Stabilization of body-centred cubic iron under Earth's core conditions

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Abstract

The Earth's solid core is mostly composed of iron. However, the stable phase of iron under inner-core conditions remains uncertain. The two leading candidates are hexagonal close-packed (hcp) and body-centred cubic (bcc) crystal structures, but the dynamic and thermodynamic stability of bcc iron under inner-core conditions has recently been challenged. We demonstrate the stability of the bcc phase of iron under conditions consistent with the centre of the core using *ab initio* molecular dynamics simulations. We find that the bcc phase is stabilized at high temperatures by a novel diffusion mechanism that arises due to the dynamical instability of the phase at lower temperatures [1]. 1. A. B. Belonoshko, T. Lukinov, J. Fu, J. Zhao, S. Davis, and S. I. Simak, "Stabilization of body-centred cubic iron under inner-core conditions", *Nature Geoscience* **10,** 312 (2017).

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