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Composition and temperature of Earth's inner core

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Abstract. We compare a theoretical prediction of the equation of state of iron at high pressures and temperatures to the properties of the Earth's inner core. The theoretical result is based on a first principles treatment of the static pressure and the pressure due to thermal excitation of electrons and an approximate ab initio (cell model) treatment of the vibrational pressure. The density of iron is found to be greater than that of the inner core even for unrealistically high temperatures of 8000 K. The isentropic bulk modulus of iron is found to be consistent with that of the inner core over a wide range of temperatures (4000–8000 K). We conclude on the basis of these comparisons that the inner core contains a substantial fraction of elements lighter than iron. Assuming ideal solutions, we find the temperature and light component mass fraction required to simultaneously match the density and bulk modulus of the inner core. For a temperature of 7000 K, 1 wt % O as FeO, satisfies the inner core observations. The temperature and mass fraction of S required depend on whether S is included as pyrite (2 wt % S, 5500 K) or as $Fe_{0.9}S$ (>8 wt % S, <3500 K). On the basis of this result and empirical mixing rules for Fe-O solutions, we argue that Fe-light element solid solutions at inner core conditions may be significantly nonideal. We derive expressions for the properties of nonideal multicomponent solutions that are valid in the limit of small amounts of impurities. These lead to general results for the properties of the alloy fraction that are required by comparisons of our equation of state of iron with seismological models.

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