

## Pressure-induced phase transition of LuSb with NaCl-type structure

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### Introduction

Using synchrotron radiation, x-ray diffraction of LnSb (Ln = Dy, Ho, Er and Tm) has been studied up to 40 GPa at room temperature.[1,2] First-order phase transitions of LnSb with the crystallographic change occur at high pressures. The structure of the high-pressure phases of LnSb (Ln = Dy, Ho, Er and Tm) is a CsCl-type structure.

Using synchrotron radiation we have studied the x-ray diffraction of LuSb with the NaCl-type structure up to 33 GPa at room temperature. The pressure-induced phase transition for the compound is observed above 24 GPa.

### Experimental

LuSb was prepared by reaction of stoichiometric amounts of each rare earth metal and antimony in a sealed silica tube at around 800 °C.

Using synchrotron radiation the powder x-ray diffraction patterns of LuSb were measured with a diamond-anvil cell and the imaging plate up to 33 GPa at room temperature. Incident beam was monochromatized by Si(111) double crystal to a wavelength of 0.6196 Å. The pressure in the diamond-cell was determined from a pressure shift in the sharp R-line fluorescence spectrum of ruby. A 4:1 methanol-ethanol solution was used as the pressure transmitting fluid.

### Results and Discussion

Figure 1 shows powder x-ray diffraction patterns of LuSb at high pressures. The profile indicates only characteristic lines of the NaCl-type structure at around 0.6 GPa. The d-values of 111, 200, 220, 311, 222, 400, 420, 422, 440, 600 and 620 lines of LuSb decrease with increasing pressure up to 21 GPa. New diffraction lines appear above 24 GPa and grow with increasing pressure. Low and high-pressure phases coexist in the wide pressure range. A single phase of the new high-pressure phase is obtained above 33 GPa. When the pressure is removed, the diffraction lines of the NaCl-type structure reappear at around 12 GPa. The x-ray diffraction pattern of the high-pressure phase of LuSb can be assigned by the index of the cubic CsCl-type structure. The lattice constant of the high-pressure phase of LuSb with the CsCl-type structure is 3.46 Å at around 33 GPa.

Figure 2 shows relative unit cell volume vs. pressure curve for LuSb. The cell volume with NaCl-type structure decreases with increasing pressure up to 21 GPa. The structural change to the CsCl-type structure occurs with volume collapse of about 1 %.

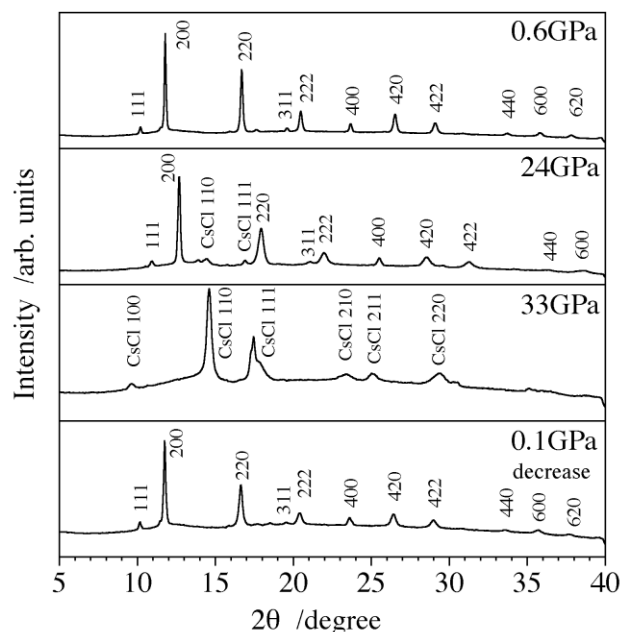


Fig. 1 Powder x-ray diffraction pattern of LuSb at high pressures.

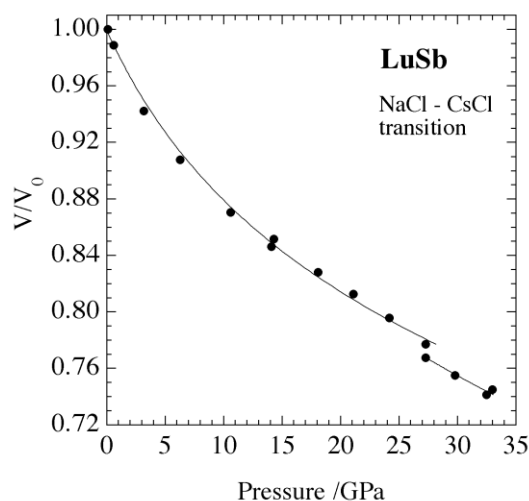


Fig. 2 Relative volume ( $V/V_0$ ) - pressure curve for LuSb at room temperature.

### References

- [1] I. Shirotni et al., Phys. Rev. **B64**, 132101 (2001).
- [2] J. Hayashi et al., Photon Factory Activity Report. **17**, 226 (1999).

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