

Thermal equations of state of MgSiO_4H_2 phase H up to 63 GPa determined by in situ X-ray diffraction measurement in a multianvil apparatus

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Hydrous minerals deliver a certain amount of water into the Earth's interior via subduction of oceanic plates. Following to the theoretical prediction on the thermodynamic stability of MgSiO_4H_2 phase H at above 35 GPa in 2013 (Tsuchiya 2013), some experimental studies have succeeded to identify the formation of this phase under high pressure and temperature conditions (Nishi et al. 2014; Ohtani et al. 2014; Walter et al. 2015). Phase H is now considered to be the key hydrous phase responsible for the water cycle in the whole mantle as the highest-pressure form of DHMS. However, the qualities of in-situ X-ray diffraction (XRD) profiles of phase H obtained in earlier studies were sometimes not enough to satisfy the precise determination of its cell parameters because phase H easily dehydrates at temperatures where spectroradiometry can be applied in laser-heated diamond anvil cell (DAC) experiments. Therefore, XRD peaks of phase H have been used basically only for its phase identification within very limited temperature ranges. Nishi et al. (2014) succeeded to obtain the cell parameters of phase H from multiple independent XRD peaks by using multianvil apparatus, which can accurately control the temperature of the sample. However, the data in limited pressure ranges of the previous study (32-42 GPa) were not applicable to construct the equation of state (EOS) of MgSiO_4H_2 phase H.

Here, we have determined the thermal equations of state of phase H by using in situ X-ray diffraction measurements in conjunction with a multi-anvil apparatus through its stability field from 34 to 63 GPa up to 1300 K. We succeeded to expand the experimental conditions up to 63 GPa by state-of-the-art high-pressure technology using sinter diamond anvils and Al_2O_3 pressure medium, which achieved higher pressures by ~20 % compared to those using the conventional MgO pressure medium in the similar design of the cell assembly used in Nishi et al. 2014. The data analysis based on the Mie-Grüneisen-Debye model using the third-order Burch-Murnaghan equations at the reference pressure of 35 GPa yielded $V_{\text{ref}} = 49.61 \pm 0.01$ (\AA^3), $K_{\text{ref}} = 344.6 \pm 4.1$ (GPa), $K'_{\text{ref}} = 3.05 \pm 0.32$, $\theta_{\text{ref}} = 974 \pm 146$ (K), $\gamma_{\text{ref}} = 1.8 \pm 0.1$, and $q = 1.79 \pm 0.55$. The compressibility of phase H observed in this study is in good agreement with that derived by theoretical calculation in the pressure regions where hydrogen bond symmetrisation is predicted to occur.

Keywords: Thermal equations of state, mantle, phase H, multianvil apparatus, water