STUDY OF MORPHOLOGY AND TOPOLOGY OF THE SURFACE OF SILICON DOPED WITH PALLADIUM ATOMS

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Abstract

In this paper, we study the morphology and topology of n-type silicon (n-Si) single crystals doped with palladium atoms at different temperatures using an atomic force microscope (AFM) and a scanning electron microscope (SEM). The AFM results show that palladium diffusion at temperatures of 1100–1200 °C leads to significant smoothing of the surface of n-type silicon single crystals. The roughness parameters decrease by 50%, the relief loses its anisotropy and becomes more isotropic. Using SEM, it was determined that doping silicon with palladium atoms at 1100 °C leads to the formation of structural microdefects with a low concentration, and the introduction of palladium impurity into Si at 1200 °C leads to the creation of smaller structural defects with a high concentration.

Key words: silicon, palladium, doping, diffusion, morphology, topology, AFM, SEM.

1. Introduction

Silicon is the main material of modern micro- and nanoelectronics due to its availability, proven technology for producing single crystals and unique electronic properties. However, in the context of the constant complication of semiconductor devices, the need to modify the surface and bulk properties of silicon increases in order to improve its electrical and optical characteristics. One of the promising areas is doping the surface with transition metals, which are capable of forming stable compounds with silicon and influencing the processes of diffusion and relaxation of the surface [1-3].

Of particular interest are Si–Pd systems, since palladium is highly chemically active with respect to silicon and can form a wide range of silicide phases. These compounds have good thermal stability and low specific resistance, which makes them in demand for the creation of barrier contacts, interconnections, and elements of nanostructured devices. The key factor determining the properties of such systems is the morphology and topology of the surface, formed during the diffusion of Pd atoms into the Si substrate at various temperatures [4–6].

To understand the mechanisms of surface modification, it is necessary to use direct visualization methods that can provide both a general picture of the distribution of defects and structural inhomogeneities, and quantitative roughness parameters. In this context, scanning electron microscopy (SEM) provides high resolution and contrast for analyzing surface morphology, while atomic force microscopy (AFM) allows quantitative investigation of topography at the nanometer level, determining the amplitude of the relief, anisotropy, and the

nature of the distribution of irregularities. The combined use of these methods opens up the possibility of a comprehensive analysis of diffusion processes and structural transformations in the Si–Pd system [7, 8].

Thus, the relevance of this work lies in the study of morphological and topological changes in the surface of n-type single-crystal silicon doped with palladium atoms by diffusion at different temperatures. The aim of the study is to establish the relationship between the conditions of heat treatment, the features of relief formation and the potential influence of the obtained structures on the functional properties of silicon materials for nanoelectronic applications.

2. Experimental part

The objects of the study were n-type silicon wafers with a specific resistance of 40 Ohm•cm (KEF-40). These wafers were made from silicon ingots grown by the Czochralski method. Silicon was doped with palladium by a diffusion method: palladium atoms were deposited on the silicon surface, after which the samples were subjected to heat treatment in evacuated quartz ampoules at a temperature of 1100–1200 °C for 3–5 hours.

The surface of single-crystal n-type silicon was investigated by atomic force microscopy (AFM) before and after doping with palladium atoms by diffusion at temperatures of 1100 °C and 1200 °C. The analysis included obtaining two-dimensional (2D) height maps, three-dimensional (3D) reconstructions and line profiles, which allowed both qualitative and quantitative assessment of the change in surface topography.

Particular attention was paid to the comparison of roughness parameters, including the maximum height range (Z-scale) and the peak-to-valley amplitude (Pt), as well as to identifying patterns in the change in morphology with an increase in the diffusion temperature. An NT-MDT atomic force microscope was used to study the morphology and topology of the surface of silicon single crystals. The microstructures formed after doping the surface of the studied samples with palladium atoms were determined using a scanning electron microscope (SEM).

3. Results and discussions

AFM images of the original sample (Fig. 1) showed that the silicon surface has pronounced anisotropy and significant roughness. The 2D map (Fig. 1a) shows elongated structures resembling parallel grooves and ridges, which may be associated with both the features of mechanical polishing and natural "step-bunching" - the aggregation of atomic steps on the surface.

In the 3D reconstruction (Fig. 1b), a relief with a sequence of ridge-like hills and deep depressions is clearly observed. The maximum relief height is about 32 nm, and the peak-valley value (Pt) reaches ~17.4 nm. The surface profile (Fig. 1c) confirms the presence of significant differences on a scale of several micrometers. Taken together, this indicates that the original surface is quite rough and has a strong relief directionality.

