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Theoretical and experimental modelling the specific resistance of vertical ohmic contacts Au–Ti–Pd–n^+-n-n^+-Si in IMPATT diodes

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Abstract. The method of electrophysical diagnostic of n^+-n-n^+ structures at the etching stage of manufacturing process of power IMPATT diodes has been proposed. A numerical method for specific contacts resistance calculation of vertical ohmic contacts with a non-uniform doping level has been developed. Vertical ohmic contacts Au–Ti–Pd–n^+-n-n^+-Si both before and after etching were used for experimental checking this model. It has been computed the value of contact resistance in the interface metal–n^+ with correction of contribution of n^+-n and n-n^+ resistances to the total resistance. The values of total effective resistances of vertical ohmic contacts Au–Ti–Pd–n^+-n-n^+-Si may be calculated using the Cox–Strack method. We used solutions of Laplace's equation for computation of specific contact resistance metal–n^+ without contribution of interfaces n^+-n and n-n^+. The values of specific contact resistance were ~10^{-6} Ohm·cm^2. This method allows to control the manufacture process by monitoring the changes in electrophysical properties of the structure between etching cycles.

Keywords: specific contact resistance, IMPATT diodes, electrophysical diagnostic, ohmic contacts.

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1. Introduction

Development of active elements for microwave electronics, in particular impact ionization avalanche transit-time diodes (IMPATT) needs in diagnostic methods at the earliest stage of device structure manufacturing. These methods allow to influence on parameters of technological processes [1]. Since the current level of IMPATT design provides an output power close to ~10 W, the value of contact resistance in it shell does not exceed 10^{-5} Ohm·cm^2 [2, 3]. Electrophysical studies are non-destructive, an express and informative diagnostic tool, so urgent is the development of diagnostic methods based on them.

However, creating test patterns on the manufactured substrate comprises a part of useful area, which restricts the use of, for example, TLM-structures for separate analysis of each layer in the p^+-p-n-n^+ structure. We propose a method of complex diagnostics of n^+-n-n^+ structure before and after the etching of the mesa-structure. In this case, we need to take into account contribution of each interface n^+-n and n-n^+ in the total contact resistance. The Cox–Strack method enables to estimate the total effective contact resistance of the vertical structure, that is the sum of the contact resistance ρ_c at the metal–n^+-Si and contribution of contact resistance section n^+-n and n-n^+ interfaces, as well as the spreading resistance in the n^+ and n layers:

$$\rho_{cs} = \rho_c + \rho_{c1}\,. \tag{1}$$

However, to separate input ρ_s, contact n-n^+ resistance, and the step of spreading resistance in the n region of n^+-n-n^+ structure, it does not allow. In this study, we investigated the contact structures of Au–Ti–Pd–n^+-n-n^+-Si before and after etching the mesa-structure and evaluated the contribution of the mentioned contact resistances.

However, it does not allow to separate contribution of ρ_c, contact resistance of n-n^+ interface and spreading resistance in the n layer of n^+-n-n^+ structure. We investigated the contact structures of Au–Ti–Pd–n^+-n-n^+-Si before and after etching the mesa-structure and calculated the contribution of each mentioned contact resistance by using our method.

2. Samples and methods

Ohmic contacts were formed by magnetron sputtering of serial layers: Pd (20 nm)-Ti (60 nm)-Au (150 nm) on the substrate heated to 350 °C. Groups of radial contacts (of radii 115, 100, 82.5, 67.5, 55.5, 47.5, 40, 27.5, and 17.5 μm) were formed at the front side of substrate. A single continuous ohmic contact was formed at the back substrate side. Two types of contacts were investigated (Fig. 1): type I – non-etched structures, and type II – mesa-structures with the etched n^+-Si layer. The parameters of layers were as follows: $h_1 = 0.1$ μm, $h_2 - h_1 = 2$ μm, $h - h_2 = 250$ μm, $\rho_{s1} = 0.01$ Ohm·cm, $\rho_{s2} = 0.08$ Ohm·cm, $\rho_{s3} = 0.01$ Ohm·cm.

