Site-selective EXAFS for Cu/ZnO Catalyst utilizing a Fluorescence Spectrometer

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Site-selective XANES utilizing a fluorescence spectrometer was reported [1 – 3]. We tried site-selective EXAFS for Cu/ZnO catalyst.

The energy resolution of fluorescence spectrometer for the emitted X-rays from sample was 1.1 eV including the contribution of beamline [4]. The Cu Kα_1 emission was analyzed by Johansson-type cylindrically-bent Ge(444) crystal. The configuration of Rowland-type spectrometer was described in ref. 5. The dwell time of one point for EXAFS measurements was 100 s.

Figure 1a illustrates the Cu K-edge EXAFS for activated Cu/ZnO catalyst (Cu 5wt%) [6] when the fluorescence spectrometer was tuned to 8045.2 eV (Cu^0 site tune). The *S/N* ratio was seriously worse over 8Å^{-1}, and curve fit was performed in *k*-space. The fit with two factors, Cu metal and Cu_2O EXAFS, was best in the case of Cu metal = 100% (Figure 1a).

The Cu^I-site tune EXAFS is shown in Figure 1b. The fluorescence spectrometer was tuned to 8049.4 eV. The *k*-space fit in the region 3.5 – 8Å^{-1} was evalulated as *R* factor (Figure 1b). The best fit was when Cu_2O : Cu metal ratio was 8 : 2.

These results support structural information obtained by site-selective XANES [6]. To improve the data quality, dwell time should be longer (Ring power down due to thunder reduced this beamtime). Measurements at Undulator beamline of SPring-8 and the increase of solid angle of bent crystal(s) to accept the fluorescence X-rays improve photon counts.

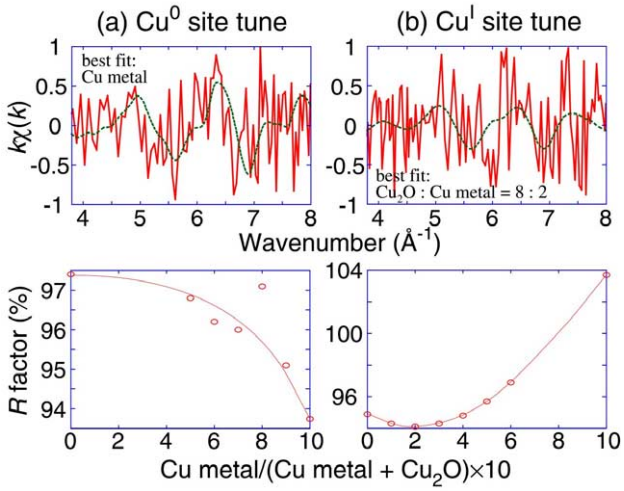

Figure 1. Site-selective EXAFS spectra for activated Cu/ZnO catalyst. Fluorescence spectrometer was tuned to 8045.2 (a) and 8049.4 eV (b). (Top) χ function weighted by k^1 (solid line) and the fit (dotted line). (Bottom) Dependence of R_f on Cu^0 : Cu^I ratio.

References

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