Symposium on Natural and Applied Sciences
Hosted Online from London, United Kingdom
Date: 5th June, 2026
Website: https://econferencia.com

INFLUENCE OF THERMAL TREATMENT ON THE Si(111) DIFFRACTION PEAK OF n-TYPE SILICON MONOCRYSTALS

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Abstract:
This thesis investigates the influence of high-temperature thermal treatment on the structural state of n-type silicon monocrystals using X-ray diffraction analysis. Particular attention is focused on the $(111)_{Si}$ diffraction peak, which is the dominant reflection for the investigated n-Si<P> samples. The XRD patterns show that the initial n-Si<P> monocrystal exhibits a sharp and intense $(111)_{Si}$ peak near $2\theta \approx 28.5°$, indicating a highly oriented crystalline structure. After annealing at 1300 °C, the intensity of the $(111)_{Si}$ reflection decreases significantly, while the peak position slightly shifts and the full width at half maximum changes from 0.144° to 0.134°. These changes indicate that thermal treatment causes structural reorganization in the silicon lattice, including redistribution of impurity atoms, partial relaxation of internal stresses, and modification of defect-related microstrain. The decrease in peak intensity suggests a reduction in the coherently diffracting volume, whereas the narrowing of the diffraction peak may be associated with partial ordering or enlargement of coherent scattering regions. The obtained results confirm that high-temperature annealing is an important technological factor influencing the crystallographic perfection and microstructural state of phosphorus-doped n-type silicon monocrystals.

Keywords: X-ray diffraction, thermal treatment, annealing, FWHM, microstrain, silicon monocrystal.

Silicon monocrystals remain one of the most important semiconductor materials for modern microelectronics, optoelectronics, radiation-resistant electronics, and sensor technologies. The functional properties of silicon-based devices are strongly related to the structural perfection of the crystal lattice, the distribution of dopant atoms, and the presence of defect-related microstrain. Therefore, the investigation of structural changes caused by high-temperature treatment is essential for understanding and controlling the properties of doped silicon monocrystals [1,2].

In this work, phosphorus-doped n-type silicon monocrystals were investigated before and after high-temperature annealing. The main attention was paid to the $(111)_{Si}$ diffraction peak because this reflection is highly sensitive to changes in the crystallographic orientation, interplanar spacing, lattice deformation, and coherent scattering regions of silicon. X-ray diffraction analysis was used as the main experimental method for evaluating the influence of thermal treatment on the structural state of the investigated n-Si<P> samples. The XRD pattern of the initial n-Si<P> monocrystal shows a sharp and intense diffraction maximum near $2\theta \approx 28.5°$, which corresponds to the $(111)_{Si}$ crystallographic plane. The high intensity of this peak indicates that the initial sample has a highly oriented monocrystalline structure. The full width at half maximum of the $(111)_{Si}$ peak for the initial sample is FWHM = 0.144°, which confirms a relatively good crystalline state, although the presence of local defects and impurity-related microstrain cannot be completely excluded.

After annealing at 1300 °C, significant changes are observed in the $(111)_{Si}$ diffraction peak. As shown in Figure 1, the intensity of the annealed n-Si<P>

sample decreases noticeably compared with the initial sample. This decrease in peak intensity can be associated with the redistribution of impurity atoms, the formation or rearrangement of defect complexes, and a reduction in the coherently diffracting volume of the silicon matrix. At the same time, the diffraction maximum slightly shifts, indicating changes in the interplanar spacing and internal stress state of the silicon lattice [3].

