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Thermal conductivity of granulated silicon doped with alkali metal atoms

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Abstract. This study presents a novel comparative method for determining the thermal conductivity coefficient of granular silicon doped with alkali metal atoms. The experimental setup utilizes a three-layer disk configuration, where the same heat flow is passed through two distinct material samples. Temperature measurements are taken separately between each heat-conducting layer, allowing for precise thermal conductivity comparisons. The method's key advantage lies in its ability to minimize experimental errors by using a comparative approach. By passing identical heat flows through different samples simultaneously, the technique effectively isolates the thermal conductivity properties of the doped silicon granules. The experimental design employs a disk with a thickness significantly smaller than its diameter. This geometry allows researchers to neglect heat loss through the side surfaces, focusing the analysis on the axial heat flow through the layered structure. This simplification enhances the accuracy of the thermal conductivity measurements for the granular silicon samples containing alkali metal dopants. This innovative approach provides a reliable means to quantify the impact of alkali metal doping on the thermal properties of granular silicon. The findings from this study have potential applications in the development of advanced semiconductor materials and thermal management solutions in electronics.

1 Introduction

Currently, there are a number of methods for manufacturing semiconductor-based, particularly silicon-based thermoelectric materials and thermocouples, based on the creation of different energy levels in the semiconductor band gap. Silicon is one of the main materials widely used in the production of semiconductor devices, and it is specially alloyed with elements of groups III and IV of the Mendeleev table in order to have the necessary electrophysical properties. These impurity atoms form an impurity layer located in the band gap of silicon. The thermal conductivity of semiconductors and metals decreases sharply as a result of the introduction of various types of dopant atoms. This is explained by the increase in structural inhomogeneity, which causes electron scattering. Currently, advanced scientific testing institutes of our republic and many countries of the world are working to increase the thermoelectric, electrophysical and radiation resistance properties of nano and micro-sized

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semiconductor materials, as well as the effect of alkali metals on them, the dependence of the physical properties of granulated semiconductors on thermal voltaic effects and the manifestation of these effects. many practical research studies are being conducted to study the mechanisms [1-2].

It is known from the powder technology that granulated silicon contains metallurgical silicon impurities (Si 98÷99%; Fe, Au, B, P, Ca, Cr, Cu, Mg, Mn, Ni, Ti, Various chemical elements (such as V 1÷2%) can be preserved [2]. We know that the introduction of alkali metal (Li, Na, K, Cs) atoms allows to obtain silicon-based r-n structures [1-3]. The sensitivity of such structures to light rays is in the spectral maximum range of 0.8÷1 μm, and the efficiency is 7.4%. The introduction of alkali metal atoms increases the radiation resistance of silicon-based semiconductor devices and QEs [3,4]. In addition, scientific studies have shown that when the size of silicon granules and the amount of input atoms are changed under the influence of temperature, the values of ZT can be improved by 100 times compared to the silicon wafer, and ZT≈1 at 200 K has been achieved. Theoretically, independent measurements of the Seebeck coefficient, electrical conductivity, and thermal conductivities show that the increase in efficiency is caused by phonons.

The thermoelectric property of semiconductor materials is related to the formation of different energy levels in their forbidden zone, and this property is widely used in the creation of thermocouples [5,6,7]. According to the analysis of the literature, the main thermoelectric property of the granular semiconductor material depends on the nature of the multi-layered heterogeneous medium consisting of accessible states or defects in two adjacent boundary regions. Under the influence of temperature, current and voltage appear due to the formation of electron-hole pairs in a heterogeneous medium. It is shown that the formation of electron-hole pairs depends on the nature and properties of accessible states, defects in multilayer heterogeneous media. Thermoelectric properties of semiconductor materials are explained by such parameters as Seebeck coefficient (α) and electrical conductivity (σ). Controllability of these parameters allows to create efficient thermoelectric materials based on granulated silicon [6,7].

2 Materials and methods

A comparative method was developed to determine the thermal conductivity coefficient of granular silicon doped with alkali metal atoms. The experimental setup consisted of a three-layer disk configuration with a thickness significantly smaller than its diameter. Two distinct material samples were placed in the disk, and an identical heat flow was passed through both simultaneously.

Temperature measurements were taken using thermocouples placed between each heat-conducting layer. The small thickness-to-diameter ratio of the disk allowed heat loss through side surfaces to be neglected, focusing the analysis on axial heat flow through the layered structure.

Granular silicon samples were prepared with various concentrations of alkali metal dopants. The thermal conductivity of these samples was measured over a temperature range of 300-600 K. A reference sample of known thermal conductivity was used for calibration and comparison.

