HIGH TEMPERATURE FEATURES OF THE POLYCRYSTALLINE SILICON PHYSICAL PROPERTIES

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The temperature dependences of the conductance, concentration, and mobility of charge carriers (CCs) in polycrystalline silicon (PCS) have been studied experimentally. It has been shown that the PCS conductance not only varies due to the thermal scattering of CCs in single-crystalline silicon (SCS) (this process is described by an exponential law), but depends, to a greater extent, on the origin of potential barriers at grain boundaries (GBs), so that the variation of the PCS parameters with temperature is nonmonotonous.

1. Introduction

Polycrystalline silicon is considered as a raw material for solar cells and other semiconductor devices. A lot of papers dealing with its optical and electric properties, measured by various technological ways, has been published [1–5]. Also promising seems the application of PCS as a constructional material with additional functionalities for space technologies, e.g., for fabricating the high-temperature mirrors with a complicated form or the electric heating units [6]. The modification of electrophysical and photoelectric properties of PCS-based semiconductor devices, solar elements, and other products subjected to some external influence is connected with the structural features of a raw material. In this connection, it is of interest to study the dependence of the electrophysical properties of PCS wafers on temperature.

In this work, the experimental results concerning the properties of PCS wafers in the temperature range $T = 20 \div 500$ °C are reported. The indicated choice, which differs from the temperature interval usually surveyed when studying semiconductors, e.g., SCS, was stimulated by the circumstance that PCS has a complicated spectrum of deep levels, which are mainly induced by charge states located at GBs, and a number of specific application regions [6–8].

2. Experimental Method

Slip-cast PCS [7] with conductivity of the p-type, the specific resistance $\rho = 1\ \Omega \times$ cm, and the average grain dimension $\gamma \approx 1000\ \mu$m was selected for studying. In order to estimate the influence of the temperature on the electrophysical properties of the material, we took advantage of the modernized four-probe method and the Hall effect. Polished 10×10-mm^2 wafers 300-μm in thickness served as specimens. In the course of experiments, the specimen temperature was monitored making use of a thermocouple, and the temperature variation was registered by a plotter. The specific resistance ρ of the specimens was measured and the concentration and the mobility of CCs in them were determined in a semiautomatic mode during both the growth of the temperature from 20 to 500 °C and its reduction. For the reliability of results, the value of ρ was determined by averaging the relevant values repeatedly measured by the four-probe method at various sections of the wafer surface.

In the figure, the temperature dependence of the electric conductance σ of the material under study and the temperature dependences of the CC mobility μ and the concentration n_v in it are depicted. The curves were plotted on the basis of the data measured in the semiautomatic mode, when the specimens were repeatedly heated up at a rate of 20 °C/min and cooled down at a rate of 10 °C/min. The experimental points correspond to additional discrete measurements at fixed temperatures.

3. Results and Their Discussion

The figure demonstrates the agreement between the temperature behaviors of the electric conductance (curve *1*) and the CC mobility (curve *2*) in the investigated material with the data reported in works [1–4]. At the same time, the temperature dependence of the CC

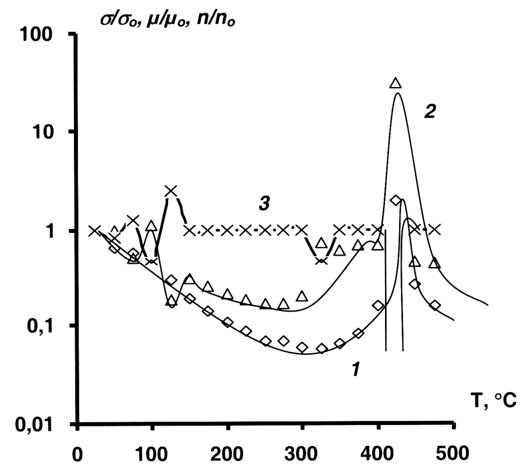
concentration (curve *3*) substantially differs from the literature data.

The reduction of the conductivity in SCS, as the temperature increases, is known to be associated with a change of the CC mobility; the growth of the conductivity, as the temperature continues to rise, is connected with the onset of the intrinsic conductivity. Such an explanation is obviously suitable for the bulk of individual crystallites, i.e. for SCS grains. However, the electrophysical properties of PCS, made up of a plenty of grains separated by interfaces, are not governed by the properties of individual crystallites only, but by the properties of their boundaries as well. Therefore, the temperature dependence of the CC concentration in PCS (curve *3*) substantially differs from that for SCS.

The atomic structure of GBs in crystals with covalent bonds has irregularities of the broken-bond type, which create additional energy levels in the energy gap [9–11]. In addition, the increase of the PCS specimen temperature makes oxygen atoms diffuse from the surface and promotes the creation of SiO_x or Si_yO_x precipitates both in the near-surface volume of grains and on the GBs [12]. The interaction between oxygen atoms and vacancies brings about the formation of various vacancy centers (*A, E, H*, and others). In our opinion, the interaction of the broken bonds, vacancies, and oxygen atoms at high temperatures ultimately results in the formation of trap clusters on the GBs, while the recombination and the emission of CCs lead to a modification of the trap energy level and, by analogy with the restructuring processes of recombination centers in PCS subjected to highly intense light radiation [8], to a change of the very nature of GBs [9, 10].

