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STRUCTURAL STUDY OF COPPER DOPED SINGLE-CRYSTAL SILICON BY DIFFUSION

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The paper presents the results of a structural study of single-crystal silicon doped with copper by thermodiffusion at 1423K. The object of the study was n-Si crystals grown by the Czochralski method, containing SiO_2 oxygen precipitates. Structural analysis was performed on an X-ray diffractometer with an improved optical scheme, which made it possible to detect weak additional reflections and changes in lattice parameters. It was established that copper doping leads to the appearance of elastic stresses in the surface layers of the crystal, a change in the interplanar distance (111) and a redistribution of the intensities of reflections (222) and (333). Diffuse scattering and additional selective reflections were detected, indicating the formation of new phases. For the first time, a direct structural method has shown the formation of CuO nanocrystals with a monoclinic structure and an average size of 14–14.5 nm and Cu_2O nanocrystals with a cubic structure and an average size of about 17 nm. Their lattice parameters were measured experimentally and are slightly different from the standard reference values, which shows that the silicon matrix and internal stresses affect their structure. It has been shown that SiO_2 oxygen precipitates create local elastic fields that promote diffusion, nucleation, and separation of copper in the form of oxide nanophases. The results obtained clarify the mechanism of structural transformations in copper-doped silicon.
Keywords: *X-ray diffraction; Subcrystallite, Nanocrystal; Copper-doped silicon; Thermal diffusion; Copper oxides; Oxygen precipitates*
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INTRODUCTION

In the production of semiconductor devices, doping is one of the most important technological processes, along with etching and deposition. The main purpose of doping is to change the type of conductivity and concentration of carriers in the semiconductor volume to obtain the specified electrical properties (conductivity and the required smoothness of the p-n junction) [1]. The introduction of foreign atoms, including those that diffuse rapidly into the silicon lattice, causes stress within the crystal and, as a result, a change in the lattice parameters. Since the movement of impurity atoms occurs with the participation of intrinsic point defects (vacancies and interstitial silicon atoms), diffusion will lead to a change in the equilibrium concentration of point defects, resulting in most cases in the formation of precipitates, usually in the form of a compound of impurities with silicon atoms [2]. Such precipitates can create sufficiently large stresses, leading to the formation of new defects. At high temperatures, particularly in the presence of SiO_2 particles, the local stresses are strong enough to attract rapidly diffusing impurities (e.g., copper, gold, and iron), which promotes their precipitation and leads to the formation of dislocation clusters. In particular, the presence of such particles is associated in the literature with the occurrence of defects in the form of a star with a central core from which complex-shaped dislocations propagate [3].

Copper impurities in silicon have attracted the attention of researchers since the advent of silicon technology. This interest is driven both by academic curiosity about the unusual properties of this *3d* transition metal and by its practical importance. The latter is determined by the fact that copper easily precipitates, forming electrically active centres that degrade the parameters of electronic devices. To avoid unwanted precipitation, it is necessary to understand, in particular, the process of nucleation. However, to date, only the properties of isolated copper atoms in silicon (interstitial Cu_i and in the substitution position Cu_s) have been studied sufficiently well, while there is no reliable identification for most even the simplest copper aggregates with background and other alloying impurities [4,5]. The concentrations at which copper and other rapidly diffusing impurities form precipitates are too low to be determined by conventional analytical methods. At the same time, even at a concentration of $2 \cdot 10^{-4}$ %, these impurities can cause noticeable structural changes after annealing the crystal at a high temperature (> 900°C). The difficulty of determining small amounts of metallic impurities in silicon (e.g., copper and similar) is a long-standing problem in semiconductor technology. Often, the presence of rapidly diffusing impurities is detected only by their effect on the distribution of crystallographic defects or on the electrical properties of the crystal [6,7].

Below, experimental results of structural studies of copper-doped silicon single crystals are presented for the first time. The aim of the work is to determine the structural perfection of single crystals, to establish the formation of copper aggregates with background impurities and their types using an X-ray diffractometer with an improved optical scheme.