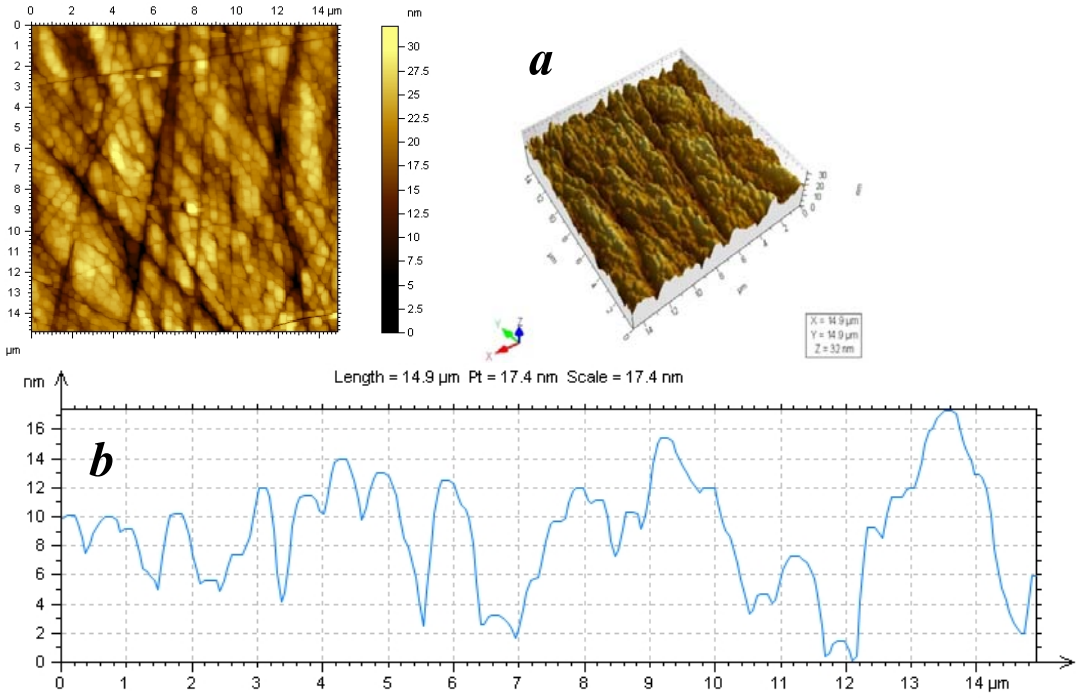

Figure 1. Typical 2D and 3D AFM images of the surface (a), cross-section profile along the main irregularities (b) of an n-type silicon single crystal.

After carrying out palladium diffusion at 1100 °C, noticeable changes in morphology are observed (Fig. 2). The elongated structures characteristic of the original sample become less pronounced, the relief becomes smoother. In 3D images, it is evident that large ridges are transformed into rounded elevations, and the depth of the depressions decreases.

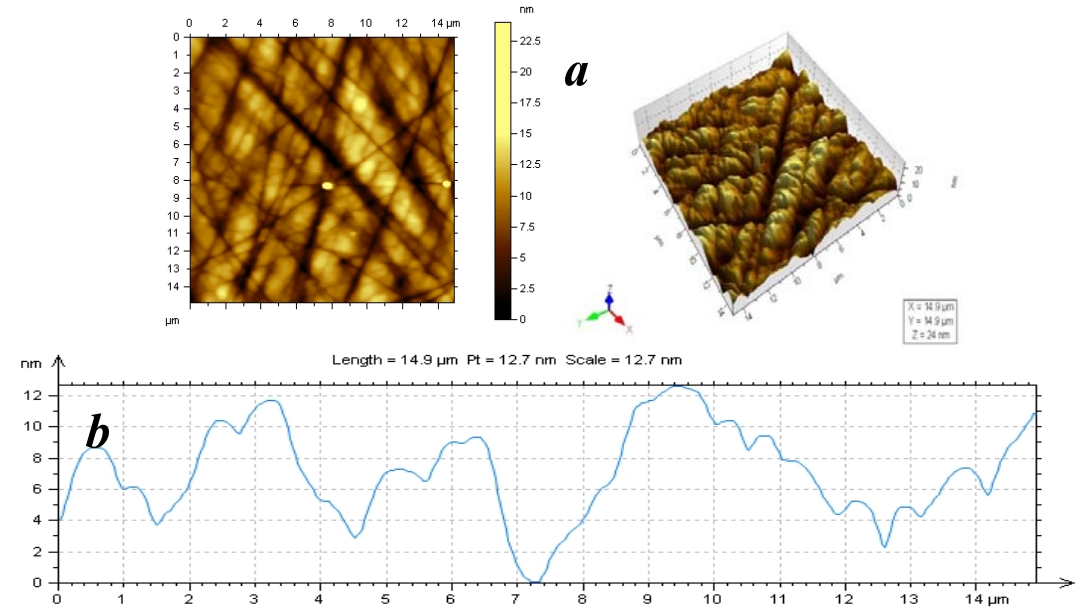

Figure 2. Typical 2D and 3D AFM images of the surface (a), cross-sectional profile (b) of a single crystal of n-type silicon doped with palladium at 1100 °C.

