

STRUCTURAL OPTIMIZATION OF SCHOTTKY DIODES BASED ON Si

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Abstract. In the paper is shown results of studying the electrophysical properties of a Schottky diode created between a monocrystalline semiconductor and a polycrystalline metal structure, focusing on the impact of thermal annealing on the non-homogeneity of the contact (separating) interface. To investigate the role of non-homogeneity of the interface, the dependence of the Schottky diode's properties on thermal annealing parameters with different contact areas was examined. It was concluded that the effect of thermal annealing on the contact area allows for a deeper understanding of the processes occurring in the metal-semiconductor contact. The processes occurring at the metal-semiconductor contact can be explained within the framework of complex systems theory, taking into account the role of the metal's microstructure and the non-homogeneity of the contact surface in determining the electro-physical properties.

Keywords: Metal-semiconductor contact, Schottky diodes, thermal annealing, interface, complex systems.

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1. Introduction

Schottky diodes are widely used in power supply systems for computers, servers, communication systems and data transmission. Serious attention to the issues of rectifier speed and the reduction of their energy losses will improve the reliability of power transistors in the primary part of the power supply unit. The use of Schottky diodes in controlled power converter circuits for electric drives ensures minimal forward recovery voltage when turning off power switches, as well as switching with low commutation losses and interference. As a result, it is possible to set a high switching frequency, reduce the number of auxiliary components and decrease their size, weight and cost (Lanin *et al.*, 2011; Asadullayeva *et al.*, 2023; Khannaa *et al.*, 2011; Lee *et al.*, 2019; Raja & Murty, 2018; Farkhadov & Abdullayeva, 2022).

The study of the reasons for the decline in the quality of devices and their premature failure is as important as the study of the physical and technological phenomena that ensure the stability and reliability of devices (Ali *et al.*, 2020; Saha *et al.*, 2025; Sistani *et al.*, 2018; Sze, 1980).

From this perspective, interest in polycrystalline metal layer electronic devices has increased recently. The ease of technological production and low cost of these layers justify the demand for polycrystalline metal layer devices (Abdullayeva & Hasanov, 2024; Askerov *et al.*, 2022; Edwards & Coleman, 2013; Askerov *et al.*, 2020; Zhu *et al.*, 2010; Askerov *et al.*, 2018; Askerov *et al.*, 2017).

For this purpose, the effect of thermal annealing on the parameters of a Schottky diode created between a monocrystalline semiconductor (Si) and a polycrystalline structured alloy (TiCu) and the non-homogeneity of the interface (boundary) has been studied.

2. Experimental section

The contact of n-type Si with a TiCu polycrystalline structure (111) oriented Schottky diode (Al-Ti_{0.9}Cu_{0.1}/n-Si Schottky diode) has been studied ($\rho = 0.7 \Omega \cdot \text{cm}$). The chip consists of 14 diodes. The geometric dimensions of the diodes vary in the range of $(1 \text{ to } 14) \times 10^{-6} \text{ cm}^{-2}$.

When studying contact, it is important to consider the complexity of a system consisting of numerous identical elementary subcontacts connected in parallel, each with different properties and parameters.

The properties of Al-TiCu / n-Si Schottky diodes have been studied, their volt-ampere characteristics ($\ln I - V$) analyzed and their electrophysical parameters calculated (Figure 1).

The relationship between terms of thermionic emission (TE) theory ($V \geq 3kT/q$) is given as (Sze, 1980; Afandiyeva *et al.*, 2007; Khannaa *et al.*, 2011; Afandiyeva *et al.*, 2018; Afandiyeva *et al.*, 2008).

$$I = I_o \left[\exp\left(\frac{q(V - IR_s)}{nkT}\right) - 1 \right] \quad (1)$$

here, V is applied forward bias voltage across the diode, q is the electronic charge, k is the Boltzmann constant, T is the absolute temperature in Kelvin.

Saturation current which is given by:

$$I_o = AA^*T^2 \exp\left(-\frac{q}{kT} \Phi_{Bo}\right) \quad (2)$$

where, A is the rectifier contact area, A^* is the effective Richardson constant that equals $264 \text{ A/cm}^2 \text{ K}^2$ for (111) orientation n-type Si (Sze, 1980; Afandiyeva *et al.*, 2017), Φ_{Bo} - barrier height (BH).

It is known that the degree of non-homogeneity is regulated by the baking temperature and the change in the contact area. It was believed that under the influence of thermal processing, the non-homogeneity of the boundary between the polycrystalline metal and the semiconductor could be altered (Abdullayeva & Hasanov, 2024; Askerov *et al.*, 2017; 2022).

It is known that under the influence of thermal processing, the device parameters and properties of objects improve (Ali *et al.*, 2020; Huet *et al.*, 2017; Nuhoğlu & Gülen, 2010; Pashaev, 2014). The dependence of the properties of the material on thermal processing and contact geometry allows a deeper study of the processes occurring at the contact.

