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Peculiarities of study of Au–Ti–Pd–n^+-n-n^+-Si multilayer contact structure to avalanche transit-time diodes

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Abstract. In this work, the method of electrophysical diagnostics of ohmic contacts to n^+-n-n^+ structures for powerful silicon impact ionization avalanche transit-time diodes has been proposed. The specific resistivity of the Au–Ti–Pd–n^+-n-n^+-Si contacts and the current-flow mechanism within the temperature range 100…360 K has been investigated. The generalized method for studying the temperature dependence of the specific contact resistance in the case of multilayer structures with non-uniform doping level has been proposed. The values of the specific contact resistance have been calculated from the temperature dependence of the total resistance of the vertical structure. The offered method can be used to control the electrophysical parameters of ohmic contacts between the etching cycles in technology of manufacturing powerful silicon impact ionization avalanche transit-time diodes.

Keywords: specific resistance, ohmic contact, impact ionization avalanche transit-time diode, thermal-field emission, thermionic emission.

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1. Introduction

Operation of powerful silicon impact ionization avalanche transit-time (IMPATT) diodes in the pulsed mode is accompanied by significant overheating. In this case, the value of the specific contact resistance (ρ_c) of the ohmic contacts to n^+-Si must not exceed $\rho_c < 10^{-5}$ Ohm·cm^2 [1]. Therefore, the control of electrophysical parameters, in particular the temperature dependence of the specific contact resistance, of vertical structures in a wide temperature range is an urgent task in technology of powerful impact ionization avalanche transit-time diodes [2, 3]. For them, it is necessary to develop express methods for controlling the temperature dependences of the parameters of semiconductor structures at the intermediate stages of the design of IMPATT diodes.

Typically, a transition layer of metal silicide is used to form ohmic (non-rectifying) contacts, it is formed by spraying metallization on the heated substrate as a result of interaction of metal with semiconductor. Properties of a solid solution are inherent to silicide. And some of its electrophysical properties distinguish it from both metal and semiconductor. Since the stability of the formed contact depends, to a large extent, on the properties of the transition layer, the control of the value of the specific contact resistance and mechanisms of current flow in the ohmic contacts is necessary to predict the stable operation of IMPATT. In this paper, we have considered the mechanisms of current flow in non-rectifying contacts Au–Ti–Pd–n^+-n-n^+-Si within the temperature range from 100 to 360 K, the peculiarities of the temperature dependence of ρ_c and method of calculating the specific contact resistance of vertical ohmic contacts with non-uniform doping level.

2. Samples and research methods

Vertical ohmic contacts on the basis of silicon with steps of doping metal-n^+, n^+-n and n-n^+ were studied. The silicon substrate was doped with phosphorus. The ohmic contacts were formed using following technology: the layers of metallization Pd (20 nm)–Ti (60 nm)–Au (150 nm) were deposited by magnetron sputtering on

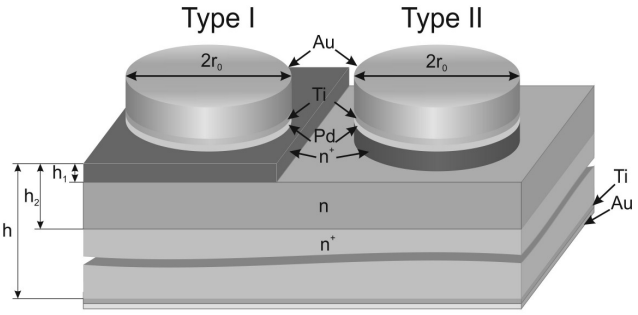

Fig. 1. The layered structure of two types of investigated ohmic contacts Au–Ti–Pd–n^+-n-n^+-Si: I – non-etched, II – etched mesa-structure.

a heated to 350 °C silicon substrate after photon cleaning in a single technological cycle. On the front side, by the method of photolithography, groups of radial contacts of different radii (115, 100, 82.5, 67.5, 55.5, 47.5, 40, 27.5 and 17.5 μm) were formed. On the other side, a solid rear contact was formed. There were investigated the contacts of two types with different technology of vertical structures: I – non-etched (Fig. 1, left side), II – etched mesa-structure (Fig. 1, right side). Parameters of layers in the n^+-n-n^+ structure are listed in Table 1.

