The 21st Global-COE International Frontier Seminar

March 1st, 2011, from 16:30, at the meeting room (#486) 4F

Fe-bearing perovskite and post-perovskite: Phase stability, spin transitions, and the consequences for the lower mantle

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Using lattice dynamical calculations based on density functional perturbation theory we are able to disentangle a part of the complex phase diagram and spin behavior of the $(Mg,Fe)SiO_3$ perovskite (pv). 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. 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. These signatures are detectable by seismic observations and they need to be taken into account in tomographic studies of the Earth's lower mantle. Then we extend the field of investigation of the pv to post-perovskite (ppv) phase transition with a study of the double substitution Mg+Si =Al+Fe. We distinguish two crystallographic cases: $AlFeO_3$ and $FeAlO_3$, corresponding respectively to two ordered cases: one with Fe and then one with Al in octahedral coordination. The pv-ppv phase transition occurs between antiferromagnetic configurations at 90 GPa and is associated with a site exchange that triggers a partial collapse of the magnetic moment. The presence of $Al+Fe^{3+}$ in perovskite/post-perovskite renders the phase transition sluggish, induces a large density jump at the transition and contributes into maintaining a residual magnetic spindown to the base of the mantle. Following this transition path the elastic moduli show positive jumps. The phase transition is marked by a small positive jump in Vp and by a smaller negative jump in Vs. The effects of the Mg+Si ⇔ Al+Fe substitution on the seismic properties of $MgSiO_3$ pv and ppv depend on the crystallography of the substitution, namely the position the exchanged cations take in the structure.

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