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Elastic properties of dysprosium orthovanadate: An in-situ powder-diffraction study

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Rare-earth orthovanadates (RVO_4) are well known as materials with possible applications mostly as laser materials [1-6]. RVO_4(R = Y, Ce-Lu) crystallize in zircon-type structure, $I4_1/amd$ space group. An irreversible pressure-induced phase transition from zircon to scheelite-type structure occurs for materials of this type in the pressure range of 5-10 GPa [7,8].

During the present investigation, structural and elastic properties of dysprosium orthovanadate were studied using the powder diffraction method. The studied $DyVO_4$ single crystal was grown by the slow cooling from molten flux. The sample for diffraction analysis was prepared by grinding in an agate mortar. Powder diffraction data at ambient pressure were obtained using a laboratory diffractometer (X'PERT MRD, Philips, with Cu X-ray tube). The lattice parameters calculated using Rietveld method are a = 7.147(2) Å, c = 6.308(2) Å, V = 322.16(6) Å^3.

In-situ powder diffraction experiment under pressure was performed at the F2.1 beamline Hasylab/DESY (Hamburg, Germany) using the MAX80 X-ray diffraction press. In this experiment applied pressure was in range from ambient up to 8.45 GPa. Energy-dispersive powder diffraction patterns were obtained with steps about 0.7 GPa. Within the studied range, the phase transition from zircon to scheelite structure was not observed. Cell parameters were calculated by Le Bail method. Above 6 GPa, a diffraction-peak broadening, apparently due to the presence of strain, was observed. In order to minimize the influence of deviatoric stresses on the derived elastic properties, we limited the calculations to the range from ambient pressure to 6 GPa. The lattice parameters vary, in this range, from a= 7.151(1) Å, c= 6.301(1) Å, V = 322.17(16) Å^3 to a = 7.0314(2) Å, c= 6.233(2) Å, V = 308.16(20) Å^3. The bulk modulus B_0 = 121(2) GPa was calculated by fitting the smooth experimental V(p) dependence using the second order Birch–Murnaghan equation of state. This value is by about 25% lower than the only published one (160 GPa) evaluated on the basis of Raman-spectroscopy data [9], but remains close to the value for a related compound, YVO_4, determined at hydrostatic conditions by Wang et al [10].

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