

The Influence of Alkali Metal Atoms on the Electrical Conductivity of Granular Silicon

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Abstract: The article discusses the physical processes associated with the influence of alkali metals on the conductivity of granular silicon. It was revealed that the presence of alkali metals at the boundary of two contacting regions is observed passivation of the recombination of centers and this leads to an increase in the conductivity value 40 times higher than that for pure silicon without alkali metals.

Keywords: electrical conductivity, charging process, charge carriers, temperature, granular silicon, alkali metal.

Study of the possibility of controlling the main thermoelectric parameters like electrical conductivity (σ) is one of the main problems in semiconductor thermoelectric materials. To date, a number of studies have been carried out in this area and it has been shown that these parameters depend on the structure of the semiconductor material, in particular on the nature of the multilayer heterogeneous medium, the formation of current and voltage with the formation of electron-hole pairs in a heterogeneous medium. For example, in article [1], identified the electron properties of silicon oxide layer, which is between two adjacent silicon and its effects on charge processes. Shown, that in the granulated semiconductor, the charging process takes place mainly in two adjacent areas, the potential barrier in the area does not negatively affect charge carriers, on the contrary, detention and re-release in their traps leads to the growth of traps, particularly, granulated semiconductor permeability. However, for effective use, the study of the temperature dependence of electrical conductivity (σ), as well as the effect of various alloying atoms on them when creating a thermoelectric material based on granular silicon is one of the unsolved problems. In this regard, in this work, the results of a study of the temperature dependence of electrical conductivity in granular silicon and the effect of alkali metal (AM) atoms on them are presented.

For the study, p-type silicon and silicon wafers doped with AM atoms were used as samples, which were used in [2÷6] to study the manifestation of the phenomenon of adsorption and desorption of AM, as well as to study the conditions for the manifestation of impurity thermal-voltaic effects. Powder technology was used to grind silicon wafers to powder particles, which is given in [1, 7]. It should be noted that the introduction of AM atoms makes it possible to obtain spectral photosensitive p-n structures based on silicon wafers [2÷6]. The presence of AM atoms, various complexes of vacancies and oxygen-containing centers are formed, for example, ($\text{Li}_x\text{-O}_y$, $\text{Na}_x\text{-O}_y$ and $\text{K}_x\text{-O}_y$) or ($\text{Li}_x\text{-V}_y$, $\text{Na}_x\text{-V}_y$ and $\text{K}_x\text{-V}_y$), and at the same passivation of recombination centers occurs [2÷4], which increases the radiation resistance of p-n structures [2, 5, 6]. Table 1 shows the results of analysis of the chemical composition of AM in silicon.

Table 1

Distribution of alkali metal atoms [2, 3]

p - type silicon	Na, %	K, %	Cs, %
	2,82	1,77	1,45

The thermoelectric properties of the samples were measured by the Egor and Disselhorst method [1, 7]. According to the test method, a mixture of granulated silicon particles using ethyl alcohol was first prepared to prepare the samples in a strained form, and they were inserted into a heat-resistant dielectric body, then compressed with a force of 30-50 kG/cm² using metal screw contacts M_A and M_B, as shown in Figure 1, on both sides. The preparation of the mixture using ethyl alcohol made it possible to tightly

place silicon particles inside the dielectric housing. Figure 1 shows a simplified scheme of samples using the Egor and Disselhorst method, and an area diagram of the charged boundary of two contacting regions.

