## Composition of the Earth's lower mantle: Results from forward and inverse mineral physics modeling

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Increased knowledge of phase transitions, chemical interactions and thermoelastic properties of mantle phases enables us to carry out an up-to-date forward modeling of the radial structure of P and S wave velocities and density to the lower mantle depths for plausible compositional models inferred from geochemical and petrological studies. We found that a pyrolite composition along 1600K adiabatic geotherm can reproduce P and S wave velocities, Poisson's ratio, and density of the averaged properties of the lower mantle (PREM, AK135) reasonably well. Discrepancies in composition and geotherm reported in previous studies may result from poorly constrained thermoelastic properties of mantle phases, magnesium silicate perovskite in particular. The relative variations of P and S wavespeed due to lateral thermal effect are close to those observed by seismic tomography, ranging from 1.8 to 2.0 from the top to the lower part of the lower mantle. However, the negative correlation of bulk sound and shear wavespeed variation, as well as density versus shear speed near the base of the lower mantle is related to chemical anomalies. Alternatively, one can also use the radial properties of the Earth obtained from seismic data to invert composition and/or temperature. In this study, we excised this approach by inverting seismic data at different depth segments to investigate the possibility of compositional layering in the lower mantle as suggested by recent tomographic and geodynamic studies. In addition to an updated view about the mantle composition, these results from forward modeling can be incorporated into future seismic and geochemical studies.

## On the sharpness of the perovskite/post-perovskite transition in the Earth's mantle

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The phase transition of pure MgSiO<sub>3</sub> perovskite (Pbnm) to the post-perovskite (Cmcm) structure has been recently reported to occur at pressures and temperatures corresponding to the Earth's lowermost mantle [Murakami et al. 2004, Tsuchiya et al. 2004, Oganov and Ono 2004]. We use ab initio calculations to assess whether this transition survives, in the Earth, for more realistic mantle compositions containing Al,  $Fe^{2+}$ , and  $Fe^{3+}$ . We estimate phase coexistence pressures as functions of minor element concentration, and from this we obtain the effects of Al and Fe on the depth and sharpness of the transition. For a pyrolitic mantle composition, with all the Al partitioned into MgSiO<sub>3</sub>, we find that Al preferentially partitions into perovskite, and increases the transition pressure by approximately 5 GPa. The transition takes place over a depth range of width 225 km. Fe competes with Al by lowering the transition pressure [Mao et al. 2004], so that post-perovskite is likely to exist in the lower mantle. However, the transition is still smooth, and not likely to explain the sharp discontinuities observed seismically at the base of the mantle. Our results suggest the geodynamical implications of the post-perovskite phase transition require reevaluation.

## References

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