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Local Structure of Ion-Bombarded α -SiC Analyzed by EXAFS

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Abstract. X-ray absorption spectroscopy on the Si k-edge was performed on α -SiC (6H) to monitor the evolution of the local structure around the Si atoms after ion bombardment. The samples were irradiated by 50 keV Na ions at fluences of 10^{13} - 10^{16} ions/cm² at a temperature of 80 K. EXAFS analysis clearly reveals that the hetero-atomic short range order of the crystalline matrix is almost completely conserved over the crystalline-to-amorphous transition as indicated by RBS-C. Further irradiation at higher fluences results in a change of the atomic coordination and formation of homonuclear Si-Si bonds.

1 INTRODUCTION

α -SiC is a very promising semiconductor materials for electronic high speed and high temperature devices [1] with a hexagonal lattice structure formed by sp^3 -bonded Si-C₄ and C-Si₄ tetrahedrons, respectively. Ion implantation is a dedicated technique for electrical doping of the ceramic. However, SiC is easily amorphized upon irradiation at damage levels as low as 0.1 dpa (displacements per atom) [2], which may strongly alter the electronic properties of the ceramic. Rutherford-Backscattering Spectroscopy studies in channeling geometry (RBS-C) [3] recently suggested that point defects are first accumulated in the still crystalline matrix until a critical damage level is reached. For a fluence of around $\Phi = 3 \cdot 10^{14}$ at/cm², the crystalline-to-amorphous transition takes place. The lattice can then be described as a random network of Si-C₄ and C-Si₄ tetrahedrons. Further implantation (in the order of $\Phi = 10^{15}$ - 10^{16} at/cm²) transform this metastable amorphous phase in a atomically amorphous state [4]. Raman scattering measurements suggest the formation of Si-Si and C-C-bonds. *Ab initio* molecular-dynamics (MD) simulation [5] have also predicted chemical short range order in amorphous SiC, with homonuclear bonds. We therefore have performed XAS-analysis on the Si k-edge to check the hypothesis given in [4].

2 EXPERIMENTAL

Single-crystalline α -SiC (6H polytype) with 4° off-axis orientation were irradiated at 80 K with Na⁺ ions of energy 50 keV at fluences of $\Phi = 2, 3, 4, 25$ and $100 \cdot 10^{14}$ at/cm². The samples were studied using RBS-C with 900 keV α particles to evaluate the amount of disorder and to analyze the damage profile. The irradiation and RBS-C were carried out at the Göttingen ion implanter IONAS [6].

Electron Yield-spectra were taken collecting the drain current of the target for incident beam energies from 1800 eV to 2400 eV in 1 eV steps on beam-line SA 32 of the 800 MeV positron storage ring SuperACO at LURE using a two-crystal type InSb(111)-monochromator (0.7 eV resolution). The photons delivered by a bending magnet were focalized using an upstream toroidal mirror of fused silica coated with 150 nm TiN. All samples were analyzed using standard procedure (linear pre-edge subtraction, third order polynomial atomic absorption, Lengeler-Eisenberger normalization algorithm) and programs [7]. Energy calibration was done using the absorption edge at 1839.1 eV of a pure Si standard. Data were then Fourier transformed using a Kaiser window function (k^2 weighting, $\tau = 2.5$) extending from $k = 2.48$ to $11.88 \text{ \AA}^{-1}$. The back-transformed contribution of the first (C) neighbors (1.14 - 1.91 Å) and second (Si) neighbors (2.23 - 3.12 Å) in SiC were fitted using single scattering approach using the experimental amplitude and phase shift functions extracted from the non-irradiated substrate.

