Japan Geoscience Union Meeting 2010
(May 23-28 2010 at Makuhari, Chiba, Japan)

SMP056-07 Room: Exibition hall 7 subroom 2 Time: May 23 10:45-11:00

Crystal structure refinement of K- and Na-hexagonal aluminous phases using the Rietveld method

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A hexagonal aluminous phase is one of candidates for an Al-rich phase in high-pressure phases of mid-ocean ridge basalt. Since potassium is contained in an hexagonal aluminous phase with natural composition, it is expected that the hexagonal aluminous phase might be a host phase of potassium in the deep Earth's mantle. A crystal structure of the hexagonal aluminous phase has been determined by Miura et al. (2000) and Gasparik et al. (2000). However, a detailed structure has not been clarified yet. In this study, we tried to synthesize a hexagonal aluminous phase in the $KAlSiO_4$-$MgAl_2O_4$system under high-pressure. Then, the crystal structures of hexagonal aluminous phases in the systems $NaAlSiO_4$-$MgAl_2O_4$and $KAlSiO_4$-$MgAl_2O_4$were refined using the powder X-ray diffraction profiles. By comparing structures among Na- and K- hexagonal aluminous phases obtained in this study and $CaMg_2Al_6O_{12}$hexagonal aluminous phase, it will be cleared how cation sites in the structure are adjusted by changing a size of accommodated cations. The K-hexagonal aluminous phase was synthesized by heating a $KMg_2Al_5SiO_{12}$gel at 20 GPa, 150 0 C for 1 hour. The Na-hexagonal aluminous phase was synthesized by holding the mixture of $MgAl_2O_4$spinel and $NaAlSiO_4$carnegieite with the composition of 40:60 mol% at 22 GPa and 1500 C for 2 hours. Compositions of recovered samples of K- and Na-hexagonal aluminous phases were determined to be $K_{1.00}Mg_{2.00}Al_{4.80}Si_{1.15}O_{12}$and $Na_{1.04}Mg_{1.88}Al_{4.64}Si_{1.32}O_{12}$, respectively, using SEM-EDS. Their powder X-ray diffraction profiles were observed using Cr K-alpha (45 kV, 250 mA) in the 2-theta range of 10 to 140 degree. RIETAN-2000 program was used for the Rietveld refinement. R factor of the Rietveld analysis for the $K_{1.00}Mg_{2.00}Al_{4.80}Si_{1.15}O_{12}$(Rwp = 11.1%) supports that it has the crystal structure of the hexagonal aluminous phase. This is the first report of the synthesis of K-hexagonal aluminous phase endmember. When a general chemical formula of the hexagonal aluminous phase is represented as $[M3][M2]_2[M1]_6O_{12}$, it was suggested that sizes of the M3 and M2 sites are adjusted by deformation of $M1O_6$octahedra rather than change of bond angles between $M1O_6$octahedra. In the $NaAlSiO_4$-$MgAl_2O_4$system, smaller ionic radius of Na^+than $K^+$and shrinkage of $M1O_6$octhahedra with the substitution reaction: Mg^{2+}+ Al^{3+}=> Na^++ Si^{4+}might allow the Na-hexagonal aluminous phase to have a relatively wide compositional range.

Keywords: hexagonal aluminous phase, crystal structure, Rietveld refinement, high-pressure phase, potassium, sodium