Element-Selective Observation of Dynamics in High-Entropy Alloy Nanoparticles with XAFS

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High-entropy alloy (HEA) is multi-principal element alloy characterized by its large configurational entropy.[1] Recent studies have demonstrated that HEA nanoparticles (HEA NPs) show characteristic catalytic activities which cannot be explained in the context of conventional alloys.[2] Although the origin of their unconventional properties remains unrevealed, the variety of local coordination environment in these multiple element alloys would have a significant importance. However, due to the difficulty in analyzing the structure of these complicated and nano-sized materials, their structure, especially dynamic structure, has been poorly understood.

Our purpose of this study is to investigate the local dynamics in HEA NPs and associate it with the intrinsic nature of constituent elements. As prospective target materials, we synthesized the HEA NPs composed of liquid metal elements (Ga, In and Sn) and platinum group metal (PGM) elements (**Fig.**), which have totally different thermodynamic properties such as melting points. To discuss the dynamics, we focused on Debye–Waller factor (DWF) accessible with X-ray spectroscopies, and performed X-ray diffraction (XRD) and X-ray absorption spectroscopy (XAS) measurements under variable-temperature conditions. Notably, the element-selective analysis based on EXAFS DWF[3] illustrated that local dynamics varies with involved elements even in the same alloy. Our results support the idea of the variety in local coordination environment in HEA NPs, and moreover offer new methodology to investigate the dynamics in multiple element materials.

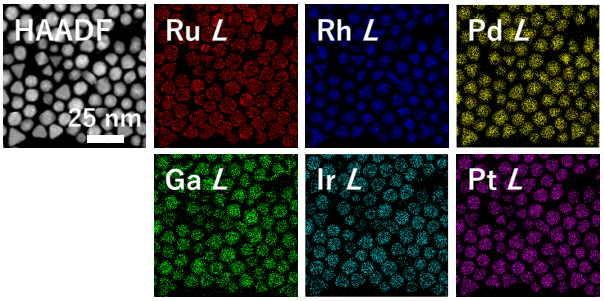

Fig. HAADF-STEM image of the Ga–PGM HEA NPs and the corresponding EDX maps.

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