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The features of temperature dependence of contact resistivity of Au–Ti–Pd_2Si–p^+-Si ohmic contacts

A.E. Belyaev[1], N.S. Boltovets[2], L.M. Kapitanchuk[3], R.V. Konakova[1], V.P. Kladko[1], Ya.Ya. Kudryk[1], A.V. Kuchuk[1], O.S. Lytvyn[1], V.V. Milenin[1], T.V. Korostinskaya[2], A.B. Ataubaeva[4], P.V. Nevolin[1]
[1]*V. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine*
41, prospect Nauky, 03028 Kyiv, Ukraine, e-mail: konakova@isp.kiev.ua
[2]*State Enterprise Research Institute "Orion", 8a, Eugene Pottier str., 03057 Kyiv, Ukraine*
E-mail: bms@i.kiev.ua
[3]*E.O. Paton Electric Welding Institute, NAS of Ukraine, Kyiv, Ukraine*
[4]*Berdakh Karakalpak State University, Nukus, Republic of Uzbekistan*

Abstract. We consider the features of formation of Au–Ti–Pd ohmic contacts to p^+-Si. Metallization was made by vacuum thermal sputtering of Pd, Ti and Au films onto the Si substrate heated up to 330 °C. It is shown that the contact resistivity increases with temperature; this is typical of metallic conductivity. We suggest that the ohmic contact is formed owing to appearance of shunts at Pd deposition on dislocations or other structural defects. The number of shunts per unit area is close to the measured density of structural defects at the metal–Si interface.

Keywords: ohmic contact, contact resistivity, metallic shunt, palladium, palladium disilicide, p^+-Si.

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1. Introduction

Reliability of the component base of solid-state microwave electronics is determined, to a large degree, by the structural properties of active elements because they are characterized by rather high residual level of intrinsic stresses. The nature of the latter is related to different physical factors. These are (i) lattice misfit for heavily and low-doped regions of *p*-*n* junctions (misfit stress), (ii) disagreement of the coefficients of thermal expansion for semiconductor and metal in the case of ohmic or barrier contact (thermal stress), (iii) various semiconductor structural defects to which local stresses are related, etc.

The external actions, such as current loads, radiation, high-frequency electromagnetic radiation, elevated temperature, lead to relaxation of intrinsic stresses. The relaxation is accompanied with appearance of new defects resulting in variation of the parameters of semiconductor devices or mass transfer in the metallization layers. This leads to appearance of extended junction layers and, ultima analysi, to contact degradation. In the last case, external actions, especially heating, are of importance [1-4]. Subjected to such actions are, e.g., high-power silicon pulse IMPATT diodes whose local areas may be overheated up to temperatures ≥350 °C [5, 6]. Therefore, the studies of interactions between phases in ohmic contacts to heavily doped p^+- and n^+-regions are topical.

2. The samples and methods of investigation

We studied interactions between phases in palladium-disilicide-based ohmic contacts to heavily doped p^+-silicon layers. The latter were formed by boron diffusion (up to concentrations of 5×10^{19}–2.5×10^{20} cm^{-3}) into an *n*-n^+-Si epitaxial structure. The *p*-*n* junction depth was ~$(3–9.8)\times10^{-5}$ cm. We studied the samples of two types: (i) test structures with continuous metallization layer and (ii) TLM-structures for measurement of contact resistivity ρ_c with the transfer length method (TLM).

The ohmic contacts were made using vacuum thermal sputtering of Pd (500 Å)–Ti (500 Å)–Au (1200 Å) onto a Si substrate heated up to 330 °C. The sputtering times were as follows: Pd (15 s) – Ti (45 s) – Au (30 s). The concentration depth profiles and phase composition of the metallization were measured using Auger electron spectroscopy and x-ray diffractometry (XRD), respectively. The Si surface morphology after removal of metallization was studied using atomic force microscopy.

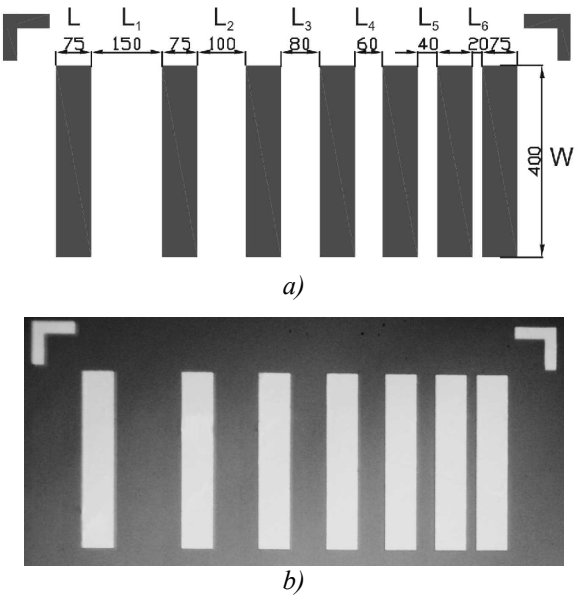

Fig. 1. A photomask for contact resistivity measurement with the TLM method: *a* – geometry of contact pads for TLM with linear contacts; *b* – photomask appearance.