Measurements of contact resistance were carried out using an automated complex based on the probe station "Zond-A5" and voltmeter B7-46/1.

3. Results and discussion

It is impossible to calculate the temperature dependence of the contact specific resistance of these multilayer structures using classical methods (Cox–Strack and Brooks–Mathes). The theoretical model for calculating the resistance in the multilayer structures described above (at T = 300 K) was considered in the work [4]. In this paper, the indicated theoretical model for studying the temperature dependences of the contact resistance was used.

To simulate the temperature dependence, it is also necessary to calculate the volume specific resistance of the semiconductor as a function of temperature. Methods for calculating the specific resistance (mobility) for Si are well known (see, for example, [5] pp. 96–104). We note only that in the region of low temperatures (T < 150 K) the scattering of carriers by charged impurities is poorly described by the Brooks–Herring potential (see p. 189 [5]). Obviously, the correct description of such processes on the whole temperature scale requires the refusal of the Born approximation. This leads to unjustifiably complex methods (for example, the method of partial phase shifts, p. 194 [5] or application of the theory of density functional [6]). In this study, we only accounted nonlinear additions to the Brooks–Herring potential [7-9], believing that the Born approximation is permissible in this area. As a result, the calculated resistance is significantly higher (5…10%) in the temperature range (T < 150 K) than the resistance calculated without taking into account the nonlinear additions.

The specific resistance is inversal to the conductance of semiconductor:

$$\rho = \frac{1}{\sigma}. \tag{1}$$

The conductance of semiconductor with the ellipsoidal law of dispersion (ellipsoid of rotation) of the main carriers can be written as:

$$\sigma = \frac{N_{val} T^{1.5}}{3} \sigma_0 \int_0^{+\infty} dk_t k_t \int_{-\infty}^{+\infty} dk_l \frac{dF(\varepsilon - \xi)}{d\xi} \times$$
$$\times \left[\frac{1}{\nu_l(k_l, k_t)} \left(\frac{k_l}{m_l} \right)^2 + \frac{1}{\nu_t(k_l, k_t)} \left(\frac{k_t}{m_t} \right)^2 \right], \tag{2}$$

where N_{val} is the number of valleys, $\sigma_0 \approx 0.542\ \mathrm{Ohm}^{-1} \cdot \mathrm{cm}^{-1}$, T – temperature in Kelvin. The remaining variables are dimensionless: ξ, $\varepsilon = \frac{k_l^2}{2m_l} + \frac{k_t^2}{2m_t}$ – the chemical potential and energy of the carrier in the units of temperature, k_l and k_t are the dimensionless impulses along the principal axes of the ellipsoid, m_l and m_t – corresponding effective masses in the units of mass of free electron, $F(\varepsilon - \xi) = [1 + \exp(\varepsilon - \xi)]^{-1}$ is the Fermi distribution, $\nu_{l,t}(k_l, k_t)$ are the pulse relaxation frequencies along the corresponding axes per one picosecond (averaging over the angles is already made).

At ultrahigh concentrations $n(\xi, T) \geq 10^{20} \mathrm{cm}^{-3}$, the effect of the nonparabolicity of dispersion law is also manifested, which is easy to account when numerical calculations by simple substitution of $m_{l,t} \to m_{l,t}\left[1 + \alpha_{l,t}\left(k_{l,t} / m_{l,t}\right)^2 T\right]$ where the parameters of nonparabolicity are $\alpha_l = 0.4 \cdot 10^{-4}$ and $\alpha_t = 0.3 \cdot 10^{-4}$.

Table 1. Parameters of layers of n^+-n-n^+ structure.

