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Study of electrophysical properties of metal–semiconductor contact by the theory of complex systems

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Abstract: The purpose of this work is to analyze the electrical properties of the metal–semiconductor contact (MSC) in the framework of the theory of complex systems. The effect of inhomogeneity of the different microstructures: polycrystalline, monocrystalline, amorphous metal–semiconductor contact surface is investigated, considering a Schottky diode (SD) as a parallel connection of numerous subdiodes. It has been shown that the polycrystallinity of the metal translates a homogeneous contact into a complex system, which consists of parallel connected numerous elementary contacts having different properties and parameters.

Key words: Schottky diode; metal–semiconductor contact; current–voltage characteristics; interfaces; heterogeneity; complex systems

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1. Introduction

Due to the fast development of the technology, the attempts at multifunctional uses of small-scale devices has significantly increased. When a metal and a semiconductor come into contact, the Schottky diode (SD), often called a "Schottky semiconductor diode"[1], completely neglects the role of metal. In other words, in most cases the metal is considered a passive partner in the metal–semiconductor contact (MSC).

It is obvious that the homogeneous model does not fully describe the real situation, since in many practical cases the interface is inhomogeneous. The interface of a real MSC is heterogeneous, mainly due to the polycrystallinity of the metal. A homogeneous model cannot describe the processes occurring in an inhomogeneous contact, where the interface, based on emission parameters, is considered to be homogeneous in two dimensions.

We believe that all of the above problems are explainable if we apply the inhomogneous model[2], where MSC is considered as a parallel connection of numerous homogeneous, elementary contacts having different parameters. Obviously, in this case, the behavior of the contact must obey the complex system laws[2, 3].

There is an opinion that the structure and state of the semiconductor surface has a decisive influence on the operation of the MSC, which can be agreed upon with the polycrystalline structure of the semiconductor[4]. However, in the case of the monocrystal structure of the semiconductor, in our opinion, the influence of metal inhomogeneity on the operation of a Schottky barrier diode (SBD) begins to dominate.

As is known from the literature, the microstructure of the film determines the important role of the metal[5, 6]. From these facts it is possible to identify the following signs of inhomogeneity[2]: a) it is impossible to find two areas with the same physical and geometrical parameters on an inhomogeneous surface; b) in nature there are no two identical inhomogeneous interfaces (or surfaces) at all. Each interface is unique, if the metal has a polycrystalline structure.

As noted above, due to the mosaic microstructure of the metal of the interface, the MSC becomes inhomogeneous, and as a result the contact becomes a complex system.

When studying the contact, it is necessary to take into account the complexity of the system, which consists of the parallel connection of numerous homogeneous elementary subcontacts with different properties and parameters[6]. The number of elementary subdiodes depends on the number of the microcrystallites on the surface of the diode (Fig. 1).

For example, the barrier height (BH) with inhomogeneous interface can be expressed by the formula[7]

$$\bar{\Phi} = \frac{\Phi_1 S_1 + \Phi_2 S_2 + \ldots + \Phi_n S_n}{S_1 + S_2 + \ldots + S_n} = \frac{\sum_{i=1}^{n} \Phi_i S_i}{\sum_{i=1}^{n} S_i} = \sum_{i=1}^{n} \Phi_i \omega_i, \qquad (1)$$

where $\omega_i = \dfrac{S_i}{\sum S_i}$, $\bar{\Phi}$ is the averaged over the surface height of the barrier, ω_i is the relative area of the subdiode and Φ_i is the height of the barrier of the i-th subdiode. It is clear that with increasing n, the number of subdiodes, i.e. the complexity, of the system grows.

The temperature dependence of the current–voltage (I–V) characteristics is an effective physical method for studying the properties of a MSC[1, 8–10].

According to the inhomogeneous model, the barrier height of systems consisting of two parallel-connected homogeneous diodes has a temperature dependence, even if the heights of the subdiode barriers do not depend on temperature, as it follows from the theory of complex systems[11]:

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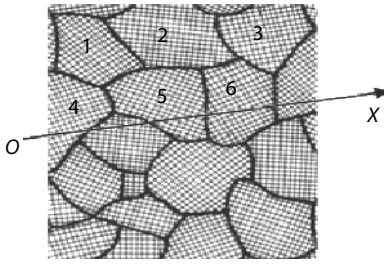

Fig. 1. Microstructure of the surface of a polycrystalline metal.

$$\Phi_B(T) = \Phi_B(0) + \alpha T, \tag{2}$$

where $\Phi_B(0)$ is the height of the contact barrier at $T = 0$, α is the temprature coefficient of the barrier height related with the inhomogeneity order of the interface that is expressed by the formula[2]

$$\alpha = -kT\ln\left[\omega + (1-\omega)\exp\left(-\frac{\Delta\Phi}{kT}\right)\right], \tag{3}$$

where $\Delta\Phi$ is the difference between heights of the potential barriers of the subdiodes, ω and $1 - \omega$ are relative areas of the subdiodes, correspondingly. In the case of the homogeneous contact, when $\Delta\Phi = 0$, α is equal to zero. In the case of the inhomogeneous contact according to Eq. (3), $\alpha \neq 0$ and depends on ω and $\Delta\Phi$. Other words in this case α is a function of microstructure.

