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REGULAR ARTICLE

Structural Models and Charge Transfer Processes of Granulated Nano Semiconductors

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It is known that the physical properties of granulated semiconductors that appear under certain conditions depend on their size or access state or defects on their surface, and their formation depends on the methods of obtaining granulated semiconductors. Structural models of granular semiconductors and charge transfer processes in them are explained in this work. Research shows that in practice, granulated semiconductor particles can be arranged in a row or next to each other. In the first case, the process of charge transfer from the first particle to the second particle is carried out through the inter-particle boundaries formed between them. In this case, J_{th} current will appear. As the temperature increases, localized traps with E_{in} energy level appear successively in the interparticle boundary regions. An increase in the amount of charges (Q_i) captured in localized traps leads to an increase in the height of the potential barrier (φ), which, in turn, leads to a decrease in electrical conductivity. In the second case, the particles are located next to each other, and the charge transfer processes occur simultaneously, as in the first case, along the adjacent interparticle boundary areas. In this case, the conductivity of the traps increases, since the charge transfer process mainly occurs along the interparticle border areas located next to each other.

Keywords: Granular nano semiconductors, Charge transfer processes, Particles, Interparticle boundaries between two adjacent particles, Energy-level localized traps, Trap conductivity.

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1. INTRODUCTION

The physical properties of granulated nano-semiconductors under certain conditions depend on the access state or defects in the volume or surface of the semiconductor, and their formation depends on the methods of obtaining granulated semiconductors [1-9]. From the analysis, it can be seen that in the process of obtaining semiconductor materials, a change in thermodynamic balance or foreign atoms or molecules entering from the external environment lead to the distortion of the crystal lattice. Such processes mainly occur strongly in micro-sized semiconductors and form boundary areas between two crystals characteristic of a polycrystalline structure. In nanoscale structures, it leads to size effects.

In this work, the theoretical and practical results of the study of the structure of two adjacent granules and the specific models and mechanisms of their explanation are proposed. The results of the research show that the surface of silicon particles consists of different unevenness and roughness of silicon dioxide. In our opinion, the processes of charge transfer in them depend on the size, structure and arrangement of the granules.

Granular silica particles can be arranged in two different ways, in a row or side by side (Fig. 1 and 2). The charge transfer processes in them are completely different from each other. Below we will consider the location schemes and structure model of granulated silicon.

2. STRUCTURE MODEL AND CHARGE TRANSFER MECHANISM

2.1 Granular Semiconductors Arranged in Series

Fig. 1a shows the structural model of a granular semiconductor with its particles arranged in a row and the corresponding zone diagram. In order to explain the scheme of sequential arrangement of particles, it is appropriate to consider the size of the base occupied by the particles and the size of the particle. For this, a heat-resistant dielectric base, for example, a ceramic tube, can be used [1-4].

When the particle size is equal to the diameter of the ceramic tube, a sequential arrangement of granular semiconductor particles is observed inside the substrate (Fig. 1a). The ohmic contacts M_A and M_B are pressed from the two ends of the dielectric case by an external force, resulting in the formation of contact areas between the silicon particles (Fig. 1a, area 5). When heat Q is given by A of the sample, an electric force appears due to the temperature difference between M_A and M_B contacts.

When the temperature is increased by one standard, electron-hole pairs are formed in area A. Charge carriers move to B side. In this case, the process of charge transfer takes place through the areas of the boundary between two adjacent silicon particles (area 5). In this case, the charge transfer processes can be explained as follows on the basis of the zone diagram of the interparticle boundary areas presented in Fig. 1b.