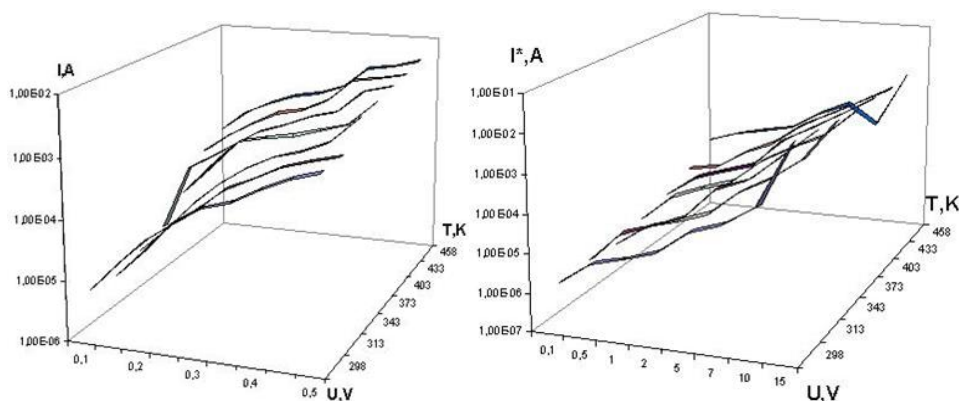


Figure 1. The $\ln I$ - V characteristics of TiCu/n-Si structure with an area $S = 4 \times 10^{-6} \text{ cm}^2$ in a) forward b) reverse directions

3. Results and Discussion

It is assumed that the interface between the metal and the semiconductor is homogeneous only when both “partners” of the contact have a monocrystalline structure. In any other case, the interface is always non-homogeneous and the degree of non-homogeneity depends on both the contact area and the thermal processing parameters.

It is clear that the processes occurring in a non-homogeneous contact cannot be described using the homogenous Schottky model (Sze, 1980), where the emission parameters of the interface are non-homogeneous in two dimensions and the emission parameters are a function of the coordinates of interface.

Experimental studies (Lee *et al.*, 2019; Askerov *et al.*, 2017; Saha *et al.*, 2005; Sistani *et al.*, 2018; Asıl Uğurlu *et al.*, 2021) show that the barrier height, breakdown voltage and other parameters of the Schottky diode are strongly dependent on the contact area and thermal parameters and cannot be explained within the framework of the homogeneous Schottky model. In this case, the application of the heterogeneous model is more appropriate: the contact is viewed as a parallel combination of numerous homogeneous discrete diodes. The number of elementary subdiodes depends on the number of monocrystals forming the contact.

It is clear that as n increases, the number of subdiodes and therefore the complexity of the system also increases (Loskutov & Mikhailov, 2007; Lu *et al.*, 2009; Cheng & Wang, 2009; Holovatch *et al.*, 2017; Askerov *et al.*, 2020; Eshqurbonov & Safarova, 2023).

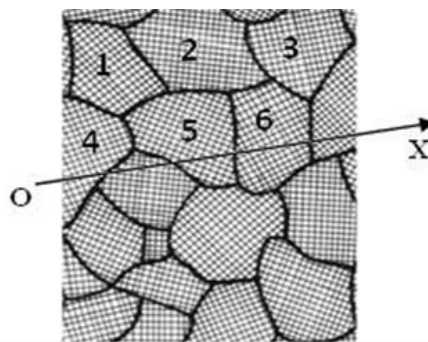


Figure 2. Microstructure of the surface of a polycrystalline structured alloy

It can be concluded that the number - n of subcontacts depends on the degree of non-homogeneity, thermoelectric parameters and the ratio of the characteristic dimensions of the diodes and crystals (Figure 2).

When, $n = 1$, the contact is formed between a monocrystalline semiconductor and a monocrystalline structured metal. The classical homogenous model of Schottky is valid here. When $n \geq 2$, the events occurring at the contact should be explained using the non-homogeneous model.

When $n = 2$ - the two-diode model of SD has been studied in the work (Askerov, 2017). It has been shown that the height of the barrier of the discrete diode system formed by two parallel connected homogenous diodes, even if the sub-diodes do not have temperature dependence, still exhibits temperature dependence:

$$\Phi_B(T) = \Phi_B(0) + \alpha T \quad (3)$$

When, $\Phi_B(0)$ and $T = 0$, the height of the contact barrier is calculated using the following formula:

$$\alpha = -kT \ln[\omega + (1 - \omega) \exp(-\Delta\Phi / kT)] \quad (4)$$

where $\Delta\Phi$ is the difference in the heights of the potential barriers of the discrete diodes. ω and $(1 - \omega)$ are the relative areas of the diodes, respectively. In the case of a homogeneous contact, when

$$\Delta\Phi = 0, \quad \alpha = 0.$$

In the case of a heterogeneous contact, according to formula (4), $\alpha \neq 0$. Also depends on $\Delta\Phi$. Where α - is the heterogeneity parameter.

4. Conclusion

The volt-ampere characteristics of TiCu/n-Si Schottky diode has been studied as a function of temperature. It was found that by changing the contact area and thermal annealing parameters, it is possible to control whether the contact behaves as a diode or an ohmic contact. The height of the barrier of the same Schottky diode before and after thermal annealing is not equal. Due to the effect of thermal annealing, the device properties of the contact improve and it can be concluded that as a result of thermal annealing, the degree of uniformity (area of ordered regions) of the contact increases and the number of subcontacts forming the contact decreases. By changing the number of subdiodes, the complex system can be modeled and its regularities can be studied using Schottky diodes.

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