American Mineralogist, Volume 103, pages 1568–1574, 2018

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

XIAOJING LAI[1,2,*,†], FENG ZHU[2,3], JIACHAO LIU[4], DONGZHOU ZHANG[2], YI HU[1,2], GREGORY J. FINKELSTEIN[2], PRZEMYSLAW DERA[2], AND BIN CHEN[2,*]

[1]Department of Geology and Geophysics, University of Hawai‘i at Mānoa, Honolulu, Hawaii 96822, U.S.A.
[2]Hawaii Institute of Geophysics and Planetology, University of Hawai‘i at Mānoa, Honolulu, Hawaii 96822, U.S.A.
[3]Department of Earth and Environmental Sciences, University of Michigan, Ann Arbor, Michigan 48109, U.S.A.
[4]Department of Geological Sciences, Jackson School of Geosciences, University of Texas at Austin, Austin, Texas 78712, U.S.A.

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