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WIDE-ANGLE XRD ANALYSIS OF THERMALLY INDUCED STRUCTURAL CHANGES IN n-TYPE SILICON MONOCRYSTALS

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Abstract:
This thesis presents a wide-angle X-ray diffraction analysis of thermally induced structural changes in phosphorus-doped n-type silicon monocrystals. The main purpose of the study is to evaluate the influence of high-temperature annealing on the diffraction behavior of the silicon matrix, with particular attention to the dominant $(111)_{Si}$ reflection. The XRD patterns of the initial n-Si<P> sample and the sample annealed at 1300 °C show that the monocrystalline orientation of silicon is preserved after thermal treatment. However, noticeable changes are observed in the intensity, position, and shape of the $(111)_{Si}$ diffraction peak. The initial sample demonstrates a sharp and intense $(111)_{Si}$ reflection, indicating a highly ordered crystalline structure. After annealing, the intensity of the main reflection decreases, while the peak position slightly shifts and the full width at half maximum changes from 0.144° to 0.134°. These variations indicate that high-temperature treatment causes structural reorganization in the silicon lattice, including impurity redistribution, partial relaxation of internal stresses, and modification of defect-related microstrain. The wide-angle XRD representation confirms that the main structural response remains associated with the silicon matrix rather than the formation of strong secondary crystalline phases. The obtained results demonstrate that annealing at 1300 °C is an important

technological factor for controlling the microstructural state and crystallographic quality of n-type silicon monocrystals.

Keywords: phosphorus-doped silicon, wide-angle XRD, $(111)_{Si}$ reflection, thermal treatment, annealing, FWHM, microstrain.

Silicon monocrystals are widely used as the main material platform in modern semiconductor technology because of their stable crystal structure, controllable electrical conductivity, and compatibility with different technological processes. The structural quality of silicon directly affects the performance of electronic, optoelectronic, sensor, and radiation-resistant devices. In particular, lattice defects, impurity atoms, microstrain, and local structural distortions can influence carrier mobility, recombination processes, electrical conductivity, and long-term stability of semiconductor devices. Therefore, the investigation of thermally induced structural changes in n-type silicon monocrystals is an important scientific and technological problem [1]. In the present work, the structural state of phosphorus-doped n-type silicon monocrystals was studied by wide-angle X-ray diffraction analysis. The main objective was to determine how high-temperature annealing affects the diffraction behavior of the silicon matrix, especially the dominant $(111)_{Si}$ reflection. The investigated samples included an initial n-Si<P> monocrystal and an n-Si<P> sample annealed at 1300 °C. The wide-angle XRD pattern was recorded in the 2θ range from 10° to 80°, which made it possible to evaluate not only the main diffraction peak but also the general phase state of the silicon matrix.

The wide-angle XRD image shows that both the initial and annealed samples are characterized by a dominant diffraction maximum corresponding to the $(111)_{Si}$ crystallographic plane. This result confirms that the monocrystalline orientation of silicon is preserved after high-temperature treatment. The presence of a strong

$(111)_{Si}$ reflection indicates that the basic diamond-type crystal structure of silicon remains stable under the applied annealing conditions. However, despite the preservation of the main orientation, noticeable changes are observed in the intensity, position, and shape of the diffraction peak after thermal treatment.

