XAFS study on gallium ions implanted in silicon carbide

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Local structure of gallium ions implanted in silicon carbide has been investigated using extended X-ray absorption fine structure on the Ga K-edge. The crystallinity of the implantation layer is compared in the samples prepared under several different conditions of implantation temperature and post-implantation annealing. It is found that significant damage is induced by the implantation at room temperature, but the crystallinity recovers by the subsequent annealing at high temperature at 1600 °C. On the other hand, the best crystallinity is obtained by the implantation at high temperature of 500 °C, but the annealing results in degrading the crystallinity. This indicates an influence of the post-implantation annealing at high temperature on the crystallinity in atomic level, which relates to the secondary defects in lattice observed by electron microscope.

Keywords: ion implantation, silicon carbide, EXAFS, fluorescence-yield detection.

1. Introduction

Silicon carbide (SiC) is a wide-gap semiconductor to be expected to replace the present silicon devices, particularly in power device applications. In the fabrication of the device structure, ion implantation is crucially important because dopant ions hardly diffuse in this material. Structural issue relevant to the ion implantation is recrystallization of damaged layer by post-implantation annealing. Ion-implantation at high temperature reduces the damage in the substrate, but the annealing at high temperature over 1600 °C is still required for electric activation. The annealing at such high temperature itself is unfavorable for a procedure in device process, and besides, recent studies have revealed additional lattice defects induced by the annealing (Laube *et al*., 1999; Ohno & Kobayashi, 2000).

Boron and aluminum are standard species for the p-type doping, but they yield unexpected deep acceptor levels (Anikin *et al*., 1985; Rybicki, 1995). From this aspect, Ga is a more preferable candidate for the p-type dopant that gives high activation rate. In this study, the local structure is investigated by extended X-ray absorption fine structure (EXAFS) using a fluorescence-yield collection technique. The local structure of the dopant Ga ions is a measure of crystallinity of the implanted layers of SiC substrate, and clearly shows the effect of implantation temperature and the post-implantation annealing.

2. Experimental

Ga-implanted layers were prepared on the commercial 4H-SiC wafers of Cree Research Inc. Multiple-energy implantation technique was utilized to fabricate a box-shaped Ga profile layer with thickness of 2000 Å and total dose of 3×10^{15} cm^{-2}. Samples were prepared under several different conditions; temperature of substrate during implantation (room temperature or high temperature at 500 °C) and with or without post-implantation annealing at 1600°C for 10 min.

EXAFS measurements were performed at beamline BL12C of the Photon Factory (KEK, Tsukuba). Samples were set in a geometry with incident angle of 2° from the surface in a close-cycled He cryostat. Fluorescence yield was collected at temperature of 80 K using the 19-element solid-state detector (Nomura, 1998).

3. Results

Figure 1 shows k-weighted normalized EXAFS, $k\chi(k)$, extracted from the fluorescence spectra and the Fourier transform, $F(r)$, for the case of implantation at room temperature. As-implanted sample shows amorphous-like feature, lacking the fine structure due to the second and further shells. The long-range order is recovered by post-implantation annealing. These results are consistent with the general view on the ion implantation; the implanted Ga ions reside at interstitial positions in the lattice and induce damages in the substrate. The post-implantation annealing stimulates the dopant atoms to occupy the appropriate positions in the lattice.

The implantation at high temperature shows a quite different feature on the local structure. As shown in Fig. 2, as-implanted sample exhibits large amplitude in $k\chi(k)$, but the subsequent annealing reduces the amplitude. This clearly indicates that the implantation at high temperature is effective to reduce the damage at implantation. If the crystallinity is evaluated with the amplitude of $k\chi(k)$, the post-implantation annealing does not improve but even