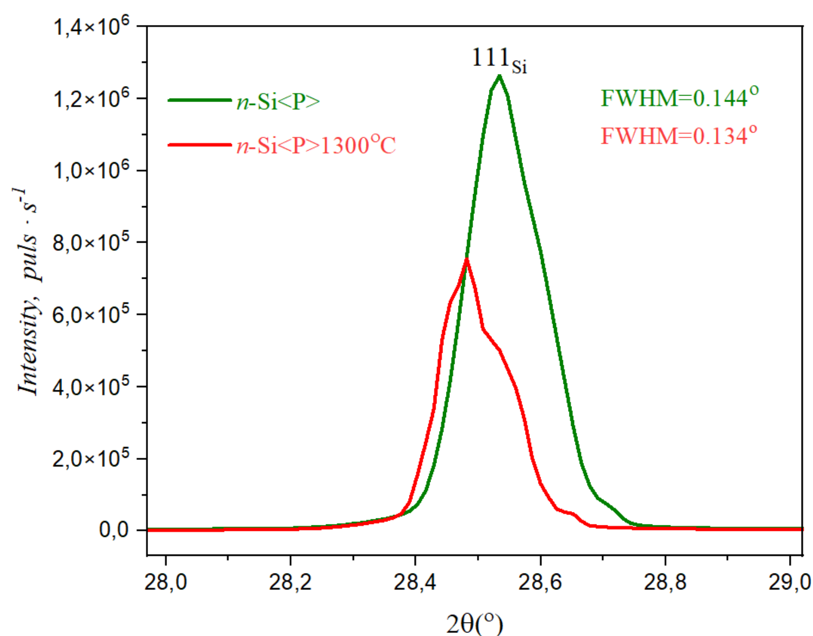

Figure 1. *X-ray diffraction patterns of the (111)$_{Si}$ peak for the initial n-Si<P> monocrystal and the n-Si<P> sample annealed at 1300 °C. The annealed sample shows a decrease in peak intensity and a change in FWHM from 0.144° to 0.134°, indicating structural reorganization in the silicon lattice.*

An important feature of the obtained result is the change in the FWHM value from 0.144° for the initial sample to 0.134° after annealing. In many cases, a decrease in FWHM may indicate partial relaxation of microstrain or an increase in the size of coherent scattering regions. However, in thermally treated doped silicon, this effect should be interpreted carefully because peak broadening is influenced not only by crystallite size but also by lattice defects, impurity redistribution, internal strain fields, and instrumental factors. Therefore, the simultaneous decrease in peak intensity and narrowing of the diffraction peak suggests a complex structural transformation rather than a simple improvement or degradation of the crystal lattice.

The observed structural changes may be explained by thermally activated processes occurring during annealing at 1300 °C. At such a high temperature, phosphorus atoms, oxygen-related background impurities, vacancies, interstitial defects, and other local imperfections can become mobile. As a result, some defect regions may be partially relaxed, while other regions may undergo impurity clustering or local lattice distortion. This leads to a redistribution of internal stresses and modifies the diffraction response of the $(111)_{Si}$ plane [4].

The shift and intensity variation of the $(111)_{Si}$ reflection confirm that high-temperature treatment affects the silicon matrix even when the monocrystalline orientation is preserved. The initial n-Si<P> sample is characterized by a more intense and sharper dominant reflection, while the annealed sample demonstrates reduced intensity and modified peak shape. These results show that the thermal treatment changes the microstructural state of phosphorus-doped silicon without destroying its main crystalline orientation.

From a technological point of view, the obtained results are important because thermal annealing is widely used in semiconductor processing. Changes in the $(111)_{Si}$ diffraction peak can influence electrophysical and photoelectric properties

of silicon-based devices through modification of defect states, impurity distribution, carrier scattering, and recombination centers. Therefore, the control of annealing temperature and duration is necessary for obtaining stable structural and functional properties in n-type silicon monocrystals [5].

Thus, the XRD analysis demonstrates that annealing at 1300 °C leads to structural reorganization of n-Si<P> monocrystals. The main evidence for this conclusion is the decrease in the intensity of the $(111)_{Si}$ peak, the slight displacement of the diffraction maximum, and the reduction of FWHM from 0.144° to 0.134°. These changes indicate that thermal treatment causes impurity redistribution, partial stress relaxation, and modification of defect-related microstrain in the silicon lattice.

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