3 Results and discussion

One of the main parameters of thermoelectric materials is thermal conductivity (χ). In order to increase the quality (Z) of thermoelectric materials, many studies are being conducted to reduce thermal conductivity. Because monocrystalline silicon has a high thermal conductivity (~150 W/m•K), it is not used as a thermoelectric material. Taking this into account, many scientific and practical research works are being conducted to reduce the thermal conductivity of silicon. For example, by making wafers by pressing silicon powders under external pressure and then baking them at a temperature of 1400 K, it was possible to reduce the thermal conductivity to ~79 W/m•K, which is almost two times compared to monocrystalline silicon [8].

$$Z = \frac{\alpha^2 \sigma}{\chi} \tag{1}$$

Z is the nobleness of materials, σ is electrical conductivity, α is specific heat, χ is thermal conductivity. With the formation of Nax-Ou, Csx-Ou or Nax-Vu, Csx-Vu complex compounds in two adjacent areas of granular silicon (Figure 1, areas 1 and 5), the atomic structure of this area changes, which, in turn, changes the electronic state of this area and causes a change in thermal conductivity. In connection with these, the thermal conductivity of the samples was also studied. The comparison method is widely used to determine the coefficient of thermal conductivity of powder. Accordingly, the same heat flow is passed through two types of material samples, and the temperature between each heat-conducting layer is measured separately [12]. For example, in the case of a multi-layer system, the temperature between each heat-conducting layer is measured separately (Figure 1).

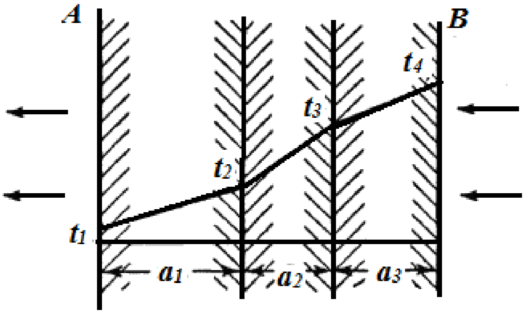


Fig. 1. Three-layer system with the thickness of layers a1, a2 and a3.

Heat flow is directed from boundary V to boundary A (shown by arrows).

Thus, in this case, it is considered that the heat flow passes through a three-layer disk, the thickness of which is small compared to the diameter, which allows to neglect the heat loss through the side surfaces. For each layer of the disk (Figure 1), the heat transfer equation can be written as follows:

$$Q = \chi S \frac{t_n - t_{n-1}}{a} \tag{2}$$

where Q is the amount of heat transferred from a layer with a temperature of tn to a layer with a temperature of t_{n-1} within a unit of time, a is the thickness of the layer, S is its surface. If heat is given from the surface of the disk (B), assuming that it first passes through all the layers and spreads to the outside environment, we can write the following for each layer of the disk with surface area S:

$$Q_1 = \chi_1 S \frac{t_2 - t_1}{a_1} \tag{3}$$

$$Q_2 = \chi_2 S \frac{t_3 - t_2}{a_2} \tag{4}$$

$$Q_3 = \chi_3 S \frac{t_4 - t_3}{a_3} \tag{5}$$

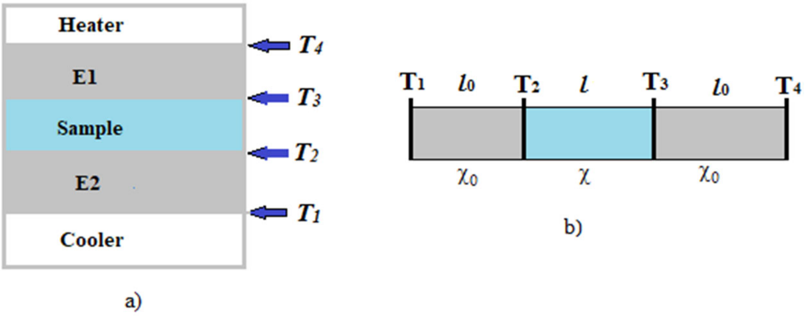
where χ_1, χ_2, χ_3 are heat transfer coefficients of each layer, respectively. Dividing expressions (4) and (5) by (6), we get the following:

$$\chi_1 = \chi_2 \frac{a_1}{a_2} \frac{t_3 - t_2}{t_2 - t_1} \qquad \chi_3 = \chi_2 \frac{a_3}{a_2} \frac{t_3 - t_2}{t_4 - t_3} \tag{6}$$

Knowing the coefficient of thermal conductivity of the first and third layers, it is possible to determine that of the middle layer. We used the comparison method to determine the thermal conductivity coefficient χ of granulated silicon with alkali metal atoms. Figure 1 shows a general and simplified view of the scheme for measuring the thermal conductivity of granulated silicon, based on the comparison of the tested sample with two reference samples [9-11].

The essence of the comparison method is that initially a sample of the material whose thermal conductivity is being studied is prepared and two standards (E1, E2) with known thermal conductivity values of similar shapes and sizes are placed between the samples. In our experiments, samples made of a special grade of brass (L63) were used as a reference, due to the thermal conductivity (110 W/m•K) being close to that of monocrystalline silicon.

The geometric dimensions of the studied samples and standards are 5 mm in length and 13 mm in diameter, and four metrologically certified XA thermocouples are placed between them as shown in Figure 1. The temperature gradient is created with the help of thermostats placed at the two ends of the system, heater and cooler.



a)

b)

Fig. 2. The scheme of measuring the thermal conductivity of granulated silicon. a) general appearance; b) simplified view.

