American Mineralogist, Volume 97, pages 1417–1420, 2012

Isothermal compression of face-centered cubic iron

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ABSTRACT

Isothermal compression curves of face-centered cubic iron (γ -Fe) were determined at high temperatures (1273 and 1073 K) up to 27 GPa by in situ X-ray diffraction experiments using synchrotron radiation and the Kawai-type multi-anvil apparatus. Fits of the third-order Birch-Murnaghan equation of state to pressure-volume data yielded $V_0 = 48.997 \pm 0.040$ Å³, $K_{T0} = 108.3 \pm 2.4$ GPa, and $K'_T = 5.8 \pm 0.2$ for 1273 K, and $V_0 = 48.600 \pm 0.098$ Å³, $K_{T0} = 88.9 \pm 5.1$ GPa, and $K'_T = 8.9 \pm 0.7$ for 1073 K, where V_0 , K_{T0} , and K'_T are unit-cell volume, bulk modulus and its pressure derivative, respectively, at ambient pressure. The relatively large values of K'_T are attributable to successive electronic spin state transitions from mixed-spin at lower pressures to low-spin at higher pressures. When discussing the constituents of Earth's (or other planets') solid inner core in terms of density and equations of state, one must carefully consider the influence of the electronic spin state.

Keywords: Face-centered cubic (fcc) iron, compression curve, high pressure, spin transition, inner core