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STUDY OF THE EFFECT OF PROTONS AND PLATINUM ATOMS ON THE CRYSTAL STRUCTURE OF SILICON USING X-RAY DIFFRACTION

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ABSTRACT

In this work, the influence of hydrogen ions and platinum atoms on the structure of silicon samples was studied. For the study, single-crystal n-type silicon samples were used, which were doped with phosphorus during growth. These samples were irradiated with protons with an energy of 600 keV and a current of 1÷1.5 μA at an irradiation dose of 9×10^{14} cm^{-2}. To study the surface layer, it was used with the X-ray diffraction method.

KEYWORDS: silicon, platinum, diffusion, doping, irradiation, proton, X-ray diffraction.

INTRODUCTION

Modern technology for the production of semiconductor microelectronic devices, which are based on ion doping of the surface layer of the substrate, has reached a level of performance at which an essential factor is the formation of defects introduced there by the proton beam and, as a result, their effect on the physicochemical characteristics of silicon substrates (Asadchikov et al., 2019).

Microdefects, which are formed as a result of coagulation of point defects, create relatively strong elastic distortion fields and lead to lateral inhomogeneity and changes in the properties of the substrate. The study of the properties of defects arising during ion implantation will expand the possibilities of modern technology for creating new devices and controlling the characteristics of microelectronic devices.

Diagnostics of the structural perfection of ion-implanted silicon samples is an important factor in the selection of the technological mode of implantation in order to obtain controlled properties of the damaged layer in terms of solving certain practical problems.

The aim of this work was to study the changes on the surface of n-Si silicon samples before and after proton irradiation and doping with platinum using X-ray diffraction.

EXPERIMENTAL PART

For the experiments, we used n-type silicon grown by the Czochralski method with a resistivity of 40 Ω cm. Silicon was doped with platinum by the diffusion method(Boltaks, 1971; Utamuradova et al., 2019).

The finished samples were polished and irradiated with protons with an energy of 600 keV and a current of 1–1.5 μA at an irradiation dose of 9×10^{14} cm^{-2}. The samples were irradiated at the SOKOL EG-2 electrostatic accelerator at the Research Institute of Semiconductor Physics and Microelectronics.

Doped and irradiated silicon samples were studied on an X-ray spectrometer with a Miniflex 300/600 goniometer and a D/teX Ultra2 detector. Cukα1 radiation, λ= 1.541 Å, was used at an accelerating voltage of 40 keV and an X-ray tube current of 15 mA. X-ray diffraction measurements were carried out in the Bragg-Brentano beam geometry in the range 2θ = from 5° to 60° continuously at a scan rate of 10 deg/min and an angular step of 0.02°.

RESULTS AND ITS DISCUSSION

Figure 1 shows experimental X-ray diffraction patterns of single-crystal n-type Si before and after doping with Pt and irradiation with protons. As can be seen, in all cases, there is an intense peak in the X-ray patterns in the range 2θ ≈ 28.5–29.5°. According to the Crystallography Open Database (COD), this diffraction peak corresponds to the (111) peak of cubic silicon space group F-43m (COD#00-080-0018). In the case of proton irradiation of a Si single crystal, the main peak shifts from silicon towards larger angles (from 28.80° to 29.25°), its intensity increases by a factor of 1.7, and its full width at half maximum (FWHM) decreases (from 0.091 ° to 0.052°), while doping leads to only a slight increase in intensity (by a factor of 1.5). In the second case, an increase in the intensity of the diffraction peak is probably due to an improvement in the degree of crystallinity of the samples due to recrystallization as a result of heat treatment during alloying (Utamuradova et al., 2021) or is associated with a change in the atomic scattering coefficient due to the presence of Pt(Katharria et al., 2006; Andrei et al., 2015). Diffraction peaks from other phases in the obtained X-ray patterns of Si<Pt>, for example, Pt, Pt-Si, are not observed. The results obtained in this work indicate that the cubic structure of the silicon single crystal is not modified by doping with Pt.

