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Phase stability and structural properties of Fe2S and its analog Co2P at high pressures and temperatures

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Earth's core is a Fe-rich alloy with a significant contribution from cosmochemically abundant light elements such as sulfur. Understanding the phase stability and structural properties of iron-rich sulfides at core conditions is critical for assessing the core's composition and dynamics. In the current study, we examined the high-pressure polymorphism of Fe_2S coexisting with Fe to outer-core pressures and high temperatures by combining in-situ powder and single-crystal X-ray diffraction techniques. We further conducted single-crystal X-ray diffraction experiments on Co_2P as a low-pressure analog of Fe_2S. Analyses of the powder X-ray diffraction patterns indicate an orthorhombic Fe_2S phase coexisting with Fe between 25 and 170 GPa at moderate temperatures. Above 85 GPa, the orthorhombic Fe_2S phase transitions to a hexagonal lattice that is stable on the liquidus to 140 GPa. Using single-crystal diffraction techniques, the orthorhombic structure of Fe_2S was solved and refined to the *C*23 structure (Co_2P type, *Pnma*, *Z*=4) at 90 GPa and quenched from 2380 K. While upon quenching at 100 GPa from 2650 K, a hexagonal lattice was identified and indexed to a unit cell compatible with a *C*22 Fe_2S phase (Fe_2P type, *P*-62*m*, *Z*=3), confirming the phase relations inferred in our powder diffraction experiments. The *C*23 Fe_2S unit-cell parameters fit between 25 and 170 GPa reveal a highly compressible *a* axis, where the *a* axis is about 3 times more compressible than the *b* and *c* axes. To 48 GPa, *C*23 Co_2P shows analogous anisotropic compression behavior to that observed at higher pressures in *C*23 Fe_2S. Structural analysis of Co_2P demonstrates that the anisotropic compression of these C23 phases is attributable to bond angle distortion and bond length compression parallel to the *a* direction and that the Co_2P-type structure is compressing towards a Co_2Si-type structure. These results display the mechanism for anisotropic compression observed in *C*23 Fe_2S and support previous observations of a *C*37-like Fe_2S phase above 190 GPa. Through this work, we determined that Fe_2S is the relevant Fe-rich sulfide to at least outer core pressures and high temperatures and assessment of the phase transition and compression behavior of the Fe_2S and Co_2P analogs provides insight into the material properties and dynamics of Earth's complex core.