Structure	h_1, μm	h_2–h_1, μm	h–h_2, μm	N_d, cm^{-3} h_1	N_d, cm^{-3} h_2–h_1,	N_d, cm^{-3} h–h_2,	Notes
Type I	0.1	2	250	10^{20}	$5 \cdot 10^{16}$	$4 \cdot 10^{18}$	Without etching
Type II							Etched mesa-structure

3.1. Contact resistance

In order to ascertain the mechanism of current flow in contact, studying the temperature dependence of the specific contact resistance ρ_c was performed. Since the donor concentration in semiconductor is quite large (~10^{20} cm^{-3}), the tunneling mechanism of the current flow through the potential barrier was expected in the whole temperature range. Indeed, when calculating the Padovani–Stratton parameter E_{00} [10], we see that it is larger than k_BT in the whole investigated temperature range:

$$E_{00} = \frac{\hbar}{2}\sqrt{\frac{N_d}{m^*\varepsilon_s}} \approx 0.076 \text{ eV}, \quad (3)$$

where $\hbar$ is the modified Planck constant, m^* – effective mass of electron, ε_s – dielectric permittivity of semiconductor, N_d – concentration of the doping impurity.

When the conditions [11] $E_{00} >> k_BT$ (k_B – Boltzmann constant) are valid, the field mechanism of current flow is implemented; in the case $E_{00} \approx k_BT$, the thermal field mechanism is realized; at $E_{00} << k_BT$ – thermoelectronic one.

At the same time, the experimental temperature dependence of the specific contact resistance in Fig. 2 can not be described by either the field nor the thermal-field function. Also, the absolute values of the specific contact resistance are much higher than the theoretical ones in the assumption of the thermal-field mechanism.

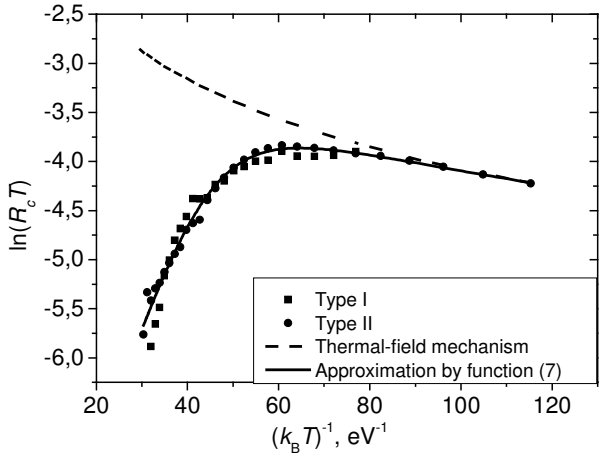

Fig. 2. Temperature dependences ρ_c plotted in the coordinates of thermionic emission, for both types of the formed ohmic contacts: ● – ohmic contacts of the type I (initial structure); ■ – ohmic contacts of the type II (etched mesa-structure); dashed line – calculated temperature dependence of the thermal-field mechanism of current flow (6); solid line – approximation by the function (7) with the used parameters from Table 1.

As can be seen from Fig. 2, at the temperatures above 300 K there is a strong temperature dependence close to the thermionic emission, that may be converted into a straight line by plotting in the coordinates $\ln(R_cT) = f(1/k_BT)$. However, if we find the height of the barrier $\varphi_{b\,\text{eff}}$ from the coefficient of inclination of this line and substitute it into the equation for thermionic emission (4), then the absolute value of the specific contact resistance will be significantly lower than the expected one:

$$R_c = \frac{k}{qA^*T}\cdot\exp\left[\frac{\varphi_{b\,\text{eff}}}{k_BT}\right] \quad (4)$$

where A^* is the modified Richardson constant.

This is possible in the case when in the current flow not the entire area is involved, but some part of it. Then the contact resistance can be calculated by introducing the coefficient B equal to the ratio of the total contact area to the area involved in the current flow:

$$R_{cs} = \frac{Bk_B}{qA^*T}\cdot\exp\left[\frac{\varphi_{b\,\text{eff}}}{k_BT}\right]. \quad (5)$$

The calculation of the parameter B shows that the area involved in thermoelectronic current flow is two orders of magnitude smaller than the total contact area.

At the same time, the current flow across the whole contact area occurs in accord with the thermal field mechanism with some effective interval, which is characterized by the thickness of the order of several lattice parameters. A simplified thermal-field dependence can be represented as:

$$R_{ct} = B_1\cdot\exp\left[\frac{\varphi_{b1}}{E_{00}\cdot\text{ctgh}(E_{00}/k_BT)}\right]. \quad (6)$$

where B_1 is the coefficient that includes the pre-exponential variables and is weakly dependent on temperature, φ_{b1} – height of the potential barrier for the whole contact area. The dependence (6) is given in Fig. 2 by the dashed line and well describes the temperature dependence of the specific contact resistance within the range of temperatures 100…150 K.

