Hydrogen bearing Calcium Silicate Perovskite Synthesized at Mantle Related Pressure-Temperature Conditions

Huawei Chen¹, Sang-Heon Shim¹, Kurt Leinenweber², Yue Meng³, Vitali Prakapenka⁴, Hans A. Bechtel⁵ and Zhenxian Liu⁶

¹School of Earth and Space Exploration, Arizona State University, Tempe, AZ
²School of Molecular Science, Arizona State University, Tempe, AZ
³HPCAT, Carnegie Institution of Washington, Argonne, IL
⁴GeoSoilEnviroCARS, University of Chicago, Chicago, IL
⁵ALS, Lawrence Berkeley National Laboratory, Berkeley, CA
⁶Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC

Perovskite-structured CaSiO₃ (Ca-Pv) is the third most abundant mineral in the lower mantle. However, the solubility of H₂O in Ca-Pv is not well constrained. We have conducted in situ Xray diffraction (XRD) measurements on Ca-Pv under H₂O saturated and undersaturated conditions in a laser-heated diamond-anvil cell at the GSECARS and HPCAT sectors of the Advanced Photon Source with a YAG laser. CaSiO₃ glass or suolunite (CaSiO₃·H₂O) as a starting material were mixed with platinum powder (10 wt%) for YAG laser coupling and internal pressure scale. We have also conducted heating without laser coupler using a CO₂ laser heating system at ASU. Cold compressed foils were loaded in the diamond-anvil cell together with Ne or water. We have measured infrared spectra of CaSiO₃ samples both in situ and after recovery at 1 bar at the Advanced Light Source.

The XRD of Ca-Pv synthesized from dry starting materials in a Ne medium are consistent with a cubic perovskite structure at high temperatures up to 2,400 K at 50 GPa. However, in the experiments with either hydrous starting materials in a Ne medium and dry starting materials in a H₂O medium, clear splitting of the 200 diffraction line appears during heating to temperatures over 2000 K and remain after temperature quench at pressure up to 60 GPa. The peak splittings were clearly observed at high temperatures to 2400 K, which is close to the melting point of water at the pressure. We have observed clear OH mode from in-situ infrared measurement. The different structural behaviors of Ca-Pv depending on environment (with or without water) together with OH vibration mode identified from infrared spectrum suggest that hydrogen enters into the crystal structure of nominally anhydrous Ca-Pv phase at high pressure and high temperature.