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MATERIALS AND METHODS

The objects of the study were n-Si (KEF) single crystals grown by the Czochralski method with a resistivity $\rho_o \approx$ (3÷10) Ω·cm, dislocation density $N_D \approx 10^1 \div 10^3$ cm^{-2}, and oxygen concentration $N_O \approx 2 \div 4 \cdot 10^{17}$ cm^{-3}. Before measurements, the samples underwent mechanical and chemical polishing with removal of a surface layer approximately 20 μm thick and had a working surface (111) with an area of 5.4 ×15.8 mm² and a thickness of 0.6 mm. The samples were doped with copper at a temperature of 1423K using the surface thermodiffusion method. The copper concentration in the samples was 10-14 cm^{-3}. Structural studies were performed on an XRD-7000 X-ray diffractometer (CuK$_\alpha$ radiation, λ = 0.15418 nm) with an improved optical scheme, according to the Θ–2Θ scheme in step scanning mode at 300 K. The angular dependence of the intensity was measured in two ways: after adjusting the samples for reflection (111) and (333). The intensity of the incident beam was approximately 5·10^5 imp·s^{-1}, and the intensity measurement error was ~ 0.6 %. The resistivity was measured using the conventional four-probe method, also at room temperature.

RESULTS AND DISCUSSION

Fig. 1 shows an X-ray diffraction pattern of copper-doped single-crystal silicon - n – Si (Cu), tuned to reflect (111) of the sample. It differs significantly from the X-ray diffraction pattern of unalloyed silicon samples, despite their similarity in appearance. The X-ray diffraction pattern of n-Si (Cu) showed no diffuse reflection at small scattering angles (2θ≈ 17.6°). The intensity of the forbidden reflection (222) (2θ = 58.9°) decreased by 9.5%, and the intensity of the structural line (333) (d/n = 0.1046 nm; 2θ = 95°) decreased by 11% compared to the intensity of similar reflections from unalloyed samples. In addition, a decrease in the intensity of the $(110)_{SiO2}$ reflection (d/n = 0.2495 nm; 2θ = 36°) of the impurity phase of crystalline quartz - SiO_2 - was also observed, by 11.5%. As for the intensity and interplanar spacing of the main reflection (111) (d/n = 0.3143 nm; 2θ = 28.4°), they increased by 2.6% and 0.7%, respectively, compared to the intensity and interplanar distance of the same reflection of the initial sample. The average level of the inelastic background of the n - Si (Cu) sample decreased by 9% compared to the level of the inelastic background of unalloyed silicon.

