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The influence of the metal microstructure on the breakdown mechanism of Schottky diodes

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ABSTRACT

In this paper, the influence of the microstructure of a metal on the breakdown mechanism of diodes with a Schottky barrier is studied. It is shown that in electronic processes occurring in the contact between a metal and a semi-conductor, the metal plays a very active role and is a more important contact partner than a semiconductor. Unlike the known mechanisms of breakdown of diodes (avalanche, tunnel and thermal), another mechanism is proposed in this paper - the geometric mechanism of the reverse current flow of Schottky diodes made using a metal with a poly-crystalline structure. The polycrystallinity of a metal transforms a homogeneous contact into a complex system, which consists of parallel-connected multiple elementary contacts having different properties and parameters.
Keywords: *Schottky diode, Metal-semiconductor contact, Interface, Barrier height, Breakdown voltage*

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1. Introduction

According to the Schottky theory [1], depending on the ratio of the work function of the metal and the semiconductor, the behavior of the metal-semiconductor (MS) contact can be either diode or ohmic. In contrast to the p-n junction, the inverse branch of the current-voltage (I-V) characteristic of the MS contact has a variety of shapes, which are presented in **Figure 1**. In **Figure 1a-Figure 1d**, the reverse branches of the current-voltage characteristic of the Schottky diodes (SD) are presented and in **Figure 1e** the current-voltage characteristic of the ohmic contact. As can be seen from the figures, along with the known diode forms of the I-V characteristic with "hard" (a) and "soft" (d) breakdowns, and I-V characteristic with breaks (b and c) is sometimes observed.

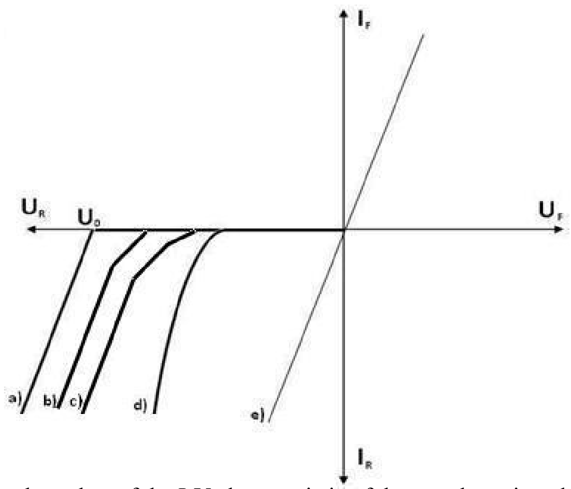

Figure 1. Reverse branches of the I-V characteristic of the metal-semiconductor contact.

The I-V characteristic with fractures was first observed in the works of Lepselter [2] and Zie [3,4]. These rare forms of I-V characteristic, in our opinion, are genetically related to each other, and secondly, they are the key to understanding the mechanism of current flow in the opposite direction.

2. Theoretical analysis

It can be suggested that the various forms of the I-V characteristics of Schottky diodes are not related to processes occurring in semiconductors, but are related to the microstructure of the metal film. The point is that, unlike devices with a p-n junction, in the case of DS, one of the "partners" of the contact, the metal usually has a polycrystalline structure, as shown in **Figure 2**.

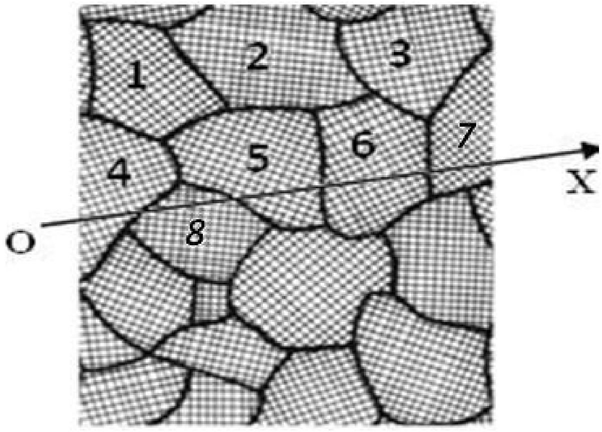

Figure 2. Microstructure of the surface of a polycrystalline metal.

In the case of a MS contact, Schottky's theory is valid only when the interface structure is homogeneous, i.e. both contacting materials have a single crystal structure. However, in most practical cases this condition is violated because of the polycrystallinity of the metal [5].

