

Chemical State Analysis of Thermally Oxidized SiC

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SiC is attracting attention as a next-generation semiconductor material because it has a larger bandgap and carrier mobility than Si, which is currently mainly used as a semiconductor, and is resistant to heat and can reduce power loss. However, when an oxide film is formed during semiconductor production, defects and irregularities appear, which scatter electrons, making it difficult to use as a suitable device [1]. The details of the elemental composition, chemical bonding state, and structure of the interface between SiC and SiO₂ generated by oxidation are not known, and the research continues [2]. In this study, X-ray Absorption Fine Structure (XAFS) was measured on a thermally oxidized SiC in air and a sample of powdered SiO₂ and SiC mixed in mol ratio. Furthermore, based on this result, the chemical state of the heated sample surface was quantitatively analyzed using the Linear Combination Fitting (LCF).

The experiments were performed at BL-13 of SR Center, Ritsumeikan University. The Si *K*-edge XAFS spectra were obtained in the total electron yield (TEY) mode. Incident energies were changed by InSb(111) double crystal monochromator. The SiC powder (Particle size: 32~75 μm) was heated in air at 300, 700 and 900 $^{\circ}\text{C}$ for 15 and 30 minute.

Figure 1 shows the results near the absorption edge for the SiC powder used for heating and the SiO₂ standard samples. As shown in Fig. 1, the SiC peak position of 1845.5 eV and the SiO₂ peak position of 1846.7 eV are clearly different. Figure 2 shows the TEY spectra near the peak position for thermally oxidized SiC. Figure 2 shows that the surface is oxidized to generate SiO₂, which changes the chemical state and shifts the peak position. At 300 $^{\circ}\text{C}$, no change was observed in the peak position or shape of the spectrum. However, heated at 700 $^{\circ}\text{C}$, the intensities of SiC and SiO₂ at 1845.5 and 1846.7 eV, respectively, were similar and the peak positions shifted. Furthermore, heated at 900 $^{\circ}\text{C}$, the peak position was completely shifted to 1846.7 eV. Assuming that the spectrum of this thermally oxidized sample can be composed as two spectra in Fig. 1, the LCF method was used to obtain the spectral intensity ratio of SiC and SiO₂ in the thermally oxidized sample. Indeed, the spectrum of the thermally oxidized sample could be reproduced by LCF one.

Figure 3 shows the TEY spectra near the peak position for SiC and SiO₂ powders mixed in some mol ratios. The mixed powder spectra for SiC : SiO₂

= 1:1, 2:1, 3:1 are very similar to that of SiC. However, as the mol ratio of SiO₂ increased to 1:2 and 1:3, it was confirmed that SiO₂ component became dominant. Similarly, the each spectrum of the mixed powder was represented by the LCF one, and the intensity ratio was obtained. From the obtained relationship, the composition ratio of the surface of the thermally oxidized SiC sample can be estimated.

It was found that SiO₂ was generated on the surface of the SiC powder by heating. In addition, quantitative analysis of the composition ratio can be performed assuming that the XAFS spectra can be expressed as a linear combination of the standard sample, and the relationship between the composition ratio and the absorption intensity ratio can be estimated.

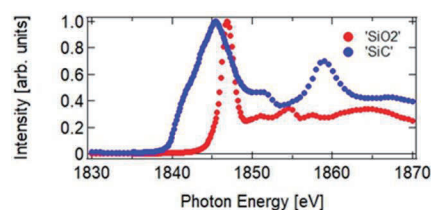


Fig. 1 Si *K*-edge XAFS spectra of SiC and SiO₂ standard samples.

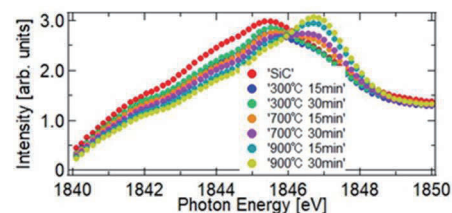


Fig. 2 Si *K*-edge XAFS spectra of thermally oxidized SiC.

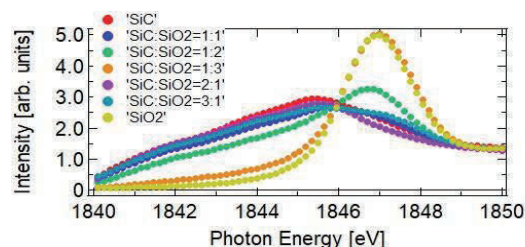


Fig. 3 Si *K*-edge XAFS spectra of mixed SiC and SiO₂ samples.

References

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- [2] A. Suzuki *et al.*, J. Electrochem. Soc., **1978**, 125, 1896.