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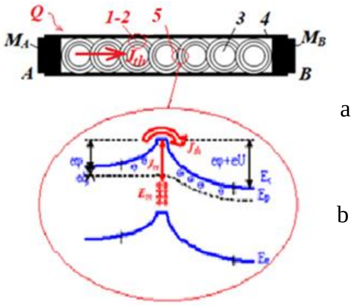

Fig. 1 – Arrangement scheme (a) and zone diagram (b) of granulated semiconductor particles arranged in series. 1-2 – rough surface area of the particle, 3 – particle core, 4 – dielectric body, 5 – interparticle boundary area

The process of transfer of charge from the first particle to the second particle is carried out through two contiguous interparticle boundary zones formed between them. In this case, J_{th} current will appear. As the temperature increases, localized traps with E_{in} energy level appear successively in the interparticle boundary regions. An increase in the amount of charges (Q_i) captured in localized traps leads to an increase in the height of the potential barrier (φ), which, in turn, leads to a decrease in electrical conductivity.

2.2 Granular Semiconductors Arranged Parallel to Each Other

Figure 2 shows the structural model of a granular semiconductor with adjacent particles and the corresponding zone diagram. This type of particle arrangement can be observed in a heat-resistant ceramic tube like the one above. For this, the size of the particles should be several times smaller than the inner diameter of the ceramic tube. In this case, the location of the particles can be described as in Figure 2a. Inside the ceramic tube, the particles form a series of particles arranged parallel to each other, as shown in Figure 1a. Their number is equal to how many times the particle size is smaller than the pipe diameter. That is, inside the tube, it forms a set of parallel and side-by-side granulated particles as shown in Fig. 2a. In contrast to Fig. 1a, an interparticle boundary (6 areas) is formed in parallel between granulated particles located in a row. also, the process of charge transfer in such a structure is fundamentally different from the process of charge transfer in a structure located in a series with each other, discussed in the previous paragraph.

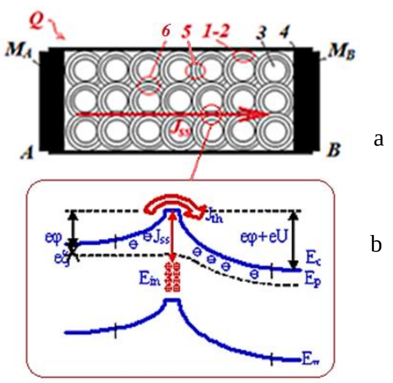

Fig. 2 – Arrangement scheme (a) and zone diagram (b) of granular semiconductor particles whose particles are adjacent to each other. 1-2 – rough surface area of the particle, 3 – particle core, 4 – dielectric body, 5 and 6 – interparticle boundary formed between consecutive and adjacent particles, respectively area, M_A and M_B are ohmic contacts in areas *A* and *B*, respectively, *Q* is the amount of heat supplied

When *Q* heat is applied, electron-hole pairs are formed in the *A* region of the sample, and they move to the *B* region. The charge transfer process takes place simultaneously through the granules connected in series and across 6 areas formed between the granules connected in parallel. In this case, the charge transfer process can be explained as follows based on the zone diagram.

According to the thermoelectric emission model, the charge carriers formed as a result of heating of the field A are trapped in the localized traps (E_{in}) above the Fermi level E_f and the J_{ss} current appears as a result of their release. J_{ss} depends on the current and E_{in} on the full conductance of the level traps (Y_{ss}).

In [9, 10], the conductivity Yss of localized traps in two adjacent areas was determined and a model was proposed to explain the charge transfer mechanisms through them. According to it, successively different energy levels under the influence of temperature, for example, at $T \sim 70 \div 420$ °C, successively $E_{in1} \sim 0.15$ eV, $E_{in2} \sim 0.17$ eV, $E_{in3} \sim 0.36$ eV, $E_{in4} \sim 0.3$ eV energy level traps can appear. The charge leaving the E_v valence zone is first trapped in E_{in1}, then E_{in2}, E_{in3}, E_{in4} energy level traps (Fig. 2b). This event continues until the traps are filled. The migration of charges across the levels leads to the generation of current J_{ss} and Y_{ss}.

