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FABRICATION, TREATMENT, AND TESTING OF MATERIALS AND STRUCTURES

The Mechanism of Contact-Resistance Formation on Lapped *n*-Si Surfaces

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Abstract—Anomalous temperature dependences of the specific contact resistance $\rho_c(T)$ of Pd_2Si–Ti–Au ohmic contacts to lapped *n*-Si with dopant concentrations of 5×10^{16}, 3×10^{17}, and 8×10^{17} cm^{-3} have been obtained. The anomalous dependences of $\rho_c(T)$ have been accounted for under the assumption that the current flows along nanodimensional metallic shunts, which are combined with dislocations with a diffusion-related limit in the supply of charge carriers taken into account. The densities of conducting and scattering dislocations in the surface region of the semiconductor are determined.

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1. INTRODUCTION

The formation mechanisms and electrical properties of ohmic contacts to various semiconductor devices based on silicon are known and well studied [1–4]. In a wide range of doping of near-contact layers, the flow of current in such contacts is described by theories and models, which have become classical [1]. At the same time, the temperature dependences of the specific contact resistance $\rho_c(T)$ for ohmic contacts to silicon devices have not been studied in sufficient detail and have not been analyzed. The anomalous dependences $\rho_c(T)$ observed in some studies (an increase in ρ_c as temperature is increased) are not accounted for by universally accepted models [4, 5]. Ascending dependences $\rho_c(T)$ were also reported in publications by Goldberg et al.; the corresponding experiments were performed with alloyed ohmic contacts to GaP and GaN with a high concentration of structural defects in the near-contact region of a semiconductor. The dependences $\rho_c(T)$ were accounted for [6–10] under the assumption that the current flows along nanodimensional metal shunts combined with dislocations. However, such a model described only the linear increase in ρ_c while the experimental dependences $\rho_c(T)$ were more complex in a number of cases. A more general explanation of the experimentally observed dependences $\rho_c(T)$ was suggested recently [11–13]. The main distinction between publications [6–10] and [11–13] is the fact that, in the latter case, the appearance of a potential well for electrons (in other words, accumulation band bending) is taken into account at the end of the metal shunt. This made it possible to consistently explain the temperature dependences of ρ_c obtained previously [6–13].

It was theoretically shown by Sachenko et al. [13] that the suggested model can be used starting from a density of conducting dislocations of $\geq 10^6$ cm^{-2} (dislocations at which the shunts are localized). Such a density of dislocations can be in fact attained on lapped semiconductor surfaces [14, 15]. Therefore, it appeared to be reasonable to check the efficiency of the model in the case of the formation of an ohmic contact to a lapped silicon surface. Ohmic contacts formed on lapped silicon are in fact model contacts since they make it possible to study the effect of dislocations on the temperature dependence of ρ_c. In addition, since lapped silicon is still used in the technology of high-power high-voltage rectifying silicon elements [16, 17], information on the dependence $\rho_c(T)$ is of interest for scientists and engineers engaged in the development of such devices.

2. THEORETICAL CONCEPTS

We now describe the theoretical approach to calculating the contact resistance in ohmic contacts to *n*-Si with a high density of dislocations. First of all, we note that the mentioned contacts are ohmic irrespective of the relation between the contact and bulk resistivities. This is possible only in the case where the current flows through regions enriched with electrons. In this situation, the entire applied voltage drops in the quasi-neutral volume, due to which the ohmic properties of the contacts are exactly realized.

The contribution of the thermionic current flowing through electron-enriched regions can decrease with an increase in temperature if limitation by the diffusion supply is taken into account; this gives rise to an increase in the contact resistance. Implementation of the condition for limitation of the current by diffusion supply is conducive to a fairly high density of scattering dislocations, which gives rise to a decrease in the mobility.

In this case, a metal–semiconductor contact is inhomogeneous with respect to the value of the contact potential. For example, in regions of the emergence of dislocations related to metallic shunts, a positive value of the contact potential φ_{c0} is established and corresponds to a potential well for electrons, while the potential φ_{c1} is negative, which corresponds to the existence of a Schottky barrier. Further, under the contact potential, we will mean the diffusion (built-in) potential φ_c, which is measured from the edge of the conduction band of the semiconductor to the bottom of the potential well or the top of the barrier [1].