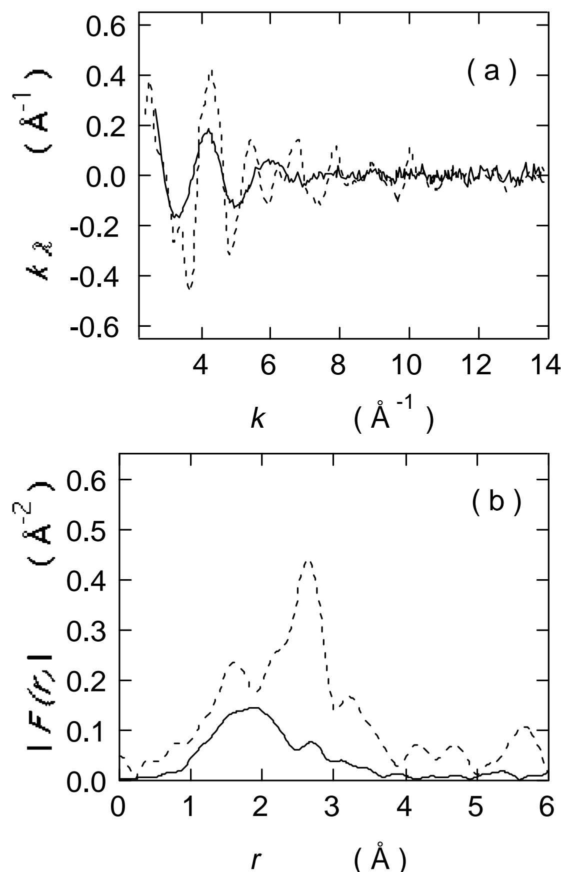

Figure 1
(a) Normalized EXAFS weighted with k, $k\chi(k)$, extracted from the fluorescence spectra and (b) the Fourier transform for the samples implanted at room temperature. Solid lines and dashed lines designate as-implantation and post-implantation annealed samples, respectively.

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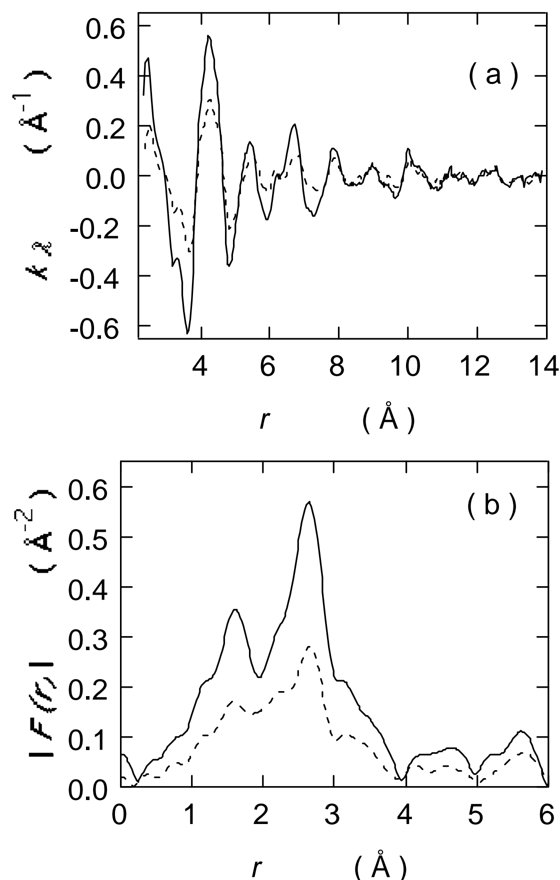

Figure 2
(a) Normalized EXAFS weighted with k, $k\chi(k)$, extracted from the fluorescence spectra and (b) the Fourier transform for the samples implanted at 500 °C. Solid lines and dashed lines designate as-implantation and post-implantation annealed samples, respectively.

degrade the crystallinity, contrary to the case of room-temperature implantation.

We determine the structural parameters for Ga ions on the assumption that Ga ions reside at the Si-sites of 4H-SiC as generally expected. There exist two types of Si-sites, quasi-cubic and hexagonal sites, and the dopant impurities can occupy both of these sites. Since the hexagonal anisotropy is small for the first 2shells, however, each position has substantially the same coordination numbers and interatomic distances; the first shell consists of four C atoms and the second shell twelve Si atoms.