It should be noted that the specific feature of such an explanation consists in that the temperature increase does not lead to a change of the total concentration of traps in the bulk of the material, but to a substantial variation of their concentration along GBs. As the temperature increases, CCs escape from the traps in the near-surface region of GBs, and, having acquired sufficiently high kinetic energies, participate in the electroconductivity, i.e. give their additional contribution to the total conductivity. Some CCs, whose kinetic energy is not high enough, can be absorbed in the near-boundary region of the following (next in the direction of the CC motion) grain, thereby leaving the CC flux. This process results in a reduction of the average CC concentration in the GB volume.

The total concentration of CCs in the PCS bulk, n_v, can be expressed as $n_v = (n_{\rm cr} + n_{\rm bgb})/2$, where $n_{\rm cr}$ and



Temperature dependences of the electroconductance of a polycrystalline silicon wafer (*1*) and the mobility (*2*) and the concentration (*3*) of charge carriers in it. The solid curves were recorded in the semiautomatic mode; the points correspond to the results of additional discrete measurements

$n_{\rm bgb}$ are the concentrations of CCs in the grains and at the GBs, respectively. As the temperature changes, $n_{\rm cr}$ is supposed to behave as the CC concentration in the bulk SCS. The quantity $n_{\rm bgb}$ is the algebraic sum of two components: the concentration n_1 of the CCs generated owing to the ionization of states in the near-boundary region and the concentration n_2 of the CCs captured by the ionized states of the next grain:

$$n_{\rm bgb} \approx \frac{n_1 - n_2}{2}. \qquad (1)$$

If the equations

$$n_2 \approx 2N_0 \exp(-q(\varphi + E)/kT), \qquad (2)$$

and

$$n_1 \approx 2N_{v1} \exp(-q\varphi/kT), \qquad (3)$$

where N_0 is the concentration of ionized traps, E the ionization energy, φ the potential barrier height, k the Boltzmann constant, T the temperature, and N_{v1} the density of states in the GB region, are used for n_2 and n_1, then, substituting Eqs. (2) and (3) into Eq. (1), we obtain the following expression which describes the CC concentration at the GBs:

$$n_{\rm bgb} \approx (N_{v1} - N_0 \exp(-qE/kT)) \exp(-q\varphi/kT). \qquad (4)$$

Since the behavior of the CC concentration in the grains was supposed similar to that in SCS, the total CC

concentration in the PCS bulk can be described, making use of Eq. (4), by the following equation:

$$\big[n_v \approx N_v \exp(-qE_g/kT)+$$

$$+(N_{v1} - N_0 \exp(-qE/kT)) \exp(-q\varphi/kT)\big]/2. \quad (5)$$

Equation (5) demonstrates that the behavior of the CC concentration in PCS is determined, first of all, by the behavior of ionized traps on the grain surface and that the component connected with GBs is more sensitive to the temperature variation. These features of the GBs substantially influence the behavior of the total CC concentration in PCS. For example, within the temperature interval $T = 50 \div 70$ °C, the variations of the CC concentration and mobility are observed, which corresponds to the averaged trap levels $E \approx 0.15$ and 0.17 eV; these results coincide with the data of work [13]. The trap levels $E \approx 0.36$ eV and $E \approx 0.3$ eV manifest themselves in the temperature ranges $T = 100 \div 170$ °C and $T = 325 \div 350$ °C, respectively. All these phenomena are observed as step-like variations of the experimentally measured CC concentration within the indicated temperature intervals.

Our experiments also revealed the step-like variations of the conductance, CC mobility, and total CC concentration near the temperature $T = 430$ °C. This result can be explained by the mutual influence of thermally generated donors both inside the grains and on their surface. The influence of thermal donors on the PCS properties (curve *1*) evidences once more for the importance of the role playing by GBs in the formation of the PCS properties, because it is onto GBs that the oxygen, which is dissolved in the melt and is responsible for the formation of SiO_4 complexes producing thermal donors, is displaced in the process of solid-state recrystallization of PCS. Broader and smoother peaks in the temperature dependences of the conductance at temperatures, where the CC mobility and concentration demonstrate a step-like behavior, testify to both the availability of separate trap levels in PCS (as it is, e.g., in SCS deeply doped with impurities) and their splitting (i.e. the availability of a wide spectrum of levels). This phenomenon once more confirms that PCS possesses the electron and crystalline structures, which are more complicated than those of SCS.

Thus, the step-like changes of the CC conductivity, mobility, and concentration in the temperature range $T = 20 \div 200$ °C are induced by the variation of trap energy levels (this conclusion is in agreement with the data of work [13]) and, in the vicinity of $T = 430$ °C, are associated with the influence of donors which are thermally generated in PCS. The total CC concentration in the PCS bulk is governed within the investigated temperature interval by the average values of the CC concentration in the grains, n_{cr}, and on the GBs, n_{bgb}.

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ОСОБЛИВОСТІ ЕЛЕКТРОФІЗИЧНИХ
ВЛАСТИВОСТЕЙ ПОЛІКРИСТАЛІЧНОГО
КРЕМНІЮ ПРИ ПІДВИЩЕНИХ ТЕМПЕРАТУРАХ

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Р е з ю м е

Експериментально досліджено температурні залежності провідності, концентрації і рухливості носіїв заряду у полікристалічному кремнії (ПК). Показано, що зміна провідності ПК відбувається не тільки за експоненціальним законом, який описує теплове розсіяння носіїв заряду у моно-Si, а в значній мірі залежить від природи потенціальних бар'єрів на межах зерен. Внаслідок цього зміна параметрів ПК із зміною температури відбувається не монотонно.