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STUDY OF THE FORMATION OF LOW-DIMENSIONAL DEFECT STATES IN SINGLE-CRYSTAL SILICON WITH THE PARTICIPATION OF OXYGEN

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This study investigates the formation of low-dimensional defect states in monocrystalline silicon involving oxygen, focusing on structural inhomogeneities and their impact on material properties. Monocrystalline silicon, a cornerstone of modern nanoelectronics, is primarily produced using the Czochralski method, which often introduces oxygen impurities. These impurities form oxide inclusions (SiO_x) and complexes ($Si–O_n$) during thermal treatments at 400–800°C, leading to defects that affect electrical and structural properties. The research employs X-ray diffraction to analyze p-type silicon samples grown by the Czochralski method, with thermal treatments at 950°C, 1050°C, and 1150°C. Results reveal that thermal processing redistributes atoms and defects, increasing lattice parameters and crystallinity, peaking at 1050°C. Subcrystalline sizes vary with temperature, reaching maximum stability at 1050°C. Oxygen and boron interactions form SiO_2 and B_2O_3 crystallites, with sizes ranging from 21–25 nm and 55 nm, respectively. Additionally, small clusters (1.6–2 nm) of SiO_x form in surface regions, indicating unsaturated silicon bonds and localized microdefects. The study also identifies SiB_6 crystallites (71–95 nm) on the surface, growing through Ostwald ripening at higher temperatures. These findings highlight the complex interplay between oxygen impurities, thermal treatments, and defect formation in silicon crystals. The research provides insights into optimizing silicon production processes to minimize defects and enhance material performance for advanced electronic applications. The results underscore the importance of controlling oxygen content and thermal processing conditions to achieve high-quality monocrystalline silicon with tailored properties. This work contributes to a deeper understanding of defect dynamics in silicon, offering practical implications for improving semiconductor manufacturing techniques. By addressing the challenges posed by oxygen impurities, the study paves the way for developing more efficient and reliable silicon-based devices in the nanoelectronics industry.
Keywords: *Monocrystalline silicon; Czochralski method; Defect states; X-ray diffraction; Crystallographic orientation; Subcrystalline structures; Microdefects; Cluster formation*
PACS: 78.30.Am

INTRODUCTION

Modern nanoelectronics requires high-purity and perfect semiconductor crystals, among which monocrystalline silicon occupies one of the leading positions due to mature technologies and low cost [1-3]. The main methods of industrial production of Si are the Czochralski method and crucible-free zone melting, with the Czochralski method being used in about 80% of cases. When growing single crystal silicon, it is important to minimise the amount of uncontrolled impurities, as their excess leads to distortion of the crystal lattice and the formation of defects that affect the properties of the material. One of such impurities is oxygen, which during crystallisation from the melt passes into silicon, partially dissolving in it and forming oxide inclusions SiO_x with the size from 1 to 50 microns [4]. During heat treatment of silicon in the temperature range of 400-800°C, supersaturated oxygen forms various complexes of Si-O_n type (n = 1-4). Part of these complexes decomposes with the release of SiO_2 or is deposited in the interstitial spaces of the Si crystal lattice in electrically neutral states. This causes the formation of defect states that affect the electrical properties of silicon [5].

The shape, type and size of such microformations depend on the technological conditions of single crystal growth and subsequent heat treatment. This problem remains unsolved until now, as it affects not only the electrophysical characteristics, but also the structural parameters of the crystal. Analysis of literature data shows that oxygen can form non-stoichiometric layers of SiO_x, microunits of precipitate type and amorphous SiO_2 particles, which significantly complicates the study of the structure and behaviour of oxygen in a silicon crystal [6-8]. The main method to investigate such characteristics of oxygen in single crystal silicon is X-ray diffraction analysis. In connection with the above, the aim of the present work is to investigate the structural inhomogeneities formed by the participation of oxygen in single-crystal silicon grown by the Czochralskii method [8].