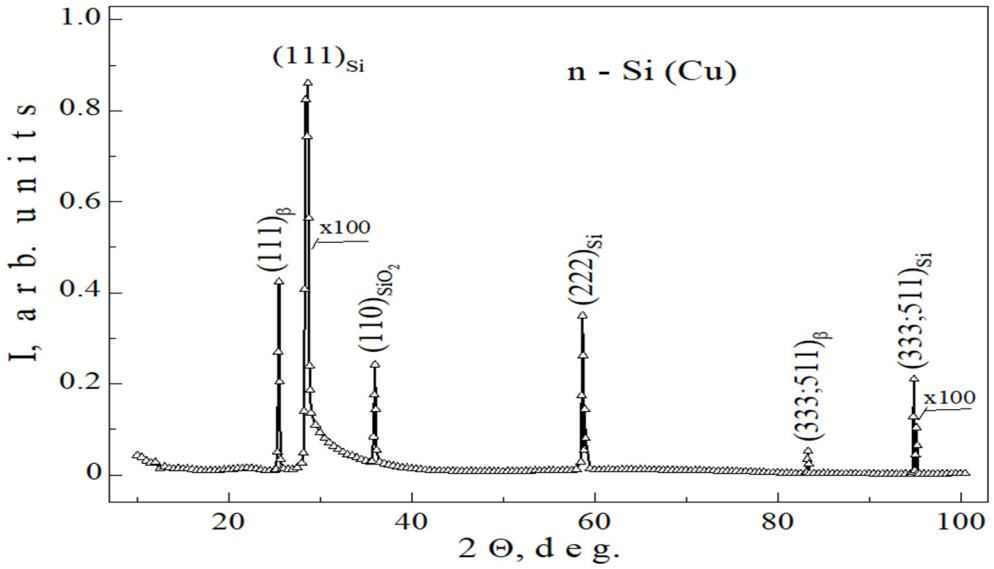

Figure 1. X-ray diffraction pattern of copper-doped single-crystal n-Si

In addition, diffuse scattering with weak intensity in the middle scattering angles with $d/n \approx$ 0.1467 nm; $2\theta \approx$ 63.4° was detected on the X-ray diffraction pattern of copper-doped samples. Precision measurement showed the presence in this angle range against the background of diffuse reflection, in addition to the forbidden reflection (222) of silicon, of three additional selective reflections (d/n = 0.1707 nm; 2θ = 53.7°; d/n = 0.1572 nm; 2θ = 58.6°; d/n = 0.1361 nm; 2θ = 69°) with weak intensity from an unknown phase. The X-ray diffraction patterns of samples tuned to third-order reflection (333) differed from those tuned to first-order reflection (111) in the presence of an additional selective reflection (d/n = 0.3079 nm; 2θ = 29°) with noticeable intensity on the right wing of the main reflection (111). This reflection is not characteristic of silicon and silicon dioxide single crystals.

The narrow width ($FWHM$ = 2.62·10^{-3} rad) and high intensity (2·10^5 imp·sec^{-1}) of the main reflection (111) indicate a high degree of perfection of the crystal lattice of doped n-Si (Cu). Structural measurements showed that the cutting plane of the samples corresponded to the crystallographic plane (111). The dimensions of subcrystals (blocks), estimated by the width of this peak using the Selakov–Sherrer method [8], were approximately ~ 57 nm. However, the slight splitting of this reflection into α_1 and α_2 emissions (Fig. 2a) indicates the presence of elastic stresses in the silicon matrix lattice associated with the presence and uneven distribution of oxygen and the possible substitution of silicon atoms by copper atoms in silicon single crystals. Since the ionic radii of silicon, oxygen and copper atoms are r_{Si}^{4+} = 0.042, r_o^{-2} = 0,140 nm

and r_{Cu}^{2+} = 0.072 nm, respectively [9]. Considering the significant chemical activity of copper towards oxygen [10], it can be assumed that molecules of silicon ion pairs are replaced by molecules of copper-oxygen ions in defect-prone areas of the silicon lattice [10]. This conclusion is confirmed by the presence of a forbidden reflection $(222)_{Si}$ with d/n = 0.1571 nm on the X-ray diffractogram (Fig. 1, 3), which should be absent for an ideal silicon lattice without elastic stress. In addition, the intensity of the main (111) reflection of doped silicon samples is 2.6% greater than the intensity of the same line in undoped samples. This fact also indicates the partial replacement of some silicon ion pairs with copper-oxygen ion molecules. Since the intensity of X-ray scattering is proportional to the atomic number (Z) of the elements, such ion replacement should lead to an increase in the intensity of this reflection in doped samples, because Z_{Si} = 14, Z_O = 8, Z_{Cu} = 29 [11]. However, with a noticeable increase in the intensity of this reflection, the X-ray diffraction pattern shows a significant decrease in the intensity of its second (222) and third (333) order reflections by 9.5% and 11%, respectively. In addition, an increase in the interplanar distance of the diffraction reflection (111) by 0.7% was observed on the X-ray diffraction pattern of the alloyed samples, which was absent in its higher orders - in the reflections (222) and (333). The almost complete splitting of the (333) reflection, close to the calculated value ($3.79 \cdot 10^{-3}$ rad) with a characteristic ratio of intensities for α_1 and α_2 radiation [I_{333} (α_1) ≈ 2·I_{333}(α_2)] (Fig. 2 b) shows the absence of distortion of the silicon lattice in the deeper layers from the surface of the doped samples [12]. All these facts indicate an uneven distribution of copper-oxygen molecules in the lattice of doped samples. Their content in the surface layer is significantly higher than in deeper layers.

