What can mineral physics tell us about the origin of ULVZs?

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The core-mantle boundary region is complex. In addition to large regions with reduced shear velocities (LLSVPs), there are small areas with shear velocities up to 30% lower than surrounding material, the so-called ultralow velocity zones (ULVZs). Although these heterogeneous regions are small (10 to 100 km), they have featured in speculation regarding an ancient global magma ocean, magnetic pole positions during reversals, core-mantle material exchange and the source of mantle plumes. Mineral physics provides important constraints in understanding the nature of ULVZs through the comparison of seismic data with experimental and computational studies of the relevant phases. Shear wave velocities are particularly important, and nuclear inelastic scattering (NIS) offers the attractive possibility to measure these velocities for iron-containing minerals in the laser-heated diamond anvil cell through direct measurement of the partial density of states (DOS). Complementary determination of the partial DOS using density functional theory (DFT) has shown the potential to identify experimental features that impact the velocity determination as demonstrated by our recent study on bridgmanite. We performed first-principles calculations to determine the iron partial DOS for $Mg_{0.75}Fe_{0.25}SiO_3$ post-perovskite. We calculated Debye sound velocities (which are closely related to the shear wave velocities) using the same approach as for experimental NIS data, and obtained velocities for $Mg_{0.75}Fe_{0.25}SiO_3$ post-perovskite that are consistent with literature values for $MgSiO_3$ and $FeSiO_3$ post-perovskite also calculated using DFT. In contrast, literature data on the Debye sound velocity determined experimentally using NIS is 35% lower than our calculated value, which led to previous suggestions that ULVZs originate from regions containing iron-rich post-perovskite. Our results show, however, that the lower NIS velocities in post-perovskite data likely arise from a similar artefact as the NIS bridgmanite data. The velocities derived from the DFT DOS of both bridgmanite and post-perovskite are consistent with seismic velocities of the bulk lower mantle, suggesting that ULVZs are likely not caused by iron-rich post-perovskite. Instead we favour previous suggestions that dense melts are a more plausible explanation.

Keywords: lower mantle, density functional theory, nuclear inelastic scattering, shear wave velocity, post-perovskite

