity over shallow donors in gallium arsenide crystals are presented in [6, 7] (and references therein) and also in [8–12]. Note that a number of studies were performed on the low-temperature-grown epitaxial GaAs with point structural defects (see, e.g., [13–15]). It was established that a conduction mechanism in such a system is the hopping conduction. Due to the deep energy level of antisite As donors (about 0.75 eV

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[3] However, in GaAs with high concentration of irradiation-induced defects dc hopping conduction is observed [5] even at a temperature of 100 K.

below the conduction band edge) the hopping conduction is possible even at room temperature. In [16], the hopping photoconduction and non-equilibrium phonon detection in p-type GaAs bolometers were studied at the temperature below 2 K. However, there are still some troubling unanswered questions. To the best of our knowledge, a quantitative description of hopping transport of the electrons is still lacking, even via hydrogen-like donors in gallium arsenide crystals.

In this paper we limit our consideration to the electron hopping regime via nearest-neighbor donors (the NNH regime). In this case, the dc hopping conductivity σ_h in covalent semiconductors is [17]

$$\sigma_\mathrm{h} = \sigma_3 \exp\left(-\frac{\varepsilon_3}{k_\mathrm{B}T}\right), \qquad (1)$$

where $\sigma_3 \equiv 1/\rho_3$ is the pre-exponential factor, ε_3 is the activation energy of electron hops via donors on the background of acceptors, k_B is the Boltzmann constant and T is the temperature.

We consider intermediate compensation ratios. For low compensation ratio and low temperature the donor–acceptor pairs can appear (donor in the charge state (+1) and acceptor in the charge state (−1)). So the hopping activation energy ε_3 is defined by the energy necessary for breaking these pairs (see, e.g., [17]).

The aim of our work is to describe quantitatively the dependences of σ_3 and ε_3 for the NNH regime with respect to the concentration of hydrogen-like donors in intermediately compensated n-type GaAs crystals at the insulator side of the insulator–metal transition.

2. Joint nonstoichiometric ‘sublattice’ of hydrogen-like donors and acceptors within the crystalline matrix

Let us consider uniform crystalline n-GaAs with the donor concentration $N = N_0 + N_{+1}$, where N_0 and N_{+1} are the concentrations of donors in the charge states (0) and (+1), respectively. There are also acceptors, all of them in the charge state (−1) with the concentration KN, where $0 < K < 1$ is the compensation ratio of donors by acceptors[4]. The electrical neutrality condition for the crystal is equal to [21, 22]

$$N_{+1} = N \int_{-\infty}^{+\infty} \mathcal{G} f_{+1}\, \mathrm{d}(E - \overline{E}) = KN, \qquad (2)$$

where $\mathcal{G}$ is the distribution of the donor energy levels E with respect to the average value $\overline{E} > 0$ relative to the bottom of the c-band, f_{+1} is the probability that a donor with the energy level E is ionized and $(1 - K)$ is the fraction of electrically neutral donors. Further, we assume that $\mathcal{G}$ is a Gaussian distribution:

$$\mathcal{G}(E - \overline{E}) = \frac{1}{\sqrt{2\pi}W} \exp\left[\frac{-(E - \overline{E})^2}{2W^2}\right], \qquad (3)$$

where W is the effective width of the donor band in the band gap. The probability that a donor with the energy level $E > 0$ below the bottom of the c-band is ionized has the form [23, 24]

$$f_{+1} = 1 - f_0 = \left[1 + \beta \exp\left(\frac{E + E_\mathrm{F}}{k_\mathrm{B}T}\right)\right]^{-1} \equiv [1 + \exp(u + \zeta)]^{-1}, \qquad (4)$$

where $\beta = 2$ is the spin degeneracy factor of the energy level of a hydrogen-like donor in n-type gallium arsenide, E_F is the electron Fermi level relative to the bottom of the c-band ($E_\mathrm{F} < 0$ in the band gap), and $u = (E - \overline{E})/k_\mathrm{B}T$ and $\zeta - \ln\beta = (E_\mathrm{F} + \overline{E})/k_\mathrm{B}T$ are the dimensionless donor energy level and the Fermi level relative to the center $\overline{E}$ of the donor band, respectively. Note that here and further the donor energy level $E > 0$ is the thermal ionization energy of the donor.