The method of numerical simulation of contact structure is based on the solution of the Laplace equation [8]. Consider a semiconductor structure n^+-n-n^+ in Fig. 1, type I, and calculate its resistance. To solve this task, it is sufficient to know the distribution of potential $\varphi(\mathbf{r})$ for each contact potential difference V in accord with the Ohm law

$$\mathbf{j} = -\frac{1}{\rho_s(\mathbf{r})}\nabla\varphi(\mathbf{r})\,. \tag{2}$$

Here, $\mathbf{j}$ is the current density. The task can be simplified, if one takes into account that the thickness of space charge is sufficiently thinner than thicknesses of corresponding semiconductor layers. In this case, we can neglect the thickness of space charge layer and assume that the contact resistance appears in an infinitely thin region. In this approximation, the continuity equation and Ohm's law reduce the task to the solution of the Laplace equation $\nabla^2\varphi(\mathbf{r}) = 0$, which is valid for all the volume of semiconductor structure except thin layers in where the contact resistance is formed. If using the cylindrical coordinate system, its origin can be placed into the center of interface with the radius r_0, then $\varphi(\mathbf{r}) \equiv \varphi(r,z)$ and $\rho(\mathbf{r}) \equiv \rho(r,z)$. There are three regions (at $r < r_m$):

$$\varphi(r,z) = \begin{cases} \varphi_1(r,z), & z \in (-h_1, 0); \\ \varphi_2(r,z), & z \in (-h_2, -h_1); \\ \varphi_3(r,z), & z \in (-h, -h_2); \end{cases}$$

$$\rho(r,z) = \begin{cases} \rho_1, & z \in (-h_1, 0); \\ \rho_2, & z \in (-h_2, -h_1); \\ \rho_3, & z \in (-h, -h_2). \end{cases} \tag{3}$$

Each of the corresponding regions should satisfy the Laplace equation

$$\left[\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2}\right]\varphi_{1,2,3}(r,z) = 0\,. \tag{4}$$

The solution can be seeked in the form

$$\varphi_k(r,z) = b_{k;0} + a_{k0}z + \sum_{n=1}^{N}\left[a_{k;n}\exp(\mu_n z) + b_{k;n}\exp(-\mu_n z)\right]J_0(\mu_n r), \tag{5}$$

$$k = 1, 2, 3\,,$$

where $N \to \infty$, $J_0(x)$ is the Bessel function of the first kind and zero order, and characteristic roots μ_n satisfy the condition that the current does not flow through the surface $r = r_m$:

$$J_0'(\mu_n r_m) = 0\,. \tag{6}$$

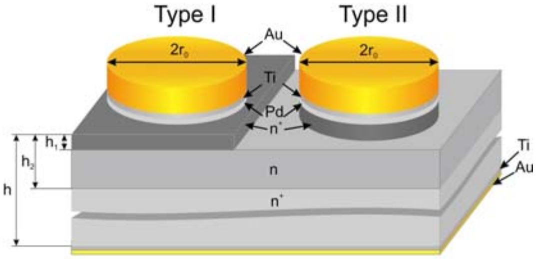

Fig. 1. The layer structure of two types for studying the Au–Ti–Pd–n^+-n-n^+-Si ohmic contact: I – non-etched contact structure, II – etched mesa-structure.

In the plane $z = -h_1$, the contact resistance of *n-n*$^+$ junction $\rho_{c\,1,2}$ leads to a potential jump

$$\varphi_1(r,-h_1) - \frac{\rho_{c\,1,2}}{\rho_1}\frac{\partial\varphi_1(r,z)}{\partial z}\bigg|_{z=-h_1} = \varphi_2(r,-h_1). \tag{7}$$

The similar jump takes place in the contact resistance inside the plane $z = -h_2$

$$\begin{aligned}&\frac{1}{\rho_k}\frac{\partial\varphi_k(r,z)}{\partial z}\bigg|_{z=-h_k} = \\ &= \frac{1}{\rho_{k+1}}\frac{\partial\varphi_{k+1}(r,z)}{\partial z}\bigg|_{z=-h_k}, \quad k = 1,2.\end{aligned} \tag{8}$$

