In situ X-ray diffraction study of aluminous phases

Toru Shinmei[1]; Daisuke Yamazaki[2]; Takeshi Sanehira[2]; takehiro kunimoto[3]; Akihiro Yamada[2]; Toru Inoue[2]; Tetsuo Irifune[2]; Ken-ichi Funakoshi[4]

[1] GRC, Ehime Univ; [2] GRC, Ehime Univ.; [3] GRC,Ehime Univ.; [4] JASRI

Many previous studies on phase relations in the subducted oceanic crust have shown that several aluminous phases (Al-rich phase or NAL phase) are formed under the lower mantle conditions. These minerals would play an important role in the deep mantle as host phases of alkaline elements especially Na and K. Aluminous phase was first reported by Irifune and Ringwood (1993) in the study of phase relations for mid-oceanic ridge basalt (MORB) composition but its structure was not fully identified. Thereafter Hirose et al. (1999), Funamori et al. (2000) and Ono et al. (2001) reported the aluminous phases occurred in MORB compositions had a calcium ferrite (CF) type structure with orthorhombic symmetry. In contrast, Akaogi et al. (1999), Miura et al. (2000) and Gasparik et al. (2000) showed the aluminous phases had a hexagonal structure. Moreover, both CF-type phase and hexagonal phase coexisted in the studies of Miyajima et al. (2001) and Hirose and Fei (2002). Aluminous phases indeed reveal rather complex solid solution and the occurrence of aluminous phases and their structure severely depend on the bulk chemical composition (Guignot and Andrault, 2004). In this manner, the stability and structural features of such aluminous phases have not been well known. In contrast, several equations of state (EOS) for such aluminous phases have been reported, however, the data were only from the room temperature compression studies. In order to understand the deep mantle phenomena, high temperature behavior is needed at all cost. In this study, we have conducted in situ X-ray diffraction experiments to clarify the stability and thermoelastic properties of aluminous phases in simple compositions, NaAlSiO4-MgAl2O4 system using a combination of multianvil apparatus and synchrotron radiation.

Oxide mixtures in proportion equal to NaAlSiO4 and NaMgAl3SiO8 were used as starting materials. Pressure was determined from the gold powder mixed with the sample using an equation of state for gold proposed by Anderson et al. (1989). Runs were conducted at pressure up to 25 GPa and temperature up to 1900 K. After taking X-ray diffraction patterns at ambient condition, samples were compressed to the desired press load at room temperature and then heated to the maximum temperature. X-ray diffraction profiles were collected on cooling stage to minimize the effect of non-hydrostatic stress stored during room temperature compression for determinations of pressure and unit cell parameters.

For NaAlSiO4 composition, an aluminous phase with CF-type structure was observed in this study. On the other hand, the diffraction patterns for NaMgAl3SiO8 composition can be refined as a hexagonal structure and no phase transition was observed in the present P-T conditions. Obtained P-V-T data sets for aluminous phases were analyzed using the high-temperature Birch-Murnaghan (HTBM) equation of state.

The fit for NaAlSiO4 CF-type phase yields the isothermal bulk modulus K0 = 184 (2) GPa, its pressure derivative K'0 = 3.5 (2), temperature derivative (dKT/dT)P = -0.024 (3) GPa K-1, thermal expansivity a (T) = 3.16 (6) x 10-5 + 8.4 (1.6) x 10-9 T and unit-cell volume at ambient condition V0 = 240.45 (5) A3. When K'0 is fixed to 4.0, K0 = 179.5 (7) GPa, (dKT/dT)P = -0.030 (2) GPa K-1, a (T) = 3.22 (5) x 10-5 + 1.1 (1) x 10-8 T and V0 = 240.52 (5) A3 are obtained. For NaMgAl3SiO8 hexagonal phase, K0 = 176 (2) GPa, K'0 = 4.9 (3), (dKT/dT)P = -0.030 (3) GPa K-1 and a (T) = 3.36 (6) x 10-5 + 7.2 (1.9) x 10-9 T are obtained with fixed value of V0 = 182.77 A3. When K'0 is fixed to 4.0, K0 = 181.7 (4) GPa, (dKT/dT)P = -0.020 (2) GPa K-1 and a (T) = 3.28 (7) x 10-5 + 3.0 (9) x 10-9 T are obtained. The derived bulk moduli of both phases reveal slightly small values compared to the previous results obtained from the room temperature compression studies using diamond anvil cell.