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ON THE KINETICS OF POLYCRYSTALLINE SILICON SINTERING

Mukhtarov E.K.
Andijan State University
e-mail: erkinmuxtarov@yahoo.com
https://orcid.org/0009-0001-5057-4905

Annotation: This paper presents the results of research into developing methods for producing purer silicon to increase the efficiency of solar cells, as well as improving sintering and crystal growth methods to obtain a more uniform structure and reduce defects.

Keywords: polycrystalline silicon, powder technology, solar energy, porosity, model, activation, diffusion.

О КИНЕТИКЕ СПЕКАНИЯ ПОЛИКРИСТАЛЛИЧЕСКОГО КРЕМНИЯ

Мухтаров Э.К.
Андижанский государственный университет
e-mail: erkinmuxtarov@yahoo.com
https://orcid.org/0009-0001-5057-4905

Аннотация: В данной работе представлены результаты исследований разработку методов получения более чистого кремния для повышения эффективности солнечных элементов, а также улучшение методов спекания и роста кристаллов для получения более однородной структуры и уменьшения дефектов.

Ключевые слова: поликристаллический кремний, порошковая технология, солнечная энергетика, пористость, модель, активация, диффузия.

Introduction

The production of various materials with different types of chemical bonds - metallic, metal-like, covalent, ionic and molecular - is an important task of modern science and technology. Currently, there are many promising materials, the production of which using powder technologies has not yet been sufficiently studied.

Semiconductors (silicon, germanium), graphene and various carbides are materials with covalent bonds. The production of such materials using powder technologies requires detailed control of the synthesis process and sintering conditions to achieve the desired properties.

For further development of powder technologies, it is necessary to focus on the following aspects:

– use of innovative methods such as mechanochemical synthesis, plasma spraying and laser sintering.

– study of the influence of temperature, pressure, atmosphere and sintering time on the final properties of materials.

- application of computer modeling to predict the behavior of materials and optimize processes.
- comprehensive study of mechanical, thermal, electrical and other properties of materials to understand their potential and application possibilities.

Research methodology

During the work, the following research methods were used:
The sintering experiments were conducted under controlled conditions with precise control of temperature, pressure, and time. The temperature range typically varied from 1000°C to 1300°C, depending on the material properties; the experiments were conducted in different atmospheres (argon atmosphere and vacuum) to investigate the influence of atmospheric conditions on the sintering kinetics; grain growth during the sintering process was measured using microanalysis methods such as SEM or TEM to track microstructure changes at different stages of the process; based on experimental and theoretical results, the optimal sintering parameters such as temperature, time, and pressure were determined to achieve high density and minimal defects.

Results and discussions

Polycrystalline silicon is one of the key materials for the production of solar cells, and its production using powder technologies is of great interest. It has a number of advantages, such as relatively low production cost and good photovoltaic characteristics. However, there are certain problems associated with improving the efficiency and reducing the costs of its production [1].

Polycrystalline silicon remains an important and promising material for solar energy, and further research in the field of powder technologies and optimization of production processes can significantly improve its characteristics and reduce the cost of solar cell production. One of the key challenges is to produce thin silicon wafers without machining, which can significantly reduce material loss and improve the cost efficiency of the process.

Conducting research in this area is of great importance for increasing the efficiency and reducing the cost of polycrystalline silicon production, which, in turn, contributes to the development of solar energy. These studies may lead to the development of new technologies and materials that will allow more efficient use of solar energy and accelerate the transition to sustainable energy sources [2].

In the process of obtaining polycrystalline silicon compressions using hydrostatic pressing from powders with an average fraction size of 5-10 microns and 40-60 microns, it gives important details about the technology and its capabilities [3]. Silicon powders with an average particle size of 5-10 microns and 40-60 microns were obtained by grinding in a ball mill. This method allows to achieve a high degree of grinding and uniform particle size. The separation of powders by size on a vibrating screen allows you to obtain fractions with a narrower size distribution, which improves the uniformity of compressions. The powders are placed in elastic

shells, which allows the pressure to be evenly distributed over the entire volume of the material during pressing. Pressing under hydrostatic pressure up to 350 MPa allows you to achieve a high density of presses and ensures uniform compression of powders, which reduces porosity and improves mechanical properties.

The dependence of the pressing density on the pressure of hydrostatic pressing is often described by a power function. If we denote the relative density by ρ and the pressure by P, then the general form of the dependence can be written as follows:

$$\rho = \rho_0 \left(\frac{P}{P_0} \right)^n$$

where ρ_0 is the initial relative density, determined experimentally, P_0 is the initial pressure, also determined experimentally, n is the exponent characterizing the internal friction of the powder mass.

