

Exploring a hydrous lowermost mantle

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The lowermost mantle (D) is characterized by high anisotropy, shear-wave splitting, and high seismic attenuation. The presence of post-perovskite (PPv) in the D layer would contribute to these seismic observables, and therefore the influence of compositional variability on the physical properties of PPv should be explored to test mineralogical models of D against the observed seismic structure. Here, we explore the influence of hydrogen on the silicate post-perovskite phase by experiment and theory. The presence of hydrogen in the core-mantle boundary region, either as primordial H diffused from the liquid outer core or added by deeply subducted slabs, could potentially influence PPv physical properties and its phase stability. The OH-storage capacity of perovskite is likely much lower than PPv so the presence of OH could also influence the structure of D. In the upper mantle, even small amounts of OH at concentrations less than 0.1 wt% can influence elastic properties and lattice preferred orientation. To study the possible influence of hydration on the mineral physics of PPv, we have used density functional theory to explore several potential hydrous post-perovskite (hPPv) structures and their associated elastic properties, 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 CO₂ laser-heating system and synchrotron-FTIR spectroscopy at the National Synchrotron Light Source.

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