We assume that the hydrogen-like impurities (both donors and acceptors) form a joint nonstoichiometric simple cubic ‘sublattice’ within the crystalline matrix[5]. The distance between the nearest impurity atoms in the sublattice is $R_\mathrm{h} = [(1 + K)N]^{-1/3}$. Note that the volume related to one impurity atom in the crystal is $[(1 + K)N]^{-1}$. In further consideration we suppose that R_h is the length of an electron hop between donors in the charge states (0) and (+1). By virtue of condition (2) the total fraction of positively and negatively charged ions at impurity sites is equal to $2K/(1 + K)$. The charge states (0) and (+1) of immobile donors migrate over the impurity sublattice, while the acceptors, in the charge state (−1), permanently occupy a fraction $K/(1 + K)$ of sites and make them unavailable for electron hops. To take into account the random distribution of the impurity atoms in the real crystal we assume that the impurity sublattice randomly and smoothly changes orientation inside a macroscopic sample, while the distance between nearest atoms and the number of the nearest neighbors remain unchanged.

The donor ‘classical’ band width, taking into account the Coulomb interaction of the ionized donor with the ions in the first coordination sphere of the impurity simple cubic sublattice, is equal to [23, 29]

$$W = \frac{e^2}{4\pi\varepsilon R_\mathrm{h}} \left(\frac{12K}{1 + K}\right)^{1/2}, \qquad (5)$$

where e is the elementary charge, $\varepsilon = 12.4\varepsilon_0$ is the low-temperature static permittivity of gallium arsenide [1, 30] and ε_0 is the electric constant.

The position of the donor band center $\overline{E} > 0$ in the band gap relative to the bottom of the c-band is [21, 23]

$$\overline{E} = I - \frac{3e^2}{16\pi\varepsilon(\Lambda_\mathrm{h} + R_\mathrm{h})}, \qquad (6)$$

where $I \approx 6$ meV is the energy level (the thermal ionizaton energy) of a single hydrogen-like donor in gallium arsenide [30, 31]: C, Si or Ge atom (substituting Ga) or S or Se atom (substituting As); Λ_h is the Coulomb field screening radius of the ion and $R_\mathrm{h} = [(1 + K)N]^{-1/3}$ is the minimum possible distance between ions in the impurity sublattice. In the Debye–Huckel approximation the screening radius is [21, 22] $\Lambda_\mathrm{h} = (\varepsilon k_\mathrm{B} T \xi_\mathrm{h}/e^2 N_\mathrm{h})^{1/2}$, where $N_\mathrm{h} = (1 - K)KN$

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[4] We consider the concentrations of donors $N < N_\mathrm{M}$, where N_M is the concentration at which in gallium arsenide the transition from the insulator state to the metallic one (Mott transition) is observed. The value $N_\mathrm{M} \approx 2 \times 10^{16}$ cm^{-3} was estimated from experimental data [18, 19]. (A model of the N_M dependence on the compensation ratio K is presented in [20].)

[5] Note that in models [25–28] the regular sublattice composed of donors only was considered for $K \ll 1$.

is the effective concentration of electrons which hop between donors and $\xi_h \geqslant 1$ is a dimensionless parameter (the ratio, in the units of k_BT/e, of the diffusion coefficient D_h of hopping electrons to their drift mobility M_h):

$$\frac{1}{\xi_h} = \frac{k_BT\mathrm{M}_h}{eD_h} = \frac{1}{K(1-K)}\int_{-\infty}^{+\infty}\mathcal{G}f_0f_{+1}\,\mathrm{d}(E-\overline{E}). \tag{7}$$

For the narrow donor band ($W \ll k_BT$) from (2), taking into account (3) and (4), we obtain $\zeta = \ln\beta + (E_F + \overline{E})/k_BT \approx -\ln[K/(1-K)]$. In this case, it follows that $\xi_h \approx 1$ from (7) and (3)–(5). For the wide donor band ($W \gg k_BT$), condition (2) along with (3) and (4) can be written as $2K \approx 1 - \mathrm{erf}(\zeta/\sqrt{2}\gamma)$, where $\gamma = W/k_BT \gg 1$. In this case, from (7), according to [22], we obtain $\xi_h \approx K(1-K)\gamma\sqrt{2\pi}\exp(\zeta^2/2\gamma^2)$. Note that, when $W \gg k_BT$, the quantity ξ_hT (and consequently the screening radius Λ_h) does not depend on the temperature T for any N and K.