For coarse–grained powder, the index of the degree of n is usually less than for fine-grained powder, which is explained by the different compactness of these materials. The degree index characterizes the ability of the powder to seal under pressure. For coarse-grained powder, a lower n indicates a lighter seal compared to fine-grained powder.

The initial values of relative density and pressure, as well as the degree index characterizing the internal friction of the powder mass, are determined experimentally and play a key role in describing the process. This model allows you to predict the density of presses at different pressures and optimize the process parameters to achieve the required material characteristics.

The compactness of silicon powders with small and large particle sizes is shown in Fig. 1. Grain size control allows you to optimize the mechanical and electrical properties of the material. This includes the development of methods to control grain growth during synthesis and sintering.

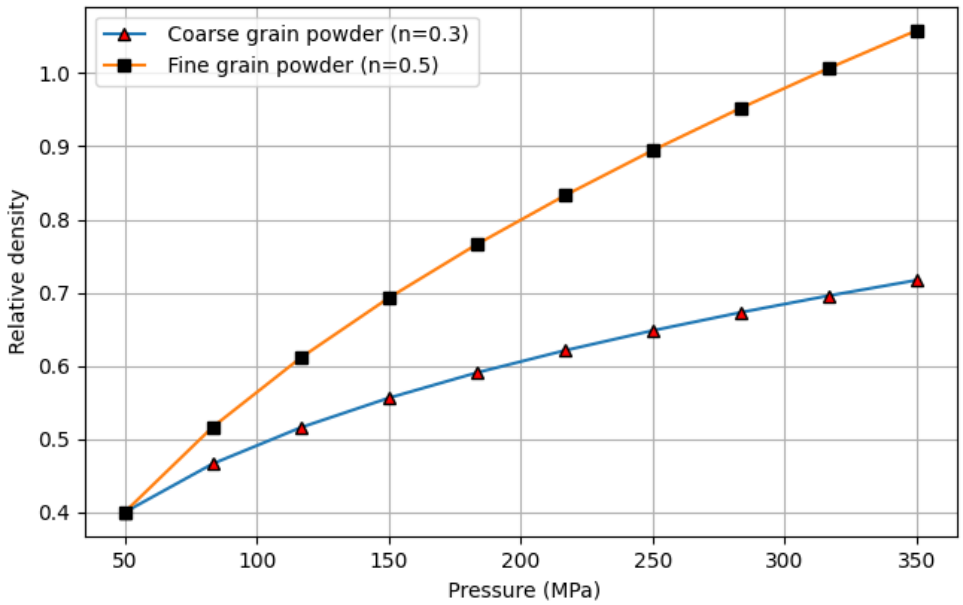

Fig. 1. The dependence of the relative density on the pressing pressure.

The constancy of the n coefficient over a wide pressure range indicates that the sealing of silicon powder occurs mainly due to interparticle slippage and rotation of particles, without significant chipping and crushing. This is an important observation for the development and optimization of pressing processes, as it provides stability and predictability of results, as well as improved mechanical properties of the final presses.

The use of additional sealing methods, such as hot isostatic pressing, can increase the relative density to 0.9 and above, which will improve mechanical and electrical properties.

A detailed analysis of the microstructure of the resulting compresses using scanning electron microscopy and X-ray diffraction will help to understand the grain distribution and possible defects, which will optimize the process.

Powders with different grain sizes will have different sintering kinetics, which must be taken into account when setting temperature conditions to obtain the best characteristics of the final material. The sintering process of polycrystalline silicon at various temperatures makes it possible to effectively control its density and structure, which is critically important for creating high-quality materials for solar cells and other applications.

Sintering kinetics is the process of changing the structure and density of a powder material when exposed to high temperatures. During sintering, changes occur related to compaction, diffusion, grain growth and other mechanisms [4].

The kinetics of polycrystalline silicon sintering includes several stages and mechanisms, such as surface and bulk diffusion, plastic flow and recrystallization. Each of these mechanisms dominates at different stages of the process and depends on temperature and time. Mathematical modeling of sintering kinetics makes it possible to predict density changes and optimize the process to achieve the required material properties.

The kinetics of sintering can be described by various mathematical models that take into account different mechanisms and stages of the process. One such model is the Henderson model, which describes the density of a material as a function of time and temperature [5]:

$$\frac{d\rho}{dt}=k(T)(1-\rho)^n$$

where ρ is the relative density, t is the time, $k(T)$ is the temperature coefficient, depending on the temperature, n is the exponent, depending on the sealing mechanism.

Let’s say the initial relative density (ρ_0) is 0.4, the temperature coefficient $k(T)$ depends on temperature and time.

