

HIGH-PRESSURE DIFFRACTION STUDY OF SELECTED SYNTHETIC GARNETS

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Crystals of synthetic garnets exhibit physical properties that may lead to various applications. These materials are characterized by high resistance for plastic flow even at high temperatures, by low thermal conductivity [1], and by Mohs hardness between 6.5 and 8.5. Garnets are applied in solid-state lasers [2]. Some of them (e.g. $\text{Gd}_3\text{Ga}_5\text{O}_{12}$, gadolinium gallium garnet – GGG) can be used for substrates for epitaxy of superconducting films [3]. Some doped oxide garnet materials can be used as optical pressure sensors [4, 5].

Mechanical properties of garnets are also 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 [6].

The general chemical formula for a garnet is $\text{X}_3\text{Y}_2\text{Z}_3\text{O}_{12}$, with divalent X, trivalent Y, and tetravalent Z cations (for example: $\text{Ca}_3\text{Ga}_2\text{Ge}_3\text{O}_{12}$) or with trivalent cations.

At ambient conditions, garnets crystallize in $Ia3d$ space group. In four-component's garnets ($\text{X}_3\text{Y}_2\text{Z}_3\text{O}_{12}$), the Z atoms are bonded to four oxygens (tetrahedral), Y atoms – to six oxygens (octahedral), and X atoms – to eight oxygens (distorted cube). In three-component garnets ($\text{X}_3\text{Y}_5\text{O}_{12}$) the five Y ions occupy two octahedral and three tetrahedral sites.

High-pressure diffraction study for selected garnets is presented in this work. 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. The lattice parameters of garnets were determined from Le Bail refinements performed with the Fullprof2k program.

Analysis of the data collected for one of the measured garnets, $\text{Ca}_3\text{Ga}_2\text{Ge}_3\text{O}_{12}$ (calcium gallium germanium garnet, CGGG) shows that the garnet structure is conserved in the studied pressure range. The lattice parameter of the garnet structure decreases with the applied pressure from 12.202(1) Å at ambient pressure to 11.995(4) Å at 8.7 GPa. The resulting bulk modulus value for the CGGG is by about 15% lower than that for gadolinium gallium garnet [7].

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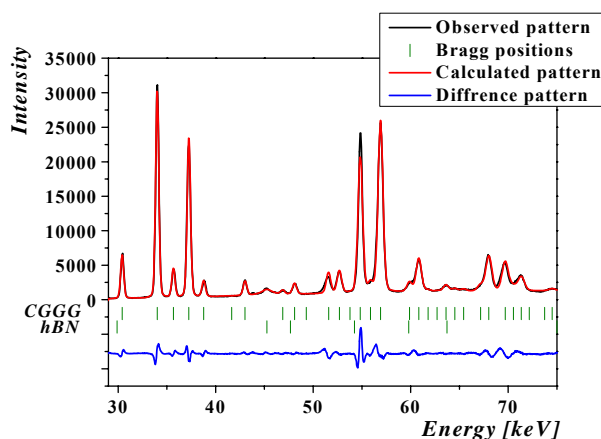


Figure 1. Le Bail refinement plot of the calcium gallium germanium garnet, sample after compression without pressure. The vertical bars refer to peak positions for CGGG and hBN.

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