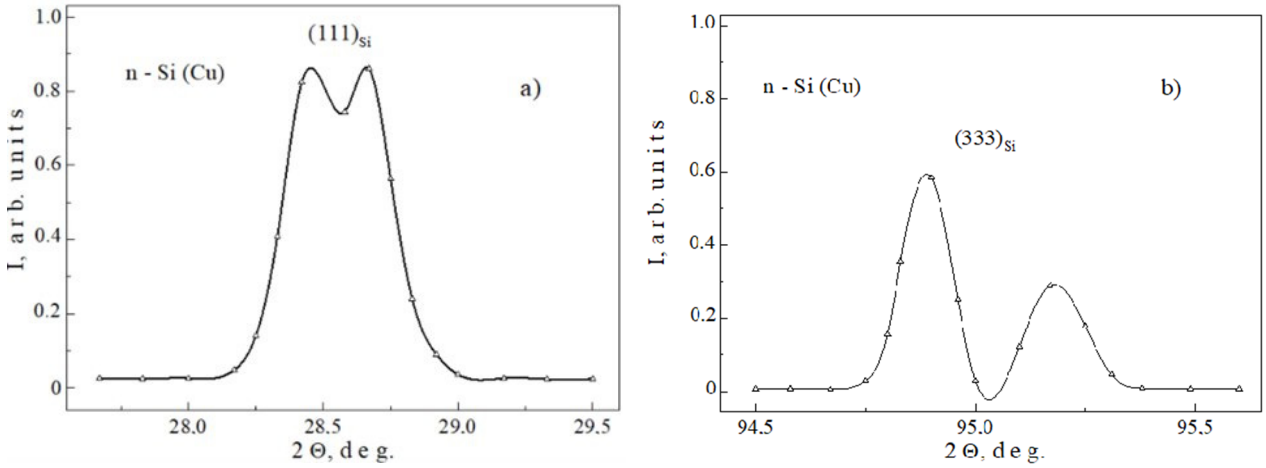

Figure 2. Reflection patterns (111) and (333) of single-crystal n-Si (Cu)

It should be noted that the observed increase in interplanar spacing in the case of structural reflection (111) shows that the arrangement of atoms in the surface layers of doped samples has a noticeable shift from their ideal position in the [111] direction while maintaining the existing initial symmetry, which cannot be said about atoms located in deeper layers. This situation leads to a partial violation of the Wolff-Bragg diffraction condition for high-order reflections (222) and (333). As a result, the normals of high-order atomic planes of the {HHH} type acquire a slightly distorted orientation with respect to the direction of the normals of the near-surface planes (111). This leads to a partial loss of intensity of the diffraction reflections (222) and (333), which is observed in the experiment. In addition, the decrease in the intensity of the (222) and (333) reflections may also be associated with a noticeable increase in primary extinction (weakening of the first-order intensity) for reflections from planes with large indices [13]. The decrease in the intensity of the diffraction reflection (110) of the SiO_2 impurity phase may also be associated with the distortion of its lattice as a result of the partial replacement of Si-O molecules by Cu-O molecules at the boundary areas between the blocks of doped samples.

