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Structure of Inter Grain Boundaries in the Granular Semiconductors and the Charge State

L.O. Olimov*, Z.M. Sokhibova, B.M. Abdurakhmanov

Andijan Machine Building Institute, Russia.

Corresponding Author:** ***L.O. Olimov, *Andijan Machine Building Institute, Uzbekistan.*

Abstract: *The article discusses the physical processes associated with the structure of the granules, their contact, and the charge-transfer mechanisms of the two connected granules.*

Keywords: *Granula, semiconductor, silicon, traps, charge transfer.*

1. Introduction

Recently, the results of the study of the electronic properties of the silicon oxide layer between two connected silicon granules and their effects on the charge transfer processes are having been discussed in the [1] work. The study showed that charge transfer in granular semiconductors occurs mainly in two adjacent areas, where potential barrier height does not affect the charge carrier, their charge carrier retention and release can increase traps, particularly granular semiconductor conductivity. Also, according to the results of this research, on thermoelements based on granulated semiconductors and their properties have been analyzed in the [2, 3] research. However, the physical processes related to the structure of the granules and, accordingly, the contact of the two connected granules and the charge-transfer mechanisms are not fully described. In this work, a detailed analysis of the physical processes related to the field is given.

2. Research Method

There are a number of methods for the production of granular semiconductor materials, of which powder technology is a promising method for producing polycrystalline semiconductor materials for solar cells or integrated schemes, as well as for thermoelements. The principal novelty of our approach is the production of silicon granules within the framework of the powder technology method, which is given in [4÷6], and we were used to produce a polycrystalline silicon plate. As a raw material of the technology, monocrystalline silicon is used, where solar cells with a coefficient of about 15% are used on their basis. The starting samples are ground in a ball mill, and it is possible to obtain a powder with a grain size of ten to a thousand nanometers with control of the grinding time. This technology is much cheaper compared to, for example, sol gel or with other methods. An electron microscope was used to study the structure of granular silicon.

3. Structure and Location Schemes of the Granule

The results of preliminary studies show that the dimensions of silicon granules are from 400 nm. up to 1000 μm, and its surface in all cases abounds in a variety of complex structures, i.e. they have a rough surface (Fig. 1). Analysis of the chemical composition of the surface of granules showed that in some areas, namely in the rough structure, oxygen-containing complexes are observed, that their concentration increases to the edge of rough structures.

It is known from powder technology that the entry of an impurity from external environments in the production of powders leads to the formation of impurity states and defects on the surface of the granule, and this simultaneously leads to contamination of the material obtained on the basis of silicon. These are the main shortcomings of powder technology. To solve these problems, the operations of vacuum drying and magnetic cleaning of granules were carried out [4÷6]. It should be noted that the grinding of the powders was carried out in ceramic mills. Since the process is carried out at room temperature, no chemical reactions between silicon atoms and impurity atoms that come from mill material or other media occur. Therefore, the magnetic method makes it possible to completely purify silicon powders from impurity atoms that come from external environments. Observations of oxygen-containing complexes on the granule surface can be related to the conditions of the technology. In our case, silicon is ground in oxygen-containing media to a powdery state. At the same time, coatings of particles with a layer of silicon dioxide are provided on the surface of the granule and this simultaneously leads to the formation of a rough structure with oxygen-containing complexes. With known assumptions, the aggregate of granular silicon powder obtained above by the indicated conditions is illustrated in the scheme shown in Fig.1.

Here, regions 1 are surface rough structures of the oxides of silicon itself. Region 2 is a boundary zone of a single crystal and, unlike its core, is abundant with growth defects, dislocations, and other structural disturbances. Areas 3 - the core of the granule, is a single crystal oriented with respect to a specific crystallization front.

