X-RAY DIFFRACTION STUDY OF THE PRODUCT OF HIGH-TEMPERATURE DIFFUSION OF MANGANESE IN CRYSTALLINE SILICON OF SAMPLE KDB-3

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The object of study was the KDB-3 sample – crystalline silicon (Si) doped with boron (B) and containing oxygen (O). During the experiments, high-temperature diffusion of manganese (Mn) into the crystalline Si structure was carried out at temperatures of 1125–1200°C.

Research Method To analyze the phase composition and structural changes in the samples, the X-ray diffraction (XRD) method was used. Measurements were carried out on a Shimadzu XRD-6100 diffractometer, which allows for qualitative and quantitative phase analysis and determines the degree of crystallinity and crystallite sizes.

Main experimental parameters:

- Radiation source: Cu Kα (λ = 1.5406 Å)
- 2θ angle range: 5.0° – 70.0°
- Scanning step: 0.025°
- Exposure time: 1.5 s
- Data processing method: phase analysis using PDF-2 and PDF-4 databases

Technical specifications of the Shimadzu XRD-6100 diffractometer:

- X-ray tube: Cu anode, power up to 2.7 kW
- Maximum voltage: 60 kV
- Maximum current: 80 mA
- Goniometer: vertical, scanning range -6°–163° (2θ)
- Detectors: scintillation counter NaI, optional – OneSight (1280 channels)
- Scanning speed: 0.1–50°/min (2θ)

Result analysis: experimental data processing was carried out using the Rietveld method to refine lattice parameters and phase composition. The main identified phases were:

- SiB_6 (silicon boride) – 87.3%
- Mn_5Si_3 (mavlyanovite, manganese silicide) – 12.7%
- Amorphous phase – 76.41%

The obtained data allowed the determination of structural changes in silicon after manganese diffusion and the influence of oxygen on the amorphization of the samples.

X-ray diffraction (XRD) analysis was conducted to determine the crystallite sizes in the studied sample. The full width at half maximum (FWHM) of the diffraction peaks was used to calculate the average crystallite sizes according to the Debye–Scherrer equation.

The results (Fig. 1, Table 1) indicate that the crystallite sizes range from 6.5 nm to 77.2 nm, with an average size of 37.5 nm. The smallest crystallite size (6.5 nm) was observed at 2θ =

9.1569°, while the largest (77.2 nm) was recorded at 2θ = 64.4229°. The dependence of peak broadening on crystallite size confirms the presence of a polydisperse structure.

Interplanar spacings obtained from XRD analysis correspond to crystalline phases SiB_6 and Mn_5Si_3. The presence of an amorphous phase (76.41%) indicates significant disruption of lattice order.

Table 1

	2θ	d	I/I_1	FWHM	The size of the crystallites	Average size of crystallites
1	43.8074	2.06488	100	0.23370	38,9nm	37,5 nm
2	64.1681	1.45021	40	0.25880	37,7 nm	
3	56.1946	1.63556	16	0.24540	39,2 nm	
4	9.1569	9.64998	12	1.29040	6,5 nm	
5	48.0118	1.89342	8	0.24220	37,9 nm	
6	43.2817	2.08874	6	0.35300	25,5 nm	
7	42.5681	2.12209	4	0.24030	37,1 nm	
8	64.4229	1.44509	5	0.12760	77,2 nm	

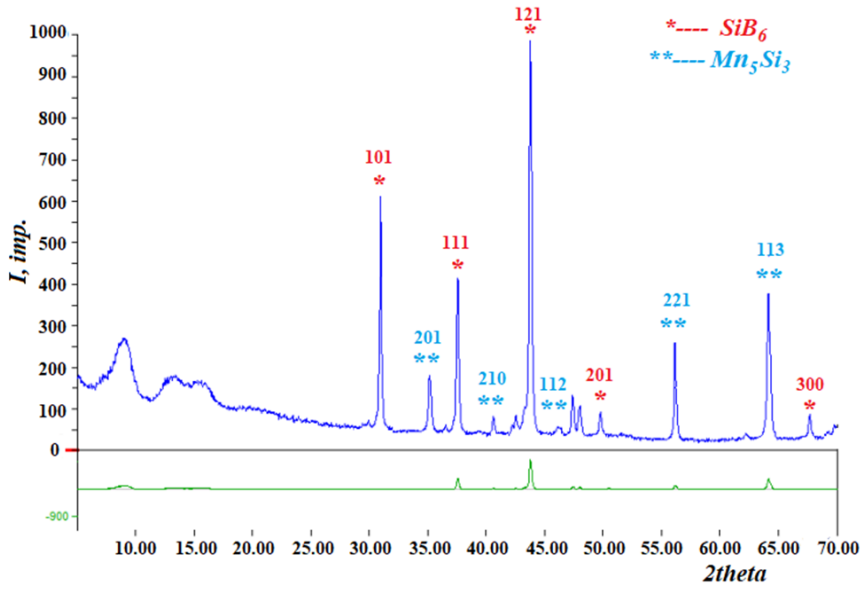

Figure 1. Dependence of I, imp on 2θ

The primary crystalline structure undergoes changes, forming Mn_5Si_3 and amorphous regions. Boron remains in the structure as SiB_6, but its excess may influence defect distribution. Oxygen contributes to local amorphization and defect formation. The interactions of B, Mn, and O in the Si crystal lattice at temperatures of 1125–1200°C, based on X-ray diffraction data and literature analysis [1-5], allow for the study of structural and electronic interactions of impurities in Si at high temperatures.