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Composition of the Lower Mantle: Predicted Properties from Atomistic Simulations

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The composition of the lower mantle is one of the most fundamental questions in geochemistry and constrains models of the Earth's formation. The density of the lower mantle, as given by PREM, does not provide a strong enough constraint to differentiate between pyrolite and chondritic earth compositions. A better approach is to fit a compositional model to the seismic velocities and total mass of the lower mantle. However, the seismic velocities of (Mg,Fe)SiO_3 perovskite and (Mg,Fe)O magnesio-wustite under lower mantle conditions are unknown. Several authors have made thermodynamic extrapolations of low pressure elastic properties to predict the seismic velocities of (Mg,Fe)SiO_3 perovskite and (Mg,Fe)O magnesio-wustite under lower mantle conditions.

An alternative, and more direct, approach is to predict mineral properties using atomistic (lattice dynamical) simulations. Such simulations, however, require accurate interatomic potentials. We derived as set of potentials in the shell and breathing-shell models by fitting to low pressure structures and elastic properties.

Our static (0 K) predicted seismic velocities and equations of state agree (within 5%) with recent first-principles calculations of the static high-pressure Vp, Vs and density for $MgSiO_3$ perovskite and MgO as obtained by Karki and Stixrude, (1999). Using lattice dynamics, however, we can predict the properties at high temperature in the quasi-harmonic approximation. We get very good predictions of heat capacities and thermal expansion coefficients at low pressure. Our high-pressure and high-temperature thermoelastic properties are also within 5% of the thermodynamic extrapolations of Hama & Suito (1999). We find that the temperature dependence of the velocities, Vp and Vs, decreases significantly with pressure. This has important consequences for the interpretation of seismic tomography data.

In order to determine the mineralogy of the lower mantle, we fit a mechanical mixture of (Mg,Fe)SiO_3, $CaSiO_3$, and (Mg,Fe)O to the PREM Vp, Vs and total lower mantle mass using a simulated annealing and downhill simplex optimization algorithm. We assumed a geotherm of 0.3K/km with a starting temperature of 2000K. Because of the small temperature dependence of the elastic properties at high pressure, our compositional model should be fairly insensitive to the chosen geotherm. We find that, within our estimated errors for the thermoelastic properties (about 5%) and densities (about 1%), a pyrolitic lower mantle is possible but a chondritic one is not. These results agree with those of Jackson & Rigden (1998) and Hama & Suito (1999).

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