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

*西 真之[1,2]、土屋 旬[1,2]、有本 岳史[1]、柿澤 翔[1]、國本 健広[1]、丹下 慶範[3]、肥後 祐司[3]、入舩 徹男[1,2]

*Masayuki Nishi[1,2], Jun Tsuchiya[1,2], Takeshi Arimoto[1], Sho Kakizawa[1], Takehiro Kunimoto[1], Yoshinori Tange[3], Yuji Higo[3], Tetsuo Irifune[1,2]

1. 愛媛大学地球深部ダイナミクス研究センター、2. 東京工業大学地球生命研究所、3. (財)高輝度光科学研究センター
1. Geodynamics Research Center, Ehime University, 2. The Earth-Life Science Institute, Tokyo Institute of Technology, 3. Japan Synchrotron Radiation Research Institute

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 $V_{ref,}$ =49.61±0.01 ($Å^3$), K_{ref}=344.6±4.1 (GPa), K_{ref}' =3.05±0.32, θ_{ref}=974±146 (K), γ_{ref} =1.8±0.1, and q = 1.79±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.

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