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## Conductivity And Seebeck Coefficient In Granular Silicon

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### ABSTRACT

The article discusses the physical processes, the related temperature dependencies of conductivity and the Zeebek coefficient in granular silicon and the influence of alkali metal atoms on them at a temperature of 300 K to 800 K. that the conductivity and Zebeck coefficient do not depend only on temperature, it depends on the crystal structure at the boundary of the two contacting regions, and the development of recombination centers in them with an increase in temperature. In the process of temperature growth, desorption of alkali metal atoms is observed, which leads to structural inhomogeneities of crystal lattices at the border of two contacting regions and at the same time increase in structural heterogeneity of crystal lattices of the desorption layer of alkali metal atoms, lead to electron scattering, which leads to a change in sign.

### KEYWORDS

Electrical conductivity, charging process, charge carriers, temperature, granular silicon, alkali metal.

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## INTRODUCTION

The study of the possibility of controlling the main thermoelectric parameters, such as specific electrical conductivity ( $\sigma$ ) and thermal eddies ( $\alpha$ -Seebeck coefficient) [1÷5] is one of the main problems in semiconductor thermoelectric materials. To date, a number of studies have been carried out in this field and it is 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 to form electron-hole pairs in the heterogeneous medium. For example, [5] shows that a thermoelectric material based on granular silicon is a multilayer heterogeneous medium. consisting of a silicon particle of micrometric dimensions, a coating substance, tunnel contacts between the particles are formed from pressed against each other; and revealed that their thermoelectric properties depend on tunnel contacts in the silica nan layer; formed on the surface of particles, as well as from local energy levels in it. Based on the results of the study, thermoelectric parameters are determined, for example,  $\alpha=500 \text{ mkV/K}$  at 400 K [5]. However, for efficient use, the study of the temperature dependence of the parameters  $\alpha$  and  $\sigma$ , as well as the effect of various alloying atoms on them when creating a thermoelectric material based on granular silicon, is one of the unresolved

problems. In this regard, the present paper provides the results of a study of the temperature dependence of these parameters in granular silicon and the effect of alkali metal atoms (AM) on them.

## EXPERIMENTAL CONDITIONS AND SAMPLES CHARACTERISTICS

For the study, the p-type silicon and flint plates of the doped AM atoms were used as samples, which in the work [6÷10], we used to study the manifestation of the phenomenon of adsorption and desorption of AM atoms, as well as to study the condition for the manifestation of impurity heat and voltage effects. For grinding silicon plates to powdered particles powder technology was used, which is given in operation [5]. It should be noted that the introduction of AM atoms allows us to obtain spectral photosensitive p-n structures based on silicon plates [6÷11]. The presence of AM atoms, various complexes of vacancies and oxygen-containing centers are formed, for example,  $\text{Li}_x\text{-O}_y$ ,  $\text{Na}_x\text{-O}_y$ ,  $\text{K}_x\text{-O}_y$  or  $\text{Li}_x\text{-V}_y$ ,  $\text{Na}_x\text{-V}_y$ ,  $\text{K}_x\text{-V}_y$ , and at the same time the passivation of recombination centers [1÷5. 11] occurs, which increases the radiation resistance of p-n structures [6÷11] Table 1 shows the results of the analysis of the chemical composition of AM in silicon.

