Poster Presentations

[MS20-P11] Structure refinement of SmVO4 at pressures ranging to 10 GPa.

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SmVO4 belongs to a family of zircon-type rare-earth orthovanadates (RVO_4, R = rare earth element). It exhibits catalytic properties useful in propane oxidative dehydrogenation [1] and photodegradation of organics [2]. In this work, the single-crystal diffraction is used in order to precisely determine the crystal structure, and high-pressure powder diffraction is applied for determination of the equation o state and phase transition point. The $SmVO_4$ single crystal was grown from PbO/PbF_2 flux by the slow cooling method. The single crystal diffraction study was performed using a Bruker-Nonius Kappa-CCD diffractometer, radiation MoK. The in-situ high-pressure measurements were conducted at I711 beamline (MAXlab, Lund, Sweden) using a membrane-driven diamond-anvil cell, with methanol-ethanol-water mixture applied as pressure transmitting medium. The radiation of vwavelength of 0.920192 Å was applied. The single crystal study yields lattice parameters of a = 7.2687(3) Å and c = 6.3887(2) Å, unit cell volume = 337.54(2), space group I41/amd. Powder diffraction gives a = 7.26659(8) Å and c = 6.3883(1) Å, both these sets compare well with the data from Ref. [4], a = 7.2647(9) Å and c = 6.384(1) Å. The experiments performed at hydrostatic pressures (at room temperature) show that $SmVO_4$ undergoes a zircon-scheelite phase transition which starts at 7 GPa and ends at about 9 GPa. The lattice parameters and axial ratios vary with pressure in a way similar to other members of the RVO_4 family. The atomic coordinates do not show a detectable variation. Fitting the Birch-Murnaghan equation of state gave the bulk modulus of the zircon type phase of 118 GPa. The above value is lower than that found in [3] for the $EuVO_4$ compound being a close neighbor of $SmVO_4$ in the RVO_4 series.

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