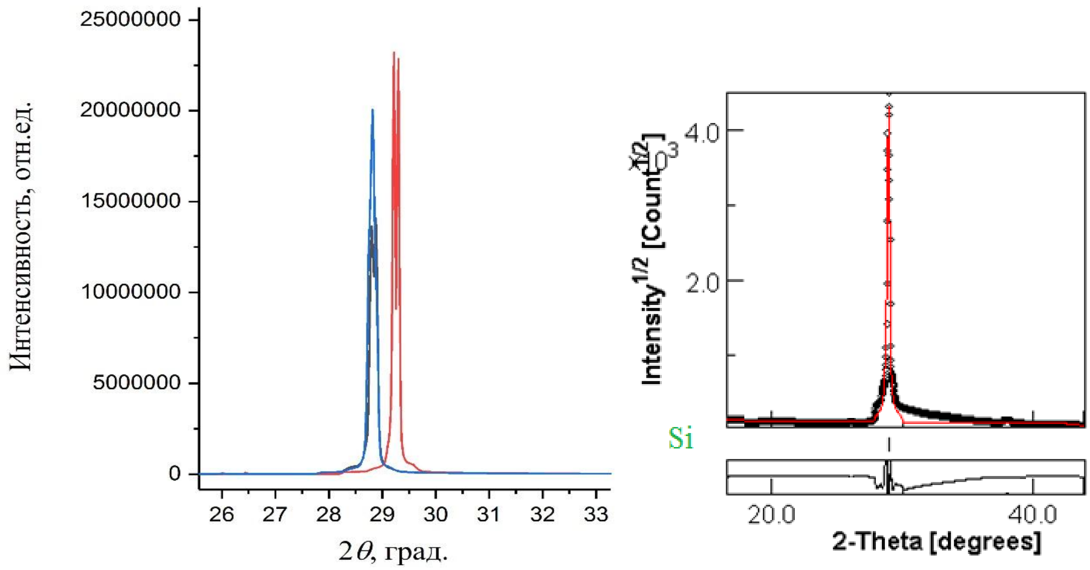

Figure 1: X-ray diffraction patterns of an n-type Si single crystal before and after doping with Pt and irradiation with protons (a). Typical X-ray diffraction pattern Si refined by Rietveld using the MAUD program (b).

Table 1 presents the calculated structural characteristics for a Si single crystal using the Material Analysis Using Diffraction (MAUD) program, which is based on the full-profile analysis of X-ray diffraction patterns by the Rietveld method. It can be seen from the data presented in the table that the unit cell constant a for the initial sample is slightly less than the theoretical value: a = 5.392 Å, V = 156.770 Å3 (COD#00-080-0018). The subsequent doping of silicon with Pt leads to a slight decrease in its unit cell constant a and, accordingly, to volume compression. This is consistent with an increase in CSR and micro deformation.

Table 1: Unit cell parameter (*a*) and volume (*V*), coherent scattering region (CSR, *D*), microstress (ε) for n-type Si single crystal before and after Pt doping and proton irradiation.

Samples	***a*, Å**	***V*, Å^3**	***D*, nm**	***ε*,**
Si	5,360	153,991	288	5 x 10^{-9}
Si<Pt>	5,342	152,444	619	3 x 10^{-5}
Si, irradiated with protons	5,486	165,108	147	5 x 10^{-5}

When a Si single crystal is irradiated with protons, the (111) peak on X-ray patterns shifts towards larger angles (up to 29.3°) and, accordingly, the interplanar distance decreases (up to 3.056 Å). In this case, an increase in the unit cell parameter and a decrease in CSR occur. In(Igor et al., 2016), the transformation of radiation defects in proton-irradiated n-type silicon crystals was studied using high-resolution X-ray diffraction analysis. It was shown that successive implantation of protons into silicon with an energy of 100, 200, or 300 keV at a dose of 2×10^{16} cm^{-2} causes the formation of a damaged layer 2.4 μm thick with a large crystal lattice parameter. The layer is formed simultaneously with the accumulation of intrinsic radiation defects, such as vacancies and interstitials. It was noted in (Skalyaux, 2015) that when silicon crystals are irradiated with protons or α-particles at room temperature, most of the formed Frenkel pairs disappear as a result of mutual annihilation, and the separated components of the pairs create more complex and stable secondary radiation defects. The dislocation density calculated by formula (1) for a silicon single crystal increases from 0.49 x 10^{-9} nm^{-2} to 0.99 x 10^{-5} nm^{-2} after irradiation. An increase in the dislocation density is associated with a decrease in CSR.

$$\rho = 15\varepsilon / a\, D \qquad (1)$$

Based on the results obtained, it can be assumed that proton irradiation of a single crystal of silicon at a dose of 9.0 x 10^{14} cm^{-2} with an energy of 600 KeV leads to the formation of defects, as noted above.

CONCLUSION

This paper presents the results of studying the effect of platinum doping and proton irradiation on the crystal structure of an n-type Si single crystal obtained by the Czochralski method. It has been found that the X-ray diffraction patterns of a Si single crystal before and after doping with Pt and irradiation with protons contain an intense peak at 2θ = 28.5–29.5°, corresponding to cubic silicon of space group F-43m. It was found that irradiation of samples with protons leads to a shift of the (111) peak from silicon towards larger angles, as well as an increase in its intensity and a decrease in its full width at half maximum, while doping does not lead to significant changes in this peak.

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