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Mechanism of contact resistance formation in ohmic contacts with high dislocation density

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A new mechanism of contact resistance formation in ohmic contacts with high dislocation density is proposed. Its specific feature is the appearance of a characteristic region where the contact resistance increases with temperature. According to the mechanism revealed, the current flowing through the metal shunts associated with dislocations is determined by electron diffusion. It is shown that current flows through the semiconductor near-surface regions where electrons accumulate. A feature of the mechanism is the realization of ohmic contact irrespective of the relation between the contact and bulk resistances. The theory is proved for contacts formed to III-V semiconductor materials as well as silicon-based materials. A *reasonable* agreement between theory and experimental results is obtained.
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I. INTRODUCTION

In recent years, a number of papers have appeared reporting on the observation of anomalous behavior of contact resistance R_c in ohmic contacts to semiconductors with high dislocation density. The following anomaly was registered: in the temperature range starting from room temperature the contact resistance increases with increasing temperature T. In particular, such temperature dependence of the contact resistance was observed for In-*n*-GaP and In-*n*-GaN contacts.[1–3] The increase of contact resistance with temperature was also observed for ohmic contacts to *p*- and *n*-InP.[4] The authors of Ref. 5 studied the temperature dependencies of contact resistance of Pt-Si-n-Si as a function of Si doping level. It was shown that for n-Si doped from 10^{16} to 10^{18} cm^{-3} experimental dependencies of $R_c(T)$ decrease with temperature increase and agree quite well with theoretical curves obtained within the frame of thermionic mechanism of current flow.

The experimental $R_c(T)$ curves obtained in the above-mentioned papers contradict the thermionic mechanism of current flow, according to which R_c must decrease with temperature. In fact, the situation is similar to the realization of the thermal-field mechanism of current flow. This case involves Schottky contacts with depletion in the near-contact semiconductor region. At the same time, the results obtained in Refs. 1–3 were explained by assuming that current flow is limited by the resistance of metal shunts on dislocations in semiconductor layers with high dislocation density. Since metal resistance increases linearly with temperature at temperatures exceeding the Debye temperature, the appearance of linear behavior of the $R_c(T)$ is expected. However, a number of experimental features in R_c behavior for metal-GaN contacts remain as yet unexplained. In particular, no interpretation was found for a specific region in the $R_c(T)$ dependence immediately before the linear increase of contact resistance with temperature at low temperatures. In addition, it was observed that the contact resistance as a function of the doping level has very weak dependence. To illustrate this, the authors studied the samples with the doping level changed by more than two orders of magnitude and demonstrated that even in a wide doping range the contact resistance at room temperature no more than doubled.

A qualitative explanation for the observed increase of contact resistance with temperature[4] is the following: In semiconductors with stepped doping ($n - n^+$ junction), the flowing current may be restricted by a diffusion mechanism supplying the electrons. For this case, it was supposed that R_c is proportional to T^2. However, a comprehensive analysis made earlier for Schottky contacts[6] with stepped doping demonstrated that the current in Schottky contacts (except for weakly doped semiconductors with electron concentration $\leq 10^{15}\,cm^{-3}$) is determined by thermionic emission rather than the diffusion limitation. Thus, the diode theory of current flow through the contact was shown to be more appropriate than the diffusion theory. In this case, the temperature dependencies of R_c in the framework of the thermionic mechanism of current flow have to be normal, i.e., decreasing resistance with temperature increase.

Here, we propose a novel concept explaining the unusual behavior of ohmic contacts in the model considering the current flow through the metal shunts along the dislocations and current limitation by a diffusion mechanism supplying electrons. An essential difference from the model developed in earlier work (Ref. 4) is the consideration of the current flow paths through the regions accumulating electrons rather than depleted regions. By combining the two above-mentioned mechanisms we can explain the behavior of $R_c(T)$ curves (decreasing with increasing temperature in

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the low temperature range and increasing as a function of temperature in a higher temperature range) not only for the metal-GaP (GaN) ohmic contacts but also for contacts fabricated for other semiconductor layers of rather high dislocation density. A comparative analysis of the theoretical and experimental results demonstrates, as a rule, very good quantitative agreement.

II. THEORETICAL BASIS FOR THE CONCEPT

Let us assume that a potential well is formed near the end of each dislocation growing into a semiconductor. Generally speaking, a Schottky layer has to appear near the end of the dislocation whose nucleus is filled with a metal. The reason for its appearance is related to the corresponding different contact potentials and surface states. An extremely high electric field appears at the end of the dislocation as a result of considerable curvature as well as the very small size of the metal shunts. The strength of the electric field can be estimated by assuming that the end of the dislocation is hemispherical, and that the charge there is determined by a small number, Z, of electrons (or ions). The strength E_s of the electric field in the semiconductor near the end is obtained from the condition of equality of electric displacements in the metal and semiconductor. Both the edge effect (which leads to a considerable increase of the electric field strength) and the effect of the mirror image forces lead to a considerable reduction of the barrier height, $\Delta\varphi$, near a shunt. Its value (in the above approximations) is

$$\Delta\varphi = \frac{q\sqrt{Z}}{4\pi\varepsilon_0\varepsilon_s r}, \tag{1}$$

where q is the elementary charge, ε_s is the semiconductor permittivity, and r is the radius of the shunt.

Assuming that $Z = 1$, $r = 2 \times 10^{-8}$ cm, and $\varepsilon_s = 10$, $\Delta\varphi$ can be estimated as 0.72 V. If the difference between the metal work function and the semiconductor electron affinity φ_{ms} is below the above value, then we have a potential well rather than a potential barrier at the shunt end. Thus, the appearance of potential wells at the ends of metal shunts formed due to dislocations has reasonable physical preconditions.

It should be noted that the influence of surface states is reduced in the case under consideration. Indeed, the shunt sectional area S_{Sh} compared with N_s^{-1} (N_s is the concentration of surface states) satisfies the following relation: $S_{Sh} < N_s^{-1}$, therefore the effective concentration of surface states that influences band bending formation at the end of the dislocation is reduced $S_{sh}N_s$ times.

The thermionic current flowing through the semiconductor regions accumulating electrons may decrease with increasing temperature, taking into account current limitation by the diffusion mechanism supplying electrons. This results in increasing contact resistance. A sufficiently high density of scattering dislocation centers leads to a decrease of electron mobility in favor of the realization of the condition for current limitation by the diffusion mechanism.