The contact resistivity measurements were performed in the 77–400 K temperature range. We used a structure involving a number of identical rectangular ohmic contacts (width $W = 400$ μm and length $L = 75$ μm) placed with a variable spacing, $L_i = (L_1, \ldots, L_6)$ (see Fig. 1a).

The total resistance between two contacts is [7]

$$R_1 = \frac{R_{SH} L_i}{W} + 2\frac{L_T R_{SK}}{W} \coth\left(L / L_T\right). \qquad (1)$$

Here $L_T = \sqrt{\rho_c / R_{SK}}$ is the transfer length; the first term in the right-hand side of Eq. (1) describes the resistance of semiconductor region with the semiconductor surface resistivity R_{SH}, while the second term is a sum of the contact resistance and that of current spreading under the contact; R_{SK} is the surface resistivity of semiconductor layer under the metal layer. If $L > 3L_T$ (which is true in our case), then $\coth\left(L/L_T\right) \to 1$. Assuming $R_{SK} \approx R_{SH}$, one obtains the following simplified expression for the total resistance:

$$R_i = \frac{R_{SH} L_i}{W} + 2\frac{L_T R_{SH}}{W}. \qquad (2)$$

By measuring the temperature dependence of the total resistance between two pairs of contacts, one obtains the temperature dependence of the surface resistance $R_{SH} = W\dfrac{R_1 - R_2}{L_1 - L_2}$; after this, it is easy to calculate the temperature dependence of contact resistivity:

$$\rho_c = L_T^2 R_{SH} = \left(WR_i - R_{SH} L_i\right)^2 / 4R_{SH}. \qquad (3)$$

The measurement was made using the current and potential probes. This made it possible to exclude the contribution from resistance of probes to the total resistance.

3. Results and discussion

The results of our measurements are as follows:

- the measured resistance of the Au–Ti–Pd_2Si–p^+-Si structure varies linearly with the spacing between contacts (see Fig. 2);
- the measured resistance increased with temperature in the 77–400 K temperature range;
- the contact resistivity increased with temperature in the 77–400 K temperature range (Fig. 3).

It is known that similar temperature dependence of ρ_c (growth with temperature) was studied earlier in [8, 9]. The authors of [8, 9] ascribed such a behavior to conduction via metallic filaments (shunts). The latter appear owing to deposition of the atoms of contact-forming metal on structural defects whose density (in the experiments [8, 9]) was $>10^7$ cm^{-2}. According to [10, 11], the dislocation density in a p^+-n-n^+ structure doped with boron up to $\geq 5\cdot10^{19}$ cm^{-3} was $\geq 10^8$ cm^{-2}. So one can assume that, in the course of palladium sputtering, the Pd atoms may deposit on dislocations and form metallic shunts that cause increase of ρ_c with temperature. Indeed, in accordance with [10, 11], the maximal dislocation density N_D in the diffuse layer is

$$N_D = 0.428\frac{\beta}{\alpha}\left(\frac{N_S}{\sqrt{Dt}}\right). \qquad (4)$$

Here β is the compression coefficient for Si lattice caused by boron doping (it equals 5×10^{-24} cm^3/atom [12]); $\alpha = \dfrac{a\sqrt{2}}{8}$, where a is the Si lattice constant (equal to 5.43×10^{-8} Å); N_S is the surface concentration of boron; D is the boron diffusion coefficient; t is the diffusion time, and

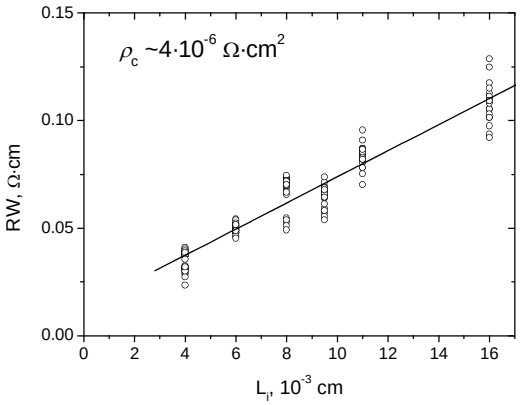

Fig. 2. Dependence of the product of the measured resistance between contacts and the contact width of the Au–Ti–Pd_2Si–p^+-Si structure (see Fig. 1) on the distance between contacts (averaged over 32 masks); $p^+ \sim 5\cdot10^{19}$ cm^{-3}.