In copper-doped samples, the presence of the silicon dioxide (SiO_2) impurity phase is indicated by the presence of a diffraction reflection (110) on the X-ray diffractogram with a slightly lower intensity (11.5%) than the intensity of this reflection in undoped samples. The characteristic size of the structural fragments - nanocrystals of the impurity phase - was ~ 75 nm. Such particles can create local elastic stresses around themselves, the magnitude of which is sufficient to attract rapidly diffusing impurities, in particular copper at elevated temperatures, and initiate processes of their separation in the form of clusters or nanoparticles. This assumption is confirmed by the presence of diffuse reflection at medium scattering angles with d/n ≈ 0.1467 nm; 2θ ≈ 63.4° and, against the background of this broad maximum, the presence of three not very narrow structural reflections with weak intensity (Fig. 3-a). Analysis of the nature of these structural lines showed that all these reflections belonged to the same newly formed impurity phase – CuO, which has monoclinic symmetry. They are caused by nanocrystals of this phase with average sizes of L_{CuO} ≈ 14–14.5 nm. The experimental values of the lattice parameters of this phase were: a_{exp} = 0.4573, b_{exp} = 0.3413, c_{exp} = 0.5239 nm and β = 98.9°, which differ slightly from the tabulated values (a_{tab} = 0.4662, b_{tab} = 0.3417, c_{tab} = 0.5118 nm and β = 99.85°, respectively) [14]. The specific volume of the CuO impurity phase is V_{CuO} ≈ 0.0808 nm^3, which is two times less than the specific volume

of silicon - $V_{Si} \approx 0.160$ nm^3. The difference in specific volume is one of the factors stimulating the formation of copper oxide nanoparticles in a silicon environment.

