Thermal Equation of State of Fe_7C_3 by Single Crystal X-ray Diffraction

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Carbon is among the leading candidates for the principle light element in the Earth's iron-rich core due to its high cosmic abundance and high solubility in Fe-Ni alloy. Fe_7C_3 is considered to be the first phase to solidify from Fe-C melt under core conditions, and is thus proposed to be an inner core candidate. However, the crystal structure of Fe_7C_3 is still controversial and its thermoelastic properties, crucial for extrapolating the room-temperature mineral physics data to high temperature conditions, were only determined below 30 GPa. Using an externally-heated diamond anvil cell and synchrotron single-crystal X-ray diffraction (XRD), we obtained lattice parameters and atomic positions of Fe_7C_3 up to 74.8 GPa and 800 K. The ambient pressure unit cell volume (V_0), bulk modulus (K_0) and its first derivative (K_0') at 300 K were determined by fitting the third-order Birch-Murnaghan equation of state. The *P-V-T* relationship could be well described by thermal equation of state based on Berman's approach, with thermal expansion described as $\alpha = \alpha_0 + \alpha_1 * (T - T_{ref})$. Furthermore, we found that the *c/a* ratio decreases up to 45 GPa and increases abruptly at around 55 GPa at 300K, probably due to the high-spin to low-spin transition of Fe_7C_3. The thermal expansivity of *c* axis is much larger than other axes. High pressure and temperature crystal data will permit stringent test of a Fe-C inner core compositional model and shed new light on the inner core anisotropy.