3. Stationary electron hopping transport via donors in the impurity sublattice

Let us consider the nonstoichiometric cubic impurity sublattice within an n-type crystalline semiconductor. This object is subjected to an external electric field of strength $\mathcal{E} = -\mathrm{d}\varphi/\mathrm{d}x$ directed along the x axis (along the edges of sublattice), $\varphi(x)$ is the electric potential (the larger value of φ corresponds to the smaller value of x). A stationary hopping current density $J_h = J_{0,+1}$ of electrons over nearest-neighbor donors has the form [22, 29, 32]

$$J_h = eN_h\left(\mathrm{M}_h\mathcal{E} + D_h\frac{\mathrm{d}}{\mathrm{d}x}\ln\frac{N_0}{N_{+1}}\right) = \sigma_{hx}\mathcal{E} + eD_h\frac{\mathrm{d}N_0}{\mathrm{d}x}, \tag{8}$$

where $N_h = N_0N_{+1}/N$ is the effective concentration of electrons which hop between donors in the charge states (0) and (+1), $\mathrm{M}_h = -\Xi R_h^2\mathrm{d}\Gamma/\mathrm{d}\varphi > 0$ is the hopping mobility of electrons, $\Xi = 1/(1+K)$ is the fraction of donors at impurity sublattice sites, $R_h = [(1+K)N]^{-1/3}$ is the length of the electron hop, $\Gamma(x+R_h;x) - \Gamma(x;x+R_h) \approx -(\mathrm{d}\Gamma/\mathrm{d}\varphi)\mathcal{E}R_h > 0$ is the difference of the average electron hopping frequency in the directions against $\Gamma(x+R_h;x)$ and along $\Gamma(x;x+R_h)$ the external electric field, $D_h = \Xi R_h^2\Gamma_h/6$ is the diffusion coefficient, $\Gamma_h/6 = [\Gamma(x+R_h;x)]_{\mathrm{eq}} = [\Gamma(x;x+R_h)]_{\mathrm{eq}}$ is the average electron hopping frequency along one of the six directions (along the edges) of the impurity sublattice for zero external field (index eq denotes equilibrium hopping frequency) and $\sigma_{hx} = eN_h\mathrm{M}_h$ is the hopping conductivity of electrons in the impurity sublattice for the orientation of the edge of the unit cell of the cubic impurity sublattice along the external electric field strength $\mathcal{E}$. Note that in impurity sublattice, $N = N_0(x) + N_{+1}(x) = N_0(x+R_h) + N_{+1}(x+R_h)$ and $N_0(x+R_h) \approx N_0(x) + R_h\,\mathrm{d}N_0(x)/\mathrm{d}x$ when $\mathcal{E} \neq 0$. In equilibrium the relation $[N_0(x)]_{\mathrm{eq}} = [N_0(x+R_h)]_{\mathrm{eq}}$ holds, i.e. $\mathrm{d}N_0/\mathrm{d}x = 0$ when $\mathcal{E} = 0$.

It follows from (8) that the dc hopping conductivity σ_h, averaged over all possible orientations of the nonstoichiometric cubic impurity sublattice with respect to the direction of the external electric field strength $\mathcal{E}$, is given (see [23]) by the expression

$$\sigma_h = \frac{\sigma_{hx}}{2} = \frac{e^2K(1-K)NR_h^2\Gamma_h}{12(1+K)\xi_hk_BT} = \sigma_3\exp\left(-\frac{\varepsilon_3}{k_BT}\right); \tag{9}$$

here we take into account that $\sigma_{hx} = eK(1-K)N\mathrm{M}_h$ and use the modified Nernst–Einstein relation $D_h/\mathrm{M}_h = (k_BT/e)\xi_h$ for $\xi_h \geqslant 1$ defined by (7); see also figure 1. Then we give formula (9) the form of (1).

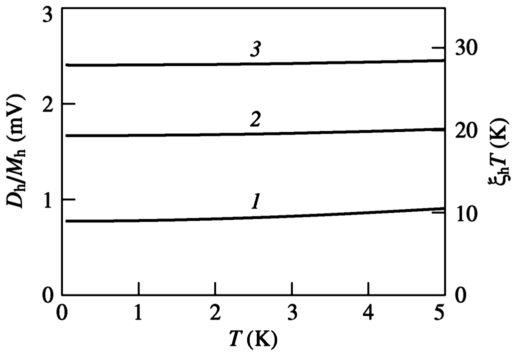

Figure 1. The dependence of the Nernst–Einstein relation D_h/M_h for electrons hopping via hydrogen-like donors in n-GaAs and the value of ξ_hT on the temperature T calculated using (7) for the donor concentrations $N = 10^{14}$ (*1*), 10^{15} (*2*), 3×10^{15} cm^{-3} (*3*) and the compensation ratio $K = 0.5$.