Let us assume that the metal-semiconductor contact potential is nonuniform. In places where dislocations enter a quasi-neutral region of the semiconductor, a positive value of band bending φ_{c0} is realized that forms a potential well for electrons. Between the dislocations, as usual, the contact potential φ_c is negative. It should be noted, that the contact potential $\varphi_c$is the diffusion (built-in) potential, determined from the edge of the conduction band of semiconductor to the top of the barrier. This corresponds to the realization of a Schottky barrier. The total current flowing through the contact interface is a sum of the current flowing through the metal shunts associated with dislocations and current flowing between the dislocations. Current flowing through the metal shunts associated with dislocations enables ohmic contacts to be realized, whose contact resistance will be calculated below.

In calculating the contact resistance, we consider that the contribution from the current flowing between the dislocations can be neglected in the case of high density of the dislocations. The reason for this is a high value (up to about 1 V) of the contact potential related to the high concentration of the surface states. The contact potential is the diffusion (built-in) potential φ_c that is measured from the edge of the conduction band of the semiconductor.

Figure 1 shows the theoretical dependencies of the diffusion potential $|\varphi_c|$ on the doping level for a metal-GaN contact with a tunnel-transparent dielectric gap calculated at different concentrations of acceptor surface states N_{sa} located in the lower half of the bandgap. The calculation was performed using the approach described in Ref. 7, pp. 139–144. It can be seen that, at $N_{sa} \geq 1.6 \times 10^{13}\,\mathrm{cm}^{-2}$, the diffusion potential values exceed 0.7 V as the doping level varies up to about $10^{19}\,\mathrm{cm}^{-3}$.

Figure 1 also shows the dependencies of $|\varphi_b| = -\varphi_c - E_f/q$ (i.e., the barrier potential determined from the Fermi level in the metal to the top of the barrier) as a function of the doping level; the concentration of surface states is $10^{13}\,\mathrm{cm}^{-2}$. The Fermi level is not pinned at the surface (otherwise φ_b would not depend on the doping level). The values of $|\varphi_b|$ (≥ 0.7 V) are high over the hole doping level range, up to concentrations of over $10^{18}\,\mathrm{cm}^{-3}$. Thus, the above-mentioned results demonstrate a fairly convincing reason for neglecting the currents flowing between dislocations.

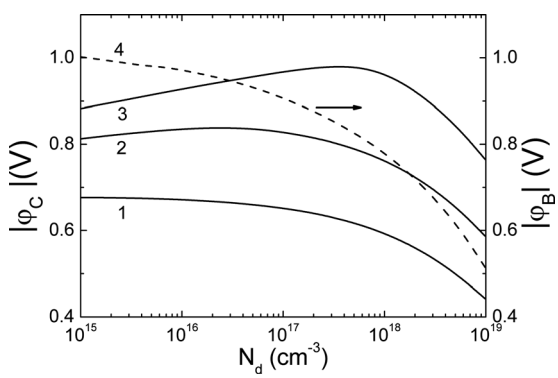

FIG. 1. The calculated dependencies of the diffusion potential $|\phi_c|$ and barrier height $|\phi_b|$ of the contact to GaN as a function of the semiconductor doping level. The following parameters are used: $\phi_{ms} = 0.5$ V, $T = 300$ K, thickness of the dielectric gap $d = 2 \times 10^{-8}$ cm, the dielectric gap permittivity $\varepsilon_d = 1$, N_{sa} (cm^{-2}): 1 -5×10^{12}; 2 -10^{13}; 3 -1.6×10^{13}; 4 -10^{13}.

Let us calculate the thermionic current flowing through a single dislocation. The current is collected from the area πL_D^2, where

$$L_D = \left(\frac{\varepsilon_0 \varepsilon_s kT}{2q^2 N_c}\right)^{0.5} \left(\Phi'_{1/2}(z)\right)^{-1/2} \tag{2}$$

is the Debye screening length for the case of an arbitrary degree of semiconductor degeneracy, N_c is the effective density of states in the conduction band,

$$\Phi'_{1/2}(z) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{\kappa}\exp(\kappa - z)}{\left(1 + \exp(\kappa - z)\right)^2} d\kappa, \tag{3}$$

where $z = E_f/kT$ is the dimensionless Fermi energy in the semiconductor, $\kappa = E/kT$ is the dimensionless kinetic energy of electrons (Ref. 8, p. 659).

The surface density J_{nc} of the thermionic current flowing through the contact at the dislocation outcrop can be determined by solving the continuity equation for electrons. The relation between the electron concentration in the bulk n_w and nonequilibrium electron concentration $n(x)$ at a point x of the near-contact space-charge region is obtained by double integration of the continuity equation over the coordinate x that is perpendicular to the metal-semiconductor interface. For a nondegenerate semiconductor,

$$n(x) = e^{y(x)} \left(n_w - \frac{J_{nc}}{qD_n} \int_x^w e^{-y(x')} dx'\right), \tag{4}$$

where $y(x) = q\varphi(x)/kT$ is the dimensionless nonequilibrium potential at a point x, D_n is the electron diffusion coefficient, and w is the width of the near-contact space-charge region.

The amount J_{nc} is determined by the following expression (Ref. 7, pp. 157, 158):

$$J_{nc} = q\frac{V_T}{4}(n_c - n_{c0}). \tag{5}$$

Here q is the elementary charge, V_T is the thermal velocity of electrons, n_c $(n_{c0} = n_w \exp y_{c0})$ is the nonequilibrium (equilibrium) electron concentration in the contact plane, and $y_{c0} = q\varphi_{c0}/kT$ is the dimensionless equilibrium potential at the metal-semiconductor interface.

Taking x in Eq. (4) as being zero and using Eq. (5) for J_{nc} it is possible to determine n_c. Then, substituting the expression for n_c in Eq. (5) and taking into account the dimensionless nonequilibrium potential $y_c = y_{c0} + \ln(qV/kT)$ (this is the condition for the contact to be ohmic), we obtain the following expression for the density of current flowing through the metal-semiconductor contact at the dislocation outcrop:

$$J_c = \frac{V}{R_{c0}}, \tag{6}$$

where

$$R_{c0} = \frac{kT}{q} \frac{\left(1 + \frac{V_T}{4D_n} e^{y_{c0}} \int_0^w e^{-y(x)} dx\right)}{\frac{qV_T}{4} n_w e^{y_{c0}}}. \tag{7}$$

When calculating R_{c0}, we took into account that

$$\int_0^w e^{-y} dx = L_D \int_{y_c}^{y_x} \frac{e^{-y}}{(e^y - y - 1)^{0.5}} dy. \tag{8}$$

The calculation shows that, at $y_x = 0.5$, the integral in Eq. (8) varies from 0.56 (for $y_{c0} = 1.5$) to 0.65 (for $y_{c0} = 3.5$) and becomes practically constant at larger y_{c0}.

