Synthesis of $LiNbO_3$-type $Mg_3Al_2Si_3O_{12}$ at 44 GPa and 2000 K using Kawai-type multianvil press with tungsten carbide anvils

*Takayuki Ishii[1], Ryosuke Sinmyo[2], Nobuyoshi Miyajima[1], Tiziana Boffa Ballaran[1], Tomoo Katsura[1]

1.Bavarian Research Institute, University of Bayreuth, 2.Earth-life science institute, Tokyo institute of technology

Garnet is one of the major constituent minerals of the upper mantle. In particular, pyrope is one of the most abundant components. Pyrope transforms to aluminous bridgmanite (Al-Brm) + corundum at about 25 GPa and Al_2O_3 content in Brm increases with increasing pressure (e.g. Kubo and Akaogi, 2000; Liu et al. submitted). Finally, Al-Brm with pyrope composition is synthesized over 40 GPa and 2000 K (Liu et al. submitted). Recently, Ishii et al. (2016) reported that recovered sample synthesized at 44 GPa and 2000 K has $LiNbO_3$ (LN)-type structure. Although there are synthesis reports of LN phase with (Mg,Fe,Ca,Mn)$Al_2Si_3O_{12}$ natural garnet (Funamori et al., 1997; Miyajima et al. 1999), synthesis with composition of pyrope end-member is first time and this structure refinement has never been made. Therefore, we made the Rietveld refinement of LN phase with pyrope composition. We also introduce high-pressure generation technique for synthesis over 40 GPa with a Kawai-type multianvil press (KMAP) in this study.
We used a 15-MN KMAP with DIA-type guide blocks carefully optimized to make a cubic compression space formed by first-stage anvils. WC anvils (TF05, Fujilloy Co., Ltd) of 1.5 mm truncation with 1.0 degree tapering were adopted for generating pressure over 40 GPa, combining a semi-sintered MgO + 5wt.%Cr_2O_3 octahedron as a pressure medium. Pressure at 2000 K was estimated with Al_2O_3 content in aluminous Brm by Liu et al. (submitted). Sintered ilmenite-type $Mg_3Al_2Si_3O_{12}$ (py-Ak) was synthesized as starting material at 26 GPa and 1200 K (Kubo and Akaogi, 2000) to minimize the pressure drop for volume change by phase transition. Sample was put in Re furnace surrounded by a $LaCrO_3$ thermal insulator. Al_2O_3 rods were placed at the both end of the sample in a heater and these were separated with Re disks. A microfocus X-ray diffractometer and an FE-SEM-EDS were used to analysis phase and composition of recovered sample. Synchrotron XRD data for Rietveld analysis were collected rotating sample at ambient conditions in SPring-8 (BL10XU). Rietveld refinement of recovered sample was performed using the RIETAN-FP/VENUS package (Izumi and Momma, 2007).
R factors for structure refinement were converged to reasonable values (R_{wp}, R_B and R_F<5). Lattice parameters of this phase with space group of R3c were determined as a = 4.8196(3) Å, b = 4.8195(3) Å, c = 12.6877(8) Å, V = 255.2(1) Å^3.

Keywords: LiNbO3 structure, Rietveld refinement, High-pressure generation technique, akimotoite, pyrope, Kawai-type multianvil press