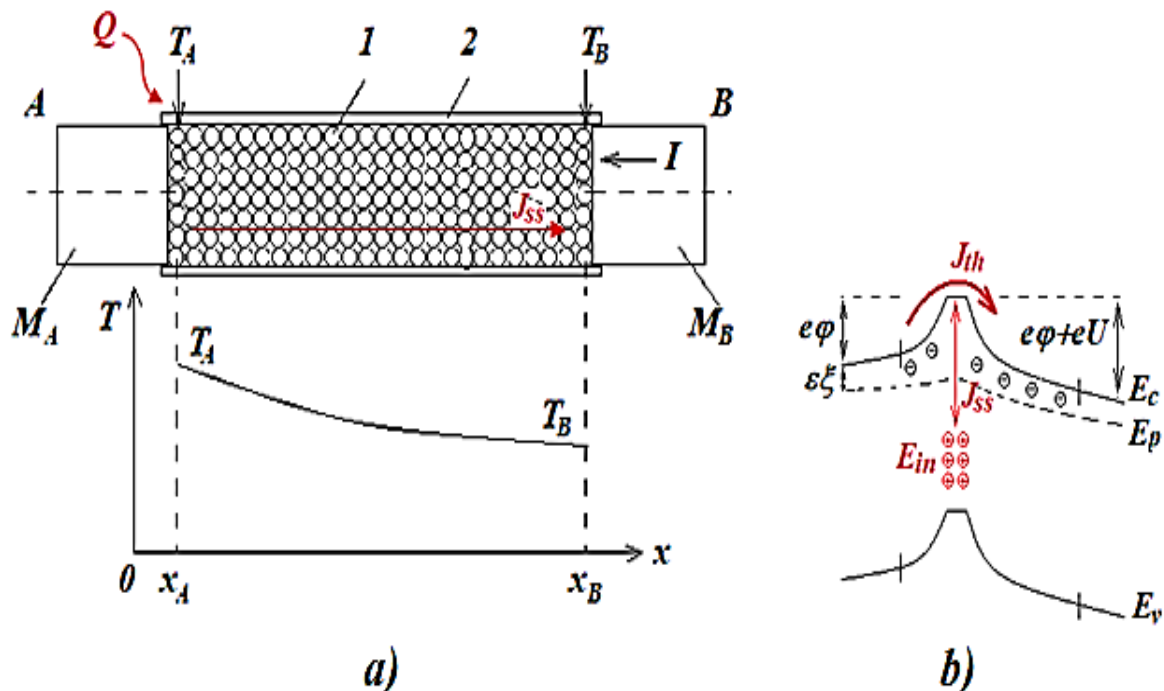


Figure 1. Scheme of measurement of samples based on the method of Egor and Disselhorsta (a) and diagram of zones (b). Here, 1 is the silicon particle, 2 is the heat-resistant dielectric housing, \$M_A\$ and \$M_B\$, and \$T_A\$ and \$T_B\$ are the ohmic contacts and thermocouples in areas A and B, respectively.

When heat \$Q\$ is applied to the sample, the charges generated in region A by temperature move to region B, and a thermoelectromotive force is generated due to the temperature difference between contacts \$M_A\$ and \$M_B\$. The temperature difference was monitored using a \$T_A\$ and \$T_B\$ thermocouple. In this case, the distance between the \$M_A\$ and \$M_B\$ contacts is 3 mm. To explain the results of the study, samples containing sodium or cesium atoms, respectively, are conventionally called “SiNa” and “SiCs”, and samples of pure granular silicon – “Si”. It should be noted that all studies were studied in the processes of increasing and decreasing temperatures. It was found that these physical phenomena are reversible processes.

In fig. 2 shows the temperature dependences of the conductivity of the samples. It is seen that the conductivity of the “Si” samples (curve 1) increases monotonically with increasing temperature. To explain the results, we will use the thermionic emission model and the structural model of the boundary of two contacting regions, as well as the mechanism for explaining the processes of charge carrier (CC) transfer in them with additions concerning the inclusion of currents arising in the process of capture and emission of CC on traps, which we formulated in [8÷10], as well as the band diagram of the charged boundary of two contacting regions (Fig. 1b) and a simplified scheme of the sample (Fig. 1a).

As shown in fig. 1b, CC are captured by states at the interface that lie above the Fermi level \$E_{in}\$, i.e. on the border of two contacting areas. The corresponding positive charge is compensated for by negatively infected acceptors in the space charge region. Based on the thermionic emission model, in addition to the main current \$J_{th}\$ due to the generation of electron-hole pairs, there is also a current \$J_{ss}\$ due to the dynamic equilibrium between the processes of capture and emission of CC associated with the conductivity of traps. \$J_{ss}\$ current is:

$$J_{ss} = Y_{ss} \delta\phi, \tag{1}$$

where \$Y_{ss}\$ is the characteristic admittance of traps, which depends both on their capture cross section and on the energy distribution, as well as on the position in space, i.e. location on the border of two contacting areas, \$\delta\phi\$ - change in the height of the potential barrier.

