

LETTER

High-pressure magnetic transition in hcp-Fe

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ABSTRACT

High-pressure experiments and ab initio calculations on the hexagonal close-packed (hcp) structure of pure iron were performed to investigate a pressure-induced magnetic transition and the equation of state in the pressure range of 0–107 and 0–400 GPa, respectively. The experimental data at room temperature showed a significant change in the cell parameter ratio at 55 GPa without any major structural changes occurring. Ab initio calculations at 0 K indicate that the change in the cell parameter ratio observed in the high-pressure experiments corresponds to a magnetic transition from an antiferromagnetic state to a nonmagnetic state. If the hcp-Fe is stable under inner core conditions, then the density of nonmagnetic hcp-Fe is ~6% denser than that of the inner core, as determined using the PREM model. This supports the view that the composition of the inner core should be composed of iron and a significant amount of lighter elements.

Keywords: Iron, high pressure, magnetic transition, inner core