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Features of temperature dependence of contact resistivity in ohmic contacts on lapped *n*-Si

A. V. Sachenko,[1] A. E. Belyaev,[1] N. S. Boltovets,[2] A. O. Vinogradov,[1] V. P. Kladko,[1]
R. V. Konakova,[1] Ya. Ya. Kudryk,[1] A. V. Kuchuk,[1] V. N. Sheremet,[1] and S. A. Vitusevich[3,a)]
[1]*V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, Kyiv, Ukraine*
[2]*State Enterprise Research Institute "Orion," Kyiv, Ukraine*
[3]*Peter Grünberg Institute, Forschungszentrum Jülich, Jülich, Germany*

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The temperature dependence of contact resistivity ρ_c in lapped silicon specimens with donor concentrations of 5×10^{16}, 3×10^{17}, and $8 \times 10^{17}\,\mathrm{cm}^{-3}$ was studied experimentally. We found that, after decreasing part of the $\rho_c(T)$ curve in the low temperature range, an increasing part is registered with increasing temperature T. It is demonstrated that the formation of contact to a lapped Si wafer results in the generation of high dislocation density in the near-surface region of the semiconductor and also in ohmic contact behavior. In this case, current flows through the metal shunts associated with dislocations. The theory developed is in good agreement with experimental results. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4752715]

I. INTRODUCTION

A number of authors draw attention to the anomalous temperature dependence of contact resistivity ρ_c in ohmic contacts to different semiconductors: as the temperature increases, the ρ_c value increases instead of decreasing. For example, such an unusual behavior was observed in Refs. 1–3 for In-*n*-GaP and In-*n*-GaN alloyed ohmic contacts. The authors of Ref. 4 reported that the contact resistance of ohmic contacts (based on AuZn and AuGe alloys) to *p*-InP and *n*-InP, respectively, increases with temperature.

In Ref. 5, anomalous $\rho_c(T)$ dependence was obtained for ohmic contacts (formed with Pd_2Si phase) to heavily doped *n*-Si with a polished surface and, as a result of this, a high concentration of structural defects resulted in the near-contact region. In this work, the authors assumed that the temperature dependence of contact resistivity may be related to current flow through the metal shunts associated with dislocations in the space-charge region (SCR). It was suggested that regions at the boundary between silicon and dislocation ends accumulate electrons, and the current value is limited by the diffusion supply of electrons.

Such a concept was considered in more detail in Ref. 6. In this work, a theoretical explanation was developed for the experimental results obtained in Refs. 1–3 as well as for new experimental data obtained by the authors of Ref. 6, by recording temperature $\rho_c(T)$ curves, which increased with temperature in the GaN- and InP-based contacts. The experimental results were explained within the proposed theory.[6]

It should be noted that no increasing $\rho_c(T)$ dependences are observed in dislocation-free silicon crystals. At the same time, it is known that the lapped silicon surface has a microrelief and contains a large number of structural defects, in particular dislocations, whose density may be in the order of 10^7–$10^8\,\mathrm{cm}^{-2}$ (see Ref. 7). Such a surface also displays pronounced adhesive and gettering characteristics, which ensure the high quality of metal contacts and *p*-*n* junctions. It also serves as an efficient sink for defects, thus reducing their number. The authors of Refs. 8–11 reported on the role of microrelief produced using photolithography in reducing dislocation density near the Si-Si interface of *p*-*n* junctions formed for power electronics by direct silicon material joining. The important role of the structural factor in the formation of *p*-*n* junctions using direct silicon joining was also underlined.[10] In Ref. 11 it was shown that, if a Si surface with a microrelief is joined to a smooth surface, then the dislocation density lowers by three orders of magnitude in the case of joining two smooth surfaces.

Lapped Si wafers are used in manufacturing technology for *p*-*n* junctions and fabrication of ohmic contacts to high-power silicon isolators.[12,13] However, the temperature dependence of ρ_c for lapped *n*-Si surfaces as well as for power-integrated circuits made using modern microelectronic technologies (including direct joining of epitaxial and other high-quality polished silicon structures[13,14]) has not yet been studied. Therefore, the investigation of the temperature behavior of ohmic contacts to lapped *n*-Si wafers is important not only for fundamental studies of the effect of dislocations on ρ_c value, but also for practical applications to obtain information about the temperature dependence of ρ_c for structures used in power electronics.

