

Electronic Properties of Granular Silicon Oxide

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Abstract: The article discusses the electron properties of silicon oxide layer, which is between two adjacent silicon and its effects on charge processes. 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.

Keywords: granule, silicon, charge carrier drift, temperature, potential barrier.

Silicon Oxide SiO_2 is about 90% of the Earth's crust, and is the basis of many minerals and materials used in construction, electronics and other spheres. Theoretical and practical research on the formation of silicon oxide SiO_2 , its electronic properties and their use in creating various devices is being carried out for over 50 years (You can get acquainted with detailed analysis in study [1]). More than 99 percent of all semiconductor devices are fabricated on silicon. Thermal silicon dioxide SiO_2 is the key insulator in silicon devices. At present, gate SiO_2 in metal–insulator–semiconductor (MIS) devices is replaced by the so-called high-k dielectrics with high permittivity, such as Al_2O_3 ($\epsilon \approx 10$), HfO_2 , Ta_2O_5 ($\epsilon \approx 25$), and ZrO_2 ($\epsilon \approx 40$). Application of high-k dielectrics does not preclude the use of silicon dioxide. In order to create a perfect interface, a SiO_2 layer with a thickness of $\approx 5 \text{ \AA}$ is grown on silicon, followed by the deposition of a high-k dielectric layer with a thickness of $\approx 50 \text{ \AA}$. Silicon dioxide has been used and studied since ancient times; however, extraordinary efforts in this field have been taken over the past 50 years in connection with the use of SiO_2 in microelectronics (silicon devices), optoelectronics (glass fibers, lasers), and acoustoelectronics (quartz).

Nonetheless, some features of the electronic structure of SiO_2 remain unclear. To date, nine allotropic modifications of silicon dioxide have been known. Eight modifications have a tetrahedral structure. In tetrahedral modifications of SiO_2 , one silicon atom is coordinated by four oxygen atoms, so that two silicon atoms are bound via the oxygen atom. The Si–O bond is formed by Si $3 sp^3$ bonding orbitals and O $2p$ -orbitals. As follows from theoretical calculations, the top of the valence band of SiO_2 is formed by a narrow band of the O $2p\pi$ nonbonding orbitals. The narrow band of the O $2p\pi$ -orbitals in SiO_2 corresponds to high values of the hole effective masses in the range $\approx (5-10)$ (heavy holes). At the same time, experiments on tunnel injection of holes into silicon dioxide have revealed the presence of light holes and the effective tunneling mass in the range $\approx (0.4-0.5)$. By now, it has been found that not only the Si $3s$, p -orbitals but also the $3d$ -orbitals of silicon contribute to the formation of the top of the valence band of SiO_2 . The contribution of the Si $3d$ -orbitals to the formation of the hole effective mass and to the charge transfer along the Si–O bond remains undetermined. The band structure calculations have demonstrated that the narrow band of the O $2p\pi$ nonbonding orbitals is separated by a band gap from the wide band of the Si $3s$, p -O $2p$ -orbitals. At the same time, the Si $L_{2,3}$, Si K, and O K X-ray emission spectra do not exhibit a band gap separating the Si $3sp^3$ -O $2p$ -bonding orbitals and the O $2p\pi$ nonbonding orbitals. The presence of the band gap in SiO_2 is also not confirmed by the experimental valence band X-ray photoelectron spectra of SiO_2 .

Oxygen atoms break bonds of silicon atoms and locate in crystalline grid nodes. Depending on their amount and their ability to form compounds, oxygen atoms form crystallographic structures of different geometric shapes, which consist of silicon and oxygen atoms on the crystal. Theoretical studies show that the diffusion of silicon-oxygen clusters forms SiO_2 tetrahedral chains of different lengths within the scope of SiO_2 [2]. Oxygen can cause Si-Si bonds on the silicon surfaces to break off to form Si-O-Si or complex forms [3, 4]. The formation or the loss of such bonds depends on external influences. For

example, the vacuum conditions and the thermal conductivity of the SiO_x at $300\div 600^\circ\text{C}$ may change the atomic structure and cause different defects [5]. In the [6] research, the process of generating local energy layers satisfying the $E_c^{\text{Si}} < E_N < E_c^{\text{SiO}_2}$ ratio on the surface of two adjacent silicon granules has been studied. The resonated tunneling of energetic layer electrons in SiO_2 have been found out. In SiO_2 , it is proposed to produce silicon-based thermoelements by providing independent changes in thermoelectric parameters. In research 7 and 8, it is recognized that physical processes in such granulated silicon thermoelements are dependent on the size, structure, and patterns of granules. According to the proposed mechanism, the charge transfer processes are mainly found in the silicic acid region between the two adjacent granules. However, despite the large number of studies in the field, the electron state of granulated silicon oxide SiO_2 and its dependence on temperature changes are one of the most unresolved problems.