To obtain the dependence of the hopping conductivity σ_h on the values of N, K and T using (9) one has to find the frequency of electron hopping Γ_h in the impurity sublattice.

For not very small and not very large ratios of donor compensation by acceptors (tentatively for $0.1 < K < 0.9$) the correlation between the position of a donor in the impurity sublattice and the donor energy level E may be neglected. Following [33], we suppose that every electron hop of length R_h between donors 1 and 2 in the charge states (0) and (+1) occurs only when their energy levels ($E_1 = \overline{E} + u_1k_BT$ and $E_2 = \overline{E} + u_2k_BT$) accidentally coincide. Such two donors at $u_1 = u_2 = u$ are resonant. We assume that the reason of the donor level coincidence is the thermal (phonon-assisted) fluctuations of donor energies and Coulomb fluctuations due to hops around this pair of donors. It is shown in [23] (see also [33]) that the average (over the impurity sublattice) frequency of the electron hops is

$$\Gamma_h \approx \frac{1}{\tau_3K(1-K)}\int_{-\infty}^{+\infty}\mathcal{G}f_0f_{+1}\,\mathrm{d}u = \frac{1}{\tau_3\xi_h} \equiv \Gamma_3\exp\left(-\frac{\varepsilon_3}{k_BT}\right), \tag{10}$$

where $\Gamma_3 = 1/\tau(u_m) \equiv 1/\tau_3$ is the probability per unit time of electron tunneling between donors in the charge states (0) and (+1) with equal energy levels $E_\tau(u_m) = \overline{E} + u_mk_BT$. The function $\mathcal{G}(u)$ is given by (3) where $E - \overline{E}$ is changed to uk_BT and W to γk_BT. The electrical neutrality condition expressed in (2) can be solved for the dimensionless Fermi level $\zeta - \ln\beta = (E_F + \overline{E})/k_BT$, where $\beta = 2$. Calculating the position of the donor band center $\overline{E}$ using (6), we find the Fermi level value $E_F = k_BT(\zeta - \ln\beta) - \overline{E} < 0$ relative to the bottom of the c-band. The value u_m is calculated from the equation (see [23])

$$u_m + \gamma^2\tanh[(u_m + \zeta)/2] = 0, \tag{11}$$

where $\gamma = W/k_BT$ and $\zeta = \ln\beta + (E_F + \overline{E})/k_BT$. It follows from (11) that if the temperature $T \to 0$ then $u_m \to -\zeta$, and if the donor band width $W \to 0$ then $u_m \to 0$.

Within the framework of the theory of the hydrogen molecular ion [34] a time of electron tunneling between two donors at the distance R_h when their energy levels coincide ($u_1 = u_2 = u$) can be estimated as [35]

$$\tau(u) = \frac{\pi\hbar}{\delta E_\tau(u)}, \tag{12}$$

where $\hbar = h/2\pi$ is the Planck constant and $\delta E_\tau(u)$ is the broadening (splitting) of the energy levels $E_\tau(u) = \overline{E} + uk_\mathrm{B}T = e^2/[8\pi\varepsilon a_\tau(u)]$ of the donors when the electron tunnels between them:

$$\delta E_\tau(u) = 4E_\tau(u) \times \frac{\rho(1+\rho)\exp(-\rho) - [1-(1+\rho)\exp(-2\rho)]S}{\rho(1-S^2)}, \tag{13}$$

$$\rho(u) = \frac{R_\mathrm{h}}{a_\tau(u)}, \qquad S(u) = \left(1 + \rho + \frac{\rho^2}{3}\right)\exp(-\rho).$$

A tunneling energy level $E_\tau(u) > 0$ below the bottom of the c-band is associated with a radius $a_\tau(u) = e^2/[8\pi\varepsilon E_\tau(u)]$ of electron localization on a donor. The Bohr radius for the center ($u = 0$) of the donor band is $a_\tau(0) = e^2/(8\pi\varepsilon\overline{E})$.