In this work, we show that the fabrication of ohmic contacts to lapped silicon wafers leads to current flow through the metal shunts associated with dislocations and ohmic contact behavior. To prove this, we made contacts to initially dislocation-free silicon with a lapped surface and investigated experimentally the dependence $\rho_c(T)$ for the contacts obtained. It was shown that, at temperatures exceeding 250 K, the $\rho_c(T)$, curves increase with temperature. The results obtained are in good agreement with the developed theory.

a)Author to whom correspondence should be addressed. Electronic mail: s.vitusevich@fz-juelich.de. On leave from Institute of Semiconductor Physics, NASU, Kyiv, Ukraine.

II. THEORETICAL MODEL

Let us consider contact resistivity in ohmic contacts to *n*-Si with high dislocation density. First of all, it should be noted that such contacts are only ohmic, no matter what the relation between the contact and semiconductor bulk resistivities is, if the current flows through the regions with accumulated electrons. In this case, the total applied voltage drops across the quasi-neutral bulk, thus realizing contact ohmicity.

The contribution of thermionic current flowing through the regions with accumulated electrons may decrease as temperature increases (with possible current limitation by diffusion supply of electrons). This results in an increase of contact resistance. A sufficiently high density of scattering dislocations leads to a reduction of charge carrier mobility, thus favoring realization of the condition of current limitation by diffusion supply of electrons.

In our case, the metal-semiconductor contact has nonuniform redistribution of contact potential. For instance, a positive value of the contact potential φ_{c0} that corresponds to a potential well for electrons (see Ref. 15, p. 207) is realized at the sites of the formation of dislocations (associated with metal shunts) to the quasi-neutral region of the semiconductor, while the negative contact potential φ_{c1} (corresponding to the Schottky barrier) is realized between the dislocations. The contact potential is the diffusion (built-in) potential φ_c measured from the conduction band edge to the bottom of potential well (or to the barrier top).

The total current flowing through the contact is a sum of the currents flowing through metal shunts associated with dislocations (the so-called conducting dislocations) and those flowing between dislocations. Current flow through shunts helps to realize ohmic contacts whose contact resistivity will be calculated below.

When calculating contact resistivity, we have to assume that, in the case of high dislocation density, it is possible to neglect the contribution from the current flowing between dislocations. The reason for this is the high contact potential (up to a value of about 1 V) because of the high concentration of surface states. Let us first calculate the thermionic current flowing through a single metal shunt associated with a dislocation. The above current is collected from the area

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

where

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

is the Debye length in the case of a semiconductor with an arbitrary degree of degeneracy (see Ref. 16, p. 659), N_c is the effective density of states in the conduction band, and

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

where $\eta = E/kT$ is the dimensionless electron's kinetic energy and $z = E_f/kT$ is the dimensionless Fermi energy in the semiconductor (see Ref. 16, p. 659).

The surface density of the thermionic current J_{nc} flowing through the contact at the site of the formation of the dislocation (at its end) is determined by solving the continuity equation for electrons. Upon double integrating that equation with respect to the coordinate x (perpendicular to the metal-semiconductor interface), we obtain a relation between the bulk electron concentration n_w and the non-equilibrium electron concentration $n(x)$ at the point x of the near-contact SCR. In the case of 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 non-equilibrium potential at the point x, D_n is the electron diffusion coefficient, and w is the near-contact SCR width.

J_{nc} is determined by the following equation (see Ref. 15, pp. 157–158):

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

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

The non-equilibrium electron concentration at the contact plane, n_c, is determined as

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

By inserting the above expression for n_c in Eq. (5) and taking into account that the dimensionless non-equilibrium potential is $y_c = y_{c0} + \ln(qV/kT)$ (this is the condition of contact ohmicity), we obtain the following expression for the density of electron current flowing through the metal-semiconductor contact at the sites of dislocation outcrop,

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

where

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

It should be noted that in calculating ρ_{c0}, we took into account

$$\int_0^w e^{-y} dx = L_D \int_{y_c}^{y_x} \frac{e^{-y} dy}{(e^y - y - 1)^{1/2}}. \tag{9}$$

The calculation shows that, in the case that $y_x = 0.5$, the value of the integral in Eq. (9) varies from 0.56 (at $y_{c0} = 1.5$) up to 0.65 (at $y_{c0} = 3.5$) and remains practically constant at higher y_{c0} values.

In the case of the diffusion supply mechanism, the contact resistivity for a contact of unit area was determined by the following expression:

$$\rho_c = \frac{\rho_{c0}}{\pi L_D{}^2 N_{D1}}, \tag{10}$$

where N_{D1} is the density of conducting dislocations. Generally speaking, the densities of conducting dislocations (associated with metal shunts) (N_{D1}) and of those taking part in electron scattering (N_{D2}) are not equal. The dislocations perpendicular to the metal–semiconductor interface mainly take part in current flow while those parallel to that interface mainly take part in electron scattering.