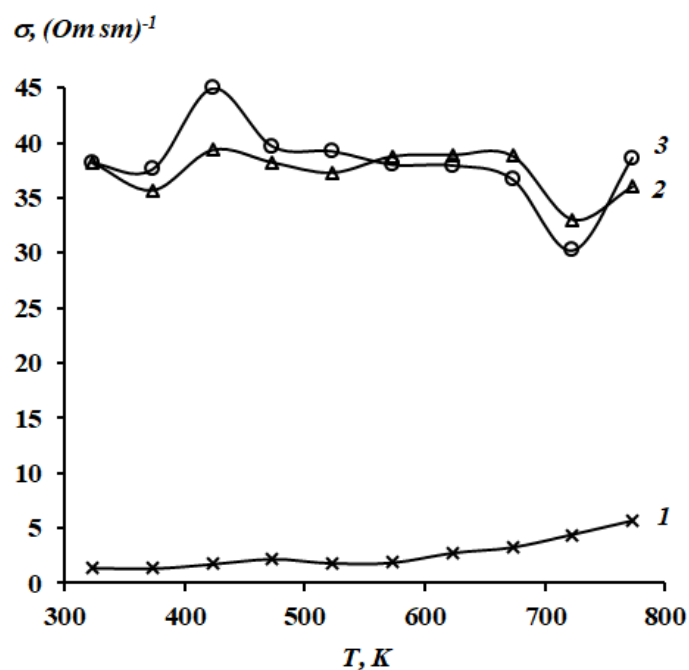


Figure 2. Dependence of the conductivity of the samples on temperature.

1 – “Si”, 2 – “SiNa”, 3 – “SiCs”.

The current J_{ss} is identically equal to the time derivative of the charge bound at the interface. At the boundary of two contacting regions, the following phenomenon takes place [1, 9, 10]: during the processes of capture and emission of CC, proceeding from the requirement of electro neutrality at the interface, the width of the space charge region should change. This, in turn, affects the entire band diagram (Fig. 1b), i.e., both the change in the barrier height $\delta\phi$ and Y_{ss} . This means that the current J_{ss} and the change in the height of the barrier $\delta\phi$ are interrelated, and the vibrational properties of this feedback are completely determined by the properties of the traps, and the connection itself arises due to the change in temperature. In addition, in (1) J_{ss} is the characteristic total conductivity of traps, which depends on their capture cross section, energy distribution, and position in space. Naturally, in the process of changing the temperature, both capture and emission of CC with the participation of traps are observed. As the temperature increases, both of these processes involve centers characteristic of the boundary of two contacting regions, for example, with $E_{in1} \sim 0.15$ eV and $E_{in2} \sim 0.17$ eV, which manifest themselves at temperatures of $323 \div 343$ K, with $E_{in3} \sim 0.36$ eV, observed up to 383 K, and with $E_{in4} \sim 0.3$ eV, which are observed up to 600 K [1, 8÷10].

An important circumstance is both the geometry of the sample and the location of the boundary of two contacting regions. As indicated, for the study we selected samples of granular silicon created from a silicon particle and with a length of ~ 3 mm (Fig. 1a). Figure 1a shows the case when ohmic contacts A and B are located on opposite sides of the sample. In this case, CC do not move from one grain to another, they are captured by traps and move along the E_{in} levels located at the boundary of two contacting regions, so the observed J_{ss} currents arise. And so, considering from these positions at elevated temperatures the generated charges due to the excitation of both shallow and deep levels, CC move in the direction from A towards B (Fig. 1a). In this case, an increase in the conductivity of the sample is observed (Fig. 2, curve 1). However, the conductivity on the “SiNa” and “SiCs” samples (Fig. 2, curves 2 and 3) changes non-monotonically, i.e., in this temperature range, a jump-like change is observed, and the conductivity value is 40 times higher than on the “Si”. This may be due to the passivation of recombination centers with AM atoms.

It is known that the presence of alkali metal atoms can contribute to the destruction of Si – Si bonds in the active zone, and silicon particles in the surface zone, i.e. in oxide layers - initiation reactions or, conversely, inhibition of the formation of polymer chains [3, 4]. As the temperature rises, desorption of AM atoms is observed at the interface of two contacting regions, various complexes of vacancies and oxygen-containing centers are formed, for example, $(Li_x-O_y, Na_x-O_y$ and $K_x-O_y)$ or $(Li_x-V_y, Na_x-V_y$ and $K_x-V_y)$ [2÷10]. These curves 2 and 3 (Fig. 2) indicate the passivation of recombination centers with AM atoms in these granular silicon samples.

Thus, the temperature dependence of the conductivity of granular silicon was studied, and the effect of alkali metal atoms on them, it was found that it depends not only on temperature, it also depends on the crystal structure at the boundary of two contacting regions, and on the manifestation of recombination centers in them when the temperature changes. and the effect of impurity state on the crystal structure.

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