The filtered $k\chi(k)$'s in the range of 0.8-3.0 Å are fitted to this model at the fixed coordination numbers. In the case of as-implantation at room temperature, significantly large disorder is involved. In this study, however, anharmonic terms are not taken into account because here we do not discuss the disordered structure but give the values only for comparison. The determined structural parameters are listed in Table 1.

The Ga-C distance of 2.0 Å is larger than that of Si-C in the host substrate by 0.1 Å, which is consistent with the difference of ionic radius in tetrahedral coordination. The mean-square relative displacements σ^2 are settled in reasonable range, by which the difference in amplitude of $k\chi(k)$ is attributable to disorder in the vicinity of Ga ions.

Table 1
Determined interatomic distances and mean-square relative displacements for the samples prepared at substrate temperature T_i and with ((b) and (d)) and without ((a) and (c)) post-implantation annealing at T_a for 10 min ((b) and (d)). The coordination numbers are fixed at 4 and 12 for the Ga-C and Ga-Si bonds, respectively.

	T_i (°C)	T_a (°C)	Ga-C r (Å)	Ga-C σ^2 (10^{-4} Å^2)	r (Å)	σ^2 (10^{-4} Å^2)
(a)	RT	——	2.11	85.7	3.03	408.
(b)	RT	1600	2.01	67.1	3.09	83.4
(c)	500	——	2.00	1.07	3.09	50.5
(d)	500	1600	2.01	122.	3.09	168.

4. Discussion

The EXAFS measurement clearly reveals the crystallinity around Ga ions depending on the implantation condition. The damage in the as-implanted layer and the effect of the post-implantation are demonstrated, which is as anticipated in the case of room-temperature implantation.

The implantation at 500 °C was shown to be effective on reducing damage significantly compared with the implantation at room temperature. The local structure of Ga ions was well explained by a model that Ga ions occupy the tetrahedral sites replacing Si atoms. The model is considered to be valid because recent Rutherford backscattering spectroscopy in the channeling mode showed that Ga ions reside at on-center positions of the lattice in the sample as-implanted at high temperature (Tanaka *et al.*, 1998).

The subsequent annealing, however, degrades the crystallinity, which was observed clearly in damping of $k\chi(k)$ and is attributed to increase in σ^2 in our model. The degradation induced by post-implantation annealing have been recognized as the secondary defects in the substrate form macroscopic point of view.

In the B-doping case, B atoms diffuse outside the implanted region by post-implantation annealing. The diffusion was explained by the kick-out mechanism (Laube *et al.*, 1999), that is, migration of B atoms is enhanced through kick-out of B atoms by interstitial Si atoms. In Al-implantation, no distinct out-diffusion takes place, but defects emerged after annealing in the images of cross-sectional transmission electron microscope. The lattice image clearly showed that extrinsic dislocation loops are induced by additional Si-C bilayer insertion. (Ohno & Kobayashi, 2000).

As shown in these studies, the secondary defects are more enhanced for lighter dopant species, but similar defects are likely to occur in the Ga-doped layer by annealing. We therefore consider that the increase of the mean-square relative distance by the post-implantation annealing is a manifestation of the secondary defects in atomic scale.

The best crystallinity is realized in the sample as-implanted at high temperature. For electric activation, however, post-implantation annealing is indispensable in this material. If Ga ions substitute for Si correctly by the implantation at high temperature, holes should be activated without annealing. Moreover, this fact means that the holes are activated in less qualified lattice layer after annealing. Reduction of lattice damage and enhancement of electrical activation were reported in the implantation of Al^+ at high-temperature at 1100-1700 °C. In this case, interstitial dislocation loop and Al precipitates were observed by high-resolution electron microscopy (Suvorova *et al.*, 1998). The mechanism and technique to improve crystallinity of the implanted layer and activate carriers effectively is a subject for future studies.

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