We find the pre-exponential factor in the temperature dependence (1) from expression (9) taking into account (10):

$$\sigma_3 = \frac{e^2K(1-K)N^{1/3}\Gamma_3}{12(1+K)^{5/3}\xi_\mathrm{h}k_\mathrm{B}T}, \tag{14}$$

where the time of electron tunneling $1/\Gamma_3 = \tau_3 = \tau(u_\mathrm{m})$ is determined using (12) for $u = u_\mathrm{m}$ from (11), and the factor $\xi_\mathrm{h} \geqslant 1$ is given by formula (7).

Using (7) we obtain that $D_\mathrm{h}/\mathrm{M}_\mathrm{h} = \xi_\mathrm{h}k_\mathrm{B}T/e$ only slightly increases in the temperature range, where the hopping conductivity is experimentally determined in n-GaAs (see figure 1). In addition, according to (12) and (11) the value of $\Gamma_3 = 1/\tau(u_\mathrm{m})$ remains almost invariable as a function of temperature. Therefore, the pre-exponential factor σ_3 does not depend on temperature. This result is in contrast to the approach [36], where it was supposed that $\sigma_3 \propto 1/T$, and the values of ε_3 were determined by plotting $\ln(T\sigma_\mathrm{h})$ versus $1/T$. This issue led to sizable overestimation of ε_3 values (almost two times) as compared with experimental data [6–12], where ε_3 was determined from the plot $\ln(\sigma_\mathrm{h})$ versus $1/T$ in accordance with (1) assuming that σ_3 did not depend on the temperature T.

The activation energy of hopping conductivity comes from (10) using (9) in the form

$$\varepsilon_3 = -k_\mathrm{B}T\ln(\Gamma_\mathrm{h}/\Gamma_3) = k_\mathrm{B}T\ln\xi_\mathrm{h} > 0. \tag{15}$$

It is seen from (15) and (7) that $\varepsilon_3 \to 0$ when the donor band width $W \to 0$. Moreover, the activation energy ε_3 decreases sublinearly upon lowering the temperature T because ξ_h increases in this case. This is the so-called gliding thermal activation energy.

Let us consider the effect of the donor level broadening on the value of ε_3 at an increase of concentration N. The averaged (over the impurity sublattice) stationary probability of coincidence (resonance) of two infinitely narrow energy levels of neutral and positively charged donors is [23, 33]

$$\int_{-\infty}^{+\infty} P(u)\,\mathrm{d}u,$$

where (see (3), (4))

$$P(u)\mathrm{d}u = \mathcal{G}(u)\frac{f_0(u)f_{+1}(u)}{K(1-K)}\,\mathrm{d}u$$

is a conditional probability that energy levels of a randomly chosen pair of donors in the charge states (0) and (+1) belong to the interval $(u, u + \mathrm{d}u)$. When the donor concentration $N = N_0 + N_{+1}$ increases, donor energy levels are broadened because the barrier for electron tunneling becomes more transparent. Thus, electrically neutral donors with energy levels within the interval $(u, u + \Delta_\tau)$ and positively charged donors with energy levels within the interval $(u - \Delta_\tau, u)$, where $2\Delta_\tau$ is a donor energy level width, are resonant.

One can assume that the quantity $2\Delta_\tau k_\mathrm{B}T$ is approximately equal to the splitting (broadening) of the energy levels δE_τ of two donors at resonance (see (13) and outlines in [36]). We assume that $2\Delta_\tau = \delta E_\tau(u_\mathrm{m})/k_\mathrm{B}T$, where u_m is defined by (11). Thus, the frequency of electron hopping via quasistationary donor levels in the charge states (0) and (+1) taking into account (10) has the form [33]

$$\Gamma_\mathrm{h}(\Delta_\tau) \approx \frac{\Gamma_3}{K(1-K)}\int_{-\infty}^{+\infty} \mathcal{G}f_0(u+\Delta_\tau)f_{+1}(u-\Delta_\tau)\,\mathrm{d}u,$$

which gives the activation energy

$$\varepsilon_3(\Delta_\tau) = -k_\mathrm{B}T\ln[\Gamma_\mathrm{h}(\Delta_\tau)/\Gamma_3]. \tag{16}$$

It is evident that $\varepsilon_3(\Delta_\tau) \leqslant \varepsilon_3$, and (16) reduces to (15) if $\Delta_\tau \to 0$. The value of $\varepsilon_3(\Delta_\tau)$ weaker depends on temperature than ε_3.