2. Materials and methods

Temperature annealing is a technological factor affecting to the microstructure and thus the degree of homogeneity of the contact between the metal and the semiconductor. The study of the properties Ni–n/Si of the SD showed that the properties and parameters of the diodes substantially depend on the area and parameters of the annealing temperature. This means that the diode or ohmic behavior of the contact can be controlled by changing the parameters of the annealing temperature and the area of the contacts.

The saturation current of the SD determined before and after thermal annealing can be expressed by the following formulas[4]

$$I_{S1} = ST^2A_1e^{-\frac{\Phi_{B1}^{(0)}+\alpha_1 T}{kT}} = ST^2Be^{-\frac{\alpha_1}{k}}, \tag{4}$$

$$I_{S2} = ST^2A_2e^{-\frac{\Phi_{B2}^{(0)}+\alpha_2 T}{kT}} = ST^2Be^{-\frac{\alpha_2}{k}}. \tag{5}$$

Here I_{S1} and I_{S2} are the saturation currents before and after annealing, respectively, S_1 and S_2 are the areas of the contact, A_1 and A_2 are Richardson's coefficients, Φ_{B1} and Φ_{B2} are the heights of the barriers of SD before and after heat treatment. B is the emission parameter of the considered interface that is expressed by the formula

$$B = A_ie^{-\frac{\Phi_{Bi}(0)}{kT}} = \text{const}. \tag{6}$$

We assume that under the influence of heat treatment, the area of the ordered contact areas increases due to the combination of crystallites (ordered areas) and atoms located in the intercrystalline space. Apparently, thermal annealing is a technological factor that changes the number of subdiodes (n) of a complex system.

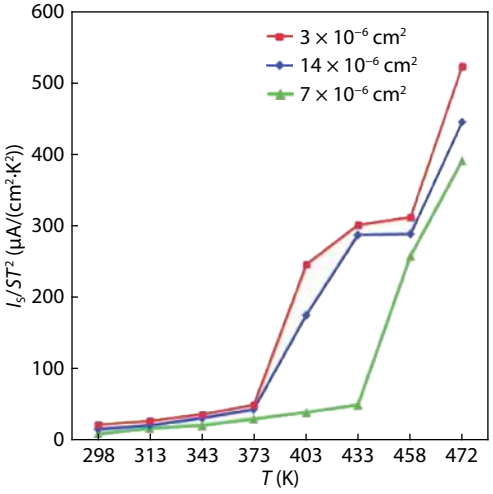

Fig. 2. (Color online) Dependence of I_S/ST^2 on the temperature for TiCu-n/Si SD with different areas.

Since $\alpha_1 \neq \alpha_2$, the saturation currents are not equal: $I_{S1} \neq I_{S2}$. As a consequence of this, the height of the barrier of the SD before and after heat treatment should not be equal to each other ($\Phi_{B1} \neq \Phi_{B2}$). This means that the difference in barrier heights for the same contact, measured by different authors, is a consequence of the uniqueness of the interface, which changes under the action of thermal annealing.

From the above it follows that Φ_B is a necessary, but insufficient parameter for the description of the emission properties of interfaces[12, 13]. To compare the results of different authors[14–16], it is necessary to take into account the experimental values of the Richardson constant A. Separately, Φ_B (or A) cannot be used as a contact parameter, since it is known a priori that the degree of homogeneity of the interface between experiments varies.

However, their product in the form of a correlation (6) can serve as a parameter of the interface, since it is constant for a given metal and semiconductor pair and does not depend on technological or design parameters such as thermal annealing or the size of contacts.

Given the correlation dependence (4), (5), for the direct current of saturation of SD, one can write the formula:

$$I_S = ST^2B. \tag{7}$$

Here B is the main emission parameter of interface between the metal and the semiconductor and expresses the saturation current density per square of temperature. The study of the temperature dependence of the saturation current of the current-voltage characteristics showed that with increasing T the saturation current increases in such a way that B remains almost constant:

$$B = I_S/ST^2 = \text{const}. \tag{8}$$

In Fig. 2 the dependence I_S/ST^2 is given on the temperature for TiCu–n/Si SD with different contact area: 3×10^{-6}; 7×10^{-6}; 14×10^{-6} cm^2. On the ordinate axis I_S/ST^2 is given in the unit μA/(cm^2·K^2), on the axis abscissa – the temperature in K. As one can see from the figure in the temperature diapason of 298–373 K, I_S/ST^2 depends weakly on the temperature.

Table 1. Dependents of B on the structure of the metal.

