

Is BCC-Fe stable in the Earth's inner core ?

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The nature of the stable phase of iron (Fe) in the Earth's solid inner core is still highly controversial, with both experiments¹ and seismology² suggesting the occurrence of an uncharacterised phase transformation in the core. Theory³⁻⁴ currently suggests that the hexagonal close packed (*hcp*) phase of Fe is stable at core pressures (P). Simulations also indicated that the body-centred-cubic (*bcc*) phase of Fe becomes elastically unstable at high-P. However, in other *hcp* metals a high-P *bcc* form is stabilized at high temperature (T). We report here the very first computational study of *bcc*-Fe able to model its behaviour at core P and T, using *ab initio* molecular dynamics free-energy calculations. We find that *bcc*-Fe indeed becomes entropically stabilised at core temperatures, but in its pure state *hcp*-Fe still remains thermodynamically more favourable. The inner core is not, however, pure Fe. Our calculations show that if the inner core contains ~8 mole% S or Si, then these impurities may stabilize *bcc*-Fe at the expense of the *hcp* form. At core P and T conditions, *bcc*-Fe has a Poisson's ratio ~0.45, and its occurrence in the upper part of the inner core could explain the seismically distinct nature of this region².