The maximum height range decreases to ~24 nm, and the Pt parameter decreases to ~12.7 nm, which corresponds to a roughness decrease of approximately 27% compared to the initial state. These changes indicate that palladium promotes an increase in the mobility of silicon atoms on the surface, activating surface self-diffusion processes [9,10]. As a result, large irregularities are "washed out", and the surface becomes less anisotropic.

With a further increase in the diffusion temperature to 1200 °C, the smoothing of the surface becomes even more pronounced (Fig. 3). The morphology loses its previous direction, and the relief acquires an almost isotropic character. Smaller and more evenly distributed irregularities are formed on the surface, which indicates a deep restructuring of the surface layer.

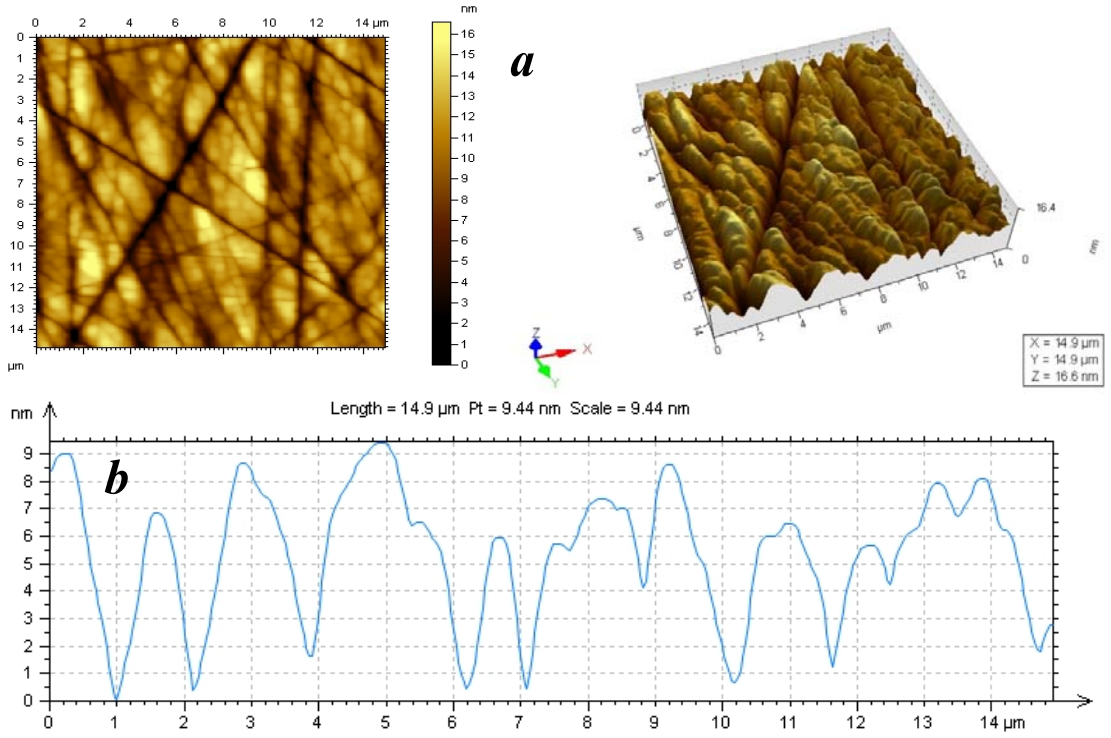

Figure 3. Typical 2D and 3D AFM images of the surface (a), cross-sectional profile (b) of a single crystal of n-type silicon doped with palladium at 1200 °C.

The maximum relief height decreases to ~16.6 nm, and Pt to ~9.44 nm, which is almost twice as low as compared to the original sample. Thus, an increase in the diffusion temperature leads to a consistent decrease in roughness and a decrease in the amplitude of surface fluctuations.

The data in the table 1 clearly demonstrate the systematic decrease in surface roughness with increasing diffusion temperature. It is especially noteworthy that at 1200 °C the roughness parameters decrease by almost 50%, which indicates the high efficiency of the smoothing process.

As the temperature increases, silicon atoms on the surface acquire increased mobility, which leads to a redistribution of the material and smoothing of large irregularities [11, 12]. Palladium can reduce the surface energy and promote an ordered redistribution of silicon atoms, which further accelerates the smoothing process [13-15]. At higher temperatures

(around 1200 °C), the interaction of Pd with Si can begin to form thin layers of silicides. This leads to additional stabilization of the surface and prevents the formation of large defects [16-18]. The transition from directed comb-like structures to a more uniform relief indicates a minimization of the free energy of the surface and the suppression of step-bunching phenomena [19].

