Chemical State Analysis of Oxidized 4H-SiC (0001) Surface

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SiC is attracting attention as a next-generation power semiconductor material. However, during the manufacturing process, defects arise at the SiO_2/SiC interface due to the formation of an oxide film, leading to a decline in device performance. In this study, we conducted research to analyze the chemical state of the interface and the local atomic structure. These states were investigated at the SR center BL-13. 4H-SiC (0001) was heated to 1100 °C in air to facilitate oxide film formation. Si *K*-edge measurements were performed on this sample using total-electron-yield mode.

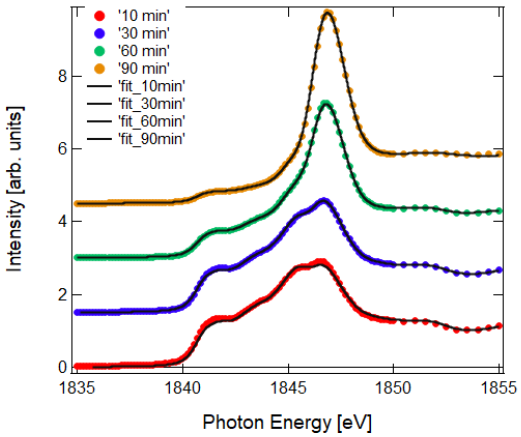

Fig. 1 XANES spectra for SiC heated in air with fitting (black).

Figure 1 shows the XANES spectra of Si *K*-edge for SiC heated in air, with the peak shifting from 1845.5 eV to 1846.8 eV, confirming the successful formation of the oxide film. Although not explicitly presented in this context, we conducted fitting using the linear combination fitting method for two experimental components related to SiC and SiO_2. Subsequently, a residual spectrum remained. We attributed this residual spectrum, observed after heating for 2 hours, to a third component. To refine our analysis, we performed a new fitting that incorporated these components, as depicted in Fig. 1. Remarkably, the fitting results aligned closely with the experimental data, suggesting the emergence of a distinct component concurrent with SiO_2 growth. Furthermore, the spectral ratio consistently indicated that SiO_2 and the third component exhibited a 1:1 growth ratio. Consequently, the existence of intermediate oxides, which may form exclusively during initial oxidation, could not be conclusively confirmed based on prior studies [1].

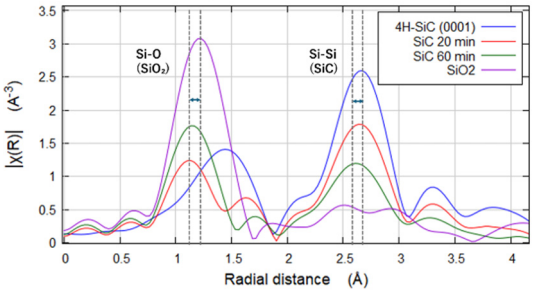

Fig. 2 EXAFS results in Si *K*-edge for heated SiC (20 min and 60 min) and standard samples.

Figure 2 shows the EXAFS results in Si *K*-edge for heated SiC. In comparison to the standard sample, a discernible alteration in local bond length occurred in the heated sample. Prior investigations have suggested that upon heating, the lattice constant of SiC tends to increase [2]. However, from Fig. 2, it becomes evident that heating induces changes in bond lengths. Specifically, Si-O (SiO_2) and Si-Si (SiC) bonds exhibit reductions of approximately 0.1 to 0.2 Å. Notably, although not explicitly depicted here, the bond lengths were consistent between the sample heated for 2 hours and the standard sample. This consistency implies that the observed change in bond length likely arises from initial oxidation or interface-related issues. Furthermore, XANES fitting revealed no compositional alterations during the oxidation stage, and the bond lengths remained unchanged during CVD for oxide film formation [3]. Consequently, we infer that this bond length modification is induced by the heating process.

References

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