

Properties of Iron and Iron alloys in the Inner Core

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Pressures (3.3 to 3.65 Mbar) and temperatures (above 5000 K) of the Earth's Inner Core (IC) still are too high for experiments. Theoretical methods, being successfully tested against reliable experimental data at comparably modest PT, can be applied at the IC conditions with the same reliability and provide valuable data on the IC material. Recent studies^{1,2} suggest that the hexagonal close-packed phase of iron, being the stable one at low T, might become less stable than the body-centered cubic phase at the high T of IC. The Gibbs energies of these phases become very close at the IC PT, perhaps beyond the resolution of what is currently available to ab initio methods³. In such a situation one needs to look at the indirect evidence. The indirect evidence tells us that the hexagonal phase becomes isotropic¹ at the IC conditions and can not be preferentially oriented to reproduce the IC elastic anisotropy⁴, while bcc phase is highly anisotropic⁵ and allows to reproduce seismic data⁶. Addition of Si promotes stability of bcc phase⁷ and deteriorates the stability of hcp phase⁸. Shear modulus of bcc phase at high T is very low and allows to reproduce PREM data^{9,10,11}. There are indirect experimental evidences for the bcc stability as well^{2,12}. Recent theoretical advances brought various estimates of iron melting T at the pressure of 3.3 Mbar to consensus of 7000 K^{13,14,15}. This might lead to higher T in the core than was thought before. This, in turn, might lead to reconsidering outer core temperatures and, thus, the temperature on the core side at the CMB.

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