

***P-V-T* measurements of Fe₃C to 117 GPa and 2100 K: Implications for stability of Fe₃C phase at core conditions**

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ABSTRACT

We report the thermal Equation of State (EoS) of the non-magnetic Fe₃C phase based on in situ X-ray diffraction (XRD) experiments to 117 GPa and 2100 K. High-pressure and temperature unit-cell volume measurements of Fe₃C were conducted in a laser-heated diamond-anvil cell. Our pressure-volume-temperature (*P-V-T*) data together with existing data were fit to the Vinet equation of state with the Mie-Grüneisen-Debye thermal pressure model, yielding $V_0 = 151.6(12) \text{ \AA}^3$, $K_0 = 232(24) \text{ GPa}$, $K_0' = 5.09(46)$, $\gamma_0 = 2.3(3)$, and $q = 3.4(9)$ with $\theta_0 = 407 \text{ K}$ (fixed). The high-*T* data were also fit to the thermal pressure model with a constant αK_T term, $P_{\text{th}} = \alpha K_T(\Delta T)$, and there is no observable pressure or temperature dependence, which implies minor contributions from the anharmonic and electronic terms. Using the established EoS for Fe₃C, we made thermodynamic calculations on the *P-T* locations of the breakdown reaction of Fe₃C into Fe₇C₃ and Fe. The reaction is located at 87 GPa and 300 K and 251 GPa and 3000 K. An invariant point occurs where Fe, Fe₃C, Fe₇C₃, and liquid are stable, which places constraints on the liquidus temperature of the outer core, namely inner core crystallization temperature, as the inner core would be comprised by the liquidus phase. Two possible *P-T* locations for the invariant point were predicted from existing experimental data and the reaction calculated in this study. The two models result in different liquidus “phases” at the outer core-inner core boundary pressure: Fe₃C at 5300 K and Fe₇C₃ at 3700 K. The Fe₇C₃ inner core can account for the density, as observed by seismology, while the Fe₃C inner core cannot. The relevance of the system Fe-C to Earth’s core can be resolved by constructing a thermodynamic model for melting relations under core conditions as the two models predict very different liquidus temperatures.

Keywords: Earth’s core, diamond anvil cell, Fe₃C, cohenite