MATERIALS AND METHODS

The object of the study was p-type single-crystalline silicon grown by the Czochralskii method with resistivity $\rho \simeq 3 \div 10$ Ω-cm, boron impurity concentration $N_p \simeq 2\text{-}10^{15}$ cm^{-3}, dislocation density $N_d \geq 10^{13}$ cm^{-2} and oxygen concentration $N_0 \simeq 2\text{-}10^{17}$ cm^{-3}. Samples with dimensions of 1.4x4x22 mm^3 were fabricated from cut wafers of single-crystalline silicon.

Control of structural and phase states, O in Si of the studied samples was carried out on the third generation X-ray diffractometer types Empyrean Malvern PANalytical L.T.D. The OriginPro2022 programme was used to determine the

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peak maximum [9]. X-ray diffraction measurements were carried out in Bragg - Brentano beam geometry in the range $2\theta_B = 15°$ to 140° continuously at a scanning speed of 0.33 deg/min and an angular step of 0.0200 (deg).

RESULTS AND DISCUSSION

Thermal treatments of single-crystalline *p-Si<B>* (control samples) were carried out at temperatures of 950°C, 1050°C and 1150°C for 5 hours. Figure 1 shows the X-ray diffraction patterns of these samples. It can be seen from the X-ray radiographs that diffraction reflections corresponding to the $(111)_{Si}$ crystallographic orientation are observed at scattering angles 2θ = 28.53°, 28.5° and 28.45°, possessing high intensity ($I_{Si,(950°C)} = 3\times10^6$ imp/s, $I_{Si,(1050°C)} = 4.7\times10^6$ imp/s and $I_{Si,(1150°C)} = 1.4\times10^6$ imp/s) and a pronounced selective character. This indicates that the surface of the control silicon samples has a crystallographic orientation (111). Also note that with increasing processing temperature, the diffraction peaks shift towards smaller angles (from 28.53° to 28.45°) and their intensity first increases by a factor of 1.6 (at 1050°C) and then decreases by a factor of 2.1 (at 1150°C). This indicates that the heat treatment for 5 hours results in the redistribution of atoms and a decrease in the number of defects in the crystal and an increase in the silicon lattice parameter: $a_{Si,(950°C)} = 0.534$ nm, $a_{Si,(1050°C)} = 0.535$ nm and $a_{Si,(1150°C)} = 0.536$ nm. Thus, the maximum degree of crystallinity is reached at 1050°C and a decrease is observed at 1150°C. In addition, diffraction reflections corresponding to $(333)_{Si}$ crystallographic orientation were recorded at scattering angles 2θ = 94.95°, 94.94° and 94.98°, with intensities $I_{Si,(950°C)} = 2.3\times10^4$ imp/s, $I_{Si,(1050°C)} = 8.9\times10^4$ imp/s and $I_{Si,(1150°C)} = 4.5\times10^5$ imp/s. In the range of scattering angles 10°÷60°, a non-monotonic character of the inelastic background level can be observed. The structural reflections of $(111)_{Si}$ are weakly separated into α_1 and α_2 components, whereas $(333)_{Si}$ shows a marked separation of these components. This indicates that the heat treatment at 950°C, 1050°C and 1150°C results in the formation of microstresses (dislocations or other defects) in the surface regions of the samples, whereas in the inner volume of the crystal lattice their stabilisation occurs[10]. In addition, at scattering angles 2θ = 25.7° and 2θ = 83.3°, β components of the first-order $(111)_{Si}$ and third-order $(333)_{Si}$ reflections are observed (see Figs. 2 a and 2 c).