Table 1. Comparative analysis of roughness parameters

Samples	**Maximum height range Z (nm)**	**Peak-to-valley Pt (nm)**	**Roughness reduction (%) relative to the original**
n-Si	~32.0	~17.4	–
n-Si<Pd> - 1100 °C	~24.0	~12.7	~27%
n-Si<Pd> - 1200 °C	~16.6	~9.44	~46%

Thus, the AFM results show that palladium diffusion at temperatures of 1100–1200 °C leads to significant smoothing of the surface of single-crystal n-type silicon. The roughness parameters decrease to 50%, the relief loses anisotropy and becomes more isotropic. These effects are directly related to the enhancement of self-diffusion processes, the surfactant effect of Pd, and the possible onset of silicide formation. The results obtained confirm the prospects of using palladium to modify the silicon surface in order to improve its electronic and optical characteristics.

Figure 4 shows micrographs of the original and doped samples. Micrographs of silicon doped with palladium (Fig. 4b, 4c) demonstrate that after the diffusion doping process, microstructures are formed on its surface.

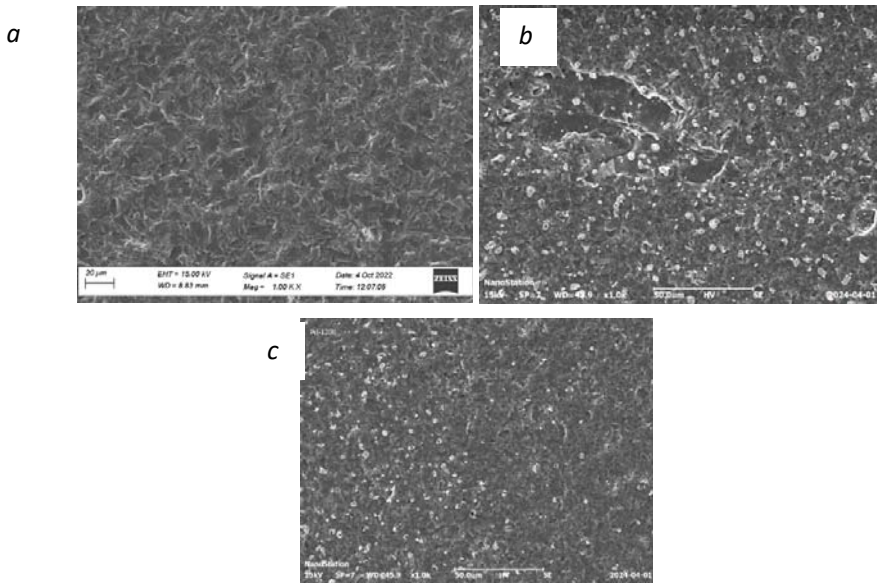

Figure 4. – Micrographs of the surface of single-crystal silicon plates before (a) and after doping with palladium (at 1100 °C (b) and at 1200 °C (c)).

According to the obtained results, doping silicon with palladium at 1100 °C (Fig. 4b) leads to the formation of structural microdefects with a relatively low density. In contrast, introducing palladium atoms into silicon at 1200 °C (Fig. 4c) results in the formation of smaller defects, but with a significantly higher concentration. It is most likely that, during diffusion doping, palladium atoms interact with technological impurities to form (Pd–O) type complexes. This interaction reduces the content of interstitial optically active oxygen (**NOopt**) in the silicon lattice \[20, 21].

4. Conclusion

In the course of the study, morphological and topological changes in the surface of single-crystal n-type silicon doped with palladium atoms by diffusion at temperatures of 1100 °C and 1200 °C were analyzed using atomic force microscopy (AFM) and scanning electron microscopy (SEM).

It is shown that the initial silicon surface has pronounced anisotropy and relatively high roughness (Pt ≈ 17.4 nm, Z ≈ 32 nm). After palladium diffusion at 1100 °C, a significant decrease in roughness (to Pt ≈ 12.7 nm), smoothing of comb-like structures and partial loss of relief directionality are observed. With a further increase in temperature to 1200 °C, the surface becomes almost isotropic, and the relief amplitude decreases almost twofold (Pt ≈ 9.44 nm, Z ≈ 16.6 nm).

Thus, it has been established that the diffusion of palladium at high temperatures leads to a systematic smoothing of the silicon surface due to the enhancement of surface self-diffusion processes and the possible onset of the formation of Pd–Si phases. These processes contribute to the minimization of the free energy of the surface and the suppression of anisotropic structures.

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