The total current flowing through the contact is the sum of currents flowing through the dislocations combined with metallic shunts (conducting dislocations) and also of currents flowing between dislocations. The flow of currents between dislocations makes it possible to implement ohmic contacts with the value of the contact resistance to be calculated in what follows.

In calculations of the contact resistance, we will assume that the contribution of the current flowing between dislocations can be disregarded in the case of a high density of dislocations. This assumption is based on a large value of the contact potential (which can be as high as on the order of one volt) which is related to a high concentration of surface states. We calculate first the thermionic current flowing through an individual dislocation. The area S_1 from which the above-mentioned current is collected is given by πL_D^2:

$$S_1 = \pi L_D^2, \tag{1}$$

where

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

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

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

here, $\eta = E/kT$ is the dimensionless kinetic energy of an electron and $z = E_F/kT$ is the dimensionless Fermi energy in the semiconductor [18].

The surface density of the thermionic current J_{nc} flowing through the contact at the site of dislocation emergence (at its face end) can be found by solving the continuity equation for electrons. Double integration of this equation with respect to the coordinate x perpendicular to the metal–semiconductor interface yields a relation between the bulk electron concentration n_w and the nonequilibrium electron concentration $n(x)$ at point x in the near-contact space-charge region (SCR). In the case of a nondegenerate semiconductor, we have

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

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

The quantity J_{nc} is defined by the expression [1]

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

where q is the elementary charge; V_T is the average thermal velocity of electrons; n_c is the nonequilibrium and $n_{c0} = n_w \exp y_{c0}$ is the equilibrium concentrations of electrons, respectively, in the contact plane; and $y_{c0} = q\varphi_{c0}/kT$ is the equilibrium dimensionless potential at the metal–semiconductor interface.

The value of the nonequilibrium electron concentration n_c in the contact plane is found from the equation

$$n_c = e^{y_c}\left(n_{c0} - \frac{V_T(n_c - n_{c0})}{4D_n}\int_0^w e^{-y(x)}dx\right). \tag{6}$$

Substitution of the obtained expression for n_c into formula (5) taking into account the fact that the dimensionless nonequilibrium potential $y_c = y_{c0} + \ln(qV/kT)$ (this is the condition for the ohmic property of a contact) makes it possible to obtain the following expression for the density of the electron current flowing through the metal–semiconductor contact at the site of dislocations emergence:

$$J_c = \frac{V}{\rho_{c0}}, \tag{7}$$

where

$$\rho_{c0} = \frac{kT}{q}\frac{\left(1 + \frac{V_T}{4D_n} - e^{y_{c0}}\int_0^w e^{-y(x)}dx\right)}{(qV_T/4)n_w e^{y_{c0}}}. \tag{8}$$

In calculation of the value of ρ_{c0}, we took into account that

$$\int_0^w e^{-y}dx = L_D\int_{y_c}^{y_x}\frac{e^{-y}dy}{(e^y - y - 1)^{0.5}}. \quad (9)$$

The calculation shows that the value of the integral in expression (9) in the case where $y_x = 0.5$ varies from 0.56 at $y_{c0} = 1.5$ to 0.65 at $y_{c0} = 0.35$ and practically remains unchanged at larger values of y_{c0}.

The value of the contact resistance determined by the mechanism of diffusion supply was found from the following formula for a unit-area contact:

$$\rho_c = \frac{\rho_{c0}}{\pi L_D^2 N_{D1}}; \quad (10)$$

here, N_{D1} is the density of dislocations involved in charge transport (conducting dislocations). Generally, the density of dislocations involved in the transport of charge carriers (N_{D1}) differs from the density of those involved in scattering (N_{D2}). The dislocations perpendicular to the interface are mainly involved in the transport of charge carriers, while the dislocations parallel to the interface mainly contribute to scattering.

The quantity $\pi L_D^2 N_{D1} S$, where S is the contact's area, has the meaning of the total area from which the current flowing through all dislocations is collected. As a rule, the value of $\pi L_D^2 N_{D1}$ is much smaller than unity even at the highest densities of dislocations on the order of 10^{10}–10^{11} cm^{-2}, except for the case of lightly doped semiconductors with $N_d \le 10^{15}$ cm^{-3}, where N_d is the concentration of shallow donor levels.