We emphasize that our simple model of the dc hopping conductivity is valid only if there is no correlation between the donor position in the impurity sublattice and the position of its energy level in the band gap of the crystalline matrix. This condition is better fulfilled for semiconductors with intermediate compensation ratios ($K \approx 0.5$) in which both acceptors and donors are uniformly distributed over bulk of crystalline semiconductor. This can be achieved, e.g., by neutron transmutation doping of semiconductors followed by thermal annealing [37].

4. Comparison of calculations with experimental data for n-GaAs

Figure 2 shows by the solid lines the dependences of the pre-exponential factor $\rho_3 = 1/\sigma_3$, calculated using (14), for the hopping resistivity $\rho_\mathrm{h} = 1/\sigma_\mathrm{h}$, on the donor concentration N in n-GaAs. Experiments [6–12] show that the compensation ratio is $K \approx 0.75$ for lightly doped samples and $K \approx 0.25$ for heavily doped samples[6]. Accordingly, we carried out calculations for the compensation ratios $K = 0.25$ (curve *1*) and $K = 0.75$ (curve *2*) and the temperature $T = 2.5$ K, which corresponds to the middle of the interval of σ_h measurements. The arrows in figures 2 and 3 mark the value of the donor concentration $N = N_\mathrm{M} \approx 2 \times 10^{16}$ cm^{-3}, which corresponds to the insulator–metal phase transition (Mott transition). When we change $N^{-1/3}$ from 40 to 110 nm the ratio $W/k_\mathrm{B}T$ changes

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[6] In [8] the concentration of electrons in the c-band n was determined by the Hall effect at $T = 300$ K. Hence, we estimated for $K \approx 0.5$ the donor concentration to be $N = n/(1-K) \approx 2n$.

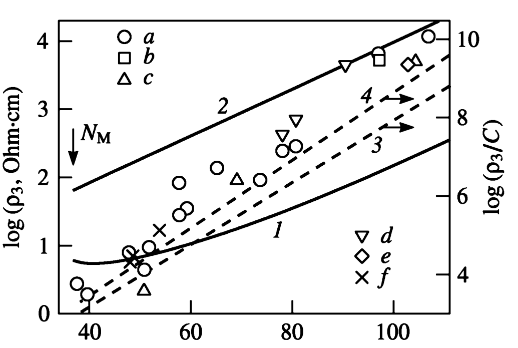

Figure 2. The dependence of the pre-exponential factor $\rho_3 = 1/\sigma_3$ on the donor concentration N in n-GaAs. The solid lines represent our calculations using (14) for the compensation ratios $K = 0.25$ (*1*) and $K = 0.75$ (*2*) at the temperature $T = 2.5$ K. Experimental data on hopping conductivity: (*a*) see [6], (*b*) see [8], (*c*) see [9], (*d*) see [10], (*e*) see [11], (*f*) see [12]. The dashed lines (right axis) represent the calculations using (17) according to the model in [17] for $K = 0.25$ (*3*) and $K = 0.75$ (*4*).

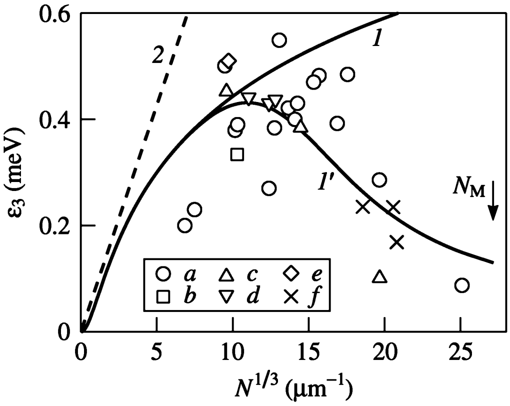

Figure 3. The dependences of the activation energy ε_3 of hopping conductivity on the donor concentration N in n-GaAs. The solid lines represent our calculation using (16) for the compensation ratio $K = 0.5$ at the temperature $T = 2.5$ K: *1*—without donor level broadening ($\Delta_\tau = 0$), *1′*—taking into account donor level broadening ($\Delta_\tau \neq 0$). Experimental data on activation energy: (*a*) see [6, 7], (*b*) see [8], (*c*) see [9], (*d*) see [10], (*e*) see [11], (*f*) see [12]. The dashed line *2* represents the calculation using the model in [17].

from 20 to 8. Then, according to (11), we obtain $u_m \approx -\zeta$. Thus, the calculation using the proposed model covers the range of known experimental data on ρ_3 for n-GaAs, which defied quantitative description so far. The experimental data values of ρ_3 move from theoretical curve *2* (for $K = 0.75$) to curve *1* (for $K = 0.25$) because the compensation ratio in GaAs usually decreases as the concentration of majority impurity increases. Note that calculations using (14) show that ρ_3 increases with K (at $K > 0.3$) at a constant N, which is in agreement with data for neutron-transmutation-doped germanium crystals [38].