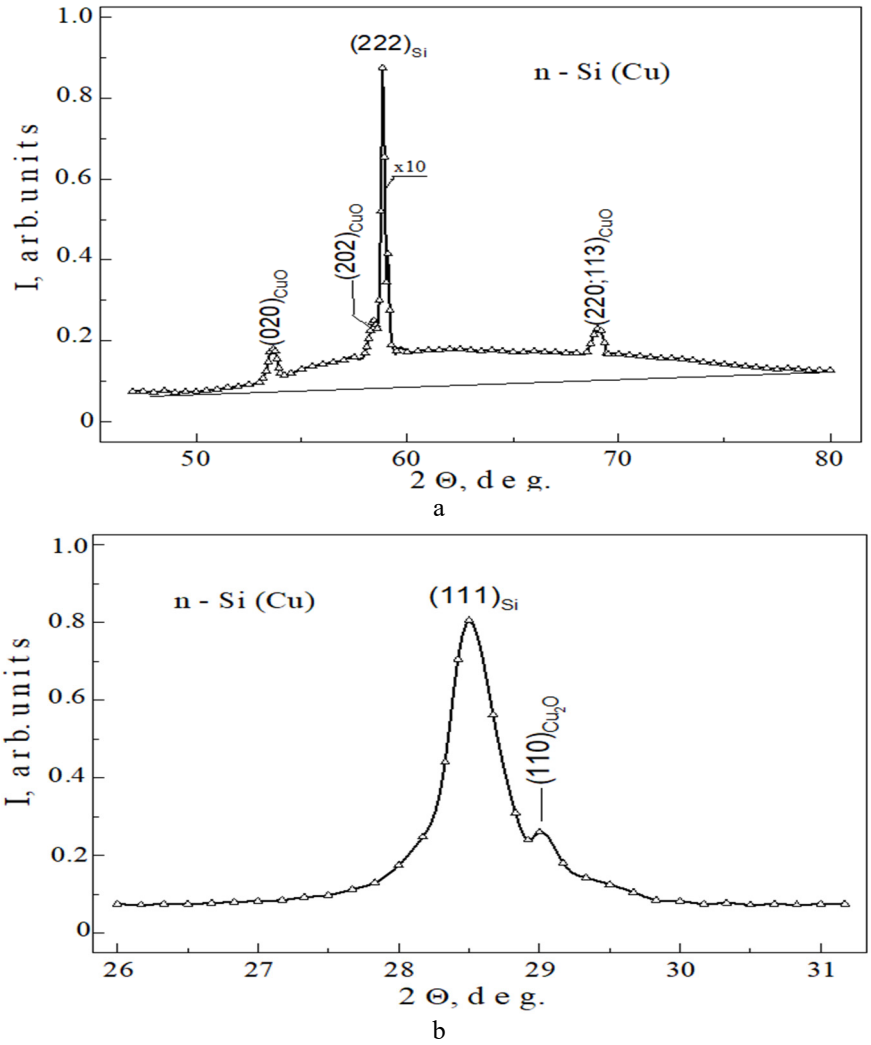

Figure 3. (a) Section of the X-ray diffraction pattern of single-crystal n-type Si doped with copper. (b) The sample is aligned for the (111) reflection

The X-ray diffraction pattern of the same sample, but tuned to reflection (333), did not differ significantly from the X-ray diffraction pattern tuned to reflection (111). Only a strong loss of intensity of the main reflection (111) (~ 3 times) and the appearance of a new selective reflection from an unknown phase on its right wing (Fig. 3-b). Analysis of the nature of the new reflection showed that nanocrystals of copper monoxide – Cu_2O, which has cubic symmetry, caused it. The characteristic dimensions of the nanocrystals are ~ 17 nm. The experimentally determined lattice parameter of copper monoxide was $a_{exp} = 0.4354$ nm, which slightly exceeds the tabulated value $a_{tab} = 0.4263$ nm [15].

CONCLUSIONS

In this work, the structure of single-crystal silicon doped with copper by thermodiffusion at a temperature of 1200°C was studied using X-ray diffraction. The results showed that when copper atoms are introduced into the silicon crystal lattice, elastic stresses arise in the surface layers and the interplanar distances change slightly. The study revealed the formation of new phases - nanocrystals of CuO and Cu_2O oxides. Their average sizes were approximately 14 - 15 nm and about 17 nm, respectively. It was also shown that SiO_2 oxygen precipitates promote copper diffusion and the formation of oxide nanophases. The results obtained provide a better understanding of the mechanism of structural transformations in copper - doped silicon and create a scientific basis for controlling such processes in semiconductor technologies.

Conflict of Interests

The authors declare that they have no conflict of interests

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СТРУКТУРНІ ДОСЛІДЖЕННЯ МОНОКРИСТАЛІЧНОГО КРЕМНІЮ, ЛЕГОВАНОГО МІДДЮ, МЕТОДОМ ДИФУЗІЇ

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У статті представлено результати структурного дослідження монокристалічного кремнію, легованого міддю методом термодифузії за температури 1423 K. Об'єктом дослідження були кристали n-Si, вирощені методом Чохральського, що містять кисневі преципітати SiO_2. Структурний аналіз проводився на рентгенівському дифрактометрі з удосконаленою оптичною схемою, що дозволило виявити слабкі додаткові відбиття та зміни параметрів кристалічної решітки. Встановлено, що легування міддю призводить до появи пружних напружень у поверхневих шарах кристалу, зміни міжплощинної відстані (111) та перерозподілу інтенсивності відбиття (222) і (333). Виявлено дифузне розсіювання та додаткові селективні відбиття, що свідчать про утворення нових фаз. Вперше прямим структурним методом показано формування нанокристалів CuO з моноклінічною структурою та середнім розміром 14–14,5 нм, а також нанокристалів Cu_2O з кубічною структурою та середнім розміром близько 17 нм. Їхні параметри решітки були виміряні експериментально та дещо відрізняються від стандартних еталонних значень, що свідчить про вплив кремнієвої матриці та внутрішніх напружень на їхню структуру. Було показано, що кисневі преципітати SiO_2 створюють локальні пружні поля, які сприяють дифузії, зародкоутворенню та розділенню міді у вигляді оксидних нанофаз. Отримані результати уточнюють механізм структурних перетворень у кремнії, легованому міддю.
Ключові слова: *рентгенівська дифракція; субкристаліт; нанокристал; легований міддю кремній; термічна дифузія; оксиди міді; кисневі преципітати*