It is known from powder technology that after pressing, sintering of formed products is carried out. Sintering of powders is made to impart the necessary hardness and strength to the product from powder materials at a temperature of 0,7÷0,9 of the absolute melting temperature of the main component of the material. For example, the melting point of silicon is ~1420 °C, but for sintering it ~1200÷1250 °C is required [4÷6]. When the powder molds or the freely poured powders are heated, a complex combination of various physicochemical phenomena occurs simultaneously or sequentially. During sintering, the size, structure, and properties of the original powder bodies change, surface, boundary and volume self- and hetero diffusion processes occur, various dislocation phenomena occur, matter transfer through the gas phase, chemical reactions, relaxation of micro- and macro voltages, recrystallization of particles, etc. take place. In our opinion, the above processes, for example, the heating process does not occur uniformly throughout the granule volume, that is, a temperature difference is observed at each region of the granules, for example, the surface temperature (regions 1 and 2) is higher than the core temperature due to mechanical friction while grinding the granules ($T3 \leq T2 \leq T1$), as shown in Figure 1. In addition, the atomic structure of these regions can vary greatly. And also, in turn, the electrical, optical and other properties of each region can differ in a wide range.

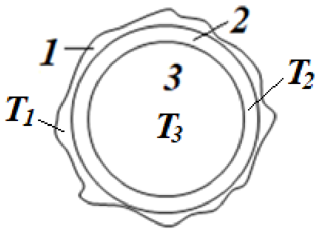

Fig1. *A simplified scheme of silicon granule.*

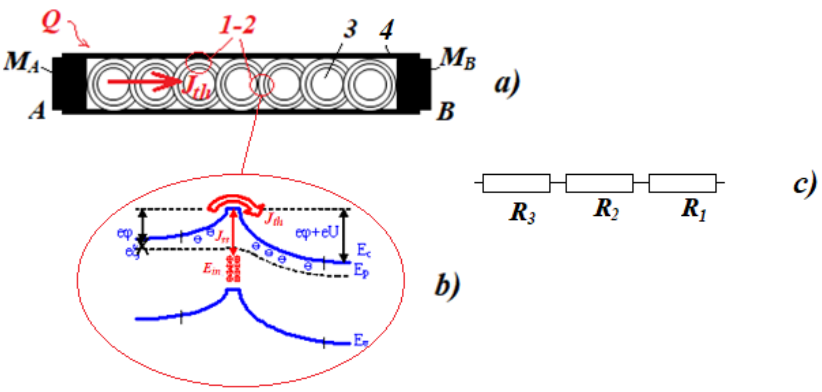

Fig2. *A simplified scheme of the method of investigation and location of the granule (a), zone diagram (b), equivalent electrical circuit. (1, 2, 3) - silicon granules, 4 - ceramic tube, M_A and M_B contacts, respectively, in the A and B regions.*

It should be noted that the study and explanation of the electrical, optical and other properties of inter grain boundaries in the granular semiconductors is more difficult, when used in practice, i.e. this may be due to the conditions of use of the granules and their location. For example, Fig. 2 illustrates a simplified scheme of two uses of granules in practice. From Fig. 2a it can be seen that the granules can be arranged in series, and a contact area can be formed between them, or the granules can be arranged side by side, as shown in Fig. 2b.

Variant 1. The positioning of the granules is consistent. If the granules are arranged in series between them, a contact region is formed in the silicon dioxide layer by pressing the silicon granules to each other and local energy levels are formed therein (region 1-2, Fig. 2a). Usually such structures are observed in larger sizes, for example, in granules with sizes of 100÷1000 micrometers.

Variant 2. The positioning of the granules next to each other. Typically, such structures are observed in smaller sizes, for example, in granules with dimensions of 400÷700 micrometers. The internal diameter of the ceramic tube is from 1 to 1.2 mm, which is several times larger than the size of the granule. In this case, granules with a size of 400-700 nanometers are placed in the tube, as shown in Fig. 3a. As a result, a region 5 is formed inter grain the granules, as in the first variant, local energy levels are formed therein. This region is formed between the granules located side by side, i.e., it differs from the first variants shown in Fig. 2a.