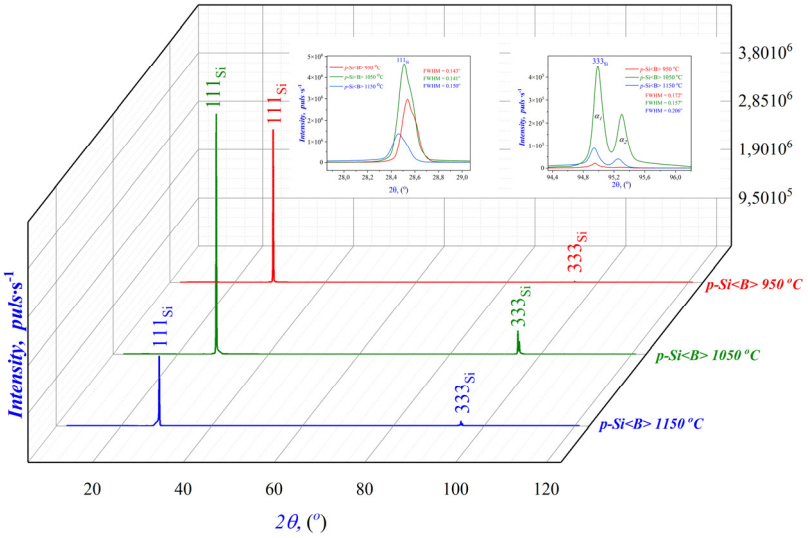

Figure 1. X-ray images of *p-Si<B>* samples subjected to heat treatment at 950°C, 1050°C, and 1150°C

According to experimental results on the diffraction reflections of $(111)_{Si}$, it was found that the subcrystallite sizes in silicon control samples, subjected to thermal treatment for 5 hours at 950°C, 1050°C, and 1150°C, were 59.7 nm, 61.1 nm, and 57.4 nm, respectively. This suggests that at 950°C, due to the relatively low diffusion temperature, the state of the subcrystallites did not undergo significant changes. At 1050°C, the size of the peak increased due to the process of recrystallization, through the attachment of subcrystallites. At 1150°C, the intensity of the peak decreased due to the activation of processes involving the removal and subsequent formation of subcrystallites. Additionally, X-ray diffraction patterns at scattering angles of 2θ = 63.2° and 105.1° reveal structural reflections corresponding to $(220)_{Si}$ and $(440)_{Si}$, indicating the presence of polycrystalline regions of various sizes (ranging from 11 nm to 87 nm) distributed on the surface and within the samples.

In addition, structural reflections corresponding to the $(222)_{Si}$ crystallographic orientation are observed at scattering angles 2θ = 58.8°, 59.0° and 58.9° in the X-ray diffraction patterns of silicon control samples heat treated for 5 h at temperatures of 950°C, 1050°C and 1150°C (see Fig. 2c). As a rule, such structural reflections are not observed in the X-ray radiograph of silicon with a crystal lattice free from various microdistortions. That is, their appearance indicates the presence of micro-distortions in the crystal lattice. There is a possibility of quantitative determination of such micro-distortions, for which the ratio of the intensity of structural reflection $(222)_{Si}$ to the intensity of the main structural reflection $(111)_{Si}$, i.e. $I_{(222)}/I_{(111)}$, is used. In our case, these values are: 3.8×10^{-4} at 950°C, 5.4×10^{-4} at 1050°C, and 6.5×10^{-4} at 1150°C. These values exceed 10^{-4}, which is characteristic of crystal lattices with a diamond-like structure in which the atoms are uniformly distributed. This, in turn, indicates that mechanical stresses in localised regions of the silicon crystal

lattice increase with increasing heat treatment temperature. This effect is due to the non-uniform distribution of oxygen entering the crystal from background impurities. This is most likely due to the difference in ionic radii of silicon and oxygen, as well as to small stresses arising during crystal growth due to the temperature gradient. Due to the difference in ionic radius, oxygen atoms are located near crystal lattice boundaries, at the interfaces of silicon subcrystallites, and in displaced lattice nodes. In doing so, they compensate for the unsaturated silicon bonds [11,12]. This, in turn, shows that silicon atoms are predominantly located in the crystal volume and this structure has high symmetry, while oxygen atoms can spontaneously form asymmetric crystallites at subcrystallite interfaces.

