

Diffusion dynamics of hydrogen atoms in PdPt nanoparticles studied by quasielastic neutron scattering

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The nanometer-sized metals attract much attention since their physical and chemical properties are substantially different from those of bulk metals. Kobayashi et al. found that the phase-separated nanoparticles of Pd-core and Pt-shell are mixed to be solid solution alloy by repeating hydrogen absorption/desorption processes at 373 K [1]. In this study, we have investigated the diffusion dynamics of hydrogen (H) atoms in solid solution PdPt nanoparticles by means of quasielastic neutron scattering (QENS). Pelican and Emu spectrometers installed at ACNS, ANSTO were used for this experiment.

Figure 1 shows the Arrhenius plot of the relaxation times (τ) for Pd_{0.8}Pt_{0.2}H_{0.47} nanoparticles together with τ for PdH_{0.47} nanoparticles obtained in our previous QENS experiments [2]. The slow and fast relaxation processes, which correspond to the motions of H atoms at the octahedral (O) and tetrahedral (T) sites, were observed. For Pd_{0.8}Pt_{0.2}H_{0.47} nanoparticles, the τ is shorter and the activation energy is smaller than those for PdH_{0.47} nanoparticles. It should be noted that the fast relaxation time is almost temperature independent below 250 K. This result suggests that the insertion of Pt atoms to the fcc lattice may deform the potential energy surface and induce tunneling diffusion of H atoms.

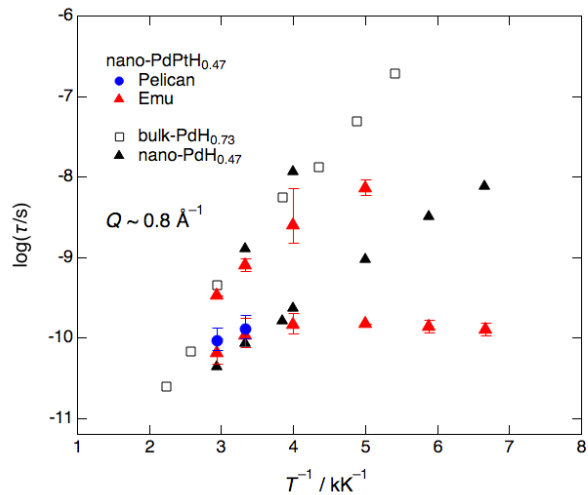


Fig. 1: Arrhenius plot of the relaxation times for Pd_{0.8}Pt_{0.2}H_{0.47} and PdH_{0.47} nanoparticles.

[1] H. Kobayashi, M. Yamauchi, H. Kitagawa, Y. Kubota, K. Kato, M. Takata, J. Am. Chem. Soc. **132**, 5576 (2010).

[2] M. Kofu, N. Hashimoto, H. Akiba, H. Kobayashi, H. Kitagawa, M. Tyagi, A. Faraone, J. R. D. Copley, W. Lohstroh, O. Yamamuro, Phys. Rev. B **94**, 064303 (2016).