The diffusion coefficient of electrons equals $D_n = kT\mu_n/q$ with the Einstein relation taken into account. We determined the electron mobility in silicon μ_n taking into account scattering of electrons in the case of three main mechanisms of charge-carrier scattering: scattering at charged impurities ($\mu_Z(n_w)$), at dislocations ($\mu_D(n_w, N_{D2})$) [19], and also at acoustic intravalley and intervalley phonons μ_a [20]:

$$\mu_n = (\mu_Z(n_w)^{-1} + \mu_D(n_w, N_{D2})^{-1} + \mu_a^{-1})^{-1}. \quad (11)$$

As a result of the fact that the depth of donor levels in silicon E_d is fairly large, the temperature dependence of the contact current and, consequently, also of the contact's resistivity at low temperatures is determined both by the dependence $\mu_n(T)$ and by the effect of the freezingout of electrons.

With the freezing-out effect taken into account, the Fermi level E_F in a nondegenerate semiconductor is determined from the equation of bulk neutrality of the type

$$\frac{N_d}{1 + \exp((E_F - E_d)/kT)} = N_{c0}\left(\frac{T}{300}\right)^{3/2}\exp\left(\frac{E_F}{kT}\right), \quad (12)$$

where N_{c0} is the effective density of states in the conduction band at the temperature $T = 300$ K.

Having calculated from (12) the Fermi energy as a function of temperature, we find the electron concentration as a function of temperature, we determine the electron concentration n_w in the neutral semiconductor bulk at an arbitrary temperature:

$$n_w(T) = N_{c0}\left(\frac{T}{300}\right)^{3/2}\exp\left(\frac{E_F}{kT}\right). \quad (13)$$

Substitution of (13) into (8) and (11) makes it possible to finally determine the temperature dependence of the quantity ρ_c: $\rho_c(T)$.

Table 1. Values of the specific resistance ρ_c, the doping-impurity concentration N_d, the density of conducting dislocations N_{D1}, and the thickness d of the studied n-Si wafers

Sample no.	Lappening		
	1	2	3
ρ_c, Ω cm	0.12	0.045	0.024
N_d, cm^{-3}	5×10^{16}	3×10^{17}	8×10^{17}
N_{D1}, cm^{-2}	10^6	7×10^6	1.2×10^6
d, μm	~350 μm		

3. SAMPLES AND METHODS OF MEASUREMENTS

We studied the Au–Ti–Pd_2Si–n-Si ohmic contacts formed by layer-by-layer vacuum thermal deposition of the metals onto n-Si:P wafers heated to 300°C and cut from ingots of dislocation-free Si obtained by crucibleless zone melting. The sample parameters are listed in Table 1.

The n-Si wafers (samples nos. 1–3) were lapped on both sides with an M10 abrasive powder. The dislocation density in the initial substrates was estimated from etch pits appearing in the Si after treatment in a selective etchant. The density of surface structural defects (including dislocations) amounted to ~10^6 cm^{-2} (Fig. 1). It was found that, after formation of the metallization layers, their subsequent removal, and etching of Si, the density of structural defects (including that of conducting dislocations N_{D1}) remained practically unchanged. These data are consistent with theoretical estimates of the density of conducting dislocations. The calculated density of scattering dislocations was 10^7–2×10^8 cm^{-2} for the lapped samples.

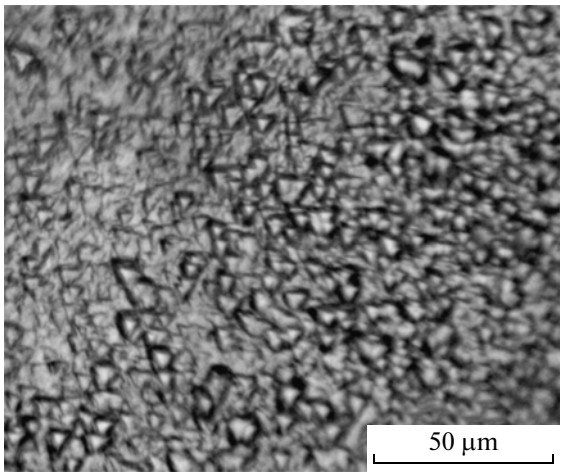

Fig. 1. Microstructure of the lapped surface of an *n*-Si wafer after selective etching.