The X-ray diffraction analysis of the *p-Si* sample revealed the presence of structural reflections corresponding to SiO_2 and B_2O_3 phases. For SiO_2, the reflections were observed at scattering angles 2θ = 20.2°, 39.1°, 42.6°, 90.8°, and 91.9°, corresponding to the crystallographic orientations (100), (102), (200), (400), and (401). The analysis of the full width at half maximum (FWHM) values indicated the formation of SiO_2 crystallites with sizes ranging from 21 to 25 nm. The crystalline parameters for SiO_2 were determined to be aexp = bexp = 0.5031 nm and cexp = 0.5527 nm, with a trigonal unit cell of space group P3221. Additionally, for B_2O_3, a structural reflection was observed at scattering angles 2θ = 23.0° to 23.6°, indicating the presence of B_2O_3 crystallites with a size of 55 nm and a trigonal unit cell with lattice parameters $a_{exp} = b_{exp} = 0.4415$ nm and $c_{exp} = 0.8812$ nm. These findings suggest the coexistence of SiO_2 and B_2O_3 phases in the *p-Si* sample.

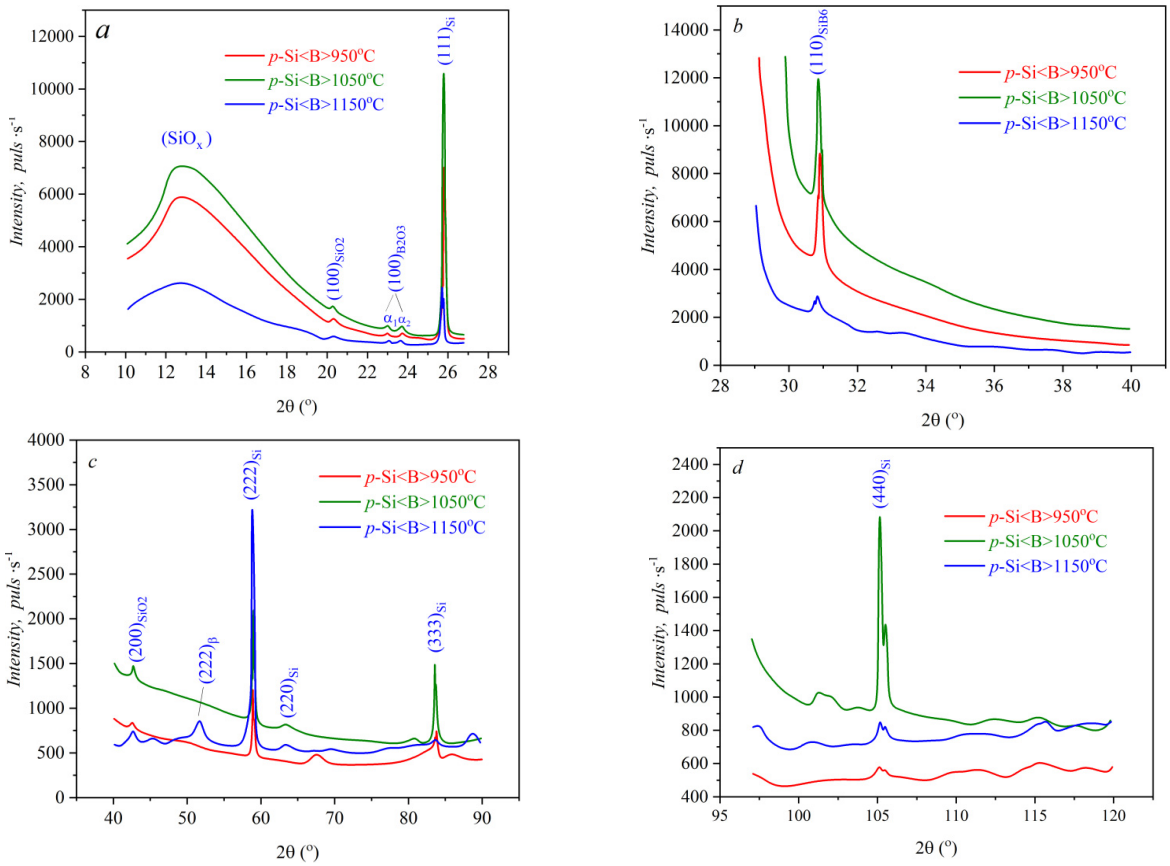

Figure 2. Variation in the inelastic background level of the X-ray image for the p-Si<B> sample at small, medium, and large scattering angles, along with the shapes of the observed structural reflections.

Moreover, in the X-ray images of silicon control samples subjected to thermal treatment for 5 hours at temperatures of 950°C, 1050°C, and 1150°C, diffuse reflections associated with the SiO_x phase are observed in the small-angle scattering region (2θ ≈ 13°) (see Fig. 2*a*). An analysis of the full width at half maximum (FWHM) values reveals the following: FWHM(950°C) = $7{,}2\times10^{-2}$ rad, FWHM(1050°C) = $8{,}7\times10^{-2}$ rad FWHM(1150°C) = $8{,}4\times10^{-2}$ rad. Based on these values, it is established that these structures are not crystallites but rather small fragments with sizes of 2 nm at 950°C, 1.6 nm at 1050°C, and 1.7 nm at 1150°C. These fragments primarily form in the near-surface regions of silicon and indicate the presence of unsaturated bonds between silicon atoms. Additionally, their small size suggests the absence of long-range order in the arrangement of silicon and oxygen atoms. Therefore, these formations are not nanocrystallites but rather clusters [13]. Since similar clusters partially form in different regions of the silicon control samples at 950°C, 1050°C, and 1150°C, variations in the inelastic background of the X-ray images are observed across small, medium, and large scattering angles. This, in turn, indicates the formation of additional microdefects in the silicon crystal lattice.

