Thermoelastic property and high-pressure stability of Fe₇C₃: Implication for iron-carbide in the Earth's core

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ABSTRACT

To investigate the physical property of Fe₇C₃, we carried out in situ X-ray diffraction experiments using a Kawai-type multi-anvil apparatus and a diamond anvil cell up to 71.5 GPa and 1973 K. The carbide was found to be stable under these experimental conditions. However, we found anomalous behavior in its isothermal compression and thermal expansivity. These anomalies could be due to the magnetic phase transition in Fe₇C₃ from a ferromagnetic (*fm*) to a paramagnetic (*pm*) phase. The Curie temperature of 523 K at 1 bar (Tsuzuki et al. 1984) decreases with pressure, and the pressure-induced magnetic transition is estimated to occur at ~18 GPa and 300 K. The pressure-volume-temperature (*P-V-T*) data set for the *pm*-Fe₇C₃ was fitted by the Mie-Grüneisen-Debye (MGD) equation of state (EOS) and the following parameters were obtained: unit-cell volume $V_0 = 184.2 \pm 0.3$ Å³, bulk modulus $K_0 = 253 \pm 7$ GPa, the pressure derivative of bulk modulus $K'_0 = 3.6 \pm 0.2$, Grüneisen parameter $\gamma_0 =$ 2.57 ± 0.05, Debye temperature $\theta_0 = 920 \pm 140$ K, and $q = 2.2 \pm 0.5$, respectively, at zero pressure. The calculated density for Fe₇C₃ provides a good explanation for the density of the Earth's inner core obtained from seismological observations.

Keywords: Fe₇C₃, Earth's inner core, equation of state, in situ XRD measurement