The contact resistance (determined by the diffusion input mechanism) for a contact of unit area was determined from the expression,

$$R_{diff} = \frac{R_{c0}}{\pi L_D^2 N_{D1}}, \tag{9}$$

where N_{D1} is the density of dislocations that take part in current flow. Generally speaking, the density of dislocations taking part in current flow (N_{D1}) and density of dislocations taking part in scattering (N_{D2}) are different. The former are mainly dislocations normal to the interface, while the latter are dislocations parallel to the interface.

The amount $\pi L_D^2 N_{D1} S$ (S is the contact area) is the total area of the current flowing through the dislocations. As a rule, the value of the relevant area, $\pi L_D^2 N_{D1}$, is far below unity, even at maximal dislocation densities $N_{D1} \sim 10^{10}$–$10^{11}\,\mathrm{cm}^{-2}$. The exception is the case of weakly doped semiconductors with $N_d \leq 10^{15}\,\mathrm{cm}^{-3}$, where N_d is the concentration of shallow donor centers.

The electron diffusion coefficient, according to the Einstein relation, is $D_n = kT\mu_n/q$. We determined electron mobility μ_n taking into account electron scattering on charged impurities (μ_Z), optical phonons (μ_o) and dislocations (μ_D),

$$\mu_n = (\mu_Z^{-1} + \mu_o^{-1} + \mu_D^{-1})^{-1}. \tag{10}$$

In our calculations, we applied the expressions for μ_Z and μ_o from Ref. 9, pp. 166, 206 and for μ_D from Ref. 10, p. 184. These expressions can be described as follows:

$$\mu_z(T) = \frac{3.68 \cdot 10^{20} \left(\frac{\varepsilon_s}{16}\right)^2 \left(\frac{T}{100}\right)^{3/2}}{n_w \left(\frac{m}{m_0}\right)^{1/2} \log\left[1 + \left(\left(\frac{\varepsilon_s}{16}\right)\left(\frac{T}{100}\right)\left(\frac{2.35 \cdot 10^{19}}{n_w}\right)^{1/3}\right)^2\right]}, \tag{11}$$

$$\mu_o(T) = \frac{31.8 \sinh\left(\frac{\theta}{2T}\right)}{\left(\frac{1}{\varepsilon_{sh}} - \frac{1}{\varepsilon_{sl}}\right)(\theta)^{0.5} \left(\frac{m}{m_0}\right)^{1.5} \left(\frac{\theta}{2T}\right)^{3/2} K_1\left(\frac{\theta}{2T}\right)}, \tag{12}$$

where θ is the temperature of the longitudinal optical phonon, m is the electron effective mass, m_0 is free electron mass, ε_{sh} (ε_{sl}) is the high- (low-) frequency permittivity of the semiconductor, and $K_1(\theta/2T)$ is the modified Bessel function of the first order,

$$\mu_D = \frac{B\exp(\eta)}{T^{1/2}N_{D2}L_D^5}K_2(\eta), \tag{13}$$

where $\eta = \hbar^2/16mL_D^2kT$ is dimensionless energy of electrons, $K_2(\eta)$ is the modified Bessel function of the second order, $B = (\hbar^2\varepsilon_0\varepsilon_{sl}c)^2/8\sqrt{2\pi k}\,q^3\sigma^2m^{5/2}$ is dimension factor, $\sigma = \lambda/2qc$ is strength factor, λ is the linear charge density of a dislocation line, c is the lattice constant in the [0001] direction.

The above expressions are valid for nondegenerate semiconductors. The quantity

$$\beta = \frac{V_T}{4D_n}e^{y_{c0}}\int_0^w e^{-y(x)}dx \tag{14}$$

is a factor that determines the degree of diffusion limitation that is essential at $\beta > 1$.

In the simplest case, all the donors (whose concentration is N_d) are ionized, and $n_w = N_d$. The theoretical $\beta(N_d)$ curves for n-GaN at different densities of the scattering dislocations are shown in Fig. 2, taking the donor ionization energy to be 15 meV, $y_{c0} = 2$, and $T = 300$ K. Thus, as a rule, the degree of the diffusion limitation mechanism is rather high for parameters varying over a wide range if accumulation is realized in the band bending region at the end of the dislocation. However, it can be seen from Fig. 1 that, as the doping level increases, the value of β decreases from a value greatly exceeding unity to a value much below unity. The reasons for such behavior are the following: (i) decrease of the Debye screening length L_D and (ii) reduction of y_{c0} due to decrease of the electric field strength at the end of the dislocation. As a result, the diode theory of current flow in the metal-semiconductor contact will be more appropriate in the case of degeneracy.

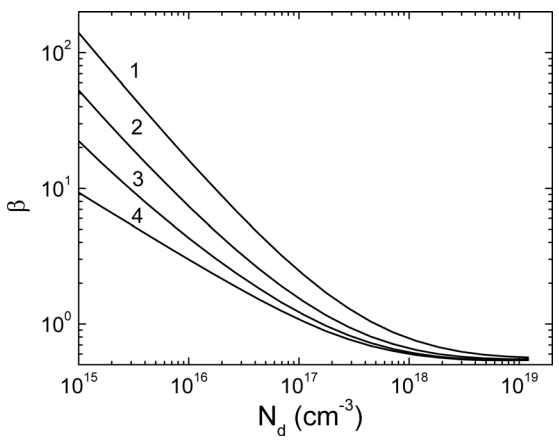

FIG. 2. The calculated dependencies of β as a function of the GaN doping level for different densities of scattering dislocations N_{D2} (cm^{-2}): $1-3\times10^9$; $2-10^9$; $3-3\times10^8$; $4-10^6$. The following parameters are used for the calculation: $y_{c0} = 2$, $E_d = -0.015$ eV, $V_T = 2\times10^7$ cm/s.