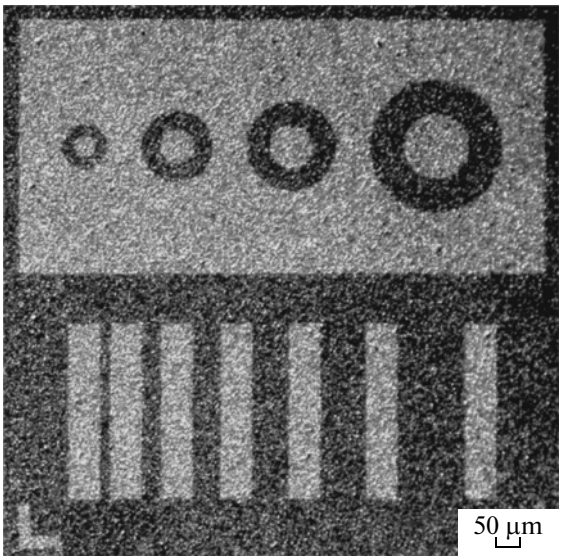

Fig. 2. Test structure for measuring the specific contact resistance. Fragment of a TLM structure $N_{D1} = 7 \times 10^6$ cm^{-2}.

An insignificant difference between the density of surface structural defects in the initial nonmetallized lapped samples and in the same samples after removal of the metallization is apparently related to the fact that the lapped surface is a more efficient sink (a getter) for structural defects appearing in the course of contact formation. The role of the microrelief in the reduction of the dislocation density in silicon structures obtained by the method of direct bonding during the fabrication of *p*–*n* junctions for high-power electronics was reported in [21–24].

It was shown by Argunova et al. [22] that the density of dislocations in the case of bonding of the microrelief silicon surface to the flat surface is lower by three orders of magnitude than that in the case of bonding of two flat surfaces.

The specific contact resistance was measured by the transmission line method (TLM) in the temperature range of 100–380 K. The test structures used in the measurements of ρ_c are represented in Fig. 2.

The phase composition of contact metallization was studied by the method of X-ray diffraction using a Philips X'Pert-MPD ($CuK_\alpha = 0.15418$ nm) diffractometer in Bragg–Brentano geometry. A typical diffraction pattern for the studied metallization layers is shown in Fig. 3.

The set of reflections from metallization is indicative of the polycrystalline structure of the separate Pd and Au metal layers. The lack of reflections from the Ti film is apparently related to the amorphous (according to X-ray measurements) state of this film, which features metallic conduction. The Pd_2Si phase is formed as a result of the interaction of Pd with Si during the course of Pd deposition onto the silicon substrate heated to 300°C; this is consistent with published data [24, 25] and with distribution profiles for components of metallization as obtained by the method of Auger electron spectrometry using a LAS-2000 spectrometer (Fig. 4). Indeed, it can be seen from Fig. 4 that not all of the palladium reacted with silicon with formation of Pd_2Si. Only a variation in the slope of the distribution profile for Si is observed, which is indicative of phase formation in the near-contact region but not of completion of the process since there are no corresponding flat regions in the profiles for Pd and Si.

4. EXPERIMENTAL RESULTS AND DISCUSSION

Figure 5 shows the temperature dependences $\rho_c(T)$ for ohmic contacts formed on lapped substrates doped

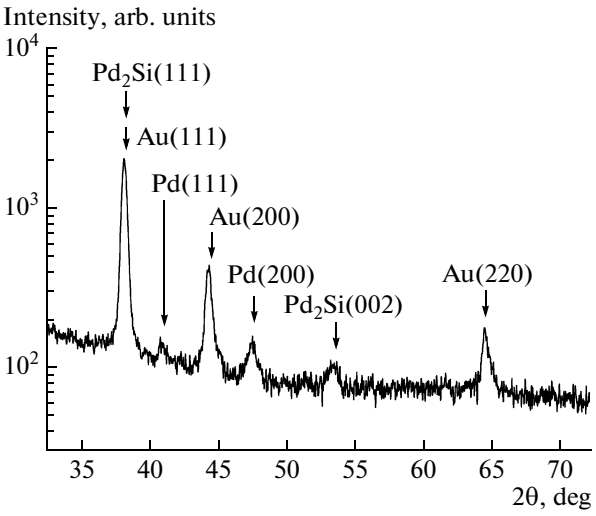

Fig. 3. X-ray diffraction patterns of contact metallization Au–Ti–Pd_2Si–*n*-Si deposited onto a lapped *n*-Si wafer heated to 300°C.