The total contact resistance is determined using the formula for the resistances connected in parallel:

$$R_c = \frac{R_{cs}\cdot R_{ct}}{R_{cs}+R_{ct}}, \quad (7)$$

Approximation by the dependence (7) is given in Fig. 2 with the solid lines. The parameters of approximation are listed in Table 2.

Table 2. Parameters of approximation for the temperature dependence of specific contact resistance.

Parameter	B	B_1, Ohm·cm^2	φ_b, eV	φ_{b1}, eV	E_{00}, eV
Value	100	$1.47 \cdot 10^{-10}$	0.1236	1.05	0.076

Estimation of the height of the potential barrier φ_{b1} was performed as the difference between the work function of electrons from Pd_2S [3] and the electron affinity to Si electron. The temperature dependences for both types of contacts are practically the same, the difference between them is only in dispersion of parameters of ohmic contacts.

It should be noted that the study of the temperature dependence of the specific contact resistance in the Au–Ti–Pd–n^+-Si contact at the thickness of the Pd layer close to 30 nm as a contact-forming layer, which were performed by the authors [12], indicates the implementation of the current flow mechanism through metallic shunts conjugated with high conductivity density dislocations (~10^7…10^8 cm^{-2}) [13]. In this case, the specified current flow mechanism is expressed in the form of a dependence increasing with the temperature of the specific contact resistance.

In our case, for both types of contacts the decreasing temperature dependence of the specific contact resistance is observed from the experimental data obtained. The possible explanation for this change in the current flow mechanism is the fact that a more thin Pd layer (20 nm) is used. As a result, formation of smaller crystallites in the polycrystalline Pd_2Si contact-forming layer occurs. Each of the crystallites is a concentrator of mechanical stresses, decrease of their sizes leads to a decrease in the values of maximum stresses, and, hence, to the probability of their relaxation with formation of dislocations. The less concentration of formed leading dislocations will lead to the predominance of other mechanisms of current flow, which is observed in our work. The obtained results are in accordance with the results obtained in [11], where analogous contacts to Si (Pd thickness is 20 nm) with a lower concentration of the dopant were considered. The temperature dependence of these contacts is also decreased. There are areas with thermal-field and field emission, that is, the mechanism of current flow by shunts is not observed.

Thus, reducing the thickness of Pd in the contact to 20 nm leads to a decrease in internal mechanical stresses at the interface and to improvement of the structure of the semiconductor layer, which is especially important in high-power silicon IMPATT diodes, where the temperature dependence of the specific contact resistance significantly influences on the output power. At the same time, the thickness of the Si p^+-layer (with a similar contact-forming Pd layer) should be minimal for optimal heat removal, whereas the vertical dislocations growing through a thin, strongly doped layer to the active region can negatively affect the reliability of these diodes [15].

4. Conclusions

The method of investigating the temperature dependence of contact resistance, which is a generalization of the Cox–Strack method in the case of multilayer semiconductor structures with a non-uniform level of doping, has been proposed.

From the study of the temperature dependence of the resistivity of the Au–Ti–Pd–n^+-n-n^+-Si contacts deposited on a substrate heated to 350 °C within the temperature range 100…360 K, it can be concluded that, at a sufficiently high concentration of the dopant (~10^{20} cm^{-3}), the typical field emission in the low temperature range is not observed. Instead, there is an prevailing mechanism of thermal-field emission. However, with the increase in the temperature for both types of contacts, the prevailing mechanism of thermionic emission with a potential barrier height of ~0.12 eV is observed. It should be noted that thermionic emission passes through local areas of much smaller area. As shown in authors' work, the use of Pd as a contact forms the layer with the thickness from the range 20 to 30 nm may affect the mechanism of current flow on the specific contact resistance through the ohmic contact.

The proposed method of studying the temperature dependence of the contact resistance can be used to control the quality of the ohmic contact both for the development of the formation modes and at the stage of forming the mesa-structure when constructing the powerful impact ionization avalanche transit-time diodes.

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