

Development and in-situ structure analysis of novel metal phosphide hydrotreating catalysts

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【 Outline of survey 】

The demand to reduce sulfur content in fossil fuels such as gasoline and diesel oil becomes stronger and stronger year by year. The sulfur compounds in fuels are converted to sulfate and cause acid rain. In addition sulfur will damage the denitrogenation catalysts which removes the NO_x produced in the engine. S. Ted Oyama has found that the metal phosphides show high activity for hydrodesulfurization reaction. We initiated the international collaboration to develop the novel metal phosphide catalysts for hydrodesulfurization reactions of fuels. The mission of our Japanese team is to develop a fast-scanned in-situ EXAFS system and to reveal the catalytic reaction mechanisms. EXAFS (Extended X-ray absorption fine structure) is an X-ray absorption spectroscopy which provides us a local structure around an X-ray absorbing atom even in the reaction conditions. We are now designing a new cell to enable high pressure and high temperature EXAFS measurements. These work will reveal the reaction intermediates and reaction mechanisms which will help to produce advanced hydrotreating catalysts. Another mission of the Japanese team is to investigate the surface reaction and its structure of Ni₂P single crystal as a model catalyst. This fundamental research will help us to understand the hydrotreating reaction in more details.

【 Expected results 】

We will reveal reaction mechanisms of the novel metal phosphides hydrotreating catalysts by taking stroboscopic pictures of metal phosphides during the reactions using fast-scanned in-situ EXAFS spectroscopy. Based on the knowledge about the in-situ structures of catalysts, one can design more effective metal phosphide catalysts. In addition, the fast-scanned in-situ EXAFS techniques are not only limited to the hydrotreating catalysts but are available in other catalytic systems. We try to apply the fast-scanned in-situ EXAFS and contribute to the development of catalytic science.

【 References by the principal researcher 】

- (1) Kawai, K. Asakura, and S. T. Oyama et al.: "In situ XAFS studies on the structure of nickel phosphide catalyst supported on K-USY", *Chem. Lett.*, **32**:956-957(2003).
- (2) Asakura, K.: "Recent development in the in-situ XAFS and related work for the characterization of catalysts in Japan.", *Cataly. Surv. Asia*, **7**:177-182(2003).

【 Term of project 】 F Y 2004 - 2008

【 Budget allocation 】 85,800,000 yen

【 Homepage address 】 <http://www.hucc.hokudai.ac.jp/q16691/index.html>