

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

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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 pyrolytic 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 σ^* (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 σ^* (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.

[1] V.R. McCrary et al. J. Chem. Phys. **88**, 5925 (1988).

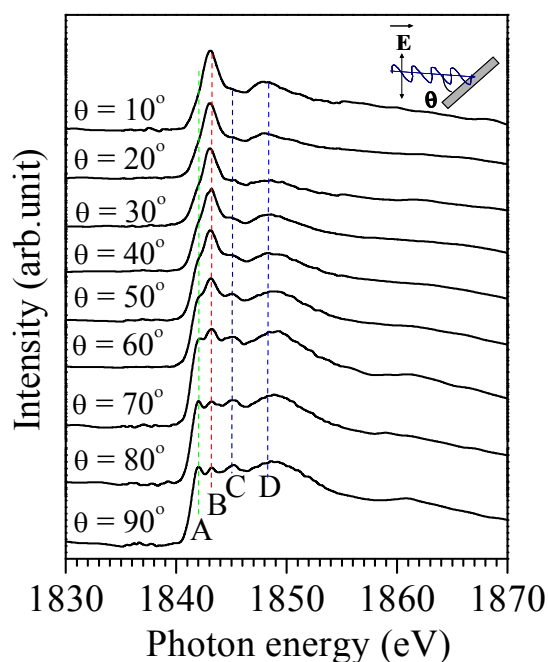


Fig.1 Si *K*-edge NEXAFS spectra for thick film on ITO surface at different incident angles of the X-ray