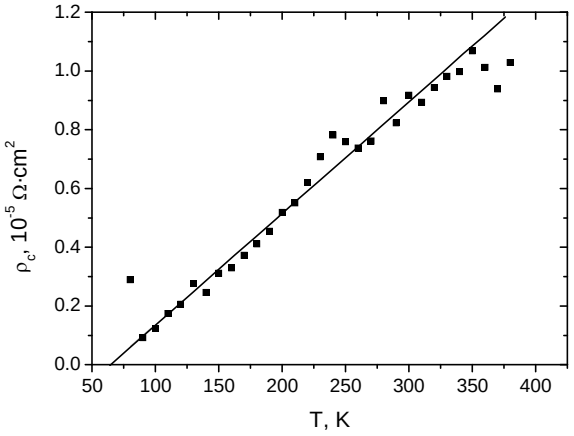

Fig. 3. Temperature dependence of contact resistivity (the measurements were performed for a single mask); p^+~ $5\cdot10^{19}$ cm^{-3}.

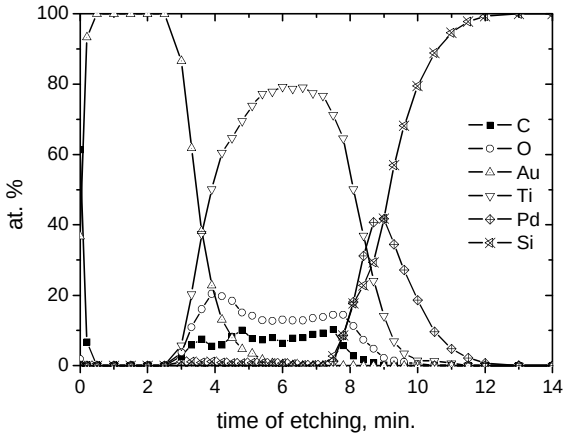

Fig. 5. Auger concentration depth profiles for components of the Au–Ti–Pd–p^+-Si metallization.

$$N_D = \frac{0.428\times5\times10^{-24}\,\text{cm}^3}{0.95\times10^{-8}\,\text{cm}}\cdot\frac{5\times10^{19}\,\text{cm}^{-3}}{0.98\times10^{-4}\,\text{cm}} =$$

$$= \frac{10.7\times10^{-5}}{0.93\times10^{-12}\,\text{cm}^2} \approx 1.1\times10^{8}\,\text{cm}^{-2}\,.$$

Let us calculate the resistance of such a shunt, $R_{sh} = \rho_{\text{Pd}}\dfrac{l}{S}$. Here l (S) is the shunt length (area); ρ_{Pd} is Pd resistivity. At T=300 K, it equals ~1.1×10^{-5} Ohm·cm. We assume that the shunt radius is close to the Si lattice constant. The atomic radius of Pd is $r \approx 1.37$ Å. The shunt area is $\pi r^2 = 3.14\times(1.37\times10^{-8}\,\text{cm})^2 = 5.89\times10^{-16}$ cm^2. If one takes the shunt length equal to the width W_l of the space-charge layer in the heavily doped Si layer ($p^+ \approx 5\times10^{19}$ cm^{-3}), then, at zero bias, $W_l = \sqrt{\dfrac{2\varepsilon_s\varepsilon_0}{q\,p^+}\left(V_{\text{D}} - \dfrac{kT}{q}\right)} \approx 5.2\times10^{-7}\,\text{cm}$. Here $\varepsilon_s = 11.7$ is the Si permittivity; $\varepsilon_0 = 8.85\times10^{-14}$ F/cm the vacuum permittivity; $V_D \approx$ (1.1–1.2) V the diffusion potential at the Pd/Si boundary. Taking into account that $l = W_l$, one obtains for the shunt resistance:

$$R_{sh} = 1.1\times10^{-5}\,\text{Ohm}\cdot\text{cm}\times\frac{5.2\times10^{-7}\,\text{cm}}{5.89\times10^{-16}\,\text{cm}^2} \approx$$

