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The 3D atomic scale and electronic structure characterization of novel fcc ruthenium nanoparticles using synchrotron light source

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Ruthenium (Ru) is a 4*d* transition metal that in the bulk adopts hexagonal close-packed (hcp) structure at all temperature ranges, and novel face-centered cubic (fcc) Ru nanoparticles (NPs) have been observed to be more efficient than conventional hcp Ru NPs larger than 3 nm. It has recently attracted much attention as a potential application in removal of car exhausts due to high catalytic activity for CO oxidation and preventing CO poisoning in fuel-cell system. We here report the 3-dimentational atomic-scale structures of fcc and hcp Ru NPs using high-energy X-ray diffraction (HEXRD), Rietveld analysis, pair distribution function (PDF), and reverse Monte Carlo (RMC) modelling. Hard X-ray photoelectron spectroscopy (HAXPES) can provide important information on the influence of NP size on electronic properties. The HEXRD and HAXPES of Ru NPs were performed at BL04B2 and BL15XU at SPring-8, the world largest third-generation (8 GeV) synchrotron radiation facility located in Hyōgo prefecture, Japan. We observed higher stability of the lattice distortion of fcc Ru NPs with increasing particle size. The PDF analysis results show that the structural disordered Ru NPs at short- to intermediate-range atomic distances. The order parameter for fcc Ru NPs decreased with increasing particle size due to the loosely packing atomic arrangement and may explain an origin of higher catalytic activity of fcc Ru NPs. In this study, the observed trend of increasing catalytic activity of fcc Ru NPs was also discussed using their core-levels and valence band electronic structures. This work was partly supported by ACCEL, Japan Science and Technology Agency (JST) and also partly supported by Ministry of Education, Culture, Sports, Science and Technology of Japan (OS: 15K04616).

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