Spin transition in Fe-bearing perovskite: implications for the lower mantle

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The Earth's lower mantle, which is the largest part by volume of our planet, is mainly formed of Fe- and Al- bearing $MgSiO_3$ perovskite (pv). The Fe-component exhibits a spin transition under pressure whose nature and outcome is still a matter of debate. Here we are using lattice dynamical calculations based on density functional perturbation theory to disentangle a part of its complex phase diagram and the spin behavior. To do this we investigate the dynamic stability of Pbnm $FeSiO_3$ pv and show the existence of unstable phonon modes. We track the eigen-displacements of the phonons modes to find low-spin and intermediate spin states. On solid-state physical basis we explore a set of hypothetical structures with various spin configurations and considerably lower enthalpy than the parent orthorhombic Pbnm structure. We show that the spin evolves along a high-spin to mixed high- and intermediate spin to low-spin transition sequence. We also analyze the thermal behavior of both high-spin and low-spin phases along the entire Mg-Fe solid solution and we discuss a first thermal phase diagram.

We discuss some of the implications of the spin transition on the physical properties of pv. We show that the elastic moduli and the bulk seismic wave velocities are weakly affected by the spin transition. However, the intrinsic differences in seismic anisotropy between the high-spin and low-spin phases of Fe-bearing pv coupled with lattice preferred orientation that can develop during mantle flow lead to distinct seismic signatures between the top and the bottom of the lower mantle [1]. These signatures are detectable by seismic observations and they need to be taken into account in tomographic studies of the Earth's lower mantle. We find that the electronic gap widens during crossover to the low-spin phase. This has a direct influence on the electrical conductivity and agrees qualitatively with in situ measurements [2]. Finally we show that the spin transitions can be observed experimentally in X-ray diffraction and Raman measurements.

References:
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[2] Ohta, K., Onoda, S., Hirose, K., Sinmyo, R., Shimizu, K., Sata, N., Ohishi, Y., Yasuhara, A. (2008), Science, 320, 89-91.