Elastic Properties of Hydrous lower mantle and D" layer minerals

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The D'' layer, above the CMB. contains strong seismic anisotropy and is characterized by an anticorrelation between the shear and bulk wave velocities, seismic discontinuity, large low-shear-velocity provinces (LLSVPs) with -1~-5% S-wave velocity anomaly, and a strong topography with laterally varying thickness from 0 to over 300km. The discovery of the phase transition from Bridgmanite (Brg) to post-Perovskite (PPv) at the pressure-temperature condition corresponding to the top of the D'' layer has been invoked to explain the seismic anomalous features within the D'' region. The effect of volatiles such as H on the Brg-PPv phase transition and physical properties has not been deeply explored yet.

In this study, the incorporation mechanisms and elastic properties of hydrous Bridgmanite (Brg) and post-Perovskite (PPv) are investigated by using first principles calculations at the lower mantle pressures. The elastic properties calculations in both (Al, Fe)-free and (Al, Fe)-bearing systems give evidences that hydrogen has less effect on the elastic wave velocities and moduli in (Al, Fe)-free and Al-bearing system. However, the elastic wave velocities and moduli, especially the shear velocity V_S and the shear modulus *G,* are remarkably sensitive to the presence of hydrogen in the Fe-bearing system. The calculated shear velocity anomaly ($\mathbf{d}V_S$) are -2.9% for $Fe^{3+}{}_{Si}H$-Brg and -3.1% for $Fe^{3+}{}_{Si}H$-PPv, which are very close to the average anomaly value of LLSVPs. This result may imply the Ferric-bearing hydrous $MgSiO_3$ is likely a dominated mineral in LLSVPs. Density functional perturbation theory (DFPT) and QHA calculation have also been performed to determine the P-T phase diagram for different hydrous systems. The phase transition boundary between Brg and PPv shifts to higher or lower pressures when the hydrogen atom substitutes in the Mg or Si sites in the lattice, respectively. The existence of volatiles such as hydrogen may account for the strong lateral chemical heterogeneity in lowermost mantle.

Reference

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