Reinvestigation of high-pressure phase sequence in ytterbium sesquioxides at room temperature

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Introduction

Since Goldschmidt et al. denominated the rare earth sesquioxides’ polymorphs as A-, B- and C-type structures, their existence in lanthanoid sesquioxides have been examined by high-pressure experiments [e.g 1]. The appearance of each phase is clearly correlated with the cationic radii of lanthanoid atoms. However, the sequence of their phase transition is still controversial. Direct transformation from C- to A-type is proposed in ytterbium sesquioxide under pressure because of the absence of B-type in their energy dispersive x-ray diffraction profiles [2]. In this work, we have reexamined the pressure-induced phase transformation of ytterbium sesquioxides using an angle dispersive x-ray diffraction method combined with LeBail profile fitting analysis.

Experimental

Powder form of ytterbium sesquioxide sample (99.99% pure: C-type structure) was prepared for the high-pressure experiments using a diamond anvil cell. The sample mixed with a small amount of gold powder was put into the hole in the rhenium gasket with a methanol: ethanol: water (16:3:1) pressure medium. The in-situ x-ray diffraction experiments were done at AR-NE1. A monochromatic x-ray beam (30keV) was focused and collimated to the sample within 30 microns size. Diffracted x-rays were detected by an imaging plate. The LeBail analysis in the GSAS package was used for the profile fitting of the x-ray profiles. Pressure was determined from the lattice parameters of gold [3].

Results and discussion

During the compression, the profile was significantly changed at 15.9 GPa. The profile fitting analysis shows that the profile consists of C- and B-types. After the further compression to 19.6 GPa, the A-type appears in addition to the B- and C-types (Fig.2b). Therefore we successfully confirmed the B-type as an intermediate phase between C- and A-type. Accordingly, the sequence of C – B – A phase transformations is established in Yb2O3. In the decompression process, the A-type reverts to the B-type at 11.9 GPa. However, the C-type did not appear after further decompression to 3.2 GPa. This is caused by a large kinetic barrier in a reconstructive transition from B- to C-type. The quick reversion from A to B-type is explained by a displacive transition, which has been already observed in Y2O3[4].

Fig. 1. :P-V data (triangles) and compression curves (solid lines) of Yb2O3 polymorphs. The right and left pointing of triangles indicate the compression and decompression, respectively. The compression curves and bulk modulas (K0) are obtained by fitting the Birch-Murnaghan equation of state to the P-V data with K0’ fixed to 4.

Fig. 2. (a) X-ray diffraction profiles from Yb2O3 samples under pressure. (b) A profile fitted pattern at 19.6 GPa with the LeBail method in the GSAS package.

References

[2] A. Fujimura et al., unpublished data collected by MAX80 at KEK-PF.

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