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Atomic-scale and electronic structure of fcc- and hcp-type Ru nanosized catalyst

NIMS/SPring-8 [1], Kyoto Univ. [2]

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Ruthenium (Ru) is a 4*d* transition metal that in the bulk adopts an hcp structure at any temperature, and novel fcc-type Ru nanoparticles (NPs) have been observed to be more efficient than conventional hcp-type Ru NPs larger than 3 nm [1]. It has recently attracted much attention due to high catalytic activity for CO oxidation and preventing CO poisoning in a fuel-cell system. The catalytic properties of Ru NPs are strongly dependent on their atomic-scale and electronic structures.

The 3-dimentational atomic-scale structures were studied using high-energy X-ray diffraction (HEXRD), Rietveld analysis, pair distribution function (PDF), and reverse Monte Carlo (RMC) modeling [2]. Hard X-ray photoelectron spectroscopy (HAXPES) provides important information on the electronic properties [3]. The HEXRD and HAXPES measurements were performed at BL04B2 and BL15XU at SPring-8, respectively.

We reported here that corresponding diffuse nature of the HEXRD patterns in terms of the total structure factor. Rietveld analysis results revealed that the lattice distortion in the fcc Ru NPs are greater than those in the hcp NPs. The PDF analysis and RMC models of fcc- and hcp-type Ru NPs show the inherited structural features of their bulk faces. As shown in figure 1(a), coordination number (CN) analysis implies enhancement of fcc-type NPs with increasing NP size.

Figure 1(b) shows the typical core-level spectra of fcc- and hcp-type Ru NPs and bulk Ru. The peaks at around 461.4 and 462.4 eV have been attributed to Ru (0) and Ru (4+). High catalytic activity of 5.4 nm fcc Ru NPs may consistent with observed higher positive shift of Ru (4+) peak with respect to hcp Ru NPs above 3 nm.

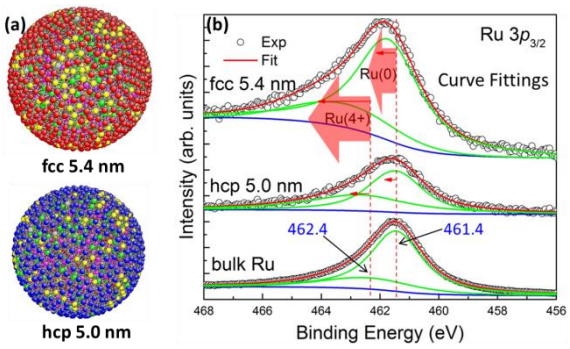

Figure 1: (a) RMC generated NP models with different CNs in highlighted colors and (b) Ru $3p_{3/2}$ core-level spectra of Ru NPs and bulk.

In this study, the observed the trend of increasing catalytic activity of fcc-type Ru NPs from atomic scale structure and electronic structures, which allows us to directly apply that novel knowledge to further development of catalyst technology.

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(1) K. Kusada et al., J. Am. Chem. Soc. **135** (2013) 5493.

(2) N. Bedford et al., J. Phys. Chem. C **111** (2007) 18214.

(3) A. L. Yang et al., Appl. Phys. Lett. **105** (2014) 153109.