We believe that the same process can occur in granular semiconductors. That is, charge carriers are trapped in traps with energy levels E_{in1}, then E_{in2}, E_{in3}, E_{in4}, which appear successively in the interparticle boundary (5 areas, Fig. 2a) and move along the traps (Fig. 2b). This in turn can lead to J_{ss} current and localized trap conductance (Y_{ss}). In granulated semiconductors, the process of charge transfer takes place in two adjacent 6 interparticle boundary zones (Fig. 2a). It should also be noted that charge carriers caught in localized traps do not move towards the core of the granule. That is, the charge carriers caught in the localized traps that appeared in the 5 interparticle boundary areas move to the localized traps that appeared in the 6 areas that are energetically close to each other. This, in turn, leads to an increase in the current Jss and Y_{ss}.

3. THERMOELECTRONIC EMISSION MODEL FOR GRANULAR NANO SEMICONDUCTORS

Above, we considered the structural models of granular semiconductors. Let's consider the charging processes in granular conductors and their production processes using the proposed models and the thermoelectronic emission model. As discussed above, when *Q* heat is applied, the temperature difference is the difference between M_A and M_B contacts. In this case, compared to the charge carriers formed due to the heating of the *A* area, the carriers of the *B* area, which have a lower temperature, move and the concentration of the charges increases under the influence of temperature. Temperature, transfer of charge carriers from area *A* with higher temperature to area *B* occurs. This process continues until a balance appears in both areas. Charge migration processes in such structures are similar to charge migration processes in polycrystalline semiconductors.

It is known from the physics of polycrystalline semiconductors that intergranular boundary areas act as localized traps for charge carriers [9-15]. The capture and release of charge carriers in localized traps leads to an increase in the potential barrier height (φ) in the intergranular boundary region, which in turn increases the resistivity (ρ) of semiconductors with a polycrystalline structure [14, 15]. Even in granular semiconductors, intergranular boundary regions act as localized traps for charge carriers. Accordingly, Figure 2b shows a zone diagram of two adjacent areas.

According to the thermoelectron emission model, a thermoelectron emission (J_{th}) current appears during the transfer of charges from left to right [12, 13]:

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

where, $\beta = e/kT$ – potential difference, A^{*} – Richardson's efficiency constant, U – given voltage, $e\varphi$ – height of the barrier on the left, $e\zeta$ – Fermi level depending on the doping concentration of the inputs in the grain.

It can be seen from the zone diagram that in addition to the J_{th} thermoelectron emission current, the second J_{ss} current is also present. This current occurs when charge carriers are captured and re-released in localized traps (E_{in}) in the intergranular boundary region above the Fermi level Ef when moving from left to right. J_{ss} current is the difference between the intensity of trapping and re-release of charge carriers in localized traps. This current depends on the total permeability of the traps (Y_{ss}), i.e., the complete permeability, which depends on the grain surfaces and energy distribution of the traps, and the potential barrier height ($\delta\varphi$).

$$J_{ss} = Y_{ss}\delta\varphi \qquad (2)$$

J_{ss} and $\delta\varphi$ have an inverse dependence due to the capture and release of charge carriers in traps. Such vibrational dependence is determined by the properties of traps.

In [9, 13-15], during temperature change from 300 K to 800 K, the capture of charge carriers in localized traps (E_i) increases the value of $\delta\varphi$ from 0.3 eV to 0.9 eV, on the contrary, during temperature decrease, $\delta\varphi$ it is determined that it leads to a decrease and that it consists of a feedback process. One of the more important properties for two connected fields is the dependence of not only Jss, but also the Jth current generated during the thermoelectronic emission process. A change in the height of the potential barrier ($\delta\varphi$) also causes a change in the current J_{th}. When the temperature changes, the trapping and re-release of charge carriers in the localized traps leads to a change in $\delta\varphi$ and J_{ss}, which leads to a change in the total current. In such cases, the total current can be expressed as:

$$J_{tot} = J_{th} + J_{ss} \qquad (3)$$

It can be seen from expression (3) that the total current depends on the trapping and re-release of charge carriers. As the temperature increases, the generation of electron-hole pairs increases. Due to them, the total current will also increase. So, the process of charge transfer in polycrystalline semiconductors mainly depends on the complete conductivity of the J_{ss} current and E_i-level traps (Y_{ss}) appearing in the two junctions, i.e., intergranular boundary areas. In [9, 10], an increase in total conductivity of E_i-level traps (Y_{ss}) was determined, which was explained on the basis of the appearance of thermo-voltaic effects with penetration in two junction areas. In our case, the processes taking place in the boundary between two adjacent granules may depend on the manifestation of voltaic effects with input heat.

4. MECHANISMS OF FORMATION OF LOCALIZED TRAPS IN INTERPARTICLE BOUNDARY AREAS

Defects formed in the intergranular boundary areas of polycrystalline semiconductors during crystallization or preserved crystalline states form deep or shallow localized traps for charge carriers [9, 11, 12]. They can appear or disappear during temperature changes. For example, in the range of ~ 20÷400 °C of thermal treatment, in series The emergence of recombination centers at E_{in1} = 0.15 eV, E_{in21} = 0.17 eV; E_{in31} = 0.36 eV and E_{in41} = 0.3 eV levels has been found to cause a disproportionate change of electrophysical parameters of polycrystalline silicon with increasing temperature [8]. In granular semiconductors, localized traps appear in the areas of the boundary between two adjacent particles.

The interparticle boundary field appears between two particles during the process of pressing the particles together. As we have seen in the previous paragraphs, the atomic structure of this field consists of various defects or entry states. The appearance of localized traps in granular semiconductors at different energy levels and the mechanism of charge transfer in them can be explained as follows.

Figure 3 shows the zone diagram of a granular semiconductor and the mechanism of charge transfer in recombination centers [9, 10]. Electrical contacts are placed in areas *A* and *B* of the sample. In order to explain the occurrence of localized traps at different energy levels and the process of charge transfer in them, we will conditionally divide it into sections I, II, III, IV, V and VI.

1. At the initial stages of temperature increase when *Q* heat is given, for example, when the temperature of section I is $T_1 < 50$ °C, the charge carriers that have passed from the valence zone to the conduction zone move from the area A with a higher temperature to the area *B* with a lower temperature. In this case, the charge carriers move along sections II, III, IV, V and VI (Fig. 3a), resulting in a current in a closed circuit.

2. As the heat energy *Q* increases, the temperatures in the sections change. For example, the temperature of section I is 50 °C < T_2 > 70 °C and the temperature of section II is increased to $T_1 < 50$ °C, let a recombination center with energy level E_{in1} ~ 0.15 eV appear in section I.

