Effect of spin transition on composition and seismic structure of lower mantle

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Spin transition of iron in ferropericlase (Fp) causes a significant softening in bulk modulus (e.g., [1] [2]), which leads to unusual positive temperature dependence of V_P. Because rapid increasing of V_P with temperature in Fp cancels out with decreasing of V_P with temperature in silica perovskite, V_P of the lower mantle becomes insensitive to the temperature variation at the depth of ~1730 km [3], which is in consistence with some seismic tomography results[4] [5]. Obviously, the insensitivity of V_P to temperature at mid lower mantle dramatically depends on the content of Fp and iron content in Fp.

The composition of the lower mantle is critical for us to understand the Earth's interior and the mantle convection. Previous reports on the composition of the lower mantle are controversial. Using the high -temperature and -pressure velocities and density data of minerals obtained from first-principles calculations, we found that the aggregate constrained well by seismic model can vary from pyrolitic composition with ~ 15wt% ferropericlase (Fp) to perovskitic-rich composition. Any composition well constrained by seismic model, however, has enough amount of Fp to exhibit positive temperature dependence of the bulk sound velocity, which results in negative correlation between bulk sound and shear velocities at mid lower mantle without involving any composition variation. Spin crossover of iron in Fp significantly reduces the temperature sensitivity of P wave velocity of the aggregate at the depth of ~1730 km along the adiabatic geotherm.

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