The work function of a polycrystalline metal is a function of the coordinate of the surface Φ(x) and can vary over a wide range. It can be assumed that the work function of the metal is constant within an individual crystallite and changes discontinuously on transition from crystallite to crystallite [6], as shown schematically in **Figure 3** by a dashed line.

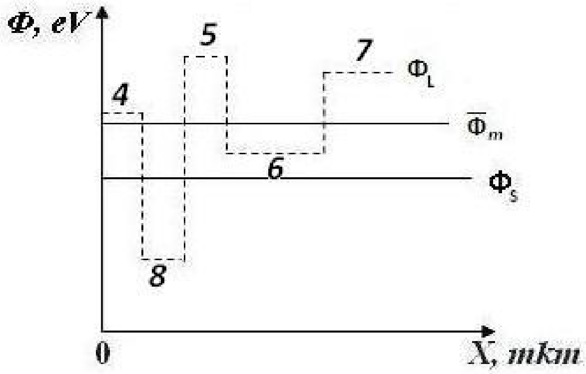

Figure 3. Dependences of the work of metal and semiconductor outlets on the surface coordinate.

Figure 3 also shows the work function of the single-crystal semiconductor Φs and the local work function of the polycrystalline metal Φ_L. Here $\overline{\Phi_m}$ is the work function of the metal averaged over the surface. The relationship between Φi and $\overline{\Phi_m}$ can be expressed by the formula [3,7,10]:

$$\overline{\Phi_m} = \frac{\sum_{i=1}^{n} \Phi_i S_i}{\sum_{i=1}^{n} S_i} \quad (1)$$

Here, Φi and Si respectively, the work function and the area of the i-th crystallite. It is obvious that the contact of such a polycrystalline metal with a single-crystal semiconductor creates an MS contact with an inhomogeneous inter- face. The barrier height of such a contact is expressed by the formula [8,10]:

$$\overline{\Phi_B} = \sum_{i=1}^{n} \Phi_{Bi} \omega_i \quad (2)$$

where, $\overline{\Phi_B}$ is the height of the barrier averaged over the interface, ω_i is the specific area of the sub diodes and Φ_{Bi} is the height of the barrier of the i-th sub diodes; **n** -is the number of sub contacts. With increasing **n**, the number of sub contacts increases.

As can be seen from formula (2), the averaged barrier height of the inhomogeneous contact $\overline{\Phi_B}$ depends on the relative area of the sub diodes and their barrier heights. In [10], the reason for the divergence of barrier height values of the same diode structures obtained by different authors is explained by the structural diversity of the interface. It is shown that each specific interface between a metal and a semiconductor is individual and unrepeatable.

In **Figure 3** shows changes in the local work function of a polycrystalline metal Φ_L and a single-crystal semiconductor Φs along an arbitrary direction of the OX surface. It also shows the experimental (or preferred) value of the work function of the metal $\overline{\Phi_m}$, which is usually given in the reference books [9].

When comparing the average metal work function $\overline{\Phi_m}$ with the work function of a semiconductor n type, we take into account that according to the Schottky theory [1] the contact has a diode property only when $\overline{\Phi_m} > \Phi s$. However, this cannot be said when comparing the local work function of a metal Φ_L with a semiconductor, since the Schottky condition is not satisfied, for example, for region 8, as is evident from **Figure 3**.

Obviously, when **n** = 1, then interface is homogeneous, that is, both contact partners have a single-crystal structure. It should be emphasized that almost all researchers of MS contact did not take into account the inhomogeneity of polycrystalline metal, and mistakenly believed that the objects they studied were homogeneous. In our works it was considered that, **n** is always more than unit [8,11]. The value of **n** was estimated as follows. If the average grain area of the polycrystalline metal is of the order of 1 μm^2 and the area of the Schottky diodes is about 1000 μm^2, then the number of parallel contacts will be of the order of **n** = 1000. It is clear that the value of n can be varied by means of thermal annealing and contact area. If each of the grains of a metal with a semiconductor creates Schottky diodes, then it is obvious that each diode has different values of barrier height, breakdown voltage, contact area, series resistance and other parameters. It is clear that when an inverse voltage is applied to such a contact, diodes with the lowest breakdown voltage will soon be first pierced, and with increasing voltage to breakdown, other diodes with higher breakdown voltage values will be connected in series. With increasing reverse voltage, the number of sub-diodes connecting in the process of breakdown increases.

