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Spin transition in Fe-bearing perovskite

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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.

Based on numerical results from first-principles calculations, we show that the spin transitions can be observed experimentally in X-ray diffraction and Raman measurements. New diffraction peaks form during the spin transition, which are explained by the associated symmetry breaking. Certain observable Raman peaks exhibit a shift at the transition; the Grueneisen parameters of certain few modes are affected by the transition.

The spin transition affects the seismic anisotropy pattern of perovskite. However it does not affect the elastic moduli and the bulk seismic wave velocities are weakly affected by the spin transition. [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.

Finally we show that the iron spin transition develops also in compressed glasses, but over a broad pressure range. More interestingly this transition can pass by an intermediate spin state configuration.

[1] Caracas, Mainprice, and Thomas (2010) Geophys. Res. Lett. 37, L13309.