The Ohm law for the whole circuit gives us an additional initial condition:

$$\begin{aligned}&\frac{\rho_c}{\rho_1}\frac{\partial\varphi_1(r,z)}{\partial z}\bigg|_{z=0} = \\ &= \left\{V - \left[\varphi_1(r,0) - \varphi_3(r,-h) + \frac{\rho_c{}'}{\rho_3}\frac{\partial\varphi_3(r,z)}{\partial z}\bigg|_{z=-h}\right]\right\} \\ &\theta(r_0 - r).\end{aligned} \tag{9}$$

The condition of equipotential contact with the radius r_m in the plane $z = -h$ is:

$$\frac{\rho'_c}{\rho_3}\frac{\partial\varphi_3(r,z)}{\partial z}\bigg|_{z=-h} - \varphi_3(r,-h) = 0\,, \tag{10}$$

where ρ_c and ρ'_c are contact resistances of metal–semiconductor junction. The equations (7) to (10) give us the following relations:

$$\begin{aligned}&a_{k;n} = \alpha_{k;n}\,a_{3;n}, \quad b_{k;n} = \beta_{k;n}\,a_{3;n}, \\ &k = 1,2,3,\end{aligned} \tag{11}$$

where

$$\alpha_{3;0} = \alpha_{3;n} = 1; \quad \beta_{3;0} = \frac{\rho'_c}{\rho_3} + h\,;$$

$$\beta_{3;n} = -\frac{\rho_3 - \rho'_c\,\mu_n}{\rho_3 + \rho'_c\,\mu_n}\exp(-2\mu_n h), \quad n = 1,2,...;$$

$$\alpha_{k;0} = \frac{\rho_k}{\rho_3}; \quad \beta_{k;0} = \beta_{k+1;0} +$$

$$+\alpha_{k+1;0}\left[h_1\left(\frac{\rho_k}{\rho_{k+1}} - 1\right) + \frac{\rho_{c\,k,k+1}}{\rho_{k+1}}\right], \; k = 1,2\,;$$

$$\begin{aligned}\alpha_{k;n} &= \frac{\alpha_{k+1;n}}{2}\left(1 + \frac{\rho_k}{\rho_{k+1}} + \mu_n\frac{\rho_{c\,k,k+1}}{\rho_{k+1}} + 1\right) + \\ &+ \frac{\beta_{k+1;n}}{2}\left(1 - \frac{\rho_k}{\rho_{k+1}} - \mu_n\frac{\rho_{c\,k,k+1}}{\rho_{k+1}}\right)\exp(2\mu_n h_k), \\ \beta_{k;n} &= \frac{\alpha_{k+1;n}}{2}\left(1 - \frac{\rho_k}{\rho_{k+1}} + \mu_n\frac{\rho_{c\,k,k+1}}{\rho_{k+1}} + 1\right)\exp(-2\mu_n h_k) + \\ &+ \frac{\beta_{k+1;n}}{2}\left(1 + \frac{\rho_k}{\rho_{k+1}} - \mu_n\frac{\rho_{c\,k,k+1}}{\rho_{k+1}}\right), \\ k &= 1,2;\; n = 1,2,...\end{aligned} \tag{12}$$

Substituting the equations (11), (12) to (5), and the result to (10), after using properties of Bessel functions one can obtain a system of linear equations for the coefficients $a_{3;n}$:

$$\sum_{n'=0}^{N} D_{nn'}\,a_{3n'} = f_n, \tag{13}$$

where the matrix in the left part of equation has the following diagonal elements

$$\begin{aligned}D_{00} &= \alpha_{1;0}\frac{\rho_c}{2\rho_1}\left(r_m^2 + r_0^2\right) + \left(\beta_{1;0} + h\right)\frac{r_0^2}{2}, \\ D_{nn} &= \left[\alpha_{1;n} + \beta_{1;n} - \exp(-\mu_n h)\left(1 - \frac{\rho'_c}{\rho_3}\mu_n\right)\right] \times \\ &\times \frac{r_0^2}{2}\left[J_0^2(\mu_n r_0) + J_1^2(\mu_n r_0)\right] + \\ &+ \frac{\rho_c}{\rho_1}\left(\alpha_{1;n} - \beta_{1;n}\right)\frac{\mu_n r_m^2}{2}J_0^2(\mu_n r_m), \quad n > 0\,,\end{aligned} \tag{14}$$