By applying the approach developed in Ref. 6, the following expression can be obtained for contact resistance in the case of degeneracy and realization of the thermionic mechanism of current flow,

$$R_{te} = \frac{k}{qA(m/m_0)T}\frac{1}{\ln[1+\exp(z+y_{c0})]}, \tag{15}$$

where A is the Richardson constant. The dimensionless Fermi energy z can be determined from the equation of bulk neutrality,

$$\frac{N_d}{1+\exp(z-E_d/kT)} = \frac{2}{\sqrt{\pi}}N_{c0}\left(\frac{T}{300}\right)^{3/2}\int_0^\infty \frac{\kappa^{0.5}}{1+\exp(\kappa-z)}d\kappa, \tag{16}$$

where E_d is the energy level of shallow donors, N_{c0} is the effective density of states in the conduction band at $T = 300$ K.

It should be noted that, for sufficiently shallow donors, Eq. (16) (written on the assumption that the donor level is discrete) does not hold at sufficiently low temperatures because in that case it does not take into account broadening of the donor levels and appearance of the impurity band. If the inequality $N_d \geq N_{c0}$ is true, then the electron concentration does not depend on temperature in the whole temperature range down to the liquid helium temperature. In that case, the equation of semiconductor bulk neutrality is determined as follows:

$$N_d = n_w = \frac{2}{\sqrt{\pi}}N_{c0}\left(\frac{T}{300}\right)^{3/2}\int_0^\infty \frac{\kappa^{0.5}}{1+\exp(\kappa-z)}d\kappa. \tag{17}$$

At strong degeneracy, the Debye screening length in the semiconductor, L_D, approaches r_0, which does not depend on temperature and weakly depends on the doping level,

$$r_0 = \frac{1}{2}\left(\frac{\pi}{3}\right)^{1/6}\left(\frac{4\pi\varepsilon_0\varepsilon_s\hbar^2}{mq^2N_d^{1/3}}\right)^{1/2}. \tag{18}$$

Thus, in the case of degeneracy, the contact resistance for the current flow mechanism associated with metal shunts can be determined by the expression,

$$R_{tw} = \frac{R_{te}}{\pi r_0^2 N_{D1}}. \tag{19}$$

In this case, averaging of relaxation time τ over electron energy E for a specific scattering mechanism at $\tau \sim E^r$ gives $\langle E_{f\lim}^r\rangle$, where $\langle E_{f\lim}\rangle = \left((3\pi^2)^{2/3}\hbar^2N_d^{2/3}/2m\right)$ is the Fermi energy for the case of full degeneracy. Since $\langle E_{f\lim}\rangle$ does not depend on temperature, the mobility for electron gas with strong degeneration does not depend on temperature either. The exception to this rule is polar optical scattering, for which the relaxation time depends on the optical phonon energy rather than on the electron energy.

Let us analyze how R_{diff} depends on the semiconductor doping level and dislocation density. For a nondegenerate

semiconductor, $R_{diff} \sim L_D/(\mu_n N_d L_D^2 N_{D1})$. In semiconductors with high dislocation density electron scattering on dislocations is predominant at low doping (Ref. 9, p. 214 and Ref. 10, p. 184). In this case, $\mu_D \sim L_D^{-1}$ and $R_{diff} \sim N_d^{-1}$. At medium doping levels, the electron mobility is determined by scattering on optical phonons and $R_{diff} \sim N_d^{-1/2}$. At higher doping levels, $\mu \approx \mu_z$ and $R_{diff} \sim N_d^{1/2}$. In the case of strongly degenerate semiconductors the analog of R_{diff} is $R_{tw} \sim N_d^{1/3}$. Thus, the dependence of contact resistance (limited by diffusion input) on the semiconductor doping level is stronger than doping dependence in the case of the thermionic mechanism in Schottky contacts. As the doping level increases, the contact resistance may not only decrease but also increase.

R_{diff} dependence on dislocation density is also nontrivial. It declines as the density of dislocations taking part in current flow, N_{D1}, increases. At the same time, R_{diff} dependence on the density of scattering dislocations is more complicated. At low doping levels, R_{diff} increases with the density of scattering dislocations due to the decrease of electron mobility, while at high doping levels, it does not depend on N_{D2}.

The total resistance of the metal shunts is in series with resistance R_{diff} (R_{tw}) in the case of a nondegenerate (degenerate) semiconductor. Therefore, taking into account the results obtained in Refs. 1–3, the total resistance of the ohmic contact in a semiconductor with a high dislocation density may be described as

$$R_{cs} = R_{diff}(R_{te}) + R_{sh}(T), \tag{20}$$

where $R_{sh}(T) = [\rho_0(1+\alpha T)/\pi r^2 N_{D1}]d_D$, ρ_0 is the metal specific resistivity at $T = 0^\circ$ C, α is its temperature coefficient, d_D is the distance traveled by electrons through dislocations from the bulk semiconductor to the contact metallization. It should be noted that all expressions in this section are obtained for contacts of unit area.

III. DISCUSSION OF RESULTS AND COMPARISON WITH EXPERIMENT

If the current is limited by the diffusion mechanism supplying electrons, then contact resistance is inversely proportional to electron mobility. Therefore, a rather strong reduction (increase) of R_{diff} should be expected as the electron mobility μ increases (decreases) considerably with T. The electron mobility increases with temperature increase in the case of electron scattering on charged impurities and dislocations, while it decreases in polar semiconductors due to scattering on polar optical phonons. In sufficiently doped semiconductors, scattering on charged impurities is predominant, while scattering on dislocations dominates at low doping levels. The efficiency of scattering on polar optical phonons is determined by the energy of a longitudinal optical phonon: the larger this energy, the higher are the temperatures at which this scattering mechanism is dominant (Ref. 9, p. 206).

Table I presents the parameters of the semiconductors: GaN, InP, GaAs, and Si are used to obtain the theoretical dependencies $\mu_n(T)$ and $R_c(T)$. Figure 3(a) shows the calculated

TABLE I. The semiconductor parameters used for calculating the theoretical $\mu_n(T)$ and $R_c(T)$ curves.

