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Thermal conductivity of minerals in the Earth's lower mantle from molecular dynamics

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Knowledge of the thermal conductivity of minerals at high temperatures and pressures is crucial for our understanding of heat transport in the Earth's lower mantle. Furthermore, the thermal conductivity of the mantle enters the Rayleigh number which determines the style of mantle convection. Despite their importance, little is known about thermal conductivities at deep-mantle conditions. Since direct measurements at the relevant temperatures and pressures are not feasible with current experimental techniques, most available data rely on extrapolations from low-P, T experiments to deep-mantle conditions. To overcome the inherent uncertainties, a computational approach is desirable.

We performed equilibrium molecular dynamics to calculate the thermal conductivities of MgO, $MgSiO_3$ perovskite (Pv), and $MgSiO_3$ post-perovskite (PPv), which are the Mg end-members of the most abundant mineral phases in the lower mantle. Using an advanced ionic interaction potential [1], the full conductivity tensor was calculated by means of the Green-Kubo approach. Our data points span a wide P, T range up to conditions representative of the core-mantle boundary. The results allowed us to parameterize the thermal conductivities of the individual phases as a function of density and temperature.

This model was then used to evaluate the thermal conductivity of the three mineral phases along a geotherm in the lower mantle. Assuming an iron-free mantle composition with mole fractions $x_{\mathrm{MgSiO_3}} = 0.66$ (in the Pv structure) and $x_{\mathrm{MgO}} = 0.34$ (corresponding approximately to volume fractions of 0.82 and 0.18, respectively), we predict that the average thermal conductivity of the two-phase aggregate raises with increasing density from 9.5 W/(mK) at the top of the lower mantle to 20.5 W/(mK) at the top of the thermal boundary layer above the core-mantle boundary. Due to the steep temperature rise across the thermal boundary layer, the thermal conductivity then drops to 16.4 W/(mK) at the core-mantle boundary. Based on experiments [2], we expect that a realistic amount of iron impurities reduces the thermal conductivity of the mineral aggregate by approximately 50%.

From the calculated thermal conductivity at the core-mantle boundary and a model geotherm, the heat flux across the core-mantle boundary can be calculated. It was found to be approximately 20 TW for an iron-free composition, and iron impurities are estimated to reduce it to about 10 TW. This relatively high core-mantle boundary heat flux is consistent with recent estimates of the heat flux required to generate and maintain mantle plumes.

[1] S. Jahn, P. A. Madden, Phys. Earth Planet. Int. **162**, 129 (2007)
[2] G. M. Manthilake *et al.*, PNAS **108**, 17901 (2011)