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The high-pressure anisotropic thermoelastic properties of a potential inner core carbon-bearing phase, Fe_7C_3, by single-crystal X-ray diffraction

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Abstract

Carbon has been suggested as one of the light elements existing in the Earth's core. Under core conditions, iron carbide Fe_7C_3 is likely the first phase to solidify from a Fe-C melt and has thus been considered a potential component of the inner core. The crystal structure of Fe_7C_3, however, is still under debate, and its thermoelastic properties are not well constrained at high pressures. In this study, we performed synchrotron-based single-crystal X-ray diffraction experiment using an externally heated diamond-anvil cell to determine the crystal structure and thermoelastic properties of Fe_7C_3 up to 80 GPa and 800 K. Our diffraction data indicate that Fe_7C_3 adopts an orthorhombic structure under experimentally investigated conditions. The pressure-volume-temperature data for Fe_7C_3 were fitted by the high-temperature Birch-Murnaghan equation of state, yielding ambient-pressure unit-cell volume V_0 = 745.2(2) Å^3, bulk modulus K_0 = 167(4) GPa, its first pressure derivative K'_0 = 5.0(2), dK/dT = –0.02(1) GPa/K, and thermal expansion relation $\alpha_T = 4.7(9) \times 10^{-5} + 3(5) \times 10^{-8} \times (T - 300)$ K^{-1}. We also observed anisotropic elastic responses to changes in pressure and temperature along the different crystallographic directions. Fe_7C_3 has strong anisotropic compressibilities with the linear moduli $M_a > M_c > M_b$ from zero pressure to core pressures at 300 K, rendering the b axis the most compressible upon compression. The thermal expansion of c^3 is approximately four times larger than that of a^3 and b^3 at 600 and 700 K, implying that the high temperature may significantly influence the elastic anisotropy of Fe_7C_3. Therefore, the effect of high temperature needs to be considered when using Fe_7C_3 to explain the anisotropy of the Earth's inner core.

Keywords: Iron carbide, thermal equation of state, anisotropy, inner core, temperature effect; Physics and Chemistry of Earth's Deep Mantle and Core