Self-ordering of silicon polymer studied by polarization-dependent NEXAFS

Md. Abdul Mannan1,2, 馬場祐治1, 関口哲弘1, 下山巖1, 平尾法恵1, 成田あゆみ1, 永野正光2, 野口英行2
1 日本原子力研究開発機構, 2 佐賀大学

Silicon polymers have high electric conductivity along the one-dimensional chain due to the smaller HOMO-LUMO band gap. Molecular orientation is quite important because the electrical and optical properties strongly depend on the backbone configuration of the polymers. In this study, the electronic structure and molecular orientation of polydimethylsilane (PDMS) film evaporated on highly oriented pyrolitic graphite (HOPG) and indium tin oxide (ITO) surfaces have been assigned. The film has been synthesized by high vacuum electron bombardment evaporation technique. The orientations and electronic structures of the films as well as those of the annealed samples were studied by Si K-edge near-edge x-ray absorption fine structure (NEXAFS) and x-ray photoelectron spectroscopy (XPS) using linearly polarized synchrotron radiation. The Si K-edge NEXAFS spectra for the thick film on ITO have at least four resonance peaks of which two peaks are found to be strongly polarization dependent (Fig. 1. peaks A and B). The lower-energy resonance peak (peak A) at 1842.0 eV has short-axis polarization corresponding to the resonance excitation from Si 1s to \( \sigma^* \) (\( p_{yz} \)), and the higher-energy resonance peak (peak B) at 1843.2 eV has long-axis polarization due to the excitation of Si 1s to \( \sigma^* \) (\( p_x \)) [1]. On the basis of the polarization dependences, it is revealed that the PDMS molecules are self-ordered and the backbones of the polymers are perpendicularly oriented to the surface. The polarization dependency disappeared for the annealed sample at about 80°C which suggests that the PDMS was almost parallel and/or randomly oriented to the surface after annealing.