for other elements, it is:

$$D_{n0} = \left[\beta_{1;0} + h + \frac{\rho'_c}{\rho_3}\right]\frac{J_1(\mu_n r_0)r_0}{\mu_n},$$

$$D_{0n} = \left[\beta_{1;0} + h + \frac{\rho'_c}{\rho_3}\right]\frac{J_1(\mu_n r_0)r_0}{\mu_n}, \quad n > 0;$$

$$\begin{aligned}D_{nn'} &= \left[\alpha_{1;n'} + \beta_{1;n'} - \exp(-\mu_{n'}h)\left(1 - \frac{\rho'_c}{\rho_3}\mu_{n'}\right)\right] r_0 \times \\ &\times \frac{J_0(\mu_{n'}r_0)\mu_n J_1(\mu_n r_0) - J_0(\mu_n r_0)\mu_{n'}J_1(\mu_{n'}r_0)}{\mu_n^2 - \mu_{n'}^2}, \\ n' &> 0, \quad n \neq n'.\end{aligned}$$

The right side of the equations (14) determined by $f_0 = \frac{r_0^2}{2}V$, $f_n = \frac{J_1(\mu_n r_0)r_0}{\mu_n}V$. The set of equations (13), (14) was solved numerically, by using Gaussian elimination (p. 128 in [9]). Finding the coefficients $\{a_{3;n}\}$ by using (3), (5), (11) and (12), we find the distribution of the potential factors for the entire semiconductor structure corresponding to Fig. 1, type I. The case, adduced in Fig. 1, type II is similar and even something easer. The contact resistance at the metal-semiconductor junction, taken as a parameter to minimize the differences between the calculated and experimental values, was determined using the method of least squares.

To measure the effectiveness of the specific contact resistance, we used the Cox–Strack method [5], which is often applied for the analysis of vertical structures. In the case of the etched mesa-structure (type II), the total contact resistance is described by the relation

$$R = \frac{\rho_{cs}}{\pi r_0^2} + \frac{\rho_3}{2\pi r_0}\arctan\left(\frac{2h}{r_0}\right) + R_t\,, \qquad (15)$$

where R_t is the resistance of continuous back contact.

3. Results and discussion

The result of theoretical calculation of the total resistance R dependence on the radius r_0 based on known parameters of specific resistances of layers for both types of ohmic contacts in the Cox–Strack coordinates $\pi R r_0^2 = f\left[2r_0 \arctan\left(2h/r_0\right)/\pi\right]$ is shown in Fig. 2.

