The Physical Properties of Lu₂O₃ under High-Pressure by X-ray Diffraction and Absorption Method

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 ${\rm Lu_2O_3}$ in-situ XANES (X-ray Absorption Near Edge Spectroscopy) measurement were performed in the SP12B1 beamline during Dec. $10{\sim}14$, 2007. ${\rm Lu_2O_3}$ has a body-centered-cubic structure ~space group Ia3)(no.206) with 80 ions per unit cell [1]. ${\rm Lu^{3+}}$ ions are distributed between two distinct crystallographic sites: 75% and 25% occupy sites with C2 and C3i symmetries, respectively [2]. ${\rm Lu^{3+}}$ ions in both C2 and C3i sites possess distorted octahedral coordination geometries. ${\rm Lu_2O_3}$ show C type in ambient pressure and B type in high pressure.

Figure 1 shows Lu L_{II} -edge XANES spectra of Lu₂O₃ at 300 K. The energy was calibrated using the data acquired simultaneously on a Lu₂O₃ foil at 300 K. The positions of the L_{II} -edge resonance peaks in the XANES spectra are shifted upward relative to that of pressure as Table I. On the other hand, x-ray-absorption spectroscopy at the L edge has been used to probe the density of states above the Fermi level as Figure 2 and Table II. We can suggest that the change of density of state in C and B type.

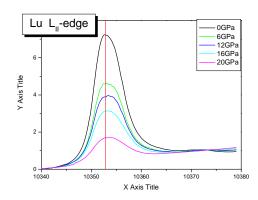


Figure 1. L_{II} -edge XANES spectra of Lu₂O₃ samples at 300 K.

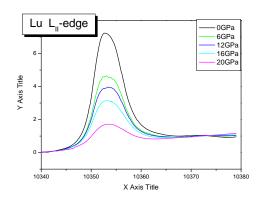


Figure 2. The density of state v.s. pressure.

Pressure (GPa)	White line (eV)
0	10352.6
6	10353
12	10353.4
16	10353.4
20	10353.6

Table I. The white line v.s. pressure.

Pressure (GPa)	Density of state
	(area)
0	75.45
6	57.15
12	52.85
16	46.43
20	34.9

Table II. The density of state vs pressure

Reference:

- 1 · L. Eyring, in Handbook on the Physics and Chemistry of Rare Earths, edited by K.A. Gschneidner, Jr. and L. Euring North-Holland, Amsterdam, Vol. 3, Chap. 27 (1979).
- 2 · M. Faucher and J. Pennetier, Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem. **36**, 3209 (1980).