Semiconductor	GaN	InP	GaAs	Si
m/m_0	0.2	0.08	0.063	1.08
$N_c/10^{18}$ (cm^{-3})	2.30	0.57	0.47	28.00
ε_{sl}	9.0	12.5	12.8	12.7
ε_{sh}	5.35	9.65	10.89	…
θ (K)	1056	494	419	…

temperature dependencies $\mu_n(T)$for GaN and InP for several values of the density of scattering dislocations and semiconductor doping level. It should be noted that the values of scattering dislocation densities used for plotting the $\mu_n(T)$ curves for GaN correspond to those used in fitting the theoretical and experimental dependencies $R_c(T)$. Both the electron mobility obtained as well as its temperature dependence are in good agreement with the experimental results (see Refs. 11–13). Indeed, for GaN, in particular, the temperature

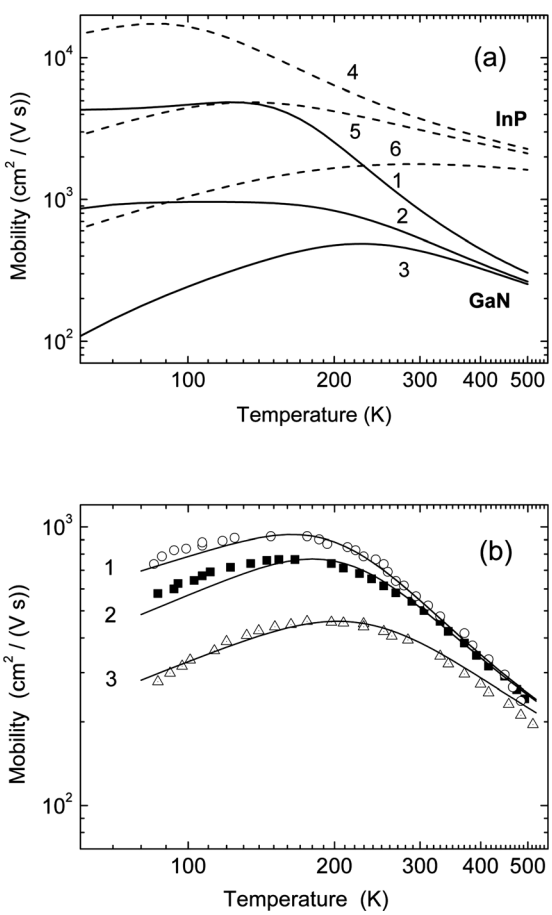

FIG. 3. (a) The temperature dependencies of electron mobility in GaN (curves 1–3) and InP (curves 4–6) calculated for different densities of scattering dislocations. The following parameters are used for the calculation: N_d(cm^{-3}): $1-5\times10^{16}$; $2-10^{17}$; $3-10^{18}$; $4-6-9\times10^{15}$. N_{D2} (cm^{-2}): $1-10^7$; $2-3\times10^8$; $3-2\times10^9$; $4-10^6$; $5-10^7$; $6-5\times10^7$. (b) The temperature dependencies of electron mobility in GaN (curves 1–3) calculated for different density of scattering dislocations and doping. The following parameters are used for the calculation: N_d(cm^{-3}): $1-3\times10^{17}$; $2-2.3\cdot10^{17}$; $3-7.4\cdot10^{17}$; N_{D2} (cm^{-2}): $1-1.07\times10^8$; $2-1.47\times10^8$; $3-4.5\times10^8$. Circles, squares, and triangles are experimental data from Ref. 11.

dependencies of electron mobility calculated at different doping levels by fitting the scattering dislocation densities can match those measured in Ref. 11 with an accuracy of 10%. The theoretical dependencies$\mu_n(T)$, calculated using Eqs. (10)–(13) are shown by solid lines in Fig. 3(b). The only fitting parameter is used, the density of scattering dislocationsN_{D2}. The experimental data (temperature dependencies of mobility $\mu_n(T)$ measured by Götz *et al.* (Ref. 11) in GaN with different doping level) are shown by circles, squares, and triangles. It should be emphasized that in the sample with doping level of $3 \cdot 10^{17}\,\mathrm{cm}^{-3}$ (curve 1) the mobility is higher than in the sample with doping level of $2.3 \cdot 10^{17}\,\mathrm{cm}^{-3}$ (curve 2). The fact is explained by higher density of dislocations in the second case. Thus, taking into account scattering by ionized impurities, optical phonons and dislocations, theoretical expressions (10)–(13) allow us to describe the experimental data obtained for GaN. Similarly, the calculated $\mu_n(T)$ curves are in good agreement with those obtained experimentally for InP.[12,13]

Let us analyze the dependencies obtained taking into account the possibility of realizing an anomalous temperature dependence of the contact resistance, i.e., increasing $R_c(T)$ with increasing temperature. To this end, the electron mobility $\mu(T)$ curve would have a decreasing share in the high temperature range starting from room temperature. It can be seen from Fig. 3, that for GaN, this occurs at a sufficiently large variation of the scattering dislocation density, from 10^6 to $2 \times 10^9\,\mathrm{cm}^{-2}$. For InP, this range is narrower, namely from 10^6 to $3 \times 10^7\,\mathrm{cm}^{-2}$. At scattering dislocation densities $\geq 5 \times 10^7\,\mathrm{cm}^{-2}$, the electron mobility of InP in the temperature range usually studied increases with increasing temperature. This corresponds to the case when the $R_c(T)$ curves have to decrease at high dislocation densities. The reason for such a distinction is the much stronger polar optical scattering in GaN that ensures a sufficiently large reduction of electron mobility at medium and high temperatures. The situation in GaAs is similar to that in InP because the optical phonon energy in GaAs is even lower than in InP.

Our analysis allows us to classify the main behavior of possible temperature dependencies of contact resistance in the case of realization of the proposed mechanism of R_c formation in semiconductors with high dislocation density. Generally, the final contact resistance value is determined by the diffusion input (i.e., R_{diff} value) and total resistance of shunts (i.e., R_{sh}). Therefore, the relationship between R_{diff} and R_{sh} may also be crucial along with the character of the dependence $\mu(T)$ for the realization of decreasing or increasing temperature dependence $R_c(T)$.

A. GaN case

Let us consider the case when the peak in the $\mu(T)$ dependence occurs and inequality $R_{diff} > R_{sh}$ is realized. The clearly pronounced descending part of the $\mu(T)$ curve occurs in polar semiconductors with high energy of a longitudinal optical phonon. In particular, polar optical scattering in GaN (where the optical phonon temperature θ is 1056 K) may reduce electron mobility at high temperatures down to 10^2 cm^2/(Vs) (Fig. 3), while in InP (where $\theta = 494$ K) the electron mobility is reduced to just 10^3 cm^2/(Vs) (see Fig. 3).

