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Polarization-dependent NEXAFS spectra for Si^+-implanted graphite

Yuji BABA, Tetsuhiro SEKIGUCHI, Iwao SHIMOYAMA
Japan Atomic Energy Research Institute, Tokai-mura, Naka-gun, Ibaraki-ken 319-1195, Japan

Introduction

There exist many stable phases of silicon carbide, such as cubic SiC and hexagonal SiC. All of the stable SiC phases are composed of only sp^3 bonds, and form three-dimensionally expanded lattices. The recent theoretical study using an ab initio tight-binding-like method showed a possibility that graphite-like two-dimensional SiC phase exists [1]. In order to check the possibility of the existence of such graphite-like SiC, we synthesized Si_xC layer where x is nearly 0.01 by the Si^+-ion implantation in highly oriented pyrolitic graphite (HOPG). The local electronic and geometric structures around the Si atoms were investigated by near-edge x-ray absorption fine structure (NEXAFS) spectroscopy at the Si K-edge using linearly polarized synchrotron beam.

Experimental

The experiments were performed at the BL-27A station. An HOPG single crystal of 12 mm ×12 mm was used as a substrate. Tetrafluorosilane (SiF_4) gas was used as ion source. A cold cathode ion gun with Wien-filter type mass separator using orthogonal electric and magnetic fields was used for the atomic Si^+-ion bombardment. The accelerating voltage was 1 keV, and the ion flux was 1×10^{11} atoms/cm^2 · sec. The NEXAFS spectra were taken by the total electron yields, which were monitored by sample drain current.

Results and discussion

Figure 1 shows the polarization dependence of the Si K-edge NEXAFS spectra for the Si^+-ion implanted HOPG. The surface [Si]/[C] ratio of this sample is about 0.01. For comparison, NEXAFS spectra for single crystals of β-SiC and Si(100) are also shown in the upper parts of the figure. For the spectra at low incidence angles, clear peaks are observed at 1839.5 eV (marked A). The concentration of Si in graphite is fairy low, thus the effect of the Si-Si bond formation on the NEXAFS spectra can be ignored. Therefore the peak A represents the local electronic structures of silicon atoms bonded by only carbon atoms. The energy of this peak is lower than the main resonance peaks for Si(100) and β-SiC. From analogy with the low-energy feature of the C $1s\rightarrow\pi^*$ resonance in graphite compared with that of the C $1s\rightarrow\sigma^*$ resonance in diamond [2], the peak A is possibly attributed to the Si $1\rightarrow\pi^*$ resonance in graphite-like Si_xC layer if this structure exists.

A remarkable feature observed in the peak A is the polarization dependence of its intensity. The intensity of the peak A increases with the decrease in the incident angles of the synchrotron beam. The peak intensity I of the NEXAFS spectra using the synchrotron beam of electric field **E** is expressed as follows,

$$I \propto |\mathbf{E}\cdot\mathbf{O}|^2 \propto \cos^2\delta \qquad (1)$$

where **O** is the direction of final state orbital and δ is angle between **E** and **O**. Considering the polarization dependence in fig.1, we can suppose that the final state orbital represented by the peak A is perpendicular to the graphite plane, i.e., parallel to the c-axis of graphite. If this final state orbital has π^* character as described above, it is presumed that the Si-C bond is parallel to the graphite plane.

References

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[2] R.A. Rosenberg et al., Phys. Rev. B **33**, 4034 (1986).

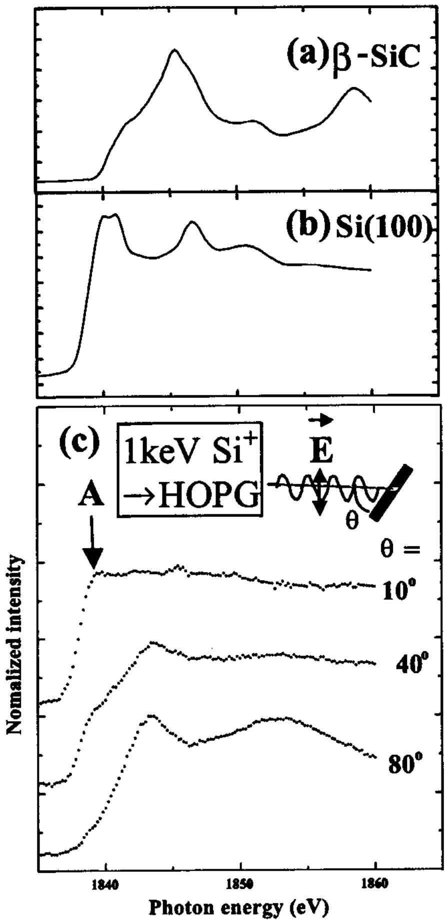

Fig.1 Si K-edge NEXAFS spectra for (a) β-SiC (b) Si(100) and (c) Si^+-ion implanted HOPG. θ is the incident angle defined by the angle between sample surface and synchrotron beam.

*** ybaba@popsvr.tokai.jaeri.go.jp**