

## The Local Structural Analysis of Sb Catalyst in PET polymers

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Polyethylene terephthalate (PET) is one of the most common polymers, and antimony compounds are used as the polymerization catalyst. In this study, the Sb local environments in PET were investigated using the technique of XAFS.

### 1. Experimental

PET resins ( $-(\text{COOC}_6\text{H}_4\text{COO}(\text{CH}_2)_2)_-$ ; about 300 ppm Sb) were melted on a flat sheet, and stacked up to 8cm thick column.  $\text{Sb}^0$ ,  $\text{Sb}_2\text{O}_3$ , Sb triacetate and Sb glycoxide, used as standards, were mixed with BN diluent respectively, pressed into 1mm thick pellets.

Measurements of the Sb K-edge were made in transmission mode, using the Si(111) double-crystal monochromator and Rh coated mirrors. X-rays were detected with ionization chambers filled with Kr gas.

### 2. Results

X-ray absorption of 0.08 was observed at Sb K-edge for a representative PET (Fig.1). Figure 2 shows the magnitude of the Fourier transforms of the  $k^3 \chi(k)$  spectra. This comparison gives rough estimation as follows. The peak found at  $2.64 \text{ \AA}$  for  $\text{Sb}^0$  (a) is due to Sb-Sb. Sb-O distance is assigned to the peak of  $1.61 \text{ \AA}$  for  $\text{Sb}_2\text{O}_3$ (b). Considering the  $k$ -space range dependence(b, c), the broad peak at  $3.30 \text{ \AA}$ , which decreased remarkably in the lower  $k$ -space range, is attributed to Sb-O-Sb(2nd). This peak can be seen at  $3.31 \text{ \AA}$  for Sb glycoxide(d), however, Sb-triacetate(e) and regular PET(f) show no peak except Sb-O.

### 3. Conclusions

Owing to the high energy of 8GeV, spectra of the Sb K-edge were obtained in transmission mode even at low concentration. Sb remained in the PET has a structure different from that of  $\text{Sb}^0$ ,  $\text{Sb}_2\text{O}_3$ , and Sb glycoxide. The detailed analyses, such as phase shift corrections, Fourier filtering and curve fitting are under way.

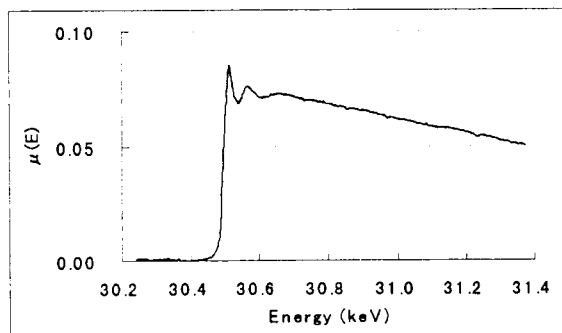


Fig.1 Measured Sb K-edge spectrum for the PET. (Background subtracted)

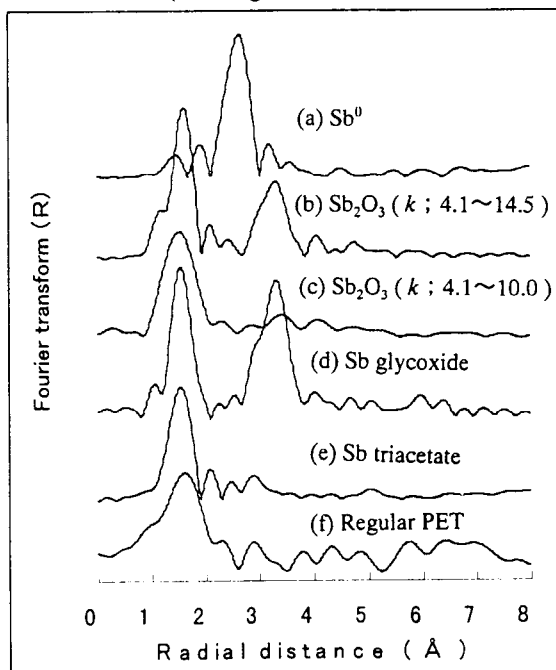


Fig.2 Magnitude of the Fourier transforms.