

## Orientation of polydimethylsilane films studied by Si K-edge NEXAFS

Yuji BABA\*, Tetsuhiro SEKIGUCHI, Iwao SHIMOYAMA, Mitsunori HONDA,  
Norie HIRAO and Ayumi NARITA

Japan Atomic Energy Agency, Tokai-mura, Naka-gun, Ibaraki-ken 319-1195, Japan

### Introduction

Thin films of organic silicon polymers have attracted much attention due to their potential applications as electric and optical devices. Compared with carbon-based polymers, silicon polymers generally have high electric conductivity along the one-dimensional chain due to the smaller HOMO-LUMO gap. Owing to this property, polysilane and its derivatives are expected to be used for various applications such as a photoconductor and a one-dimensional electric conductor. Since the electric properties of one-dimensional polymers are strongly dependent on the backbone conformation, it is quite important to elucidate the ordering as well as electronic structures of polymers. Here we present the electronic structures and molecular orientations for polydimethylsilane, one of the most simple polysilane derivatives, deposited on an ITO (indium tin oxide) surface.

### Experimental

The experiments were performed at the BL-27A station. Polydimethylsilane molecules (M.W.~2000) were deposited on a clean surface of ITO using Knudsen-cell evaporator. The thickness of the deposited film was estimated by the peak intensities in X-ray photoelectron (XP) spectra. The near-edge X-ray absorption fine structure (NEXAFS) spectra were recorded by total electron yield mode. For the measurements of the polarization dependences, the sample was rotated around the vertical axis.

### Results and discussion

Fig.1 shows the wide scan XP spectra for thin and thick films of polydimethylsilane. The thickness of the thin sample was calculated to be about 5 layers. In a small inset, the Si 1s narrow scan for thick film is displayed. A single Si 1s peak is seen and its binding energy is almost the same as previously reported one for powdered sample [1]. This confirms that polydimethylsilane molecules were evaporated as a polymer form and deposited on the ITO surface without decomposition.

Fig.2 shows the Si K-edge NEXAFS spectra for thick sample at various incident angles. The spectral features are almost the same as those previously reported [2]. McCrary et al. have reported the peak assignments of similar polymer and showed that the lower-energy resonance (peak A) has short-axis polarization corresponding to the resonance excitation from the Si 1s to  $\sigma^*$ (pyz), and the higher-energy resonance (peak C) has

long-axis polarization due to the excitation to  $\sigma^*$ (px) [3]. The intensity of the peak A is enhanced at the grazing incidence, while the peak B is enhanced at the normal incidence. On the basis of the polarization dependences, it was revealed that the backbones of polydimethylsilane molecules are well ordered and they are nearly parallel to the surface even in multi-layered film.

### References

- [1] K.G. Nath, I. Shimoyama, T. Sekiguchi and Y. Baba, *J. Electron Spectrosc. Relat. Phenom.* **144-147**, 323 (2005).
- [2] K. Seki et al, *J. Electron Spectrosc. Relat. Phenom.* **78**, 403 (1996).
- [3] V.R. McCrary et al., *J. Chem. Phys.* **88**, 5925 (1988).

\*baba.yuji@jaea.go.jp

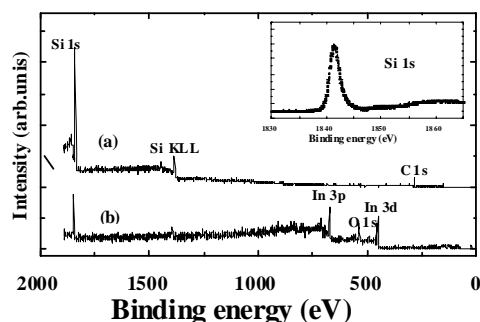


Fig.1 XPS spectra for (a) thick film and (b) thin film of polydimethylsilane deposited on ITO. Si 1s narrow scan for thick film is shown in the inset.

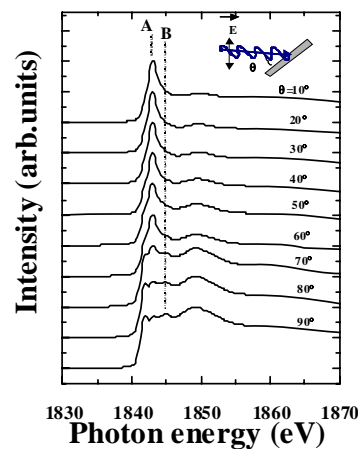


Fig.2 Polarization-dependent NEXAFS spectra for thick film of polydimethylsilane deposited on ITO. The incident angle of X-rays is shown in each spectrum.