Equation of state of fcc-Fe up to 23.5 GPa and 1873 K

Noriyoshi Tsujino[1]; Yu Nishihara[2]; Yoichi Nakajima[3]; Eiichi Takahashi[4]; Ken-ichi Funakoshi[5]

[1] Dpt. Earth Plant. Sci.,Tokyo Inst. Tech.; [2] GRC, Ehime Univ.; [3] Earth Planet. Sci., Tokyo Inst. Tech.; [4] Earth and Planetary Sci., Tokyo Inst. of Tech.; [5] JASRI

In-situ synchrotron X-ray diffraction experiments were conducted using the SPEED- Mk.II multi-anvil apparatus of SPring-8 on fcc-Fe which is one of the possible candidate material for Earth's inner core, and its pressure-volume-temperature (P-V-T) data were collected up to 23.5 GPa and 1873 K. At 1 bar, fcc-Fe is known as one of Anti-invar which shows anomalously high thermal expansivity, and mixed spin state is considered to be stable at high temperature. Since it is expected that the thermal expansivity is lowered to normal value with increasing pressure due to successive transition from mixed spin to low spin state, determination of thermal equation of state of fcc-Fe is quite important for understanding of its electronic spin state. The analysis of the derived P-V-T data using the lattice dynamical approach by Mie-Gruneisen-Debye EOS yielded V_0 = 49.028 +- 0.0027 A^3, K_{T_0} = 111.2 +- 1.8 GPa, K'_T = 5.23 +- 0.21, Gruneisen parameter = 2.30 +- 0.04 with fixed value of Debye temperature = 340 K. Detailed analyses of present P-V-T data give no clear evidence for pressure effect on Anti-invar effect. P-V-T measurements at higher P-T conditions are needed for accurate estimate of density of fcc-Fe at conditions of Earth's inner core.