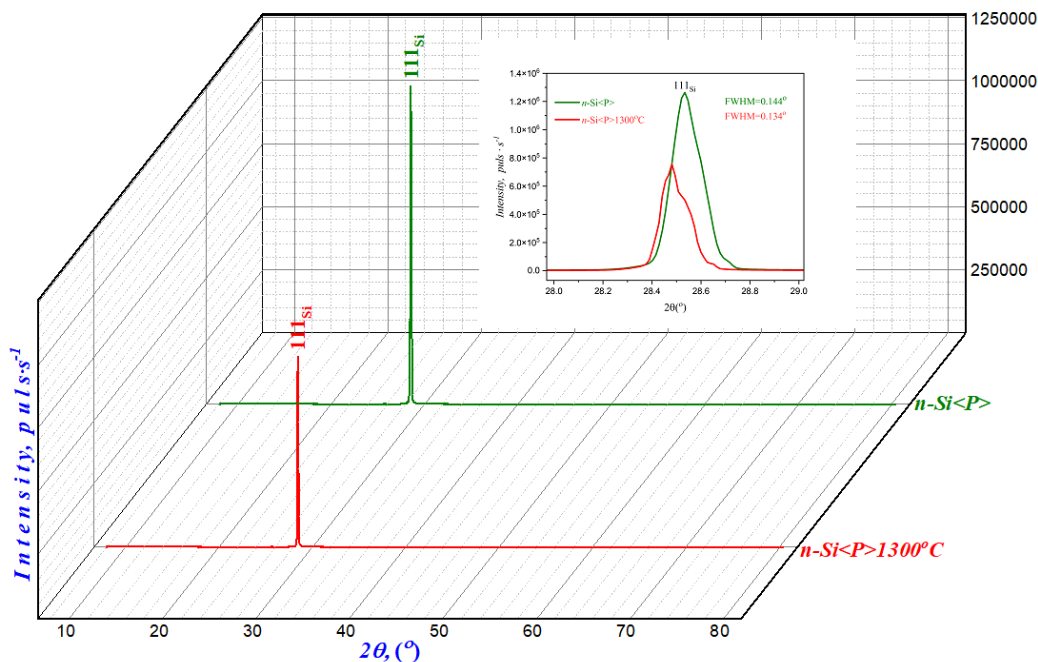

Figure 1. *Wide-angle X-ray diffraction patterns of the initial n-Si<P> monocrystal and the n-Si<P> sample annealed at 1300 °C. The inset shows the high-resolution comparison of the Si(111) diffraction peak, demonstrating the decrease in intensity and the change in FWHM from 0.144° to 0.134° after thermal treatment.*

As can be seen from Figure 1, the initial n-Si<P> sample demonstrates a sharp and intense $(111)_{Si}$ reflection near $2\theta \approx 28.5°$. The high intensity of this peak indicates a high degree of crystallographic orientation and a relatively ordered silicon lattice. The full width at half maximum of the initial sample is FWHM =

0.144°, which characterizes the width of the diffraction maximum and provides information about coherent scattering regions, microstrain, and defect-related lattice distortions. In monocrystalline silicon, FWHM should not be interpreted only as a crystallite-size parameter, because peak broadening can also be caused by internal stresses, dislocations, impurity complexes, oxygen-related defects, and instrumental broadening [2]. After annealing at 1300 °C, the $(111)_{Si}$ diffraction peak undergoes significant modification. The intensity of the main reflection decreases compared with the initial sample. This decrease indicates that thermal treatment changes the state of the coherently diffracting silicon matrix. The reduction of intensity may be related to impurity redistribution, the formation or rearrangement of defect complexes, and the appearance of local strain fields. At high temperature, phosphorus atoms and background impurities can become more mobile, and this mobility may lead to the formation of impurity-rich regions or local structural inhomogeneities. As a result, part of the crystal volume may contribute less effectively to coherent diffraction, causing a decrease in the intensity of the $(111)_{Si}$ peak [3].

Another important feature observed in the inset of Figure 1 is the change in FWHM from 0.144° for the initial sample to 0.134° after annealing. A decrease in FWHM may indicate partial relaxation of microstrain or an increase in the size of coherent scattering regions. However, this result should be interpreted together with the decrease in intensity. If only the FWHM change is considered, one may conclude that annealing improves the crystal structure. However, the simultaneous decrease in intensity suggests a more complex structural process. This means that some local distortions may be relaxed during annealing, while other regions may experience impurity redistribution and defect reorganization. Therefore, the thermal treatment does not simply improve or degrade the lattice; instead, it causes a mixed structural transformation in the silicon monocrystal.

The slight shift of the $(111)_{Si}$ peak after annealing is also important. According to Bragg's law, a shift in the diffraction angle indicates a change in interplanar spacing. If the peak shifts toward lower 2θ values, the interplanar distance increases, which can be associated with lattice expansion or tensile microstrain. In phosphorus-doped silicon, such changes may arise due to thermally activated redistribution of dopant atoms, oxygen-related complexes, vacancies, and other point defects. The Czochralski-grown silicon material may contain background oxygen, and during annealing oxygen can participate in the formation of oxide-related complexes or precipitates. These processes can modify the local lattice parameter and produce additional internal stress fields [4].

The wide-angle representation of the XRD pattern is especially useful because it shows that the main structural response remains concentrated around the silicon matrix reflection. No strong competing crystalline phase dominates the diffraction pattern in the presented angular range. This means that the high-temperature treatment mainly modifies the internal structural state of the silicon matrix rather than causing complete phase transformation. The inset provides a detailed view of the $(111)_{Si}$ peak shape, while the full wide-angle diffractogram gives broader structural context. Thus, the combination of the wide-angle pattern and the high-resolution inset makes the interpretation more reliable. From the technological point of view, the obtained results are significant because annealing is one of the most commonly used processes in semiconductor device fabrication. High-temperature treatment can improve some structural properties by reducing certain defects, but it can also activate impurity redistribution and generate new defect complexes. For n-type silicon, these changes may influence electrical conductivity, carrier lifetime, recombination behavior, and the stability of device parameters. Therefore, controlling annealing temperature, duration, and cooling

conditions is necessary for obtaining silicon materials with predictable structural and functional properties [5].

In summary, the wide-angle XRD analysis confirms that high-temperature annealing at 1300 °C causes noticeable structural changes in phosphorus-doped n-type silicon monocrystals. The main $(111)_{Si}$ orientation is preserved, but the diffraction peak intensity decreases, the peak position slightly changes, and the FWHM decreases from 0.144° to 0.134°. These results indicate structural reorganization of the silicon lattice, including partial stress relaxation, impurity redistribution, and modification of defect-related microstrain. The presented XRD data demonstrate that thermal treatment is an important technological factor for controlling the crystallographic quality and microstructural state of n-type silicon monocrystals.

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