In the X-ray radiographs of silicon control samples heat treated for 5 h at temperatures of 950°C, 1050°C and 1150°C, a structural reflection is observed at a scattering angle of 2θ = 30.8° referring to the SiB_6 (silicon hexaboride)

phase with crystallographic orientation (110) at a scattering angle of 2θ = 30.8° (see Fig. 2 b). This phase is formed by cubic unit cells with lattice parameters: aexp = 0.4156 nm. The crystallite size corresponding to this phase is: 75 nm at 950°C, 71 nm at 1050°C and 95 nm at 1150°C. This, in turn, indicates the following processes: at 950°C, crystallite formation and growth occur; at 1050°C, reorganization and fragmentation are observed, which leads to a temporary decrease in their size; at 1150°C, atomic mobility increases and crystallite enlargement occurs due to the intensification of the Ostwald Ripening mechanism.

CONCLUSION

Based on the X-ray structural analysis of single-crystal p-Si samples, the following conclusions have been drawn:

It has been established that the surface of the p-Si single-crystal samples corresponds to the crystallographic orientation (111). Through thermal treatment at 950°C, 1050°C, and 1150°C, there is a redistribution of atoms and defects, leading to an increase in the lattice parameter: $a_{Si,(950°C)}$ = 0,534 nm $a_{Si,(1050°C)}$ = 0,535nm and $a_{Si,(1150°C)}$ = 0,536 nm. Furthermore, the crystal perfection is increased at 1050°C and decreased at 1150°C.

During the thermal treatment at 950°C, 1050°C, and 1150°C, micro-stresses (dislocations and other defects) are formed in the surface areas of the samples, while their stabilization occurs within the bulk of the samples.

It has been found that at 950°C, due to the relatively low diffusion temperature, sub-crystals (59.7 nm) do not undergo significant changes. At 1050°C, a recrystallization process takes place, resulting in their enlargement to 61.1 nm. At 1150°C, due to the destruction and subsequent reformation of sub-crystals, their size is reduced to 57.4 nm.