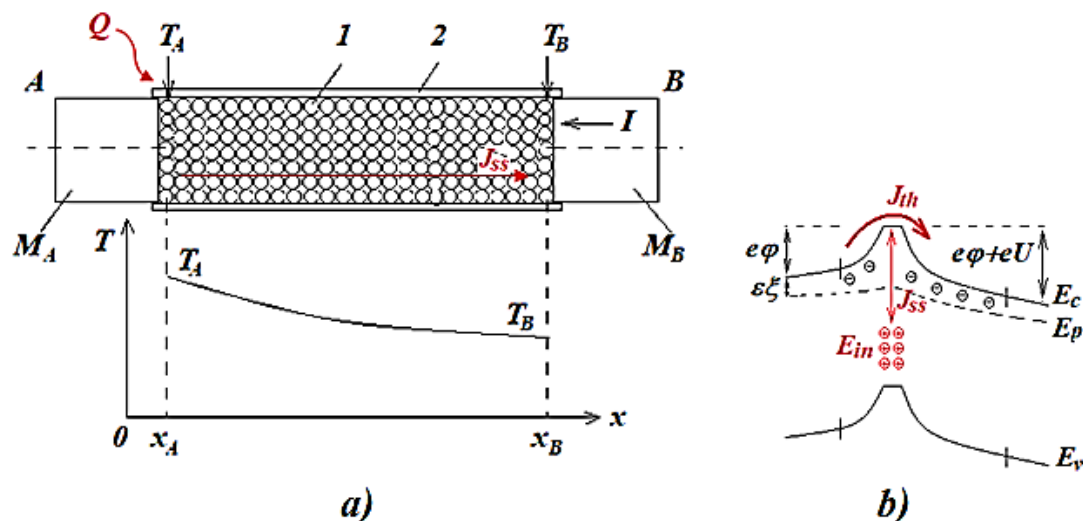
Table 1

*Distribution of alkali metal atoms [6, 7]*

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 [12]. 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/sm<sup>2</sup> 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.

## RESULTS OF EXPERIMENTAL INVESTIGATIONS AND DISCUSSION

### Conductivity

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 [13÷15], 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).

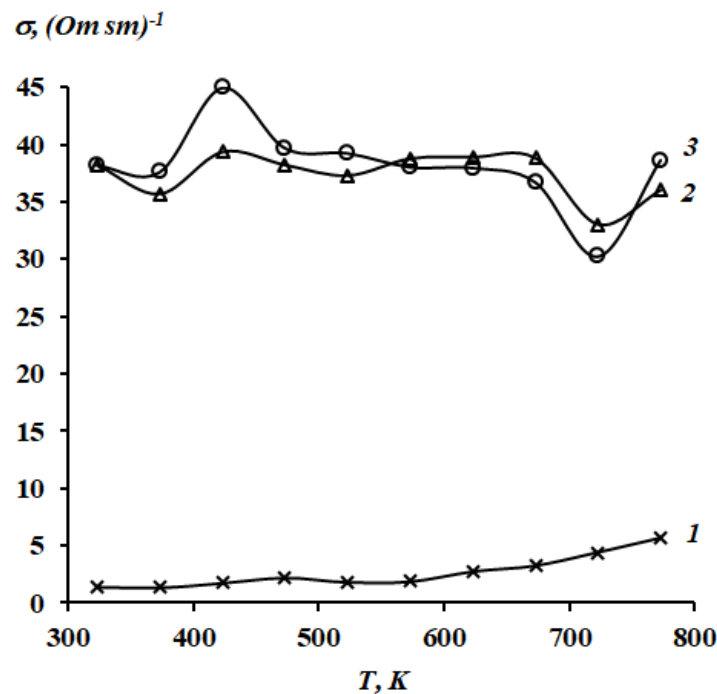


Figure: 2. Dependence of the conductivity of the samples on temperature. 1 – “Si”, 2 – “SiNa”, 3 – “SiCs”.

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:

$$J_{ss} = Y_{ss} \delta \varphi, \quad (1)$$

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.

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 [14, 15]: 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  $\sim 3$  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.

### Seebeck coefficient

Figure 3 shows the temperature dependence of the Zeebeka coefficient ( $\alpha$ ). It should be noted that unlike metals in semiconductors, the Seebeck coefficient decreases with increasing temperature. It can be seen that with an increase in temperature on the samples “Si” of the coefficient Zeebeka ( $\alpha$ ) exponentially decreases (curve 1). At  $\sim 400$  K, its value is 500 mK/K, which corresponds to the results obtained in operation [5]. However, on the samples “SiNa” and “SiCs” there is growth and decline. For example, on samples “SiNa”  $\alpha$  increases by 1.2 times at 475 K compared to the original state, and on samples

“SiCs” increases by 1.3 times, then decreases, even if  $T \geq 700$  K, its sign changes to "negative."

