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

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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