The quantity $\pi L_D^2 N_{D1} S$ (S is the contact area) corresponds to the total area from which the current flowing through all metal shunts associated with conducting dislocations is collected. As a rule, the $\pi L_D^2 N_{D1}$ value is considerably below unity (even at maximal dislocation densities about 10^{10}–10^{11} cm^{-2}), except in the case of slightly doped semiconductors with $N_d \leq 10^{15}$ cm^{-3} (N_d is the concentration of shallow donor levels).

According to the Einstein relation, the electron diffusion coefficient is $D_n = kT\mu_n/q$. We determined the electron mobility in silicon, μ_n, taking into account the three main mechanisms of electron scattering: on charged impurities ($\mu_Z(n_w)$), on dislocations ($\mu_D(n_w, N_{D2})$) (see Ref. 17, pp. 166, 214), and on acoustic phonons, both intra- and inter-valley (μ_a)[18]

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

The donor level in silicon, E_d, is sufficiently deep. Therefore, the temperature dependence of the current (as well as of the contact resistivity) at low temperatures is determined by both the dependence $\mu_n(T)$ and the effect of electron freezing-out. Taking into account the above-mentioned effect, the Fermi level E_f in a nondegenerate semiconductor is determined from the bulk neutrality equation,

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

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

By calculating the Fermi energy as a function of temperature from Eq. (12), we can determine the electron concentration n_w in the neutral semiconductor bulk at an arbitrary temperature

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

The insertion of Eq. (13) in Eqs. (8) and (11) allows us to determine the dependence $\rho_c(T)$.

TABLE I. Resistivity ρ, impurity concentration N_d, dislocation density N_{D1} and thickness d of the n-Si wafers under investigation ($T = 300$ K).

Number of sample	1	2	3
ρ (Ω·cm)	0.120	0.045	0.024
N_d (cm^{-3})	5×10^{16}	3×10^{17}	8×10^{17}
N_{D1} (cm^{-2})	1.0×10^6	7.0×10^6	1.2×10^6
d (μm)	~350	~350	~350

III. SAMPLES AND METHODS OF MEASUREMENT

We studied the Au-Ti-Pd_2Si-n-Si ohmic contacts fabricated using layer-by-layer vacuum thermal deposition of metals onto n-Si (doped with phosphorus) wafers heated to 300 °C. The wafers were cut from the dislocation-free n-Si ingots obtained using crucibleless melting. The sample parameters are given in Table I.

The n-Si wafers (samples 1-3) were lapped on both sides with abrasive powder M10. The dislocation density was estimated from the density of etch pits that appeared in Si after treatment in the selective etchant CrO_3 (100 g per 200 ml H_2O):HF:H_2O = 1:2:3 (Fig. 1). The concentration of near-surface structural defects (including dislocations) in the lapped specimens was 1×10^6–7×10^6 cm^{-2}. The N_{D1} values calculated from the temperature dependence of ρ_c were in good agreement with those determined from the density of etch pits. The calculated values of both scattering and conducting dislocation densities are given in Table II. The ohmic contact was formed by the palladium silicide phase Pd_2Si that appeared in the course of metal deposition onto a Si wafer heated to 300 °C.

Owing to the mismatch of both the coefficients of thermal expansion and lattice parameters of materials (see Table III), stresses appeared in the Si near-contact region. Relaxation of those stresses increased the density of structural defects in the near-contact region of silicon as compared to the case of the initial lapped surface. The calculated density of scattering dislocations grew and reached 1×10^7–2×10^8 cm^{-2}.

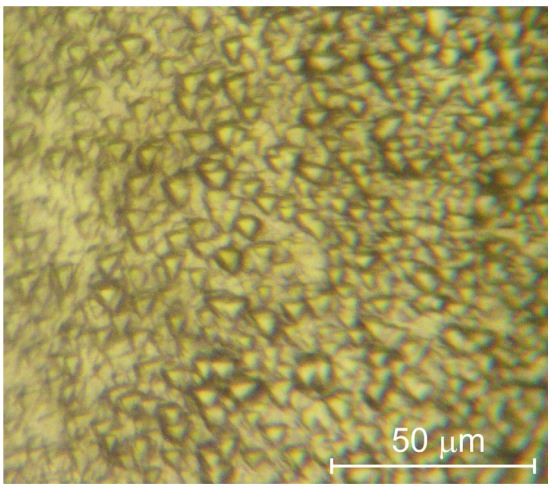

FIG. 1. Surface microstructure of lapped n-Si wafer after selective etching (a fragment); density of conducting dislocations is $N_{D1} = 7 \times 10^6$ cm^{-2}.

