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XPS and NEXAFS observations on low-dimensional silicon-carbon mixed compounds

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Introduction

Carbon materials have lots of stable low-dimensional structures such as fullerene and nanotube. Compared with second-row elements, low-coordinated silicon compounds, graphitic or cage-like structure, are predicted to be unstable. As to the mixed silicon-carbon systems, recent theoretical work has shown that the stoichiometric SiC nanotubes are stable, and one of the structures has smaller band gap than that of bulk SiC [1]. However, no unambiguous experimental data are available as to the structures of low-dimensional silicon-carbon mixed compounds. In this work, we present the results for core-level spectroscopic observations on SiC thin films as well as SiC corpuscles, one-dimensional silicon polymer (polydimethylsilane), and adsorbed alkylsilane derivatives; tetramethylsilane (TMS) and hexamethyldisilane (HMDS) in order to elucidate the structures in low-dimensional silicon-carbon mixed systems.

Experimental

Experiments were performed at the BL-27A station. SiC_x thin films (x~3) were synthesized by ultra-low-energy ion beam deposition on graphite and sapphire at 800°C using tetramethylsilane as source gas. Silicon polymer and corpuscles were attached on indium plate. Alkylsilane molecules were adsorbed on Cu substrate at 80 K. Thickness of the layer was 300 monolayer. The electronic structures were analyzed in-situ by X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS).

Results and discussion

Fig.1 shows the Si 1s-XPS spectra excited by 2200 eV photons. The Si 1s binding energy shifts to higher-energy side with the decrease in the molecular size, i.e., E_B(bulk-SiC)<E_B(polymer)<E_B(TMS). For SiC_x thin films of 0.06 nm thickness, two peaks are clearly observed. The lower-energy peak (marked A) corresponds to the bulk SiC. The peak position of higher energy one (marked B) is close to those of alkylsilane molecules, which suggests that a part of SiC_x film has low-dimensional structure.

Fig.2 displays the Si *K*-edge NEXAFS spectra. A sharp peak is observed at 1840 eV (marked A) for SiC_x film. Such low-energy peak is never observed for bulk SiC or low-dimensional Si compounds ((a)-(e)). For second-row elements like carbon, it was established that the energy of the resonance excitation from 1s to unoccupied π^* orbitals is lower by several eV than that from the 1s to unoccupied σ^* orbitals. We consider that the peak A is due to resonance from Si 1s to π^*-like orbitals deduced from carbon case. This implies that the SiC_x thin film has two-dimensional structure whose configuration is similar to that of graphite.

References

[1] M. Menon et al., Phys. Rev. B **69**, 115322 (2004).

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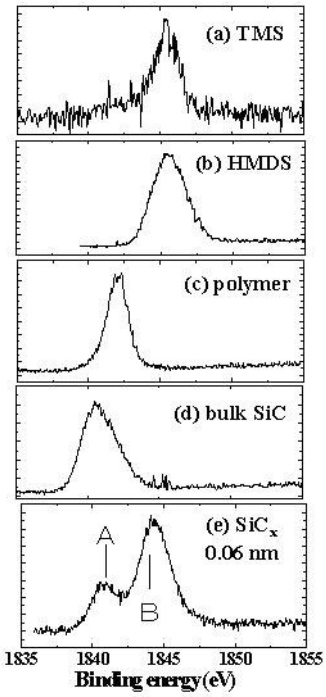

Fig. 1 Si 1s XPS spectra excited by 2200 eV photons for silicon-carbon compounds.

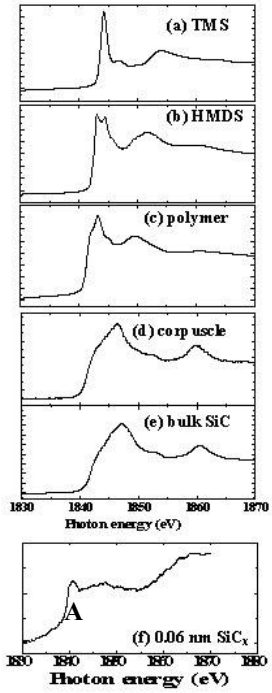

Fig.2 Si K-edge NEXAFS spectra for silicon-carbon compounds.