HIGH-PRESSURE DIFFRACTION STUDY OF SELECTED FOUR-COMPONENT SYNTHETIC GARNETS

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The synthetic garnets exhibit physical properties that may lead to various applications. These materials are characterized by low thermal conductivity [1] and by Mohs hardness between 6.5 and 8.5. The garnets containing *e.g.* Fe or Mn as components exhibit anti-ferromagnetic proprieties [2]. Some of these materials (for example, gadolinium gallium garnet – GGG) can be used for substrates for epitaxy of superconducting films [3]. The garnet-based single crystal films, grown on the garnet substrates (*e.g.* $Y_3Al_5O_{12}$) can be used as scintillation detectors [4]. The doped garnets are applied in solid-state lasers [5], also they can be used as optical high-pressure sensors [6,7]. Elastic properties of garnets (hardness, bulk modulus) are of interest from the point of view of Earth science, because minerals of garnet structure are considered as one of major components of the deep interior of the Earth [8].

Bulk moduli of synthetic three-component garnets are relatively high, for example that for gadolinium gallium garnet equals K_0 = 169(15) GPa [9]. Those for four-component garnets (chemical formula $X_3Y_2Z_3O_{12}$, with divalent X, trivalent Y, and tetravalent Z cations, for example: $Ca_3Fe_2Ge_3O_{12}$, or with trivalent cations, *e.g.* $Gd_3Sc_2Al_3O_{12}$) remain unknown, giving a motivation for the present study.

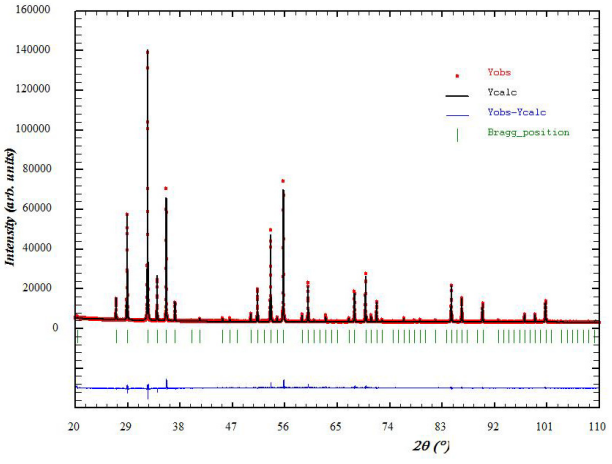

Figure 1. Rietveld refinement plot of the calcium iron germanium garnet (21ºC, ambient-pressure data). The lattice parameter for the sample studied is 12.3288(2) Å.

The $Ca_3X_2Ge_3O_{12}$ garnets, where X = Fe, Ga, were characterized at the ambient pressure by X-ray diffraction using a Philips X'pert MRD diffractometer (an example is shown in Fig. 1). The *in-situ* X-ray diffraction experiments were conducted using the energy-dispersive method at the F2.1 beamline equipped with a large-anvil diffraction press, MAX80. The pressures ranging to 8.7 GPa were calibrated using a NaCl equation of state. Lattice parameters of garnets were determined from Le Bail refinements performed with Fullprof2k program.

The analysis of the data collected for the measured garnets shows that their crystal structure is conserved in the studied pressure range. The bulk moduli obtained by fiitting the Birch–Murnaghan (BM) equation of state (EOS) are found to be comparable with the values of some other members of the garnet family.

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