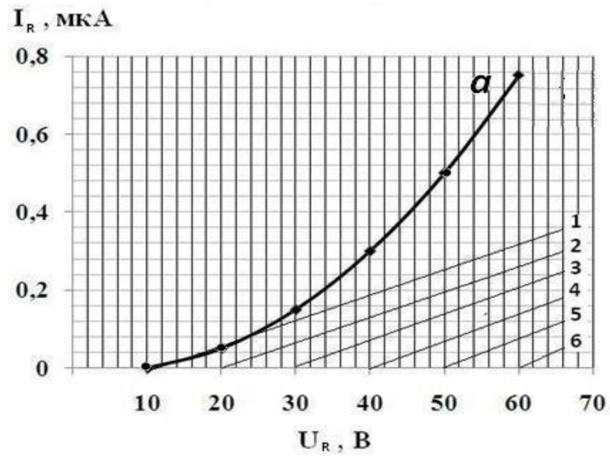

Figure 4. Reverse I-V characteristic (a) of several parallel connected Schottky diodes having different breakdown voltages.

Method To verify the validity of the foregoing assumption, **Figure 4** presents the results of model calculations of the I-V characteristic SD produced using a metal with a polycrystalline structure. It was assumed that the breakdown voltages of the sub-diodes have different values (10V, 20V, 30V, 40V, 50V). For simplicity, it was considered that other parameters of the diodes, such as the area, barrier height and the series resistance, as well as the mechanism of the flow of charges particles though the contact, are the same. It is clear that when applying revers voltage greater than

10V, a diode 1 will break through, in which the current increases linearly with increasing voltage. When the reverse voltage reaches 20V, diode 2 also breaks through, as a result of geometric summation of currents, the slope of the **I_R (U_R)** dependence grows. Obviously, with the further growth of the reverse voltage, other (3,4,5,6) sub-diodes are connected to the breakdown process. Thus, with increasing reverse voltage, the area of contacts participating in the breakdown process increases.

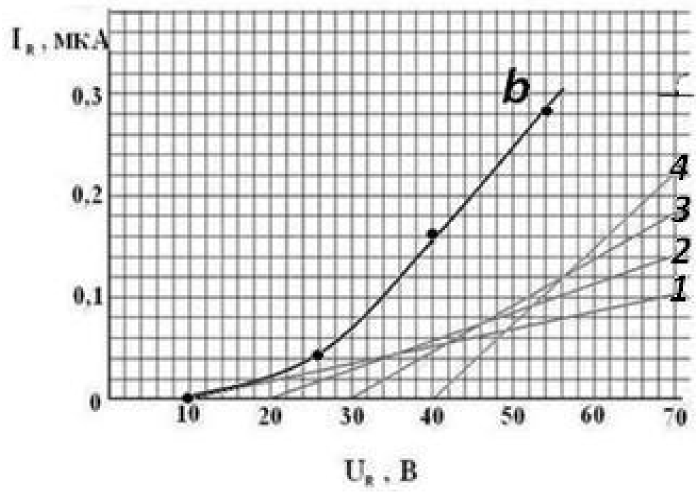

Figure 5. Reverse I-V characteristic (b) of several parallel connected Schottky diodes having different breakdown voltages and areas.

Figure 5 shows the results of another model calculation, where the DS consists of 4 sub-diodes having different areas and breakdown voltages. It is assumed that all the parameters of the sub-diodes are identical, in addition to the breakdown voltage and the areas, and diodes having high breakdown voltages have a large area. As is easy to see from Fig. 5, with increasing reverse voltage, the reverse current of the sub-diodes increases linearly, and diodes with high breakdown voltages and areas are connected to the breakdown process. As a result of the geometric addition of linear reverse currents, the current-voltage characteristic of the DS in the opposite direction (b) becomes nonlinear.

3. Results and discussion

The relationship between the total reverse current and the reverse voltage can be expressed by the formula:

$$I_R = k(U_R - U_0)^{\mu} \qquad (3)$$

Here, Uo is the diode breakdown voltage, μ indicates the degree of nonlinearity of the inverse I-V characteristic. To determine the degree of nonlinearity, the inverse I-V characteristic is constructed on a logarithmic scale and is shown in **Figure 6**. In this case, it is equal to μ = 2.09 (a) and μ = 2.46 (b). The value of μ depends on the degree of inhomogeneity of the metal film.

