Properties of ultra-high pressure hydrous silicates: experiment and theory

Joshua P. Townsend[1†], Jun Tsuchiya[2], Zhenxian Liu[3], Craig R. Bina[1], Steven D. Jacobsen[1]*

1. Dept. Earth and Planetary Sci., Northwestern University, Evanston IL 60201-3130
2. Geodynamics Research Center, Ehime University, Matsuyama Japan
3. Geophysical Laboratory, Carnegie Institution of Washington, Washington D.C.

*: Principal Investigator

†: Email: joshua@earth.northwestern.edu

Abstract Category: Materials

Abstract:

Here we present results of combined first-principles calculations using density functional theory (DFT) and high-pressure experiments to investigate the properties of dense silicate structures and the effect of small impurities of hydrogen on their physical properties, with applications to planetary interiors. In the Earth's lower mantle (P~120 GPa, T~3000-4000 K) the dominant mineral, perovskite, undergoes a phase transition to a recently discovered 'post-perovskite' (PPv) phase. Although PPv has only been synthesized in the laboratory, it is often invoked to explain deep seismic reflectors above the core-mantle boundary, however PPv alone cannot explain all the seismic observations. In the upper mantle, many minerals can accommodate small amounts of hydrogen (usually by means of a cation exchange defect), which greatly affects their physical properties such as elasticity. Therefore, to study the possible influence of hydrogen on the physical properties of PPv, we have used density functional theory to explore several potential hydrous post-perovskite (hPPv) structures and their associated elastic properties (fig1.), thermal stabilities, and IR signatures. We will present a comparison of the observed elastic properties of the D" region with the calculated elastic properties of hPPv, as well as calculated FTIR spectra for comparison to ongoing experiments using a new CO_2 laser-heating system and synchrotron-FTIR spectroscopy at the National Synchrotron Light Source.

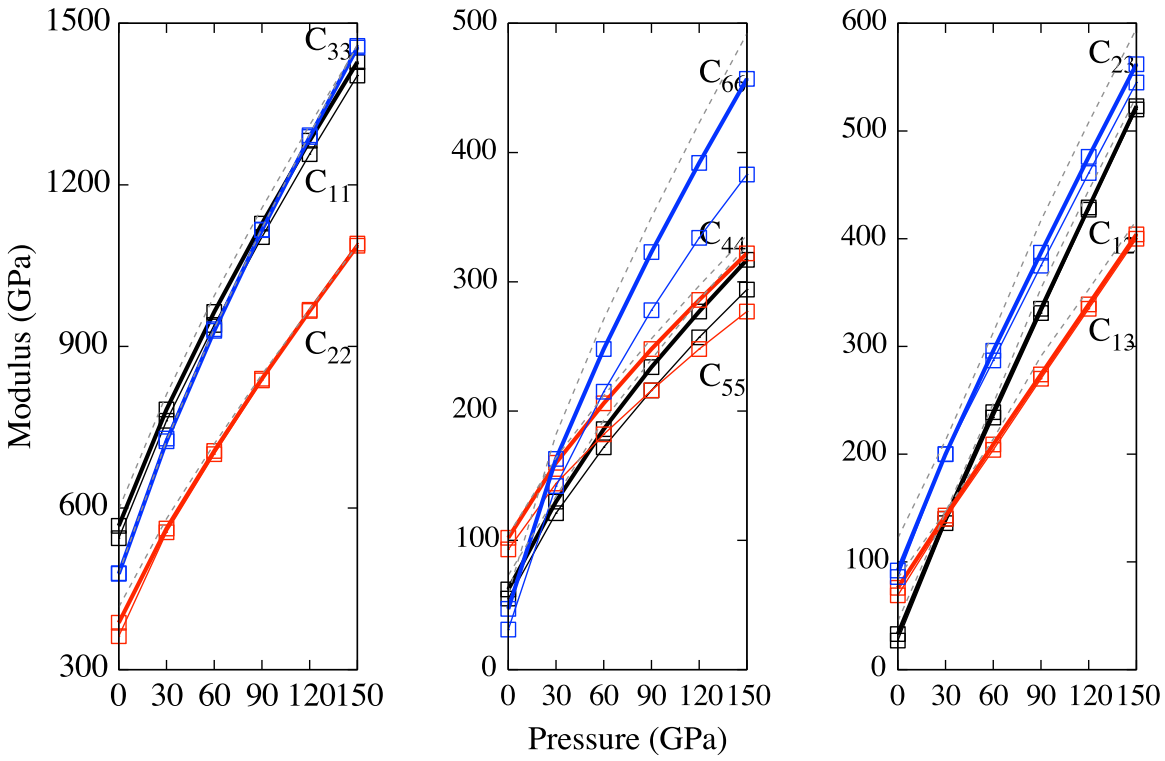

Figure 1: Elastic tensor components for hPPv (solid lines), compared to dry PPv (dashed lines). Addition of 800 ppm H to PPv reduces stiffnesses by ~3-20%