In *n*-Si, as in GaN, the electron mobility decreases rather strongly (proportionally to $T^{-2.5}$) at high temperatures. This is related to the contribution to carrier mobility of scattering on acoustic phonons and two intervalley phonons (whose temperatures are 190 and 630 K, respectively).[14] Thus, a stronger increase of $R_{diff}(T)$ should be expected in the region of mobility reduction in silicon than in InP. In both cases considered, an increased region has to be realized in the $R_{diff}(T)$ curves (as well as a minimum that appears under certain conditions).

Figure 4 shows the experimental $R_c(T)$ dependencies for the In-GaN structures measured in Ref. 3 on the samples with a total dislocation density of about $10^8\,\mathrm{cm}^{-2}$ as well as the results of our calculations of $R_{diff}(T)$ for three electron concentrations, 5×10^{16}, 10^{18}, and $10^{19}\,\mathrm{cm}^{-3}$. In Fig. 4 (as well as in the other figures), the density of conducting dislocations N_{D1} was used as a parameter when plotting the calculated curves. The data demonstrate that there is rather good agreement between the theoretical and experimental results.

A particular situation with a semiconductor doping level of $10^{19}\,\mathrm{cm}^{-3}$ should be noted. In this case, the thermionic mechanism of R_c formation is valid. Therefore, we used in our calculations Eqs. (15), (18), and (19) in the approximation made for degenerated semiconductors. It was found that, at sufficiently strong semiconductor degeneracy and action of the thermionic mechanism, there is practically no temperature dependence of the parameters obtained. A similar situation also occurs for the Debye screening length at strong semiconductor degeneracy. Good agreement is obtained between the calculated and experimental contact resistance values in the degenerate semiconductor. It should be emphasized that both the calculated and experimental values of contact resistance weakly depend on the semiconductor doping level.

Figure 5 shows the experimental and calculated $R_c(T)$ dependencies for the Au-TiB$_x$-Al-Ti-*n*-GaN structure. The GaN

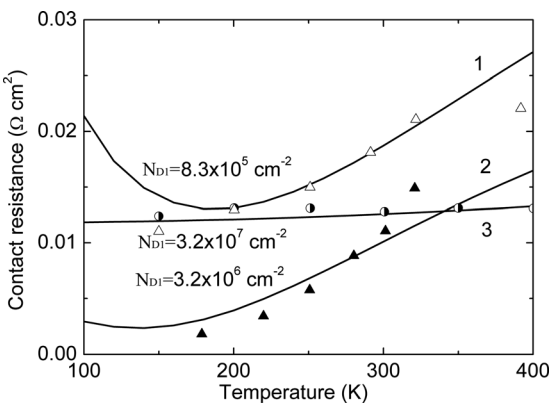

FIG. 4. The temperature dependencies of In-GaN ohmic contact resistance for different densities of conducting dislocations. Circles and triangles, experimental data from Ref. 3, curves, theory. Experimental N_d (cm^{-3}): open triangles, 5×10^{16}, filled triangles, 10^{18}, circles, 10^{19}. The following parameters are used for the calculation: $E_d = -0.015$ eV, $V_T = 2 \times 10^7$ cm/s, $y_{c0} = 3$; N_d (cm^{-3}): $1 - 5 \times 10^{16}$; $2 - 10^{18}$; $3 - 10^{19}$; N_{D2} (cm^{-2}): $1 - 10^7$; $2 - 3 \times 10^8$.

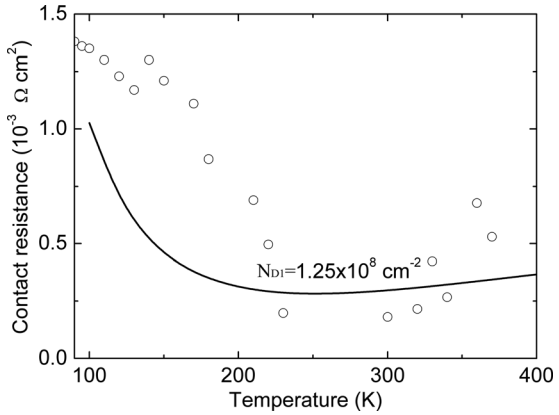

FIG. 5. The temperature dependencies of GaN ohmic contact resistance (the doping level is $10^{17}\,\mathrm{cm}^{-3}$). Circles, our experimental data, curves, theory. The following parameters are used for the calculation: $E_d = -0.015$ eV, $V_T = 2 \times 10^7$ cm/s, $y_{c0} = 3$; $N_{D2} = 1.9 \times 10^9\,\mathrm{cm}^{-2}$.

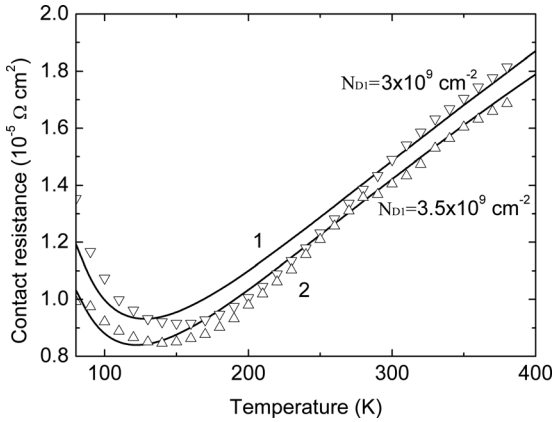

FIG. 6. The temperature dependencies of Au (2000 Å)-TiB_2 (1000 Å) -Au (250 Å)-Ge (250 Å)-n-$n^+ - n^{++}$-InP ohmic contact resistance. Triangles, our experimental data, curves, theory. The following parameters are used for the calculation: $N_d = 9 \times 10^{15}\,\mathrm{cm}^{-3}$; $V_T = 4 \times 10^7$ cm/s; $E_d = -0.007$ eV, $y_{c0} = 2$; $N_{D2} = 1 \times 10^{10}\,\mathrm{cm}^{-2}$; $\alpha = 3.9 \times 10^{-3}\,\mathrm{K}^{-1}$. Alloying temperature, T (°C): 1, triangles down, 420; 2, triangles up, 450.