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 circuits, 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 [6-8], and we were used to produce a polycrystalline silicon plate. As a raw material of the technology, single-crystal silicon used, where solar cells with a coefficient of about 15% are used on their basis. The starting samples are ground in a ball mill, wherein the powder can be obtained with a granules size of ten to a thousand nanometers controlling the grinding time. In order to research structure of the granular silicon electronic microscope was used and to assess the transfer of charge carriers the specific resistance (ρ) of the granules was measured by two-probe method in a temperature range of 20 to 300°C [1]. The measurements were conducted in semi-automatic mode directly with the granules heated, as in a temperature rise from 20 to 300°C , and at the stage of its decrease.

The results of preliminary studies show that the dimensions of silicon granules are from 400 nm. up to $1000\ \mu\text{m}$, and its surface in all cases abounds in a variety of complex structures, i.e. they have a rough surface [7]. 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 [6-8]. 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.

The location of the granules corresponds to the polycrystalline structure. The intergrain boundary areas consist of silicon oxide, inlet, or defects, which form a barrier effect [9]. This effect is explained by the electron states of the two adjacent areas. The electron states of the two adjacent areas depend on the successive recombination centers in the course of the temperature rise, where the release of chargers leads to a change in potential barrier height (φ). By selecting the conduction (σ) of the Setto model, it is possible to define φ [9]:

$$\sigma = \frac{q \langle a \rangle A^* T}{k} \exp\left(-\frac{q\varphi}{kT}\right) \quad (1)$$

here q - electron charge, k - Boltzman constant, $\langle a \rangle$ - grain size, A^* - the effective Richardson constant, T - temperature.

Figure 1 shows the temperature dependence of φ and σ . As you know, as the temperature rises, recombination centers appear in the grain boundary areas of the polycrystalline semiconductors. In

them, the capture of charge holders will increase ϕ , which in turn will decrease the σ . In our case, on the contrary, σ was initially stable, and then suddenly, ϕ decreased. The thermionic emission model [9] can explain the results.

Figure 1c depicts the zones diagram of the two adjacent industries [9]. Besides the J_{th} thermionic emission current the second J_{ss} current is also presented. These sluggish local traps (E_{in}) appear in the process of retaining and recharging of chargers. J_{ss} is dependent on the actual permeability of the pit traps (Y_{ss}) and ($\delta\phi$.)

$$J_{ss} = Y_{ss} \delta\phi \tag{2}$$

This means that the current J_{ss} and the change in the barrier height $\delta\phi$ are interrelated, and the vibrational properties of this interrelation are determined by the properties of the traps. [10] proposed a model for explaining this mechanism of vibration-dependence and explaining the mechanisms of charging them. According to him, with increasing temperature, various types of energy-saturated traps appear. Charges from the valence band are sequentially caught in E_{i1} energy-saturated trap, followed by E_{i2} , E_{i3} , E_{i4} energy-saturated traps (Figure 1). This phenomenon will continue until the traps fill. When the charge is moving along the surface, ϕ increases. Relocation of the charge over the surface causes the appearance of J_{ss} and Y_{ss} . In our case, the occurrence of localized trapezoidal permeability (Y_{ss}) causes it to be constant up to $T \sim 100^\circ\text{C}$ and then results in a sudden increase in permeability. In our opinion, $T < 125^\circ\text{C}$; Different energy-intensive traps, close to each other at $T \sim 125 \div 275^\circ\text{C}$ and $T > 275^\circ\text{C}$, appear in series. They quickly fill up with chargers and move along the traps. In this case, the change of σ belongs to the trap permeation of the two adjacent fields, that is, SiO_2 . The closeness of the energy levels of sequentially occurring traps can lead to the reduction of ϕ . The value of the detected ϕ corresponds to the energy between E_{i1} , E_{i2} , E_{i3} , E_{i4} .

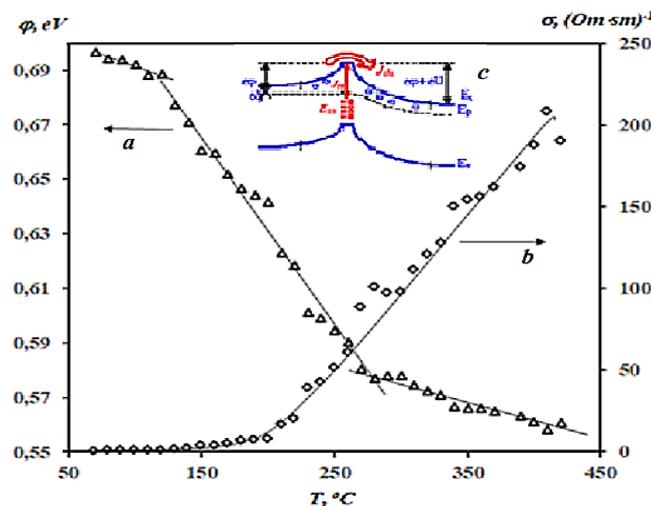


Figure 1. Temperature dependence of ϕ (a) and σ (b) between two adjacent granules, c - zones diagram.)

Thus, 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. This phenomenon increases the opportunity to produce semiconductor devices, solar cells and thermoelements based on granulated silica. The results can also play an important role in the study of physical properties of granular semiconductors, including physical processes occurring within two adjacent areas.

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