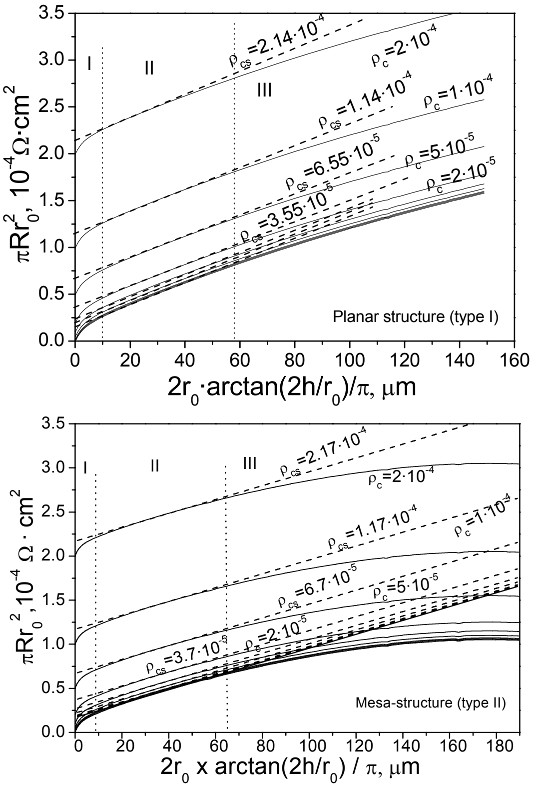

Fig. 2. Calculated dependences in Cox–Strack coordinates $\pi R r_0^2 = f\left[2r_0 \arctan(2h/r_0)/\pi\right]$ both for type I (up) and type II (down) structures. Solid lines from the top to bottom correspond to values of contact resistances: ρ_c = $2\cdot10^{-4}$, 10^{-4}, $5\cdot10^{-5}$, $2\cdot10^{-5}$, 10^{-5}, $5\cdot10^{-6}$, $2\cdot10^{-6}$, 10^{-6}, and 0 Ohm·cm². Dotted lines corresponds to values of effective contact resistances calculated from the linear region II by using the Cox–Strack method. The maximum values of the argument are matched to r_0 = 280 μm.

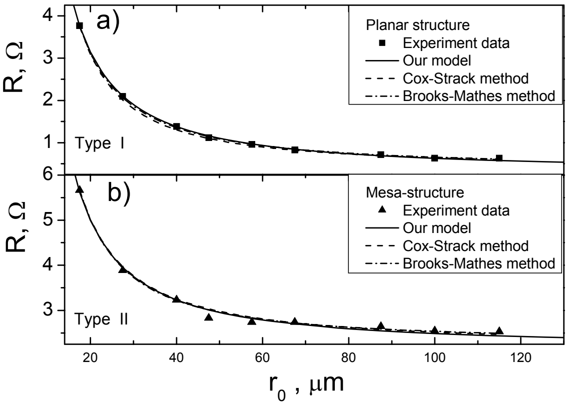

Fig. 3. Resistance versus radius $R(r_0)$ of vertical ohmic contacts Au–Ti–Pd–n^+-n-n^+-Si, formed for the planar contact (a) and for etched mesa-structure (b); markers – experimental values, the solid line – theoretical calculation by using our method, dotted line – by using Cox–Strack, and dash-point line – by Brooks–Mathes methods.

It is easy to see that the dependence has three specific regions (Fig. 2), namely:

- first, of low values of the contact radius related with nonlinear correlation between the increase in radius and spreading currents;
- second, of linear dependence on the contact radius related with the region of correct using the Cox–Strack method for dependence of contact effective specific series resistance and substrate specific resistance with both types of formed contacts;
- third, of large diameters affects the error associated with the Cox–Strack method.

The calculated value (Table) of the specific contact resistance (ρ_c) of the interface layer metal–semiconductor without the contribution of the contact resistance at the boundaries of n^+-n and n-n^+ (ρ_{c1}) ohmic contacts for planar ohmic contacts is $\rho_c = 0.8\cdot10^{-5}$ Ohm·cm² and for mesa-structures is $\rho_c = 1.6\cdot10^{-6}$ Ohm·cm².

Table. The results of calculation of the specific contact resistance by the numerical method based on the solution of the Laplace equation.

Contact type	h_1, μm	$h_2 - h_1$, μm	$h - h_2$, μm	ρ_{s1},Ohm·cm (h_1)	ρ_{s2}, Ohm·cm ($h_2 - h_1$)	ρ_{s3}, Ohm·cm ($h - h_2$)	R_t, Ohm·cm	ρ_c, Ohm·cm²
Planar structure (type I)	0.1	2	250	0.01	0.08	0.01	0.5	$0.8\cdot10^{-5}$
Mesa-structure (type II)	0.1	2	250	0.01	0.08	0.01	2.2	$1.6\cdot10^{-6}$

4. Conclusions

The method of determining the specific contact resistance of vertical structures has been proposed. It is based on the solution of the Laplace equation and describes the contact structures metal-n^+ and structures with doping steps n^+-n and n-n^+. In accord with this calculation, the contact resistance ρ_c of ohmic contacts Au-Ti-Pd-n^+-n-n^+-Si was determined as $\sim 10^{-6}$ Ohm·cm^2. This method allows anyone to control the process of forming the mesa-structure by tracking changes in the electrical properties of the structure between the etching cycles.

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