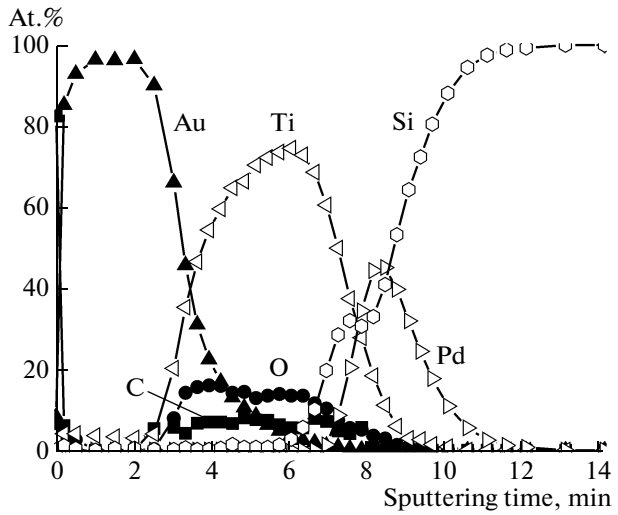

Fig. 4. Distribution profiles for components in the ohmic contact Au–Ti–Pd_2Si–*n*-Si after rapid thermal annealing at $T = 300°C$.

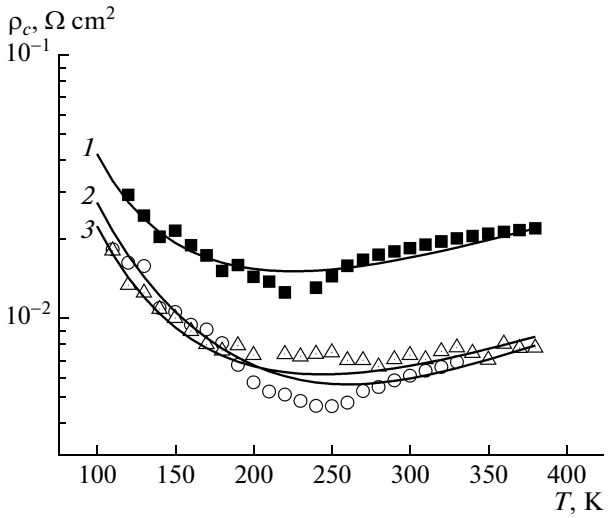

Fig. 5. Temperature dependences of ρ_c for Au–Ti–Pd_2Si–*n*-Si ohmic contacts: solid lines represent theory and symbols correspond to experimental data for samples 1–3 (curves *1*–*3*, respectively). $N_d = (1)\ 5 \times 10^{16}$, $(2)\ 3 \times 10^{17}$, and $(3)\ 8 \times 10^{17}$ cm^{-3}.

with 5×10^{16}, 3×10^{17}, and 8×10^{17} cm^{-3} of impurities. It can be seen that the value of ρ_c for lapped samples varies nonmonotonically with an increase in temperature. The observed dependences $\rho_c(T)$ in this case are consistent with the previously suggested [11–13] mechanism for the formation of an ohmic contact with a high density of structural defects in the near-contact region of the semiconductor under the assumption that there are two types of dislocations in this region: scattering dislocations, which are parallel to the interface, and conducting dislocations, which cross the SCR. In our modeling experiment, the nature of the latter dislocations is related to the polishing of the Si surface, while scattering dislocations predominantly appear as a result of mechanical stresses in the contact, which are related to the mismatch of the thermal-expansion coefficients and lattice parameters for Pd_2Si, Pd, and Si [26–28] and also to local concentrators of stresses. However, in this case, we cannot exclude also the possibility of the appearance of conducting dislocations.

