Synthesis of LiNbO$_3$-type Mg$_3$Al$_2$Si$_3$O$_{12}$ 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$_2$O$_3$ 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$_2$Si$_3$O$_{12}$ 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$_2$O$_3$ octahedron as a pressure medium. Pressure at 2000 K was estimated with Al$_2$O$_3$ content in aluminous Brm by Liu et al. (submitted). Sintered ilmenite-type Mg$_3$Al$_2$Si$_3$O$_{12}$ (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$_2$O$_3$ 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 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/VEENUS 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