Size-dependent hydrogen-storage properties in Rh nanoparticles, revealed by various synchrotron based X-ray techniques: HEXRD, EXAFS

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Study on the reaction of hydrogen with nano-sized metals has attracted much attention due to the potential applications as effective hydrogen storage materials. Kusada et al. reported that the hydrogen absorption ability of Rh nanoparticles (NPs) is closely related to their enthalpy of hydrogen storage, which is changed from endothermic to exothermic with decreasing particle size, with a critical size between 7.1 and 10.5 nm [1]. However, the origin of the hydrogen-storage properties of Rh NPs can hardly be described as one parameter, changeover of the thermodynamic behavior, and has not been unveiled yet.

In this study, we have investigated the structural characterization of Rh NPs with various particle sizes (2.4, 4.0, 7.1, 10.5 nm), using the synchrotron based X-ray techniques. To unveil the origin of their hydrogen absorption ability, we used the particle size dependence of lattice distortion, coordination number, mean-square displacement and volume fraction of cavities for Rh NPs. From the HEXRD and EXAFS, it is found that the lattice distortion/mean-square displacement (Fig. 1) increase and coordination number decreases with decreasing the particle size. This result suggested that the hydrogen absorption ability of Rh NPs is more closely related to mean-square displacement for local structure (EXAFS) than that for mean structure (HEXRD). From the cavity analysis, we confirmed that the cavities are distributed over the whole particle and hydrogen can be trapped on the entire volume for the smallest Rh NPS.

The obtained structural information will contribute to designing and improving the functionality of nano-sized metals.

Fig.1. Relation between mean-square displacement and particle size for Rh NPs.


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