Post-Rh_2O_3(II) phases in A_2O_3 (A=Ga, In) compounds: experiments and theoretical calculation

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Since the structural transformation from corundum to Rh_2O_3(II) structure was found in Al_2O_3[1,2], the post corundum phases in various sesquioxides, (*i.e.* Fe_2O_3[3,4], and Cr_2O_3[5]) have been actively surveyed by in-situ x-ray diffraction experiments under high pressure. Last year, we have reported Rh_2O_3(II) structures as post corundum phase in IIIB sesquioxides (*i.e.* Ga_2O_3 and In_2O_3) by experimental and theoretical methods[6]. Here, we report the further structural changes in their compounds.

In advance of the high P-T experiments, high-pressure phase stabilities of $CaIrO_3$ phase, which is a candidate for post Rh_2O_3(II) phases, were calculated using density functional theory with local density approximation (DFT-LDA)[7].

The high P, T experiments have been done at BL-10XU (SPring-8) using a symmetrical diamond anvil cell (DAC) combined with Nd:YLF or Nd:YAG 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 Ga_2O_3 (beta-Ga_2O_3), and In_2O_3 (C-type rare earth 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 Rh_2O_3(II) phase in Ga_2O_3 persists up to 108 GPa at 2300 K. However, after heating at 164 GPa, the x-ray diffraction pattern drastically changed. The new peaks are assigned by *Cmcm* symmetry isostructural to the $CaIrO_3$ phase. The pressure is well consistent with the transition pressure (c.a. 130 GPa) calculated by DFT-LDA. Volume reduction associated with the transition is calculated to be 2.3 %, which is comparable to 2.8 % in Al_2O_3 . In case of In_2O_3, 45 GPa is expected for the transition pressure from Rh_2O_3(II) to Cmcm phase. However, we could not observe *Cmcm* phase, although we conducted several laser heating experiments at 40 - 57 GPa. Instead of *Cmcm* phase, an unexpected phase appears above 40 GPa. A primitive orthorhombic unit cell is suggested by indexing with dichotomy method (DICVOL04). The volume reduction from Rh_2O_3(II) phase amounts to 5.7 %, which is significantly larger than that associated with the Rh_2O_3(II) - Cmcm transition. Therefore, the new phase would be one of the densest structures in the known sesquioxides[8]. The details about the structure will be presented at the conference site.

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