SD	Structure	Area of SD (cm^2)	T (K)	B (A/(cm^2·K^2))
Al–n/Si	Polycrystalline	7×10^{-6}	298	5.8×10^{-10}
TiCu–n/Si	Polycrystalline	7×10^{-6}	298	6.4×10^{-6}
TiCu–n/Si n/Si	Polycrystalline	14×10^{-6}	298	11×10^{-6}
TiCu-n/SiSi	Polycrystalline	3×10^{-6}	298	6.3×10^{-6}
PtSi–n/Si	Monocrystalline	9×10^{-6}	298	5.3×10^{-7}
TiW–n/Si	Amorphous	5×10^{-6}	298	5×10^{-8}

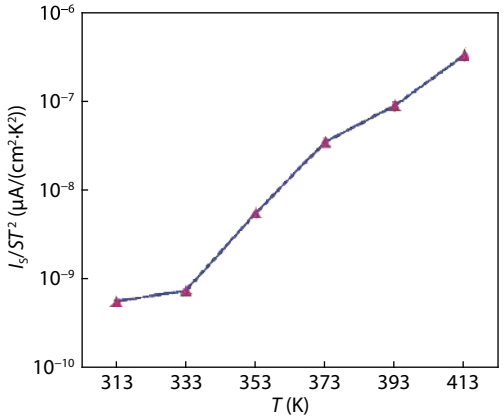

Fig. 3. (Color online) Dependence of I_S/ST^2 on the temperature for SD Al -n/Si with the area 7×10^{-6} cm^2.

Weak growth is likely due to the multiplier $\exp\left(-\frac{\alpha}{K}\right)$ related with the microstructure:

$$\frac{I_S}{ST^2} = B\exp\left(-\frac{\alpha}{K}\right), \tag{9}$$

that demonstrates the influence of the inhomogeneity order of the interface. With a further increase of temperature 373–472 K, I_S/ST^2 increases significantly with the increase of T.

Apparently, this is due to the reconstruction of the microstructure of interface under the influence of the temperature exposure. According to Eq. (8), when $\exp\left(-\frac{\alpha}{K}\right)=1$, then $B_0 = B_T$. This is possible only if $\alpha = 0$, i.e., when interface is homogeneous. In other cases, Eq. (8) is expressed by the formula

$$B_0 = B_T\exp\left(-\frac{\alpha}{K}\right). \tag{10}$$

The new emission parameter B varies over a wide range depending on the nature and structure of the metal. Fig. 3 shows the dependence of I_S/ST^2 on the annealing temperature for the SD Al–n/Si with the area of 7×10^{-6} cm^2. From the comparison of Figs. 2 and 3, it can be noted that at the room temperature for SD Ti Cu–n/Si with an area of $S = 7\times10^{-6}$ cm^2, the value $B = 11$ μA/(cm^2·K^2), and in the case of SD Al–n/Si SD with the same area, the value $B = 50$ μA/(cm^2·K^2) is obtained.

Thus, we can conclude that, depending on the nature of the metal, the emission parameter B varies in a wide range from 5.83×10^{-10} to 6.3×10^{-6} A/(cm^2·K^2) (Table 1).

From the foregoing, it can be concluded that metal plays a more active role in the electronic processes occurring in the MSC, and the polycrystallinity of the metal converts the contact into a complex system, where MSC consists of numerous elementary and homogeneous parallel connected subcontacts, the number of which varies due the parameters of thermo annealing and the contact area.

3. Conclusion

From the foregoing, we can conclude that in physical processes occurring in the contact of a metal with a single-crystal semiconductor, the metal plays a more active role than the semiconductor if the metal has a polycrystalline structure. The polycrystallinity of the metal translates the MSC into a complex system[9], where the contact is represented as a set of numerous elementary and homogeneous discrete contacts connected in parallel[4]. The number of subcontacts can be varied by thermal annealing and contact area. With decreasing n, the uniformity of the interface increases. Under the influence of thermal annealing and the contact area, the physicochemical behavior (composition and structure) of the contact can also change, such as, for example, the degree of uniformity of the interface, the relationship of the sections with diode and ohmic properties.

Schottky diodes made with the use of polycrystalline metals is a convenient object for checking the conclusions of the theory of complex systems. Many complex[17–19] phenomena in the real world are not reproducible, but in the case of SD with a polycrystalline metal film, complex systems can be reproduced.

The use of Schottky diodes allows one to study a number of laws of a complex system with a change in the number of subcontacts.

Our study allowed us to draw the following conclusions:

1. It was shown that the height of the SD barrier with an inhomogeneous interface has a temperature dependence, even if the height of the barrier of sub-diodes is temperature independent, as follows from the theory of complex systems.

2. It is believed that Φ_B is a necessary but insufficient parameter for describing the emission properties of interfaces. Separately, both PV and A cannot perform the functions of the MSC parameter, since their values are a function of surface coordinates. However, their product in the form of correlation (6) can serve as an interface parameter, since it is constant for a given metal and semiconductor pair.

3. To describe the emission properties of MSCs, it is proposed to use a metal and a semiconductor B constant for the given pair, which expresses the density of the saturation current per square temperature. Parameter B varies over a wide range depending on the nature and structure of the metal.

4. It is proposed to study the nature of complex systems using SD. It is known that many complex phenomena are difficult to reproduce in the real world. However, the use of SD allows one to study a number of patterns of a complex system when changing the number of subcontacts.

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