The obtained results can be described in the following way.

(i) In the case, where ρ_c is limited by diffusion supply, the nonmonotonic dependences of ρ_c on temperature are typical of a nondegenerate semiconductor (curves *1*–*3*). As can be seen from Fig. 5, curve *3* for $N_d = 8 \times 10^{17}$ cm^{-3} carries on somewhat above the curve *2* for $N_d = 3 \times 10^{17}$ cm^{-3}. As follows from the theoretical dependences $\rho_c(T)$ described by expressions (10) and (11), the value of ρ_c depends on the densities of both conducting and scattering dislocations in the near-contact region. It is noteworthy that the value of ρ_c decreases as the density of conducting dislocations is increased and increases as the density of scattering dislocations is increased. As can be derived from the data listed in Table 2, the densities of scattering dislocations for samples 2 and 3 are equal to each other, whereas the density of conducting dislocations for sample 2 is higher by a factor of 1.2 than that in sample 3. This results in a decrease in the value of $\rho_c(T)$ for sample 2 compared to sample 3 in spite of the fact that a higher level of doping is conducive to a decrease in ρ_c. In addition, at low temperatures, the run of the dependence $\rho_c(T)$ is significantly affected by the value of y_{c0}. The larger y_{c0}, the more intense the increase in the value of $\rho_c(T)$ with decreasing temperature in the region of low temperatures. For example, the fitting value of y_{c0} was found to be equal to seven for curves *1* and *2*, while this value equals five for curve *3*.

(ii) As the measurement temperature is further increased, the value of ρ_c increases for all samples under study; this is caused by both a decrease in the contribution of scattering dislocations to the temperature dependence of mobility and an increase in scattering at phonons, which results in a decrease in μ_n as temperature is increased.

Table 2. Densities of scattering and conducting dislocations in the contacts for samples nos. 1–3

Sample no.	Density of scattering dislocations, N_{D2}, cm^{-2}	Density of conducting dislocations, N_{D1}, cm^{-2}	
	calculation	calculation	experiment
1	2×10^8	1.05×10^6	10^6
2	10^7	1.2×10^6	10^6
3	10^7	1.45×10^6	1.2×10^6

(iii) A comparison of the temperature dependences of ρ_c for ohmic contacts formed on nondegenerate samples of Si (Fig. 5) with those of ohmic contacts to degenerate n^+-Si (see [11]) shows that a portion with anomalous variation in ρ_c with increasing temperature is observed for both types of samples. This portion is caused by flow of the current through regions enriched with electrons and formed at ends of metal shunts in the case of current limitation by the diffusion supply of electrons.

Taking into account that depletion band bending is formed in the space between dislocations and the height of this bend is large due to a high concentration of surface states in the metal–Si contact, then, at a fairly high density of dislocations combined with metallic shunts, the current flowing through the dislocations becomes much higher than the current flowing between dislocations. As a result, the contact becomes ohmic. Another feature of the current flow through carrier-enriched SCRs in a semiconductor is the fact that the flowing current is often limited by diffusion supply, i.e., diffusion theory of the current flow takes place. In this case, the flowing current is directly proportional to the mobility of charge carriers μ_n, while $\rho_c \sim 1/\mu_n$. Since the temperature dependence of μ_n features, as a rule, a maximum and the value of μ_n decreases in the regions of both low and high temperatures, it may be expected that the value of ρ_c decreases, in particular, in the region of fairly high temperatures.

Theoretical dependences in Fig. 5 were drawn using expressions (1)–(13). Agreement between the theory and experiment is fairly good. In this consideration, the density of conducting dislocations N_{D1} amounts to $\sim 10^6$ cm^{-2} for all three samples, which is consistent with the density of structural defects estimated from etch pits. It is worth noting in this case that, in addition to dislocations crossing the SCR, other types of extended defects can appear during the course of contact fabrication; these defects can be conducive to the formation of metallic shunts.

5. CONCLUSIONS

Thus, the results of theoretical and experimental studies of the temperature dependences $\rho_c(T)$ for ohmic contacts to *n*-Si fabricated with the use of lapped samples, showed that the mechanism of contact-resistance formation characteristic of contacts with a high density of dislocations takes place in such contacts.

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