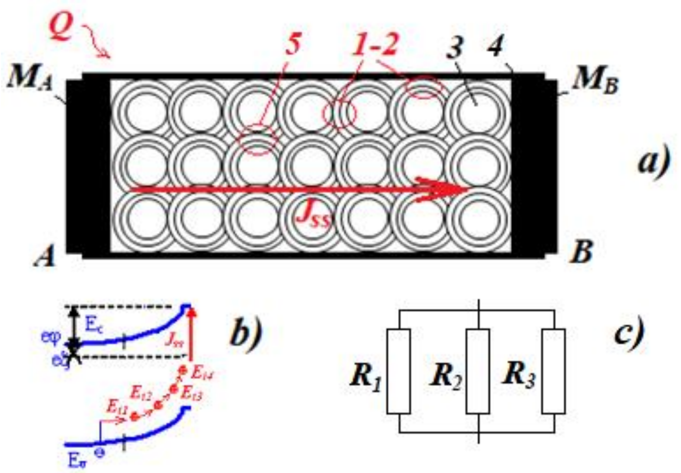

Fig3. *A simplified scheme of the method of investigation and location of the granule (a), zone diagram (b), equivalent electrical circuit. (1, 2, 3) - silicon granules, 4 - ceramic tube, MA and MB contacts, respectively, in the A and B regions.*

It should be noted that in both cases the granules do not contact the nuclei (3), they contact only the surfaces, i.e., those caused by regions 1 and 2, where it is shown in Fig. 1. For both cases location or view of regions 1, 2, 3 and 5 are shown in Fig. 3a.

4. MECHANISM OF THE PHENOMENON

It is known that when a thermoelement is heated (Q), a temperature gradient is observed in the contact between M_A and M_B. In this case, in semiconductors, electrons at the hot (A) end acquire higher energies and velocities than on (B) cold, and an increase in the concentration of charge carriers with temperature is observed. As a result, there is a stream of electrons from the hot end to the cold. At the cold end, a negative charge accumulates, while on the hot end there remains an uncompensated positive charge. The process of charge accumulation continues until the resulting potential difference causes the flow of electrons in the opposite direction equal to the primary, so that balance is established. In this case, in a closed circuit, the current and voltage depend on the specific resistance of the semiconductors. Knowing the specific resistance, we can determine the mechanisms of carrier charge transfer. In our opinion, in both cases the mechanisms of charge carrier transfer between themselves vary very strongly.

Variant 1. It is known from the physics of polycrystalline semiconductors that between grain boundaries in polycrystalline semiconductors are the centers of accumulation of defects and residual impurities from the feedstock. This congestion creates localized charge states [7]. Filling the charge state on the between grain boundaries leads to a change in the height of the potential barriers, which substantially affects the drift of the charge carriers, and, consequently, a change in ρ [5, 6, 8]. In connection with this, in our first case, that is, when the granules are arranged in series, the transfer of charge carriers into such structures, as well as the behavior of the specific resistance (ρ), can be explained within the framework of the modified thermionic emission model [7].

It is known that, according to the model of thermionic emission, the zone diagram of the charged between grain boundaries can be represented in the form as shown Fig. 2b. As shown in Fig. 2, daylight carriers come from one grain to another, causing seizure is observed, and emission of charge carriers. Thus the total current J_{th} major carriers flowing from left to right can be written as follows [7]:

$$J_{th} = A^* \cdot T^2 \exp(-\beta(\zeta + \varphi))(1 - \exp(-\beta U)) \tag{1}$$

Here, $\beta = e/kT$ – reverse thermal potential difference, e – electron charge, k – Boltzmann constant, T – temperature, A^* – the effective Richardson constant, U – the applied voltage. Shifted in the forward direction barrier is denoted by $e\varphi$, and $e\xi$ - depending on the concentration of the doping, the Fermi level in the crystal grains.

