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Effect of pressure on the crystal structure of dense hydrous magnesium silicate Al-phase E

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A single crystal of Al-phase E, was synthesized by Kawamoto et al. (1995)[1] using a multi-anvil apparatus at conditions of 9.3 GPa and 875 ˚C. Electron microprobe analysis of the specimen showed a chemical composition of 39.7wt% SiO_2, 4.9 wt% Al_2O_3, 9.5 wt% FeO, and 45.9 wt% MgO, yielding at total (H_2O excluded) wt% of 87.2 If the difference of the total weight is ascribed to H_2O, the unit cell content is calculated to be $Mg_{1.98}Fe_{0.23}Al_{0.17}Si_{1.15}H_{2.47}O_6$. A blue transparent single crystal fragment, 59x35x24μm in size, was placed in the modified Merrill-Bassett type diamond anvil pressure cell. The 4:1 fluid mixture of methanol and ethanol was used for pressure medium and SUS301 plate was used for gasket. The pressure was calibrated using the ruby fluorescence method. Sets of X-ray diffraction intensities at high pressures up to 3.8 GPa were measured using synchrotron radiation at the beam line BL-10A, Photon Factory, High Energy Accelerator Reasearch Organization, Tukuba, Japan. The wave length λ=0.6984 Å) was calibrated by the unit cell constants of a ruby standard crystal. Data at room pressure were measured with MoKα radiation using another fragment, 94x47x24μm in size, of the same single crystal. Table 1 lists the mode of data collection. Lattice constants at various pressures are presented in Table 2. The Al-bearing phase E has significantly short c-axis repeat period compared to that of the Al-free phase E. Kudoh et al. (1993) reported the lattice constants, a=2.9701(1) Å, c=13.882(1) Å, V=106.06(4) $Å^3$ for phase E , $Mg_{2.08}Si_{1.16}H_{3.20}O_6$, and a=2.9853(6) Å, c=13.9482(7) Å, V=107.65(4) $Å^3$ for phase E , $Mg_{2.17}Si_{1.01}H_{3.62}O_6$. Yang et al. (2002) reported the lattice constants, a=2.981(1) Å, c=13.898(3) Å, V=107.0(1) $Å^3$ for phase E , $Mg_{2.22}Fe_{0.52}Si_{0.98}H_{2.08}O_6$. The short repeat period of the Al-bearing phase E is considered to be due to the occupation of Al^{3+} at octahedral site by replacing Mg^{2+}. As pointed out by Yang et al. (2002)[2], the following three mechanism may be the most important and common for the substitution of trivalent cation into phase E:

(1) $2R^{3+} + \square \rightarrow 3Mg^{2+}$;
(2) $R^{3+} + H^+ \rightarrow Si^{4+}$;
(3) $2R^{3+} \rightarrow Mg^{2+} + Si^{4+}$;
'□' means vacancy.

In the case of Al-phase E, $R^{3+}= Al^{3+}$. Since the ionic radii of $^{iv}Al^{3+}$(=0.39Å) > $^{iv}Si^{4+}$ (=0.26 Å) and $^{vi}Al^{3+}$(=0.53Å) < $^{vi}Mg^{2+}$ (=0.72 Å), the facts that the unit cell volume of Al-bearing phase E is smaller than that of Al-free phase E at room pressure and the compressibility of the c-axis is slightly larger than that of the a-axis indicate that mechanism (1) should dominate for the formation of Al-bearing phase E.

Table 1. Mode of data collection

Size of the crystal	59x35x24μm
Wave length	0.6984 Å
$2\theta_{max}$	85°
Scan mode	ω scan

Table 2. Lattice constants at various pressures

P (GPa)	a (Å)	c (Å)	V ($Å^3$)
0.0*	2.968	13.798	105.3
1.5	2.956	13.731	103.9
3.4	2.945	13.678	102.7
3.8	2.938	13.642	102.0

*Data at room pressure were measured with MoKα radiation.

Table 3. Lattice compression at various pressures

P (GPa)	a/a_0	c/c_0	V/V_0
1.5	0.9960	0.9951	0.9867
3.4	0.9923	0.9913	0.9753
3.8	0.9899	0.9887	0.9687

References

[1] T. Kawamoto, K. Leinenweber, R. L. Hervig, J. R. Holloway , *Proceedings of Conference of Volatiles in Deep Earth and Planets*, American Institute of Physics, (1995)

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