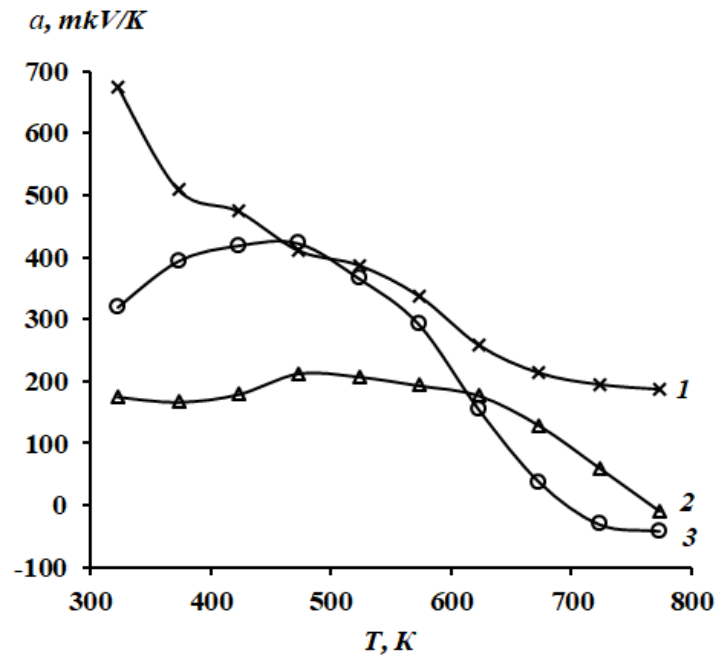


Figure: 3. The Seebeck coefficient ( $\alpha$ ) of samples depends on temperature. 1 – “Si”, 2 – “SiNa”, 3 – “SiCs”.

It is known that the thermoelectric properties of granular materials depend not only on temperature, it depends on the structure, nature, and state of matter, and the Zeebek coefficient depends on the semiconductor material, as well as on the temperature gradient [1÷3, 12]. It should be noted that for the study we selected samples of granular silicon created from a silicon particle and a sample length of  $\sim 3$  mm (Figure 1a). As defined above, conductivity changes are associated with manifestations by new recombination centers relating to a crystal lattice at the border of two contacting regions. In our opinion, with the manifestation

of recombination centers, the heat flux or conductivity changes, and this leads to a simultaneous decrease in the Seebeck coefficient (Figure 2, curve 1). As for the samples “SiNa” and “SiCs”, for example, at  $T \sim 300 \div 475$  K, the presence of alkali metal atoms in the surface zone of the silicon particle, passivation of recombination centers is observed at the energy levels  $E_{in}$  (Figure 1b), at the border of the two contacting regions with AM atoms, and this simultaneously leads to an increase in the Seebeck coefficient.

According to the literature analysis, the presence of alkali metal atoms can contribute: in the core - to the destruction of Si-Si bonds,



and in the surface zone of silicon particles, i.e. in oxide layers - to the initiation reactions or, conversely, inhibition of the formation of polymer chains [7, 8]. In the process of temperature growth, desorption of AM atoms is observed at the border of two contacting regions, various complexes of vacancies and oxygen-containing centers are formed, for example, ( $\text{Li}_x\text{-O}_y$ ,  $\text{Na}_x\text{-O}_y$ ,  $\text{K}_x\text{-O}_y$ ) or ( $\text{Li}_x\text{-V}_y$ ,  $\text{Na}_x\text{-V}_y$ ,  $\text{K}_x\text{-V}_y$ ) [6÷11]. At the same time, the crystal lattice of the desorption layer changes, forming inhomogeneous structures, which leads to a decrease in  $\alpha$  at  $T \sim 423 \div 700$  K. Also, according to literary analysis, the Zeebek coefficient in some cases, the sign of the coefficient can vary depending on the temperature [1÷3, 15]. In our opinion, with an increase in the structural inhomogeneity's of the desorption layer of alkali metal atoms, they lead to electron scattering, which leads to a change in the sign of the Zeebeck coefficient at a further temperature,  $T \geq 700$  K.

## CONCLUSIONS

The study of conductivity and Zebeck coefficient in granular silicon and the influence of the AM atoms on them were studied with a change in temperature from 300 K to 800 K. It was shown that the conductivity and Zebeck coefficient depends not only on temperature, it depends on the crystal structure at the border of the two contacting regions, and the development of recombination centers in them with a change in temperature. It was revealed that passivation of recombination centers by AM atoms leads to an increase in conductivity and Zeebek coefficient. In the process of temperature growth, desorption of AM atoms is observed, which leads to

structural in homogeneities of crystal lattices at the border of two contacting regions and at the same time increase in structural heterogeneity of crystal lattices of the desorption layer of alkali metal atoms, lead to electron scattering, which leads to a change in the sign of the Zeebek coefficient.

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