$$\approx 0.97\times10^{4}\,\text{Ohm} \approx 10^{4}\,\text{Ohm}\,.$$

It is easy to show that the calculated contact resistance at T = 300 K coincides with the experimentally observed one if one assumes that there are ~10^9 metallic shunts per 1 cm^2 of contact area. This value is close to the dislocation density generated in the course of p^+-layer formation in the diffusion layer, as well as to the density of structural defects revealed at the metal–Si boundary after removal of the metallization layers (Fig. 4). The latter fact indicates that, in the course of sputtering, some amount of Pd penetrates into Si (Fig. 5), with possible formation of Pd_2Si phase. This is confirmed by the results of x-ray phase analysis (Fig. 6).

However, we do not exclude a possibility that not all amount of Pd is spent for formation of the Pd_2Si phase. Some Pd atoms may deposit on the structural defects (without generating a new phase) and form a mixed interface. The authors of [2, 13] denoted a possibility of such processes. In that case, shunt formation and increase of planar nonuniformity of the contact junction are possible (see Fig. 4).

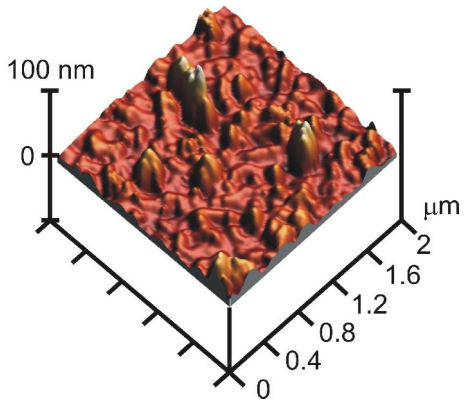

Fig. 4. Surface morphology of the metal–Si interface after removal of the metallization layers.

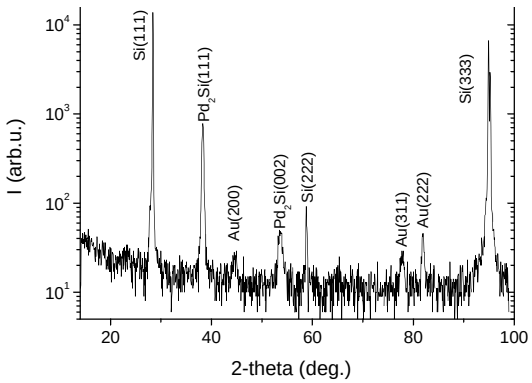

Fig. 6. XRD pattern of the Au–Ti–Pd–p^+-Si contact metallization.

A difference between the densities of dislocations and shunts may be related to the intrinsic stresses because of distinctions in the lattice constants of Si ($a \approx 5.43$ Å), Pd ($a \approx 3.89$ Å), Pd_2Si ($a \approx 6.49$ Å, $c \approx 3.43$ Å), and Pd atomic radius (1.37 Å). Such a factor was observed often in the contact systems. The authors of [8] believe that it may increase, by 1–2 orders of magnitude, the density of defects at which the shunts are localized. Absence of the corresponding titanium peaks in the XRD pattern may be related to presence of its compounds in the amorphous state.

As temperature at which ρ_c is measured grows, the number of shunts does not change considerably. To illustrate, at $T = 400$ K, with allowance made for the temperature dependence of ρ_{Pd} (the temperature coefficient of Pd resistivity $\alpha = 38\times10^{-4}$ deg^{-1}), the shunt resistance is $\sim1.36\times10^4$ Ohm, while their number is $\sim1.2\times10^9$ per 1 cm^2. The character of temperature dependence of ρ_c does not change as the doping level of p^+-Si layer is increased up to 2.5×10^{20} cm^{-3}.

4. Conclusion

The obtained temperature dependence of contact resistivity ρ_c is determined by variation of the metallic resistivity of the contacting metal with temperature and, possibly, by presence of a thin junction layer at the metal–semiconductor interface. The origin of such a layer, as was shown in [2, 13], may be related to a thin metastable layer of "metallic glass" that is a mixture of metal and silicon atoms. According to the model for the metal–Si interface that was advanced in [14], the metal atoms generate interstitial defects in silicon. This results in appearance of dangling covalent Si–Si bonds, i.e., the state of a Si atom is converted from covalent one to that similar to metallic. This factor, along with the shunts, causes metallic-type conductivity in an ohmic contact.

Our results confirm the notion existing in the literature that every silicide can be used as ohmic contact to heavily doped silicon [2, 13, 14].

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