Prediction of a new phase transition pathway for Fe under pressure

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Abstract:

Iron is the main component of the earth's core (the solid inner-core below the liquid outer-core which is liquid) [1-3], thus, the understanding of the physical phenomena relative to this earth's area remain up to now a subject of great scientific interest in geophysics. The nature of the stable phase of iron in the Earth's solid inner core is still highly controversial. Many experimental studies suggest the possibility of other phase transformation in iron at the core conditions. Experimental observations [4, 5] have indicated the possible presence of complex, inner-core layering. In the other side, the theoretical studies [6, 7] suggest that the *hcp* phase of iron is stable at core pressures and that the *bcc* phase of iron becomes elastically unstable at high pressure [8].

In this work, a density functional theory is applied to investigate the relative stability of Fe in different phases (*bcc*, *fcc* and *hcp*) for both the nonmagnetic (NM), ferromagnetic (FM) and anti-ferromagnetic (AFM) states as well as the effect of pressure. From the calculated enthalpy as a function of pressure, we predict the phase transition pathway for Fe at T = 0 K as: *bcc* (FM) $\xrightarrow{10GPa}$ *hcp* (AFM2) $\xrightarrow{30.2GPa}$ *hcp* (NM) $\xrightarrow{116GPa}$ *fcc* (FM). A new intermediate, which is the *hcp* (AFM2) phase, was obtained. The resulting enthalpy of each phase indicates that the *hcp* AFM2 phase is more favorable than the *hcp* NM phase, thus we suggest the existence of novel transition under pressure from *bcc* FM to *hcp* AFM2 phase around 10 GPa. The calculated elastic constants C_{ij} for the preferred pressure induced transition phases satisfy the criteria for elastic stability. Also these phases are dynamically stable based on the phonon dispersion and phonon total density of states considerations.

Keywords: Density functional theory; Phase transition; Ferromagnetism; Phonon; Transition elements.

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