The amount of heat passing through the cross-sectional surface of the substance is directly proportional to the thermal conductivity of the substance (χ), the surface area (S), the temperature gradient $\frac{\delta T}{\delta x}$ and time (t):

$$Q = -\chi S\left(\frac{\delta T}{\delta x}\right)*\mathrm{t} \tag{7}$$

The amount of heat passing through each layer in a unit of time (2b) is determined by the following expressions:

$$Q_1 = \chi_0 S\frac{\Delta T_{12}}{l_0} \qquad Q_2 = \chi S\frac{\Delta T_{23}}{l} \qquad Q_3 = \chi_0 S\frac{\Delta T_{34}}{l_0} \tag{8}$$

where χ is the thermal conductivity of the examined layer χ_0 is the thermal conductivity of reference layers 1 and 3.

$$Q_2 = \frac{1}{2}(Q_1 + Q_2) \tag{9}$$

If it is assumed that, then the thermal conductivity of the investigated layer χ is equal to the following:

$$\chi = \frac{\chi_0 l_1}{2l_0}\frac{\Delta T_{12}+\Delta T_{34}}{\Delta T_{23}} \tag{10}$$

In our experiments, l_0=l_1 follows from the fact that the geometric dimensions of each layer are the same. Then formula 10 will look like this:

$$\chi = \frac{\chi_0}{2}\frac{\Delta T_{12}+\Delta T_{34}}{\Delta T_{23}} \tag{11}$$

Table 1. Measured thermal conductivity of granulated silicon with alkali metal atoms under different temperature gradient conditions.

#	Si			Si+Na			Si+Cs		
	$t_{н}$,°C	t_c,°C	χ	$t_{н}$,°C	t_c,°C	χ	$t_{н}$,°C	t_c,°C	χ
1	31.2	23.09	15.36	31.5	23.5	11.02	31.5	23.5	10.46
2	40.8	23.09	16.2	40.1	23.9	11.48	40.1	23.9	9.14
3	51.6	23.2	15.9	50.3	24.1	10.71	50.3	24.1	10.69
4	61.6	22.2	16.23	60.1	24.5	9.62	60.1	24.5	9.29
5	61.6	32.0	16.76	70.2	28.3	12.14	70.2	28.3	10.25
6	61.6	42.07	16.43	70.2	37.1	12.2	70.2	37.1	9.86
7	61.6	51.55	15.34	70.2	45.2	11.81	70.2	45.2	9.54

Table 1 also presents the results of calculating the thermal conductivity of granulated silicon containing alkali metal atoms measured in conditions with different temperature gradients. In our experiments, the temperature of the hot side started from 30ºC and reached 70ºC with a difference of about 10ºC. Experiments were conducted separately for each sample, for samples containing monocrystalline silicon, cesium and sodium atoms, and each time the value of thermal conductivity χ was calculated using 11 formulas.

According to the data presented in Table 1, the results obtained for granular silicon are consistent with the results presented in the work, that is, when the temperature of the hot side reaches 60 ºC, the temperature of the cold side has changed by 10 ºC. In the experiments conducted on granulated silicon containing alkali metal atoms, when the temperature of the hot side reached 70ºC, the temperature of the cold side also changed by 10ºC. Comparing all the obtained results, the thermal conductivity (χ) of granulated silicon with dimensions of 400 nm ÷ 60 µm in the temperature range of 20 ÷ 70 ºC is from 15.34 to 16.76 W/m•K, which corresponds to the results of work [4], which is a single crystal at least 9 times smaller than silicon [9,12].

The thermal conductivity (χ) of granulated silicon with alkali metal atoms of the same size in the temperature range of 20 ÷ 70ºC is 9.62 to 11.81 W/m•K for the sample with sodium atoms, which is at least 12.5 times smaller than monocrystalline silicon, cesium 9.14 to 10.69 W/m•K for the sample containing atoms, which is at least 14 times smaller than that of monocrystalline silicon. thermoelectric parameters of granulated silicon with different electrophysical properties were studied in the work, according to which it was determined that the thermal conductivity (χ) of granulated silicon depends primarily on the size of its constituent particles.

4 Conclusion

In our experiments, the thermal conductivity of granulated silicon depends not only on the particle size, but also on the composition of the sample. In the two adjacent areas of granulated silicon (Figure 2, areas 1 and 5), Nax-Ou, Csx-Ou or Nax-Vu, Csx-Vu complex compounds are formed. as a result of this, it was found that the electronic state and thermal conductivity of this field will change. Based on the scientific researches considered in this way, it is possible to say that the precursors and alkali metal atoms form donor surfaces in granulated silicon. This, in turn, causes a change in the electrophysical and thermoelectric properties of the granules during the temperature change. The given considerations serve as a useful source for solving the existing problems in explaining the physical properties of granulated semiconductors under certain conditions, including the structure of granules, the formation of two adjacent areas, charge transfer processes between them, as well as other kinetic phenomena in micro- and nano-sized semiconductors. Taking these into account, to sum up, the results obtained in the study of the thermoelectric properties of granulated silicon are important in obtaining new types of thermoelectric materials and explaining the physical processes occurring in them.

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