

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

Hitoshi YUSA¹, Takumi KIKEGAWA², Taku TSUCHIYA³

¹NIMS, Tsukuba, Ibaraki 305-0044, Japan

²KEK-PF, Tsukuba, Ibaraki 305-0801, Japan

³GRC, Ehime. Univ., Matsuyama, Ehime 790-8577, Japan

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].

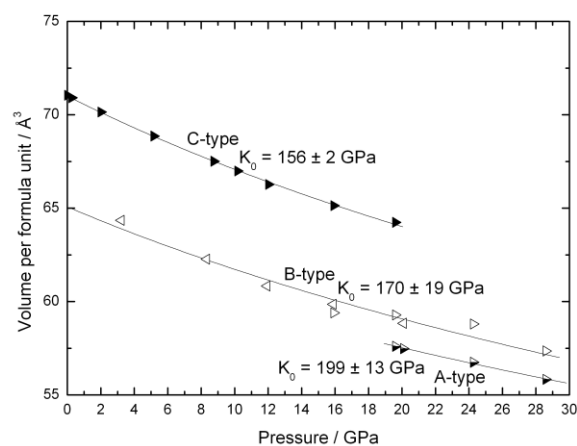


Fig.1. :P-V data (triangles) and compression curves (solid lines) of Yb₂O₃ polymorphs. The right and left pointing of triangles indicate the compression and decompression, respectively. The compression curves and bulk modulus (K_0) are obtained by fitting the Birch-Murnaghan equation of state to the P-V data with K_0' fixed to 4.

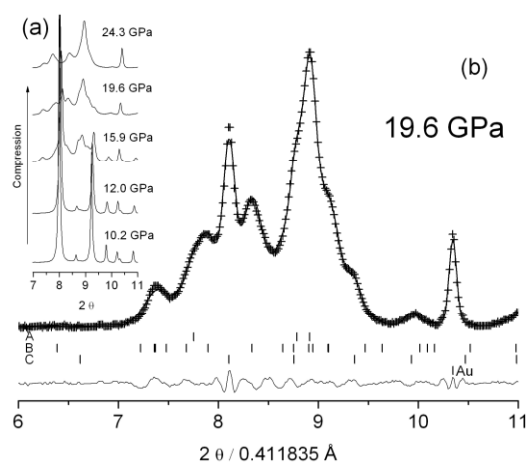


Fig. 2. (a) X-ray diffraction profiles from Yb₂O₃ samples under pressure. (b) A profile fitted pattern at 19.6 GPa with the LeBail method in the GSAS package.

References

- [1] H.R. Hoekstra, Inorg. Chem., 5, 754 (1966).
- [2] A. Fujimura et al., unpublished data collected by MAX80 at KEK-PF.
- [3] O.L. Anderson et al., J. Appl. Phys., 65, 1534 (1989).
- [4] H. Yusa et al., Inorg Chem., 49, 4478 (2010).

* yusa.hitoshi@nims.go.jp