3 RESULTS AND DISCUSSION

In Fig.1 we show the damage profiles calculated from the RBS-C spectra. The crystalline-to-amorphous transition in the surface region occurs at a critical fluence of $\Phi = 3.5 \cdot 10^{14}$ at/cm², while the width of the damaged region slowly increase for higher fluences. The Fourier transforms of the EXAFS-oscillations in Fig.2 show that the first C neighbor do not change significantly up to $\Phi = 4 \cdot 10^{14}$ at/cm², while the induced disorder is clearly visible in the decreased amplitude of the second Si neighbor. That shows, that the Si-C₄ and C-Si₄ tetrahedrons are still present just after

the crystalline-to-amorphous transition and therefore confirming the interpretation of this state as a random network of those tetrahedrons. For high fluences of $25 \cdot 10^{14}$ at/cm² there is a strong reduction of the amplitude of the first C neighbor, while the second Si neighbors of SiC has nearly disappeared. In addition, a new neighbor bond is detected at a distance corresponding to the Si-Si distance in amorphous Si. The radial distribution remains almost the same for further implantation ($100 \cdot 10^{14}$ at/cm²).

Figure 1: Damage-profiles from RBS-C

Figure 2: Fourier Transform of SiC in comparison to a-Si

The results of the quantitative analysis are given in the following table:

Φ [10^{14} at/cm ²]	first neighbor (C)			second neighbor (Si)			new bond (Si)		
	N	σ [Å]	R [Å]	N	σ [Å]	R [Å]	N	σ [Å]	R [Å]
0	4	1.888	0.02	12	3.083	0.02	-	-	-
2	3.8(3)	1.890(4)	0.049(3)	8.5(3)	3.080(2)	0.049(3)	-	-	-
3	3.6(2)	1.893(2)	0.051(3)	8.4(3)	3.093(2)	0.057(2)	-	-	-
4	3.4(2)	1.896(3)	0.062(5)	7.4(3)	3.099(3)	0.074(4)	-	-	-
25	1.8(4)	1.945(15)	0.108(9)	2.1(3)	3.13(2)	0.09(1)	0.9(2)	2.34(2)	0.09(2)
100	1.5(4)	1.916(15)	0.10(1)	2.0(3)	3.13(2)	0.14(2)	0.8(2)	2.36(2)	0.09(2)

This values underline the given interpretation on the local environment of the Si-atoms: Nearly no change in the number of C-neighbors up to $\Phi = 4 \cdot 10^{14}$ at/cm² accompanied by an increase of static disorder. The first neighbor distance increases slightly as a function of the fluence. This is also observed for the second neighbor (Si), of which the number decreases significantly with increasing fluence. For the high fluence regime, only around 2 next C neighbors are found. 3 next Si neighbors are detected, where two thirds are corresponding to the Si-Si distance of the crystalline SiC and the rest forming direct Si-Si bonds at distances in agreement with amorphous Si. The increase of the distances with increasing damage can be explained by an increase of the number of dangling bonds.

We like to note that the creation of new Si-bonds is also clearly visible in the near edge structure: While the absorption edges of crystalline Si and crystalline SiC are separated by 1.2 eV, the maximum of the derivative of the edge of the irradiated samples is shifting in direction to the value of Si with increasing fluence [8]. The observed values of next neighbors are in very good agreement with the results of MD simulations [5]. The authors calculate around 2.1 C neighbors at 1.89 Å. The simulations predict a first Si neighbor at 2.32 Å, followed by a broad maximum around 3 Å. As the two peaks overlap, the number of next Si neighbors is not well defined, but also around 2.

In conclusion, we showed via EXAFS analysis, that α -SiC amorphized by Na⁺ ion irradiation in the range of $\Phi = 2 - 100 \cdot 10^{14}$ at/cm² shows a local order which is in agreement with the interpretation of a random network for low irradiation fluences. For higher fluences around $10^{15} - 10^{16}$ at/cm², Si-Si bonds are formed, while only 2 next C neighbors are detected and around the same amount of second Si neighbors. The ion-beam amorphized state shows therefore a local Si environment with a chemical order in very good agreement with MD simulations.

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