Post-corundum phases in A2O3 (R=Ga, In) compounds under high P-T condition

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It is known that corundum is a representative structure in various sesquioxides such as Cr2O3, Ga2O3, Rh2O3 and Fe2O3. Recently, the post corundum phases of Fe2O3 have been investigated for their significance in the Earth's interior (Ono et al., 2005; Ito et al., 2006). They proposed GdFeO3-type structure or Rh2O3(II)-type structure as the post corundum phase.

We performed the high P-T experiments of Ga2O3 and In2O3 to determine the post corundum structures. Before performing the high P-T experiments, high-pressure phase stabilities of the post corundum candidates were investigated using density functional theory static lattice energy calculations (e.g. Tsuchiya and Tsuchiya 2006).

The high P, T experiments have been done at BL-10XU (SPring-8) using a symmetrical diamond anvil cell (DAC) combined with Nd:YLF laser. The angle dispersed x-ray diffraction (30 keV) was detected by an imaging plate and an x-ray CCD camera. The powdered samples of Ga2O3 (beta-Ga2O3), and In2O3 (C-type RE structure) were used as starting materials. A small amount of gold or platinum powder was mixed with the samples to make an effective absorption of the laser beam.

The structure of the Ga2O3 sample heated below 40 GPa was identified as a corundum structure. Whereas, if it was heated beyond 65 GPa, the x-ray diffraction pattern was completely changed to a new phase. The attempt of Rietvelt analyses on this phase suggests that the structure was assigned to Rh2O3(II)-type phase rather than GdFeO3-type structure, judging from the disagreements of the (110) reflection of the perovskite. The transition pressure determined by a reversal experiment is located at 39-37 GPa, which is consistent with 35 GPa by the theoretical calculation. The transition pressure from C-type RE to corundum structure in In2O3 has been proposed by static (Shannon, 1966) and dynamic compression experiments (Atou et al. 1990) to 6.5 and 15-25 GPa, respectively. However, we could not determine the stability fields of corundum structure because the corundum structure was only confirmed in the recovered samples after releasing pressure. We only observed the transition from C-type RE to Rh2O3(II) structure in the present in-situ experiments under high pressure. The corundum converts to C-type RE structure after heating in the recompression experiment at about 3GPa. Hence, we could conclude that the corundum structure is metastable phase in In2O3.