Synthesis and Compression study of orthorhombic $Fe_7(C, Si)_3$: A possible constituent of the Earth's core

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Earth is understood to have a solid inner core predominantly consisting of Iron or its alloy with other light elements, such as Si, C, S etc. Several experimental studies have reported the presence of iron carbides with different composition and crystal structure [1,2,3]. A recent, theoretical simulation study [4] comparing the hexagonal, orthorhombic pure phases of Fe_7C_3 and silicon (Si) doped hexagonal, orthorhombic phases of Fe_7C_3 showed that values of density and Poisson's ratio of orthorhombic(*o*) Fe7(C, Si)$_3$ at inner core to be very close to the Preliminary Reference Earth Model (PREM) data [5]. The above study proposed orthorhombic Si-doped Fe carbide (*o*−Fe7(C, Si)$_3$) with 3.2 wt % of Si at C cite to be one of the most important component of the Earth's inner core.

In the present work we have synthesized orthorhombic Si doped Fe_7C_3, by creating conditions of Earths interior using laser heated diamond anvil cell. Orthorhombic phase of Si-doped Fe carbide is characterized using Transmission Electron Microscopy (TEM), Raman spectroscopy, and X-ray diffraction (XRD) measurements. Mapping of the chemical composition of the sample using transmission electron microscopy suggest that 17% of C site is replaced by Si. We have carried out high pressure X-ray diffraction analysis to map out the equation of state of the sample and found that the material remains in its parent phase. But High-pressure compression behaviour of our sample reveals two anomalies around 28 and 75 GPa and anisotropic compression of the unit cell. Isothermal bulk modulus shows elastic stiffening around 28 GPa followed by an elastic softening around 75 GPa. We attribute these anomalies to the magnetic transitions. Estimation of bulk modulus values at inner core pressures using the obtained equation of state parameters, gives values those match within 6-7% of PREM data. Extrapolation of density of the high pressure orthorhombic phase to inner core conditions suggest values lower by 1-2% with respect to PREM data. Our results indicate that the present orthorhombic phase to be a strong contender for the composition of Earths inner core.

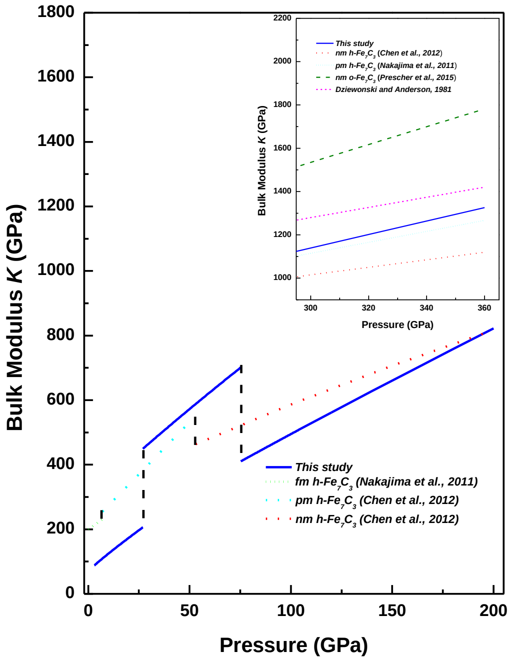

Figure. 1. *K* value of o − Fe7(C, Si)$_3$ at 300 K as a function of pressure, estimated using parameters obtained from fitted 3rd-order B − M EOS in our study (blue lines), ferromagnetic (fm)- phase of h − Fe_7C_3 (green short dashed line, *Nakajima et al.* (2011) [1]), paramagnetic(pm)-phase of h − Fe_7C_3 (cyan dotted line, *Chen et al.* (2012)), and nonmagnetic (nm)-phase of *h* − Fe_7C_3 (red dotted line, *Chen et al.* (2012) [2]). Inset: *K* extrapolated to core pressure at 300 K of our study (blue line), pm-phase of h − Fe_7C_3 (cyan short dotted line, *Nakajima et al.* (2011) [1]), nm-phase of *h*−Fe7C3 (red dotted line, *Chen et al.* (2012) [2]), nm-phase of *o*−Fe_7C_3 (olive dashed line, *Prescher et al.* (2015) [3]), PREM data (Magenda short dashed line, *Dziewonski* & *Anderson* (1981) [5]).

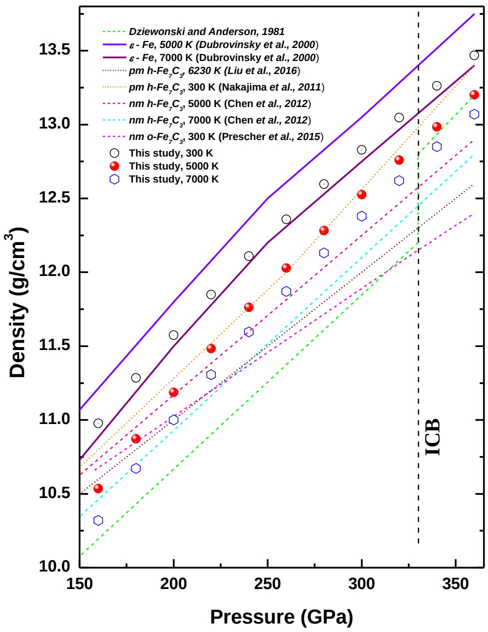

Figure.2. Comparison of densities of ε − Fe, Fe_7C_3, and *o* − Fe7(C, Si)$_3$ at the Earth's core pressures. Green short dashed line is density profile of PREM (*Dziewonski* & *Anderson*, 1981 [5]). Violet and purple solid curves represent isothermal density profile ε − Fe at temperatures 5000 K and 7000 K (*Dubrovinsky et al.*, 2000 [6]). Orange and wine short doted lines show density profile of pm-*h* − Fe_7C_3 at 300 K (*Nakajima et al.*, 2011 [1]) and 6230 K (*Liu et al.*, 2016 [7]). Pink and cyan short dashed lines are the density profile of nm *h* − Fe_7C_3 at 5000 K and 7000 K (*Chen et al.*,2012 [2]). Magenta short dashed line represents density profile of nm *o* − Fe_7C_3 at 300 K (*Prescher et al.*, 2015[3]). Black circles, filled red circles, and blue diamonds represent the density profile at 300 K, 5000 K, and 7000 K in our study obtained by extrapolating the density.

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