As shown in Fig.2b, the holes are trapped at the interface states lying above the Fermi level E_{ip}, ie in the between grain boundaries. Corresponding positive charge is compensated by a negative infected acceptor in the space charge region. Thermionic emission current creates J_{th}, the current from left to right. In addition to current J_{th} at the between grain boundaries, there is also a second current J_{ss}, shown in Fig.2b and 3b. This current is determined by the difference between J_{ss} intensities capture and emission holes. Current J_{ss} identically equal to the time derivative of the associated interfacial charge. At the between grain boundaries of the following phenomenon occurs [7] in accordance with the processes of capture and emission of charge carriers at the interface, to maintain full electro neutrality, changing the width of the space charge region. This in its turn affects the entire band diagram (see Fig. 2b) and the change in the barrier height $e\varphi$. That is, between the currents J_{ss} and change the barrier height has $e\varphi$ feedback. A vibrational property of this feedback is completely determined by the properties of traps, and the link itself arises due to changes in temperature. Increasing the height of the potential barrier leads to increased electrical resistance the total resistivity of the granules increases. The observed electrical resistance temperature change can be described within the frame of the modified Seto model:

$$\rho = \frac{k}{q\langle a \rangle A^* T} \exp\left(\frac{q\varphi}{kT}\right) \tag{2}$$

where $<a>$ is the grain size, φ is the potential barrier height on the grain boundary.

The potential barrier height

$$\varphi = \frac{Q_i^2}{8\varepsilon\varepsilon_o q N_G} \tag{3}$$

Here, Q_i is the boundary derivative charge in the grain boundaries, N_G - is the concentration of an electrically active dopants, ε_o and ε – dielectric constant.

It is seen from (2) that an increase of the trapped charge Q_i on localized traps in grain boundaries leads to an increase of φ, and this simultaneously leads to an increase of ρ. In our case, this process occurs between granules, ie, in two contacting regions of the granule (regions 1-2, Fig. 2a). An equivalent circuit of such a structure is shown in Fig. 2c. It can be seen that the equivalent circuitry consists of the series-connected resistances of the granule (R_1) and the two contacting regions of the granule (R_2). In this case, the total specific resistance is determined with the summary specific resistivities (R_1, R_2).

Variant 2. Charge carrier transfer in the second variant, as shown in Fig. 3a, is very different from the first one. In the same way, one can explain the process of transfer of charge carriers within the framework of thermionic emission. In work [5, 8, 9], we have studied the behavior of the current J_{ss} and the total conductivity of the traps (Y_{ss}), arising from the thermionic emission.

The current J_{ss} is:

$$J_{ss} = Y_{ss}\delta\varphi \tag{4}$$

The principal novelty of the approach is to take into account, principal changes of the conditions for the current in the framework of the thermionic emission model, (J_{ss}), which arise while capturing and emitting of a charge on traps, and working with the model in these conditions (Fig. 3). For example, it is shown that when the number of charge captures is larger than the emission, the charge moves along the levels (E_i) of the traps along the boundary of the two contacting grains (Fig. 3b), then the total conductivity of the traps (Y_{ss}) is increasing. Using the shown mechanism of the J_{ss} current generation, it becomes possible to consider the processes of charge carrier transfer in region 5 (Fig. 3). Figures 3a and 3b schematically depict the granule arrangement and the zone diagram, respectively. In this case, the charge carriers do not move from one granule to another, they are trapped in traps and move along the E_i levels (Fig. 3b) in region 5, so the observed J_{ss} currents appear (Fig. 3). An equivalent electrical circuit of such a structure is shown in Fig. 2c. It is seen that the equivalent electrical circuitry consists of the parallel-connected resistance of the granule (R_1) and the region 5 of the pellet (R_2). In this case, the total specific conductivity is determined with the summary specific conductivities (R_1, R_2).

5. Conclusion

Thus, in terms of the structure of granular semiconductors, the surface has different levels of roughness, and the charge transfer processes depend on the size of the granule and the layout scheme. If the granules are arranged sequentially, the charge transfer processes occur through the granules. Conversely, if the granules are parallel to each other, the charge carriers do not travel through the granules, which are caused by the traps formed between the granules.

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