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Thermal Conductivity of Earth's Liquid Outer Core from First-Principles Calculations

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The ability of liquid iron to transport heat and electric charge by conduction at extreme pressure and temperature is of paramount importance to the thermal history of the core. Thermal conductivity determines the amount of heat conducted along the core adiabat, i.e. heat not available for generation of the magnetic field, and also strongly controls the time required for the inner core to reach its current size. Electrical conductivity sets the rate of magnetic field dissipation, and consequently the amount of energy required to sustain the geodynamo. Also, because these properties tightly control the heat budget within the core, they dictate the extent to which radiogenic heat need to be invoked to obtain thermal history models that are in agreement with geophysical and paleomagnetic observations.

Current estimates for electrical conductivity of iron at conditions characteristic of Earth's core are rather uncertain, constraining the value only to within a factor of three. Thermal conductivity values are subsequently obtained by applying the Wiedemann-Franz relation, the validity of which has not been rigorously shown at extreme pressures. In addition, electronic transport properties are expected to depend strongly on pressure (P) and temperature (T), as well as on the concentration (X) of light elements in the liquid metal. However, with no data available on these variations, geophysical studies in which these values are applied invariably assume them to be constant.

In an effort to improve our understanding of the P-T-X behavior of electronic transport properties in the core, and also to test the various assumptions made in their determination, we have performed first-principles calculations of the electrical and thermal conductivity of liquid iron over a large range of pressure and temperature conditions, including those characteristic of Earth's core. Compositions respectively doped with silicon, oxygen and sulphur are also considered. These calculations involve using first-principles molecular dynamics to generate a series of uncorrelated liquid structures at constant temperature and density, for which the electronic transport properties are then computed using the Kubo-Greenwood equation.

Our aim is to construct a parameterized model for the thermal and electrical conductivity of liquid iron as a function of pressure, temperature and light element composition, which can be applied in geodynamo simulations and thermal history models for planetary cores. Preliminary results indicate a strong pressure and temperature dependence, with the Wiedemann-Franz relation only approximately satisfied. Implications of these results for models of the thermal history of the core will be considered and discussed.