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Pressure-induced *C*23–*C*37 transition and compression behavior of orthorhombic Fe_2S to Earth's core pressures and high temperatures

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Abstract

The phase stability of orthorhombic Fe_2S was explored to 194 GPa and 2500 K using powder and multigrain synchrotron X-ray diffraction techniques. Between 30 and 120 GPa, a *C*23-like (Co_2P, *Pnma*, $Z = 4$) Fe_2S structure is observed and determined to exhibit a highly compressible *a* axis. A softening of the *a* axis occurs between 120 and 150 GPa and a relative stiffening of the *b* and *c* axes accompanies this compressibility change. Above 150 GPa, the *a* axis stiffens as the *b* and *c* axes soften, and a *C*37-like (Co_2Si, *Pnma*, $Z = 4$) Fe_2S unit cell is measured. On the basis of these changes in unit cell geometry, a pressure-induced *C*23–*C*37 Fe_2S phase transition is inferred between 120–150 GPa. The *C*23 and *C*37 (*Pnma*, $Z = 4$) structures are closely related and share the same site symmetries. Forming the *C*37 structure from the *C*23 structure requires a shortening of the *a* axis and lengthening of the *b* and *c* axes accompanied by a four- to fivefold coordination change. The softening of the *a* axis above 120 GPa may therefore indicate the onset of a coordination change, and the final compressibility change above 150 GPa may mark the completion of this phase transition. The presented pressure-temperature (*P-T*) stabilities of *C*23 and *C*37 structures of Fe_2S are in agreement with and resolve the differing observations of two previous studies (Tateno et al. 2019; Zurkowski et al. 2022). As *C*37 Fe_2S is observed to core-mantle boundary pressures and high temperatures, the *C*37 Fe_2S density profile through Earth's outer core was determined by fitting the *C*23 Fe_2S equation of state (<120 GPa) and applying a 1.6% volume reduction based on the *C*37 Fe_2S volume residuals to this fit. Comparing the density of liquid *C*37 Fe_2S with that of liquid hcp-Fe (Dewaele et al. 2006) and the seismologically determined density deficit of Earth's core (Irving et al. 2018), 13.9 ± 1.5 wt% and 8.6 ± 0.8 wt% sulfur are required to match the densities at the CMB and ICB, respectively, for a purely Fe-S core.

Keywords: Fe-sulfide, Earth's core, high pressure, diamond anvil cell, equation of state, phase transition, iron alloys, high temperature