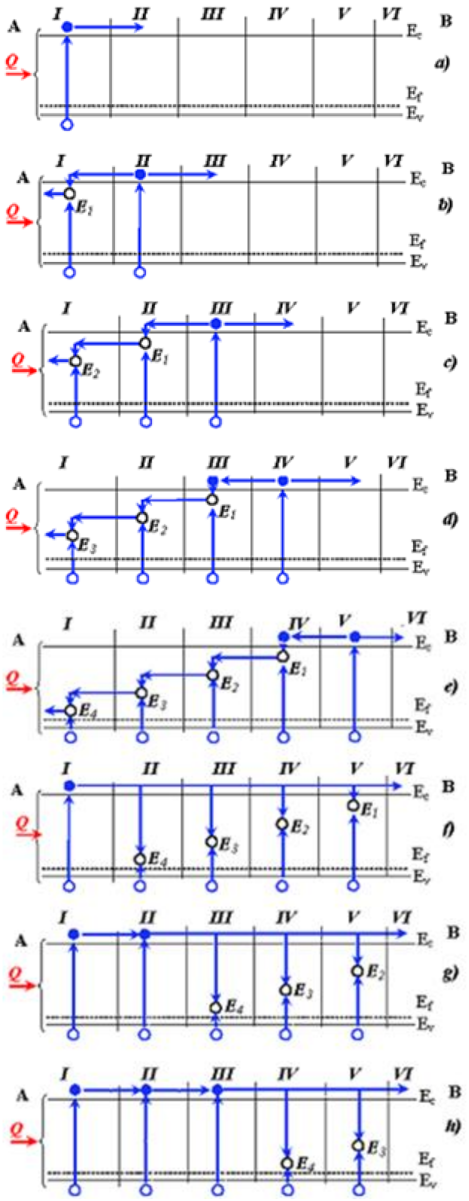

Fig. 3 – Zone diagram of granular semiconductor and mechanism of charge transfer in recombination centers

In this case, the migration of generated charge carriers depends on the concentration of recombination centers. If the recombination centers are greater than the concentration of charge carriers generated in the II section, the charge carriers are caught in localized traps with an energy level of E_{in1} ~ 0.15 eV and move towards the I section (Fig. 3b). On the contrary, if the concentration of recombination centers is less than the concentration of charge carriers generated in section II, charge carriers move from A to area V.

3. If the temperature of section I is 70 °C < T_3 > 100 °C, that of section II is 50 °C < T_2 > 70 °C, the temperature of section III is T_1 < 50 °C, as well as the energy level E_{in2} ~ 0.17 eV in section I, Let a recombination center with an energy level of E_{in1} ~ 0.15 eV appear in section II. The charge carriers generated in sections I and II are trapped in the recombination centers of levels E_{in2} ~ 0.17 eV and E_{in1} ~ 0.15 eV, respectively. Even in this case, charge migration depends on the concentration of recombination centers. That is, if the concentration of recombination centers is greater than the concentration of charge carriers generated in section III, charge carriers move towards sections I and II along the levels that appear in these sections (Fig. 3c). In this case, charge carriers move from area B to area A of the sample. Otherwise, charge carriers move from A to B.

4. If the temperature of areas I, II and III changes to 100 °C < T_4 > 250 °C, 70 °C < T_3 > 100 °C, 50 °C < T_3 > 70 °C, respectively, in these sections, E_{in3} ~ 0.3 eV, E_{in2} ~ 0.17 eV and E_{in1} ~ 0.15 eV energy level recombination centers should appear, and the IV region temperature should increase to T_1 < 50 °C. In this case, as mentioned in point 3, the generation and migration of charge carriers is observed (Fig. 3e, 3f, 3g and 3h). In this case, charge carriers move from B to A area. This process continues until the process of manifestation of recombination centers stops or the levels disappear. With the loss of successive recombination centers in sections I, II, III, the direction of charge carriers changes from area A to area B.

At the next stages of temperature increase, such processes are observed that, due to the increase in the concentration of charge carriers generated in sections I, II and III, and the appearance of the above-mentioned recombination centers in sections IV, V and VI, correspondingly, charge carriers move from A to B area. it accelerates. The amount of current in the closed circuit increases. In addition, the generation of charge carriers in localized traps can be observed at later stages of temperature increase. This process also accelerates the transfer of charge carriers from A to B area. The considered considerations play an important role in the explanation of thermal voltaic effects in a granular semiconductor.

5. CONCLUSIONS

Thus, in practice, charge transfer processes depend on the arrangement of granular semiconductor particles. If the granulated semiconductor particles are located in a row, charge transfer processes take place from the first particle to the second particle through the interparticle boundary areas formed between them. In this case, such a process occurs that localized traps with energy level E_{in} appear successively in the interparticle boundary areas as the temperature increases. An increase in the amount of charge carriers trapped in localized traps (Q_i) leads to an increase in the height of the potential barrier (φ), which in turn leads to a decrease in electrical conductivity. On the contrary, if the granular semiconductor particles are located next to each other, the charge transfer processes simultaneously, as noted above, from the first particle to the second particle in the interparticle boundary areas formed between them. through and along the interparticle boundary areas. In this case, as the temperature increases, localized traps with an energy level of E_{in} appear successively in the interparticle boundary areas. Charge carriers are trapped in localized traps. With the appearance of localized traps with a new energy level, charge carriers move along the localized traps. This process leads to an increase in the permeability of localized traps. That is, localized traps participate in conductivity.