The interaction of silicon, boron, and oxygen atoms results in the formation of crystallites SiO_2 and B_2O_3, belonging to the trigonal elementary cell with spatial group $P3_221$. The dimensions of the SiO_2 crystallites are $a_{exp} = b_{exp}$ = 0,5031 nm and c_{exp} = 0,5527 nm, with a size of 21-25 nm. The B_2O_3 crystallites have dimensions $a_{exp} = b_{exp}$ = 0.4415 nm, c_{exp} = 0.8812 nm, and a size of 55 nm.

After thermal treatment at 950°C, 1050°C, and 1150°C, clusters with sizes of 2 nm, 1.6 nm, and 1.7 nm are formed in the surface regions of monocrystalline p-Si samples. These clusters are formed due to unsaturated silicon-oxygen (SiO_x) bonds, leading to the formation of additional microdefects in the crystal lattice.

Furthermore, thermal treatment at the same temperatures leads to the formation of nanocrystallites with sizes of 75 nm, 71 nm, and 95 nm on the surface of p-Si samples. These nanocrystallites consist of cubic elementary cells with lattice parameters a_{exp} = 0.4156 nm.

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ДОСЛІДЖЕННЯ ФОРМУВАННЯ НИЗЬКОВИМІРНИХ ДЕФЕКТНИХ СТАНІВ В МОНОКРИСТАЛІЧНОМУ КРЕМНІЇ ЗА УЧАСТЮ КИСНЮ

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В цій роботі досліджується формування низьковимірних дефектних станів у монокристалічному кремнії за участю кисню, зосереджуючись на структурних неоднорідностях та їхньому впливі на властивості матеріалу. Монокристалічний кремній, наріжний камінь сучасної наноелектроніки, виробляється переважно методом Чохральського, який часто вводить домішки кисню. Ці домішки утворюють оксидні включення (SiO_x) та комплекси (Si–On) під час термічної обробки при 400–800°C, що призводить до дефектів, які впливають на електричні та структурні властивості. У дослідженні використовується рентгенівська дифракція для аналізу зразків кремнію p-типу, вирощених методом Чохральського, з термічною обробкою при 950°C, 1050°C та 1150°C. Результати показують, що термічна обробка перерозподіляє атоми та дефекти, збільшуючи параметри решітки та кристалічність, досягаючи піку при 1050°C. Розміри субкристалічних структур змінюються з температурою, досягаючи максимальної стабільності при 1050°C. Взаємодія кисню та бору утворює кристаліти SiO_2 та B_2O_3 розмірами від 21 до 25 нм та 55 нм відповідно. Крім того, в поверхневих областях утворюються невеликі кластери (1,6–2 нм) SiO_x, що вказує на ненасичені кремнієві зв'язки та локалізовані мікродефекти. У дослідженні також виявлено кристаліти SiB_6 (71–95 нм) на поверхні, що ростуть шляхом дозрівання Оствальда за вищих температур. Ці результати підкреслюють складну взаємодію між домішками кисню, термічною обробкою та утворенням дефектів у кристалах кремнію. Дослідження дає уявлення про оптимізацію процесів виробництва кремнію для мінімізації дефектів та підвищення характеристик матеріалу для передових електронних застосувань. Результати підкреслюють важливість контролю вмісту кисню та умов термічної обробки для досягнення високоякісного монокристалічного кремнію з індивідуальними властивостями. Ця робота сприяє глибшому розумінню динаміки дефектів у кремнії, пропонуючи практичні наслідки для вдосконалення технологій виробництва напівпровідників. Вирішуючи проблеми, що виникають через домішки кисню, дослідження прокладає шлях для розробки більш ефективних та надійних пристроїв на основі кремнію в наноелектронній промисловості.

Ключові слова: *монокристалічний кремній; метод Чохральського; дефектні стани; рентгенівська дифракція; кристалографічна орієнтація; субкристалічні структури; мікродефекти; утворення кластерів*