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P-V-T measurements of Fe_3C to 117 GPa and 2100 K: Implications for stability of Fe_3C phase at core conditions

Chris McGuire[1,*], Tetsuya Komabayashi[1], Samuel Thompson[1], Geoffrey Bromiley[1], Takayuki Ishii[2], Eran Greenberg[3,†], and Vitali B. Prakapenka[3]

[1]School of GeoSciences and Centre for Science at Extreme Conditions, University of Edinburgh, Edinburgh EH9 3FE, U.K.
[2]Bayerisches Geoinstitut, University of Bayreuth, 95440 Bayreuth, Germany
[3]Center for Advanced Radiation Sources, The University of Chicago, Chicago, Illinois 60637, U.S.A.

Abstract

We report the thermal Equation of State (EoS) of the non-magnetic Fe_3C 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 Fe_3C 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) Å^3, K_0 = 232(24) GPa, K'_0 = 5.09(46), γ_0 = 2.3(3), and q = 3.4 (9) with θ_0 = 407 K (fixed). The high-*T* data were also fit to the thermal pressure model with a constant αK_T term, $P_{Th} = \alpha K_T(\Delta T)$, and there is no observable pressure or temperature dependence, which implies minor contributions from the anharmonic and electronic terms. Using the established EoS for Fe_3C, we made thermodynamic calculations on the *P-T* locations of the breakdown reaction of Fe_3C into Fe_7C_3 and Fe. The reaction is located at 87 GPa and 300 K and 251 GPa and 3000 K. An invariant point occurs where Fe, Fe_3C, Fe_7C_3, 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: Fe_3C at 5300 K and Fe_7C_3 at 3700 K. The Fe_7C_3 inner core can account for the density, as observed by seismology, while the Fe_3C 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, Fe_3C, cohenite