Using percolation theory, the following equation was obtained for the NNH regime in [17]:

$$\frac{\rho_3}{C} = \exp\left(\frac{\delta}{a_i N^{1/3}}\right), \tag{17}$$

where C is an unknown power function of N and T, the dimensionless parameter $\delta(K)$ only slightly increases with the compensation ratio K (for example, $\delta(0.25) = 1.78$ and $\delta(0.75) = 1.94$), and $a_i = \hbar/(2mI)^{1/2}$ is the state radius of an electron on a single donor (the Bohr radius), $m = 0.066m_0$ is the effective electron mass in the c-band of gallium arsenide, $I = 6$ meV [1, 30]. The calculations of the values ρ_3/C using (17) for $K = 0.25$ and 0.75 are shown in figure 2 by the dashed lines *3* and *4*, respectively. However, as seen in figure 2 the experimental data are within four orders of magnitude, while the calculations using the model in [17] span over seven orders of magnitude. (In order to decrease this deviation we estimate that the factor $C \propto N^{-b}$, where $2 < b < 3$, should be used.)

Figure 3 shows the dependence of the activation energy ε_3 of hopping conductivity on the donor concentration N for the average compensation ratio $K = 0.5$. The calculation was performed using (16) at the temperature $T = 2.5$ K: the curve *1*—without donor level broadening ($\Delta_\tau = 0$), the curve *1′*—taking into account donor level broadening ($2\Delta_\tau = \delta E_\tau(u_m)/k_B T$). Note that $\delta E_\tau(u_m)$ is determined using (13) for $u = u_m$ obtained by solving (11). The calculation of $\varepsilon_3 \approx 0.74e^2N^{1/3}/(4\pi\varepsilon)$ according to the NNH model [17], for $K \approx 0.5$ and $\varepsilon/\varepsilon_0 = 12.4$, is shown in figure 3 by the dashed line. It can be seen that the calculation according to (16) agrees with the experimental data [6–12], while the calculation using the model in [17] gives overestimated values of the activation energy ε_3. In the donor concentration interval, where in figure 3 the curve *1′* is split up with the curve *1* (from $N \approx 5 \times 10^{14}$ cm^{-3} to $N_M \approx 2 \times 10^{16}$ cm^{-3}), the ratio of quantum-mechanical broadening $\delta E_\tau(u_m)$ of donor levels to the donor classical band width W changes from 10^{-3} to 0.3. Thus, it is essential to take into account donor level broadening due to the finite time of electron localization on them.

5. Conclusions

We have developed a model of dc nearest-neighbor hopping conductivity of electrons via shallow donors in the crystals of n-type gallium arsenide with the intermediate compensation ratio ($K \approx 0.25$–0.75). It was supposed that donors with the concentration N and the compensating acceptors with the concentration KN form a joint nonstoichiometric simple cubic sublattice within the crystalline matrix. The distance between nearest impurity atoms in the impurity sublattice is $R_h = [(1 + K)N]^{-1/3}$. In this case, the total fraction of ions of both types in the impurity sublattice is $2K/(1 + K)$. Only electron hops of length R_h between donors at the instances of accidental alignment of their energy levels due to thermal fluctuations were taken into account. The hopping conductivity was averaged over all possible orientations of the nonstoichiometric cubic impurity sublattice with respect to the direction of the external electric field strength. It was taken into account that the energy levels of donors were distributed due to the Coulomb interaction between the ions in the first coordination sphere of the impurity sublattice, and were broadened due to the finite time of electron localization on each donor. Calculations of the pre-exponential factor σ_3 and the activation energy ε_3 of the electron hopping dc conductivity σ_h over donors depending on their concentration were performed. They agree with known experimental data [6–12] for intermediately compensated n-type gallium arsenide crystals.

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