

Abstract Submitted
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On the stability of body-centered cubic Fe at Earth's core conditions VEKILOVA OLGA, SIMAK SERGEI, ABRIKOSOV IGOR, Linköping University, Linköping, Sweden — Elucidation of Earth's core content and structure is extremely important for understanding Earth's behavior influencing human life, from geodynamics to earthquakes. Though cosmochemical and geochemical studies strongly suggest that solid Fe is the main constituent of the inner core, its exact content and crystal structure are still a matter of debate. The recent experiments reported controversial results of phase stability. Dubrovinsky *et al.* showed stabilization of the body centered cubic (bcc) phase of Fe alloyed with 10 at. % of Ni at pressures above 225 GPa and temperatures over 3400 K [1]. Tateno *et al.* on pure Fe at up to 377 GPa and 5700 K, no bcc phase was observed [2]. We offer a resolution of this contradiction based on finite temperature first-principles molecular dynamics calculations of elastic properties of both bcc Fe and Fe₉₀Ni₁₀ alloy at high-temperature high-pressure conditions. We indicate the stability range for the bcc phase of high-pressure high-temperature Fe and show how experimental conditions may cause diverse phase stabilization. REFERENCES [1] L. S. Dubrovinsky *et al.* Body-centered cubic iron-nickel alloy in Earth's core. *Science* **316**, 1880-1883 (2007). [2] S. Tateno, K. Hirose, Y. Ohishi, Y. Tatsumi. The structure of iron in Earth's inner core. *Science* **330**, 359-361 (2010).

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