

P-19

Equation of state of monazite-type lanthanum orthovanadate: *in situ* high-pressure powder diffraction and *ab initio* calculations

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Lanthanum orthovanadate (LaVO₄) is one of a few of the RVO₄ compounds which can crystallize in the monazite-type structure. In the present study, equation of state of the monazite-type of LaVO₄ is studied using *in situ* high-pressure powder diffraction at room temperature, and *ab initio* calculations within the framework of the density functional theory.

A polycrystalline LaVO₄ sample was prepared by solid state reaction between dried La₂O₃ (Auer-Remy 4N) and V₂O₅ (Alfa Aesar 4N5) oxides mixed at equimolar ratio. Mixed and ground oxides were compressed into pellets and sintered in air at 1300°C during 6 hours. After the sintering process, the sample was re-ground, pressed into pellets and sintered at 1300°C for 6 h again.

In situ high-pressure powder diffraction experiment was performed in a diamond anvil cell at the I711 beamline of the MAX IV synchrotron (Lund, Sweden). A preindented steel gasket of 100 μm thickness with a 200 μm hole was used for the encapsulation between the diamond anvils of the studied sample using the ethanol-methanol-water pressure-transmitting medium. The experiment was performed in hydrostatic conditions up to pressure of 9.1 GPa. Applied pressure was calibrated by the laser-excited ruby fluorescence peak position. To perform the Rietveld analysis with the Fullprof.2k 5.30 package, the 2D data were converted to 1D patterns with the Fit2D program. The calculated dependence of the unit cell volume on pressure was used in the fitting of a third-order Birch-Murnaghan equation of state with EOSfit52 program.

The fitted parameters of a third-order Birch-Murnaghan equation of state are found to be in good agreement with theoretical ones.

P-20

Mechanochemical synthesis of the scheelite-type PrVO₄ and HoVO₄

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At ambient conditions, rare-earth orthovanadates adopt zircon-type structure (space group *I4₁/amd*) except LaVO₄ which typically crystallizes in monazite-type structure. Zircon-type RVO₄ can be prepared in single crystal form using several crystal growth techniques or in powder form e.g. as a product of solid state reaction between rare-earth and vanadium. It is known, that at high-pressure conditions (5-10 GPa) RVO₄ materials with zircon structure undergo a transformation to the scheelite-type structure (space group *I4₁/a*). Tojo *et al.* [1] have shown, for selected RVO₄ (R = Y, Nd, Sm, Gd, Dy and Er) crystals that the scheelite-type phase can be obtained via mechanochemical reaction between R₂O₃ and V₂O₅ oxides.

In the present work, we describe successful attempts to obtain scheelite-type PrVO₄ and HoVO₄ by means of ball milling of zircon-type samples. Experiments were performed using a ball grinder. The primary sample of HoVO₄ was grown in single crystal form by Czochralski method, the PrVO₄ sample was prepared by solid state reaction between Pr₆O₁₁ and V₂O₅ oxides. Both samples were ground for 1, 2, 4, 8 and 16 hours of milling. All specimens were studied using a laboratory X-ray powder diffractometer. The diffraction patterns demonstrate that the scheelite-type structure appears after 1 hour of milling and that its content in the specimen grows with increasing duration of mechanochemical reaction. After 16 hours of milling the scheelite-type phase dominates in both, HoVO₄ and PrVO₄, samples, as shows the example for HoVO₄ (Fig. 1): after 16 h only two reflections of the zircon-type polymorph remain.

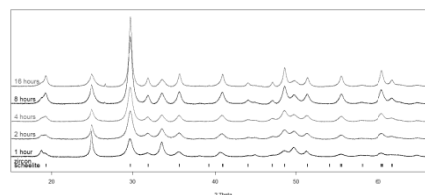


Figure 1. Variation of phase composition for ball milling of zircon-type HoVO₄ sample. Small vertical bars at the bottom part mark the diffraction peaks of the scheelite type phase.

[1] T. Tojo, Q. Zhang, F. Saito, *J. Alloys Compds* **427** (2007) 219.