American Mineralogist, Volume 107, pages 739–743, 2022

The crystal structure of Fe_2S at 90 GPa based on single-crystal X-ray diffraction techniques

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Abstract

The Fe-S system was explored in a laser-heated diamond-anvil cell at 89(2) GPa and 2380(120) K to better understand the phase stability of Fe_2S. Upon temperature quenching, crystallites of Fe_2S were identified, and their structure was investigated using single-crystal X-ray diffraction techniques. At these conditions, Fe_2S adopts the *C*23 structure (anti-$PbCl_2$, Co_2P) with space group *Pnma* ($Z = 4$). This structure consists of columns of corner-sharing, FeS_4 tetrahedra, and columns of edge-sharing FeS_5 square pyramids linked along edges in the *b* direction. Sulfur is in ninefold coordination with Fe. This study marks the first high-pressure structural solution and refinement of Fe_2S synthesized in a multigrain Fe+FeS sample at 90 GPa and 2400 K and establishes the stability of *C*23 Fe_2S at these conditions. A previous powder diffraction study reports an orthorhombic Fe_2S phase with a *C*37, Co_2Si-like unit cell above 190 GPa. A *C*23–*C*37 structural transition is inferred to explain the previously observed unit-cell parameters at higher pressures and temperatures. These results highlight the utility of applying single-crystal X-ray diffraction techniques to high *P*-*T* multigrain samples to explore the structural properties of iron-rich phases in Earth and planetary cores.

Keywords: Crystal structure, iron sulfides, Earth's core, diamond anvil cell, single crystal, high pressure, high temperature, iron alloys