The considered considerations can be of great importance in explaining the kinetic phenomena occurring in granular semiconductors and two adjacent boundary fields.

REFERENCES

1. F.L. Omonboev, A.T. Mamadalimov, L.O. Olimov, *J. E3S Web Conf.* **413**, 04013 (2023).
2. F.L. Omonboev, A.T. Mamadalimov, *J. E3S Web Conf.* **458**, 01022 (2023).
3. L.O. Olimov, U.A. Akhmadaliev, *J. E3S Web Conf.* **458**, 02014 (2023).
4. L.O. Olimov, U.A. Akhmadaliev, *J. E3S Web Conf.* **458**, 02016 (2023).
5. L.O. Olimov, B.M. Abdurakhmanov, A. Teshaboyev, *Materialovedeniye* No 1, 14 (2014) [In Russian].
6. L.O. Olimov, U.A. Akhmadaliev, *Journal Genius Repository* **12** No 6, 1 (2023).
7. L.O. Olimov, I.T. Khojimatov, *J. Sci. Prog.* **3** No 2, 357 (2023).
8. U.A. Akhmadaliev, L.O. Olimov, *IX International Scientific Conference*, 23 (London. Great Britain: 2023).
9. L.O. Olimov, *Inter Grain boundaries in polycrystalline silicon: microstructure, charge states and p-n transitions*, Doctor diss. (2016).
10. L.O. Olimov, B.M. Abdurakhmanov, F.L. Omonboyev, *Am. J. Eng. Technol.* **3** No 25, 28 (2021).
11. *Polycrystalline semiconductors. Physical Properties and Applications* (Ed. by G.M. Harbeck) (M.: Mir: 1989).
12. *Thin polycrystalline and amorphous films.: Physics and applications* (Ed. by L. Kazmersky) (M.: Mir: 1983).
13. L.O. Olimov, *Geliotekhnika* No 2, 39 (2010).
14. L.O. Olimov, *Uzbekistan Physics Journal* No 5-6, 361 (2007).
15. L.O. Olimov, *Uzbekistan Physics Journal* No 3, 231 (2005).

Структурні моделі та процеси переносу заряду у гранульованих нанонапівпровідниках

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Відомо, що фізичні властивості гранульованих напівпровідників, які виникають за певних умов, залежать від їх розміру або дефектів на їх поверхні, а їх утворення залежить від методів отримання гранульованих напівпровідників. У роботі представлені структурні моделі зернистих напівпровідників і процеси переносу заряду в них. Дослідження показують, що на практиці гранульовані напівпровідникові частинки можуть бути розташовані в ряд або поруч. У першому випадку процес перенесення заряду від першої частинки до другої здійснюється через утворені між ними міжчасткові межі. У цьому випадку з'явиться J-й струм. Зі збільшенням температури в областях міжчасткових меж послідовно виникають локалізовані пастки з рівнем енергії E_{in}. Збільшення кількості зарядів (Q_i), захоплених локалізованими пастками, призводить до збільшення висоти потенційного бар'єру (φ), що, у свою чергу, призводить до зменшення електропровідності. У другому випадку частинки розташовані поруч, і процеси перенесення заряду відбуваються одночасно, як і в першому випадку, уздовж суміжних міжчастинкових граничних ділянок. Процес перенесення заряду відбувається в основному вздовж міжчастинкових ділянок, розташованих поруч.

Ключові слова: Гранульовані нанонапівпровідники, Процеси перенесення заряду, Частинки, Міжчастинкові межі.