

## Local structure analysis of the active site of Co-Mo sulfide catalysts using selenophene as a probe molecule by means of XAFS

Takeshi KUBOTA\*<sup>1</sup>, Masataka ITO<sup>1</sup>, Takeshi KADONO<sup>1</sup>, Yasuaki OKAMOTO<sup>1</sup>

<sup>1</sup>Department of Material Science, Shimane-Univ.,  
Matsue, Nishikawatsu, Shimane 690-8504, Japan

### Introduction

Development of ultra-deep hydrodesulfurization (HDS) catalysts is one of the most urgent issues in petroleum industry for environmental protection. We need to get information on the active site structure of HDS catalysts and microscopic reaction mechanism on them for more efficient developments of the catalysts. In this study, we investigated Co-Mo(W) catalysts prepared by a CVD method, which synthesize selectively the Co-Mo-S phase, after hydrodeselenium (HD-Se) reaction [1].

### Manuscript preparation

Supported Co/MoS<sub>2</sub> catalysts were prepared by a CVD method using Co(CO)<sub>3</sub>NO[2-3]. The sample was sulfided at 673 K. The HDSe reaction of selenophene was performed using a closed circulation system at 523 K. Co K-edge EXAFS spectra for catalysts after HDSe reaction were measured at BL-9C in a fluorescence mode. The synchrotron radiation was monochromatized by a Si(111) monochromator.

### Results and Discussion

Changes of the local structure of Se and Co caused by the HDSe reaction were followed by the XAFS measurements. Figure 1 shows Fourier Transform (FT) of Co K-edge EXAFS for CVD-Co/MoS<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> and CVD-Co/MoS<sub>2</sub>/SiO<sub>2</sub> after the HDSe reaction. It is observed from Figure 1 that with the reaction proceeds, Co-S contribution is replaced to Co-Se shell. Figure 2 shows Fourier Transform (FT) of Se K-edge EXAFS for CVD-Co/MoS<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> and CVD-Co/MoS<sub>2</sub>/SiO<sub>2</sub> after the HDSe reaction. It is observed from Figure 2 that local structure around Se atoms is not changed with the reaction proceeds, indicating the sulfur defect sites of the catalysts are preferentially adsorbs organo-selen compounds.

### References

- [1] T. Kubota et al., Chem. Phys. Lett., 370, 813 (2003).
- [2] T. Kubota et al., Applied Catal. A, 290, 17 (2005).
- [3] Y. Okamoto et al., J. Catal., 222, 143 (2004).

\* kubotake@riko.shimane-u.ac.jp

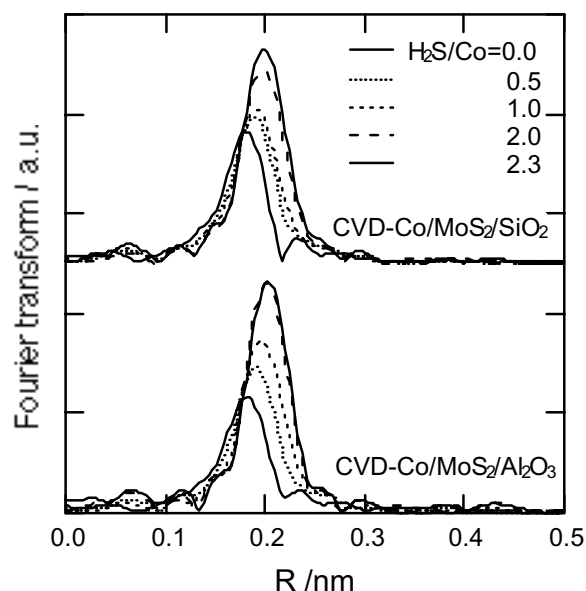


Figure 1 Fourier Transform of Co K-edge EXAFS for CVD-Co/MoS<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> and CVD-Co/MoS<sub>2</sub>/SiO<sub>2</sub> after the HDSe reaction i.

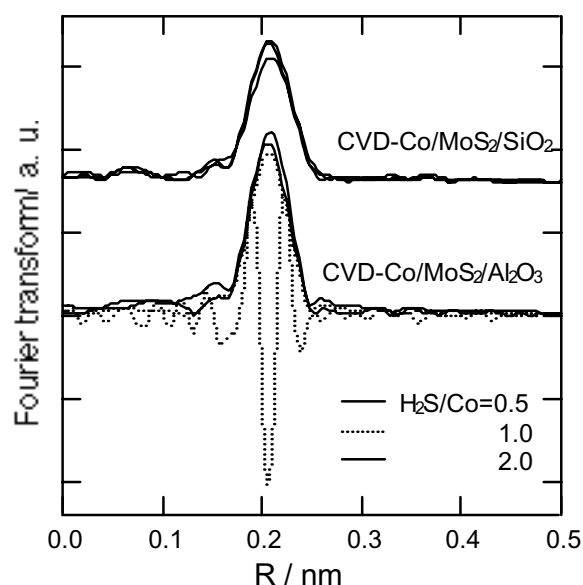


Figure 2 Fourier Transform of Se K-edge EXAFS for CVD-Co/MoS<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> and CVD-Co/MoS<sub>2</sub>/SiO<sub>2</sub> after the HDSe reaction.