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Size-effect of Pd and Ru nanoparticles revealed by Rietveld analysis using high-energy X-ray diffraction

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Nano-sized metal catalysts, which can be controlled the structure and particles size, exhibit higher surface area and more densely populated unsaturated surface coordination sites. Their excellent properties can be resulted in significantly improved catalytic activity over conventional catalysts. However, the origin of the nano-effects in the catalytic activity of metals is still debated and conclusion has not been reached. Kusada *et al.* firstly reported the face-centered cubic (fcc) Ru nanoparticles obtained by a chemical reduction method in 2013, while the bulk Ru has a hcp structure. The catalytic activity for CO oxidation of the fcc Ru nanoparticles was higher with increasing particle size, despite the decrease in surface area, which lacks physical intuitiveness. Therefore it is very important to secure an information of metal nanoparticles depended on their structure and size. In addition, there is a lack of report on the size-effect of Pd nanoparticles, which have also attracted much attention as a catalyst for CO oxidation and hydrogen-storage.

We present the particle size dependence of structural information of fcc-structured Pd and Ru nanoparticles to understand the origin of their catalytic activities for CO oxidation. It is found from Rietveld analysis using high-energy X-ray diffraction that the average domain size linearly increase with increasing particles size for fcc Pd nanoparticles. In contrast, for the fcc Ru nanoparticles, the average domain size saturates at about 1.4 nm despite the increase in particle size. It is also demonstrated that the lattice distortion of the close-packed (111) plane is decreased with increasing particle size for fcc Pd nanoparticles. The lattice distortion is, however, nearly independent of particle size for fcc Ru nanoparticles (Fig.1). It is also found that the B factors of fcc Ru nanoparticles are larger than that of fcc Pd nanoparticles. The obtained structural information will contribute to designing and improving the functionality of nano-sized catalysts.

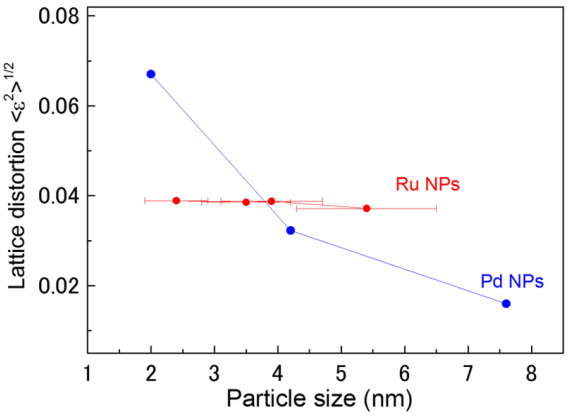

Fig.1. Relation between lattice distortion and particle size for fcc-Pd and fcc-Ru nanoparticles.

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