samples were prepared using MOCVD epitaxial growth on a sapphire substrate at $T = 1050$ °C with a doping level of $10^{17}\,\mathrm{cm}^{-3}$ and a dislocation density of the order of $10^8\,\mathrm{cm}^{-2}$.[15] The agreement between theory and experiment in this case was not as good as in the previous case due to the variation in the structure parameters at the interfacial plane. We believe, however, that this agreement is fairly good because it enabled us to obtain correct values for both the position of the minimum of the $R_c(T)$ curve and the minimal R_C value. In particular, the realization of an $R_c(T)$ minimum at a temperature of about 270 K indicates a high density of scattering dislocations (of the order of $10^9\,\mathrm{cm}^{-2}$). The results are also supported by X-ray measurements. In summarizing the results obtained for GaN, it should be emphasized that the presence of a well-pronounced descending part in the $\mu(T)$ dependencies (see Fig. 3) is sufficient to explain the increase of $R_c(T)$.

B. InP case

Let us next consider the cases when either the $\mu(T)$ dependencies contain a peak or they increase to high temperatures at an arbitrary interrelation between R_{diff} and R_{sh}. Such a situation is fairly typical of InP-based structures. To illustrate this, in Fig. 6 we present our experimental and calculated $R_c(T)$ data obtained for the Au-TiB_x-AuGe-n-n^+-InP structures with high dislocation density and a semiconductor doping level of $9 \times 10^{15}\,\mathrm{cm}^{-3}$ (circles and triangles, experimental data; curves, calculated dependencies $R_c(T)$ obtained using Eq. (20) for two samples with different alloying temperature of ohmic contact). Since in this case the resistances $R_{diff}(T)$ and $R_{sh}(T)$ are in series, the total resistance is determined by their larger value. In the case of the relation $R_{sh}(T) > R_{diff}(T)$, the mechanism proposed in Ref. 1 is valid.

To ensure the required increase in $R_c(T)$ with temperature, the R_{sh} value has to be proportional to the distance d_D that electrons travel through a dislocation from the bulk semiconductor to the metal contact, and inversely proportional to r^2. In Refs. 1–3, it was assumed that $d_D = w$. However, the electrons can enter a shunt only at the end of the dislocation where the required value of the electrostatic potential is realized. Thus they have to travel over the whole dislocation length. With this assumption for this case, the required R_{sh} value may be ensured by varying either the conducting dislocation density or metal shunt diameter.

According to Ref. 16, p. 223, the diameter of the dislocation nucleus may be sufficiently large (>1 nm). Therefore, several needles composed of metal atoms can be located in it. Let it be gold that penetrates into a dislocation. For gold, resistivity $\rho \approx 2.25 \times 10^{-6}$ Ω·cm and its temperature coefficient $\alpha = 3.9 \times 10^{-3}\,\mathrm{K}^{-1}$. Taking into account that the conducting dislocation density is $\sim 10^{10}\,\mathrm{cm}^{-2}$, good fitting can be obtained by setting $d_D \approx 1$ μm and $r \approx 2.8 \times 10^{-8}$ cm (i.e., two atomic radii of gold). An analysis of the obtained data (Fig. 6) demonstrates that the agreement between the theory and experiment for R_{sh} is fairly good.

C. GaAs case

If there is no peak in the $\mu(T)$ curve (the electron mobility increases with T up to the highest measured temperatures) and the inequality $R_{diff} > R_{sh}$ holds, then if the proposed mechanism of diffusion limitation is realized the temperature dependencies of R_c will demonstrate the decrease, as in the case of the thermionic mechanism for Schottky contact. Figure 7 shows the experimental and calculated $R_c(T)$ curves for the case of contact to GaAs-based material with a doping level of $4 \times 10^{15}\,\mathrm{cm}^{-3}$. The experimental curves were obtained for an In-GaAs alloyed contact.[17] The authors of Ref. 16 suggested that the presence of decreasing dependencies $R_c(T)$ proves that the thermionic mechanism of current flow is realized in the contact. They determined the barrier height (which turned out to be anomalously low) from the slope of the $R_c(1/T)$ curve. It should be emphasized that we obtained the satisfactory agreement between the theory and experiment in the framework of the mechanism proposed by us in this work assuming that the density of conducting dislocations is of the order of $10^7\,\mathrm{cm}^{-2}$. In this case, both characteristics, i.e., the value of contact resistance and its temperature dependence, can be theoretically described. A large increase of contact

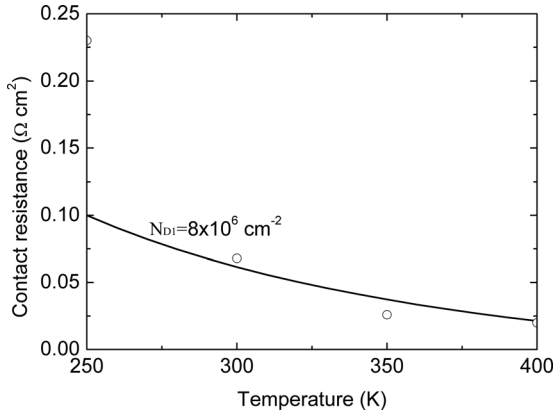

FIG. 7. Temperature dependencies of In-GaAs ohmic contact resistance. Circles, our experimental data, curves, theory. The following parameters are used for the calculation: $N_d = 4 \times 10^{15}\,\mathrm{cm}^{-3}$; $V_T = 4 \times 10^7$ cm/s; $y_{c0} = 0.8$.

resistance is due to the restriction of the current flow to a relatively small area. Our estimate shows that the relative area, $\pi L_D^2 N_{D1}$, is of the order of 10^{-3} at a semiconductor doping level of $4 \times 10^{15}\,\mathrm{cm}^{-3}$ and $N_{D1} \sim 10^7\,\mathrm{cm}^{-2}$. The reduction of contact resistance at low temperatures in our model is correlated with a comparatively weak freezing-out because of low donor energy and electron scattering on dislocations. Combining the above factors allows us to explain the results obtained in this work. The estimated resistance of indium shunts using the values $d_D = 5 \times 10^{-5}\,\mathrm{cm}$, $r = 5 \times 10^{-8}\,\mathrm{cm}$, and $N_{D1} = 2.5 \times 10^7\,\mathrm{cm}^{-2}$ gives a value that is smaller than the experimental R_c value by a factor of 7 at $T = 400\,\mathrm{K}$. Thus, the relation $R_{sh}(T) < R_{diff}(T)$ that is required to realize decreasing dependencies $R_c(T)$ is valid in this case.

