

Configuration of self-assembled silicon polymer films studied by polarization-dependent NEXAFS

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Introduction

Thin films of organic silicon polymer have excellent optical and electric properties such as high electric conductivity and high heat resistance. Silicon polymers are also considered as ideal one-dimensional molecular wires due to their small σ - σ^* gap compared with carbon-based polymers. Since the electric and optical properties in thin films of polymers strongly depend on the molecular configuration of one-dimensional chain, it is important to precisely determine the orientation of the polymers on solid surfaces. In the previous report, we have shown that the polydimethylsilane (PDMS) grown on indium tin oxide (ITO) are self-ordered and stand-up on the surface [1]. In this report, we present the precise configuration of PDMS molecules on the ITO on the basis of the polarization-dependent NEXAFS spectra.

Experimental

All the experiments were performed *in situ* at the BL-27A station. The evaporation was performed by electron-bombardment heating. The evaporation rate was precisely controlled by monitoring the positive current of the shutter. The electronic structures and molecular orientations were investigated by XPS and NEXAFS measurements. The NEXAFS spectra were taken with the total electron yield mode.

Results and discussion

Fig.1(a) shows the Si *K*-edge NEXAFS spectra taken at different incident angles. The NEXAFS spectra show at least four resonance peaks of which two peaks are found to be strongly polarization dependent. The peak A is due to the resonance excitation from Si 1s to σ^* p_{yz} orbitals localized at the Si-C bond, and the peak B corresponds to the resonance from Si 1s to σ^* p_x orbitals localized at the Si-Si bond [2]. Fig.1(b) displays the normalized intensity of the peak A as a function of the incident angle θ [3]. It was shown that the experimental data follow the line $\gamma=40^\circ$ where γ is the polar angle of the plane-type σ^*_{Si-C} orbitals (peak A)

Fig.2 shows the images of the standing-up orientation of PDMS molecules. The left image shows *all-trans* zig-zag while right one shows *all-trans* helical conformation. In the case of zig-zag conformation, the Si-C bonds are parallel to the surface, so the polar angle of the plane type σ^*_{Si-C} orbitals should be 0° . In the case of helical conformation, on the other hand, the Si-C bonds are not

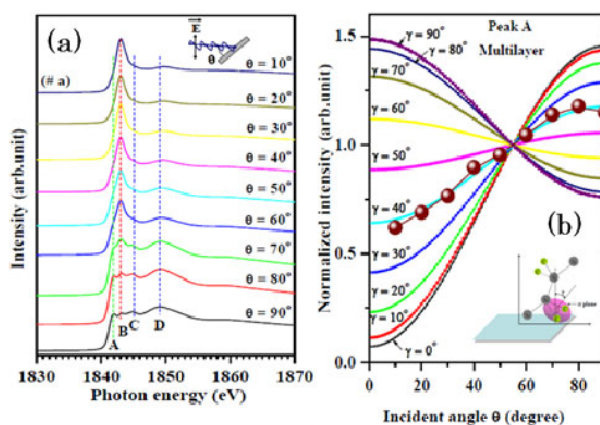


Fig.1 (a) Si *K*-edge NEXAFS spectra taken at different incident angles for multilayered PDMS film on ITO. (b) Normalized intensity I of the peak A in the NEXAFS spectra as a function of the incident angle θ . The filled circles are the experimental values.

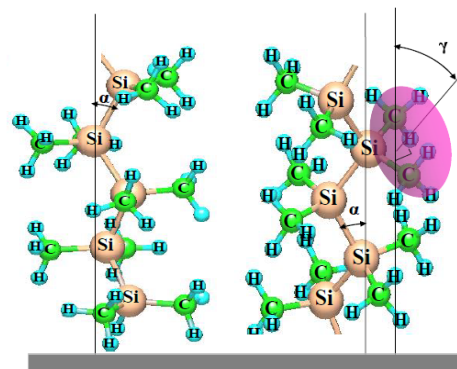


Fig.2 Images of two types of conformation for a PDMS molecule standing-up on the surface.

parallel and the polar angles of Si-C orbitals were calculated to be 41.5° and 48.5° , respectively. Thus it was elucidated that the multilayer film is composed of helix structure and perpendicularly oriented on the ITO surface.

References

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