Elastic properties of zircon- and scheelite-type praseodymium orthovanadate

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Rare-earth orthovanadates (RVO4) form a group of materials with various possible applications [1-6]. Typically, RVO4 adopt the zircon structure (space group I41/amd, Z = 4) at ambient conditions. Up to now, most studies on structure and physical properties were focused on optical characteristics, low temperature Jahn–Teller effect and structure investigations including structural phase transitions which are typical for these materials at high pressure. It has been shown for selected RVO4 materials that below 50 GPa they undergo two structural phase transitions at high-pressure conditions. The first one is the zircon – scheelite phase transition which starts at about 5-10 GPa [7,8,9], the second one is the scheelite – fergusonite transition starting at about 30 GPa [9]. As far as we know, no literature data for praseodymium orthovanadate equation of state have been published.

Figure 1: The unit cell volume as a function of applied pressure. Solid lines correspond to fitted Birch–Murnaghan equation of state.

The aim of present investigation was to experimentally determine the equation of state parameters for zircon and scheelite phases of praseodymium orthovanadate (PrVO4) at pressure range from ambient up to 6 GPa, using synchrotron radiation and MAX80 large-anvil press at F2.1 beamline (Hasylab, DESY). The zircon-type sample used in this study was grown in single crystal form by slow cooling method from PbO/PbF2 flux. The metastable scheelite structure was obtained from polycrystalline zircon sample via pressing at 7 GPa with simultaneous heating up to 700°C for 15 min. The heating was followed by fast cooling. As a result of this treatment, the scheelite structure was obtained with an admixture of zircon phase. For present investigation both samples were finely
ground in an agate mortar, mixed with vaseline in volume ratio 1:1 and placed inside a hexagonal boron nitride tube which was mounted in a boron-epoxy cubic gasket of 6 mm edge. NaCl powder was used for applied pressure calibration. Energy dispersive data for both samples were carried out at pressures from ambient up to 6 GPa at room temperature. Unit cell parameters for each pressure point were refined using Le Bail method using the Fullprof program.

The unit-cell parameters values measured at ambient conditions are in good agreement with data obtained for these samples using a laboratory diffractometer. The parameters smoothly decrease with pressure as it is shown in Figure 1. Bulk moduli for studied samples were calculated from 2-nd order Birch-Murnaghan equation of state using EosFit52 software.

References