TABLE II. Densities of scattering and conducting dislocations in contacts to samples (1-3).

Number of sample	1	2	3
Density of scattering dislocations (cm^{-2}) (calculation)	2.00×10^8	1.00×10^7	1.00×10^7
Density of conducting dislocations (cm^{-2}) (calculation)	1.05×10^6	7.00×10^6	1.45×10^6
Density of conducting dislocations (cm^{-2}) (experiment)	1.0×10^6	7.0×10^6	1.2×10^6

The contact resistivity was measured in the 100–380 K temperature range by the transmission line method.[21] The phase composition of contact metallization was studied by the x-ray diffractometry technique in the Bragg-Brentano geometry using an x-ray diffractometer, Philips X'Pert–MRD ($Cu_{K\alpha} = 0.15418$ nm). To separate phases of thin layers, the experimental diffraction patterns were taken at different angles of x-ray incidence. Figure 2 shows the diffraction pattern obtained for the Au-Ti-Pd_2Si-*n*-Si contact metallization.

Phase analysis of the metallization layers showed that the following reflections were observed: Au (111; 200; 220), Pd (111; 200), and Pd_2Si (111; 002). The presence of the families of reflections from metallization indicates the polycrystalline structure of single Au and Pd layers. The absence of reflections from the Ti film can be related to its x-ray amorphous state having metallic conductivity. The Pd_2Si phase is formed upon Pd interaction with Si in the course of Pd deposition onto the wafer heated to 300 °C. This conclusion correlates with the data from x-ray diffraction and Auger electron spectrometry presented in Ref. 22.

TABLE III. Lattice parameters and coefficients of thermal expansion for Si, Pd, and Pd_2Si ($T = 300$ K).[19,20]

Material	Lattice parameters (nm)		Coefficient of thermal expansion α (K^{-1})
	A	*c*	
Si	0.543		2.54×10^{-6}
Pd	0.389		11.75×10^{-6}
Pd_2Si	0.6497	0.3437	

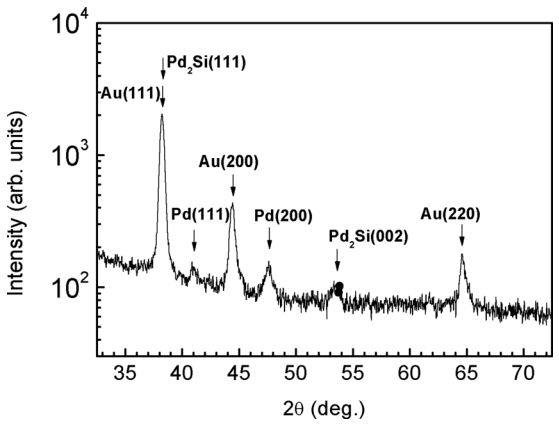

FIG. 2. X-ray diffraction pattern of the Au-Ti-Pd_2Si-*n*-Si contact metallization deposited onto a lapped *n*-Si wafer heated to 300 °C.

IV. EXPERIMENTAL RESULTS AND DISCUSSION

Curves 1-3, shown in Fig. 3 correspond to the $\rho_c(T)$ dependences of the Au-Ti-Pd_2Si-*n*-Si ohmic contacts made on the lapped *n*-Si wafers with impurity concentrations of 5×10^{16}, 3×10^{17}, and 8×10^{17} cm^{-3}, respectively. It can be seen that the resistivity ρ_c of the samples under investigation is a nonmonotonic function of temperature. The $\rho_c(T)$ curves calculated using Eqs. (1)–(13) agree well with the experimental $\rho_c(T)$ dependences (dots). The calculated density of conducting dislocations, N_{D1}, in the near-contact region varies within the range from 1×10^6 up to 7×10^6 cm^{-2} and practically coincides with the results of the metallographic analysis (see Table II). The density of scattering dislocations, N_{D2}, is about 10^7 cm^{-2}, except for one case where it is about 2×10^8 cm^{-2} (see curve 1 in Fig. 3). We explain such an increase of N_{D2} as being produced by contact alloying.