If we denote by *dS* the contact area, where the breakdown voltage varies in the range from *Uo* to *Uo + d Uo*, then it is obvious that *dS* can be expressed by the formula:

$$dS = So\, f\,(U)\; dUo \qquad (4)$$

Here, *f (U)* is the distribution function of the interface with respect to breakdown voltages; *So* is the total contact area. By changing the microstructures by the method of technology, one can change *f (U)* and, accordingly, the shape of the I-V characteristic of the DS in the opposite direction.

From the above, it can be concluded that the current-voltage characteristic of the DS in the opposite direction with a single break (**Figure 1b**) is a consequence of parallel connected two sub-diodes (**n** = 2) having different values of the breakdown voltage, area and height of the barrier.

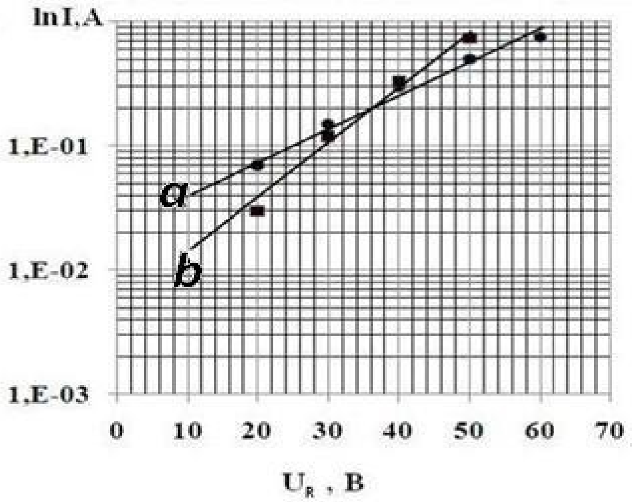

Figure 6. Dependence of the reverse branch of the I-V characteristic curve on a logarithmic scale.

After the breakdown the first diode, the reverse current rises according to the avalanche breakdown, and when the reverse voltage reaches the breakdown voltage of the second diode, the second diode breaks and, accordingly, the reverse currents of the diodes are added geometrically, as a result of which a bending appears in the current-voltage characteristic (**Figure 1b**). In the same way, it is possible to explain the I-V characteristic of a DS with a double bend (**Figure 1c**). In this case, the number of sub-diodes is n = 3.

Thus, as a result of the parallel connection of the diodes, the linear I-V characteristic of the DS becomes nonlinear, that is, it has new properties not inherent in discrete sub-diodes. A similar property is inherent in complex systems [12]. Naturally, we can conclude that DSs made with the use of polycrystalline metals can serve as an experimental object for testing a number of problems of complex systems, since many complex phenomena and processes are not experimentally "reproducible" even in real conditions.

It is known that the contact of a metal with a semiconductor is sometimes called a Schottky semiconductor diode.
In view of the foregoing, with equal justification, we can assume that DS is a "metal" Schottky diode.

4. Conclusion

It is shown that in electronic processes occurring in the contact between a polycrystalline metal and a semiconductor, the metal plays a more important role, and is an active contact partner than a semiconductor. It is suggested that many questions of the MS contact can be explained within the framework of the theory of complex systems, since the complexity of the system grows with the growth of the number of sub-diodes. An analogously complex system, in the case of diode Schottky with increasing n, the contact acquires new properties that are absent at the subsystem level.

The various forms of the I-V characteristic of Schottky diodes in the reverse direction are explained by the geometric mechanism of the breakdown, according to which they are a consequence of the influence of the microstructural inhomogeneity of the interface initiated by the polycrystallinity of the metal. Changing the microstructure of the metal by the technology, it is possible to change the degree of inhomogeneity and the number of sub-diodes forming the contact. The number of sub-diodes can be varied by the shape of the I-V characteristic. At n = 1, the Schottky diode has an ideal "sharp", and at n> 4, a "soft" breakdown. When n = 2 or 3, there are volt-ampere characteristics with one or two bends. As a result of geometrical addition of linear reverse currents I-V characteristics, the general current-voltage characteristic becomes soft, i.e. nonlinear.

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