Initial stage (up to 1390 K) (Fig. 2):

$$k(T)=k_1\exp\left(\frac{-Q_1}{RT}\right)$$

where k_1 is the pre–exponential factor for surface diffusion, Q_1 is the activation energy for surface diffusion, R is the universal gas constant, T is the temperature.
Middle stage (1440 K – 1610 K) (Fig. 2):

$$k(T)=k_2\exp\left(\frac{-Q_2}{RT}\right)$$

where k_2 is the pre–exponential factor for volumetric diffusion and plastic flow, Q_2 is the activation energy for volumetric diffusion and plastic flow.

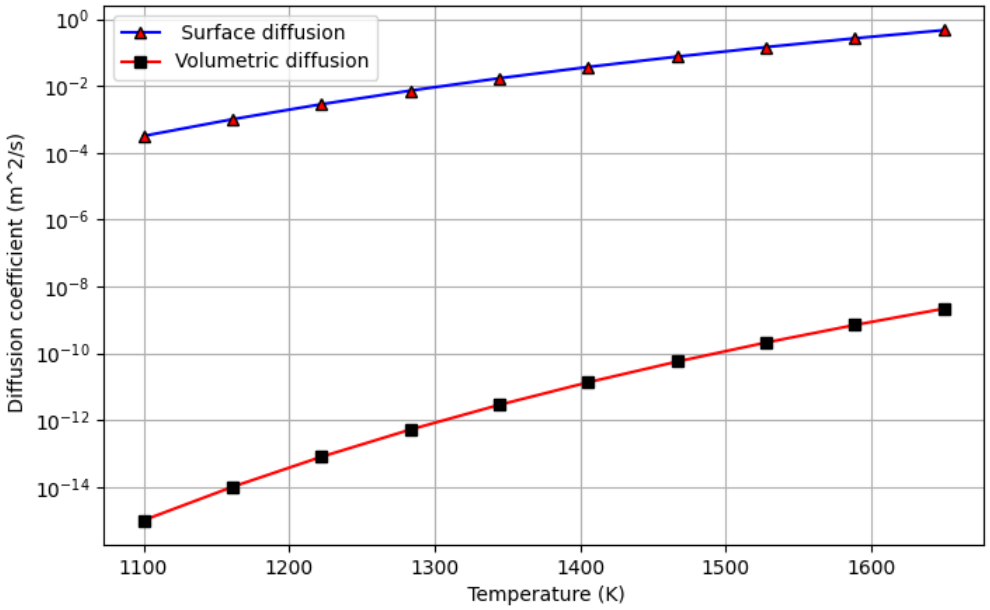

Fig. 2. Dependence of diffusion coefficient on temperature.

Various mathematical models are used to simulate sintering kinetics, which include parameters describing temperature, time, particle sizes and other characteristics of the material. One of the widely used models is the K–model, which describes the dependence of changes in the size of contacts between particles on time and temperature:

$$r(t)=r_0\left(1+\frac{t}{\tau}\right)^n$$

where $r(t)$ is the contact radius at time t, r_0 is the initial contact radius, τ is the characteristic time depending on the temperature and properties of the material, n is the coefficient depending on the sintering mechanism.

The characteristic time τ depends on the temperature and properties of the material, and is determined as follows:

$$\tau=\frac{\gamma a^m}{D}$$

where γ is the surface energy, a is the radius of the initial particle, m is the coefficient depending on the diffusion mechanism, D is the diffusion coefficient depending on the temperature according to the Arrhenius law:

$$D = D_0 \exp\left(\frac{-Q}{RT}\right)$$

where D_0 is the pre–exponential factor, Q is the activation energy, R is the gas constant, and T is the absolute temperature.

The high values of the relative temperature of active sintering of silicon powder in comparison with powders of metals and other studied substances can be explained by the peculiarities of the structural and energy characteristics of silicon. The main factors influencing this process are the low contribution of the volume energy of dislocations and the dominant role of grain boundary diffusion.

For silicon, the activation energy of volumetric diffusion can be quite high, which necessitates high temperatures to significantly accelerate diffusion processes. Typical activation energy values for bulk diffusion in silicon are in the range of 3.5-4.0 eV.

The calculation shows that at a given temperature, the surface diffusion coefficient will be significantly higher than the volume diffusion coefficient. This means that at a temperature of 1473 K, surface diffusion will occur much faster than bulk diffusion, which contributes to the rapid growth of contact points between particles and improved sintering in the initial stages.

Conclusion

The hydrostatic pressing process of silicon powders is an effective method for producing polycrystalline silicon with high density and satisfactory strength. Optimization of process parameters and the use of additional technologies can lead to improved material performance, which will open up new opportunities for its application, especially in the field of solar energy.

Energy factors play a key role in the sintering process of silicon powder. Controlling the surface energy, selecting suitable temperatures and taking into account the activation energy makes it possible to optimize the sintering process and obtain a material with the required properties. This is especially important for high-tech applications such as electronics and solar energy.

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