Figure 8 shows the experimental and calculated temperature dependencies of contact resistance for the Au-Ti-Pd_2Si-n^+-Si structures. Si has $\rho \approx 0.0025\ \Omega\cdot$cm that corresponds to the doping level of $1.5 \times 10^{19}\,\mathrm{cm}^{-3}$. In calculating the theoretical $R_c(T)$ curves, we used the expressions for Debye screening length and electron diffusion coefficient taking into account semiconductor degeneracy. The temperature dependence of electron mobility in n-silicon was used from Ref. 18, p. 132 for the doping level of $10^{19}\,\mathrm{cm}^{-3}$. A very good agreement between the theory and experiment is found. It was achieved by suggesting appropriate semiconductor degeneracy at temperatures $\leq 200\,\mathrm{K}$.

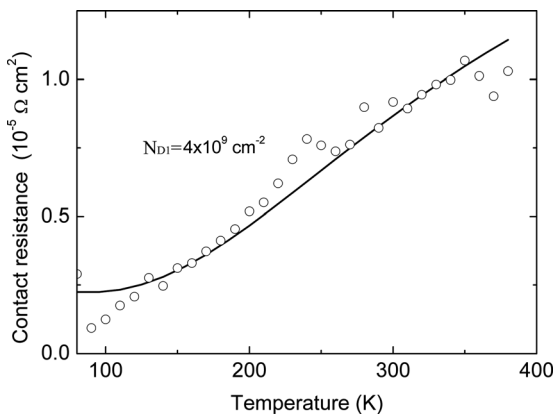

FIG. 8. Temperature dependencies of Au-Ti-Pd_2Si-n^+-Si ohmic contact resistance. Circles, our experimental data, curves, theory. The following parameters are used for the calculation: $N_d = 1.5 \times 10^{19}\,\mathrm{cm}^{-3}$; $V_T = 10^7$ cm/s; $y_{c0} = 2$.

The results allow us to determine the densities of scattering and conducting dislocations by comparing the theoretical and experimental dependencies of contact resistance as a function of temperature. Thus, the proposed concept has a heuristic capability for the determination of new parameters of metal-semiconductor contacts.

It should be noted that no averaging was applied when fitting the experimental dependencies using calculated ones. This demonstrates that the scattering in parameters related to lateral nonuniformity of contact does not play a crucial role.

IV. CONCLUSIONS

The mechanism of formation of metal-semiconductor contact resistance proposed here may take place, first of all, in wideband-gap semiconductors with a high density of dislocations and surface states in the contact. It seems paradoxical because, according to this mechanism, current flows through the depletion rather than accumulation regions.

At the same time, there are a number of facts definitely supporting this mechanism. The theory developed is in good agreement with the experimental results such as increasing contact resistance R_c with increasing temperature, weak dependence of contact resistance on the semiconductor doping level as well as strong dependence of R_c and the position of the minimum in the temperature dependence of R_c on the dislocation density. The above agreement was obtained for the contacts not only to III–V semiconductors but on heavily doped silicon as well.

The realization of the proposed mechanism does not exclude the possibility of contact resistance decreasing with temperature increase over the whole measurement range. This is more likely in the structures with low-energy optical phonons and the mechanism has been demonstrated in weakly doped gallium arsenide.[17] Characteristic features in this case are high contact resistance and extremely low contact barrier height obtained on the assumption that the traditional thermionic mechanism of current flow is predominant.

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[1]T. V. Blank, Yu. A. Gol'dberg, O. V. Konstantinov, V. G. Nikitin, and E. A. Posse, Tech. Phys. Lett. **30**, 806 (2004).
[2]T. V. Blank and Yu. A. Gol'dberg, Semiconductors **41**, 1263 (2007).
[3]V. N. Bessolov, T. V. Blank, Yu. A. Gol'dberg, O. V. Konstantinov, and E. A. Posse, Semiconductors **42**, 1315 (2008).
[4]T. Clausen, O. Leistiko, I. Chorkendorff, and J. Larsen, Thin Solid Films **232**, 215 (1993).
[5]G. Y. Chang, Y. K. Fang, and S. M. Sze, Solid-State Electron. **14**, 541 (1971).
[6]R. K. Kupka and W. A. Anderson, J. Appl. Phys. **69**, 3623 (1991).
[7]S. M. Sze and Kwok K. Ng, *Physics of Semiconductor Devices*, 3rd ed. (John Wiley and Sons, 2007).

[8]V. L. Bonch-Bruevich and S. G. Kalashnikov, *Physics of Semiconductors*, 2nd ed. (Nauka, Moscow, 1990) (in Russian).
[9]K. Seeger, *Semiconductor Physics* (Springer-Verlag, Vienna-New York, 1973).
[10]J. H. You and H. T. Johnson, Solid State Phys. **61**, 143 (2009).
[11]W. Götz, N. M. Johnson, C. Chen, H. Liu, C. Kuo, and W. Imler, Appl. Phys. Lett. **68**, 3144 (1996).
[12]W. Walukiewicz, J. Lagowski, L. Jastrzebski, P. Pava, M. Lichtensteiger, and G. H. Gatos, J. Appl. Phys. **51**, 2659 (1980).
[13]V. V. Galavanov and N. V. Siukaev, Phys. Status Solidi **38**, 523 (1970).
[14]D. K. Ferry, Phys. Rev. B **14**, 1605 (1976).
[15]V. P. Klad'ko, S. V. Chornen'kii, A. V. Naumov, A. V. Komarov, M. Tacano, Yu. N. Sveshnikov, S. A. Vitusevich, and A. E. Belyaev, Semiconductors **40**, 1060 (2006).
[16]H. F. Matare, *Defects Electronics in Semiconductors* (Wiley-Interscience, 1971).
[17]T. V. Blank, Yu. A. Gol'dberg, O. V. Konstantinov, V. G. Nikitin, and E. A. Posse, Tech. Phys. **52**, 285 (2007).
[18]V. I. Fistul', *Heavily Doped Semiconductors* (Plenum Press, New York, 1969).