The results obtained can be explained in the following way:

1. If the ρ_c value is limited by a diffusion supply of electrons, then a nonmonotonic temperature dependence of ρ_c is typical of nondegenerate semiconductors (see Refs. 5 and 6). It can be seen from Fig. 3 that, at low temperatures, curve 3 for $N_d = 8 \times 10^{17}$ cm^{-3} passes above curve 2 for $N_d = 3 \times 10^{17}$ cm^{-3}. It follows from the theoretical $\rho_c(T)$ dependences described by Eqs. (8), (10), and (11) that contact resistivity ρ_c is a function of the density of conducting as well as scattering dislocations. As the density of conducting (scattering) dislocations grows, the ρ_c value decreases (increases). It can be seen from the data presented in Table II that the densities of scattering

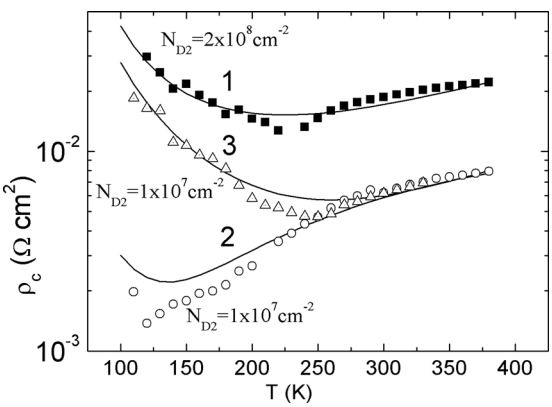

FIG. 3. Temperature dependence of contact resistivity ρ_c for three samples (1-3) of Au-Ti-Pd_2Si-*n*-Si ohmic contact (full curves-theory; symbols-experiment). Impurity concentration N_d, cm^{-3}: 1–5×10^{16}; 2–3×10^{17}; 3–8×10^{17}. The equilibrium dimensionless potential at the metal-semiconductor interface: y_{c0}: 1-5; 2-2; 3-5. Densities of scattering dislocations N_{D2} are indicated.

dislocations for samples 2 and 3 are the same, while the density of conducting dislocations for specimen 2 is five times greater than that for sample 3. This leads to a reduction of the $\rho_c(T)$ value for sample 2 in comparison to that for sample 3 despite the fact that the higher doping level favors a reduction of ρ_c. Besides, at low temperatures the value of accumulation band bending at the dislocation end, y_{c0}, essentially affects the $\rho_c(T)$ curves. The larger the band bending y_{c0}, the stronger is the increase of $\rho_c(T)$ at low temperatures as the temperature decreases. As an illustration, the fitting value of y_{c0} for curves 1 and 3 is five, while for curve 2 it is equal to two.

2. With a further rise in temperature (curves 1 and 3 after $T > 240$ K, curve 2 after $T > 125$ K), the contact resistivity ρ_c increases. The reason for this is that the contribution from scattering dislocations and charged impurities to the temperature dependence of electron mobility μ_n decreases, while that from scattering by phonons (leading to a reduction of μ_n with temperature) increases.
3. An analysis of the temperature dependences of ρ_c for ohmic contacts formed on lapped wafers of rather high-resistance nondegenerate silicon (curves 1–3) showed that a portion of the $\rho_c(T)$ curve corresponding to the anomalous temperature dependence of ρ_c was observed for all the samples under investigation. This portion is due to current flowing through the regions of electron accumulation. Those regions appeared at the metal shunt ends under the condition of current limitation by the diffusion supply of electrons.

The observed $\rho_c(T)$ dependences indicate the mechanism of ρ_c formation proposed in Refs. 5 and 6. The theory considers two types of dislocations in the near-contact region, namely, scattering dislocations (parallel to the metal–semiconductor interface) and conducting dislocations (crossing SCR). The origin of the latter dislocations is related to the lapping of Si surface, while the scattering dislocations are related to stress relaxation in the contact. The stress is result of mismatch of both the coefficients of thermal expansion and parameters of the Pd_2Si and Si lattices.

It should be noted that the increase of contact resistivity with temperature may be also realized, in principle, if the near-contact region contains a large number of other extended defects, on condition that they favor the formation of metal shunts penetrating into the semiconductor bulk.

V. CONCLUSION

The results of experimental studies and theoretical analysis of the temperature dependence of contact resistivity, $\rho_c(T)$, of ohmic contacts to samples fabricated using lapped *n*-Si wafers indicate the mechanism of contact resistance formation that is typical of contacts with high dislocation density. This is supported by anomalous (increasing with temperature) $\rho_c(T)$ curves at sufficiently high temperatures as well as by the results of metallographic analysis reflecting rather high dislocation density.

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