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High-pressure diffraction study of structural and elastic properties of zircon-type and scheelite-type RVO_4 (R = Nd, Eu)

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Rare-earth orthovanadates (RVO_4, with *R* = Sc, Y, La-Lu) crystallize, typically, in $I4_1/amd$ space group (zircon type structure). They transform to the scheelite-type structure ($I41/a$ space group) under high-pressure conditions of several GPa. As the transition is irreversible, it is possible to study the properties of scheelite polymorph at ambient pressure. The first detailed information on transition of this kind at hydrostatic conditions was reported for YVO_4 [1, 2]. Physical properties of zircon-type rare-earth orthovanadates are better recognized, and various applications have been proposed for them, in particular they can be applied as catalysts. The orthovanadates with the scheelite structure attract attention because some representatives such as $EuVO_4$ show strong luminescence [3] creating an opportunity for application in optoelectronic devices. The above-mentioned features resulted in an increasing interest in structural phase transitions, their mechanisms and in equations of state for both RVO_4 polymorphs.

The aim of the present investigation was the *in-situ* observation of the zircon-scheelite phase transition under pressure and determination of elastic properties for two members of the RVO_4 family, $NdVO_4$ and $EuVO_4$, for both zircon and scheelite type polymorphs. The samples of zircon structures were obtained by solid state reaction between R_2O_3 (R = Nd, Eu) and V_2O_5 at temperatures of 1100°C for $NdVO_4$ and 950°C for $EuVO_4$. The samples transformed to scheelite-type structure after compression of zircon-type phase at elevated temperature.

In-situ high-pressure X-ray diffraction experiments were performed in the range up to 15 GPa at I711 beamline MAX II (Lund, Sweden) using a diamond-anvil cell. The samples studied were placed in a hole drilled in a pre-indented stainless-steel gasket which was subsequently clamped between two diamond anvils having 0.3 mm diameter culets. A water-ethanol-methanol mixture was used as pressure-transmitting medium providing hydrostatic compression conditions up to about 10 GPa. The applied pressure was measured by laser-excited ruby luminescence. Data acquisition was carried out using MAR165 area detector. Using the aforementioned experimental approach, the zircon-type $NdVO_4$ and scheelite-type $EuVO_4$ were studied. The acquired experimental data were analyzed using Rietveld method providing the information on structure of the material. For $NdVO_4$, the zircon-scheelite phase transition was observed in the pressure range from 4.35 to 5.75 GPa. Bulk modulus values were calculated for both materials from the volume-pressure relationship.

References

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