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Updated Fe-FeS phase diagram under high pressure

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The distribution and behavior of sulfur in the interiors of Earth and other terrestrial planets are largely governed by phase relations in the Fe-FeS system. While Fe and FeS form a simple binary eutectic system at ambient pressure, the Fe-FeS phase diagram becomes significantly more complex under high-pressure conditions. Under elevated pressures, a series of intermediate iron sulfide phases, including Fe_3S, Fe_2S, and the recently discovered $Fe_{12}S_7$ [1], Fe_5S_2 [2], and $Fe_{4+x}S_3$ [3], emerge across varying pressure-temperature conditions and bulk compositions. In this study, we investigated the Fe-FeS system up to 60 GPa using a combination of *in situ* synchrotron and *ex situ* characterization techniques. Several novel Fe sulfide phases were identified through high-pressure single-crystal structure analyses in a diamond anvil cell following in situ syntheses through laser heating. Additionally, subsolidus and melting phase relations were examined using multi-anvil presses with well-controlled temperature fields, within synchrotron beamlines and in-house facilities, covering the compositional range where Fe, FeS, and intermediate iron sulfide phases are stable. The findings provide new insights into the stability of Fe sulfide phases in the deep mantle and the solidification processes of sulfur-bearing planetary cores.

Reference

[1] Zurkowski, C. C., et al. Geochemical Perspectives Letters 21 (2022).

[2] Zurkowski, Claire C., et al. Earth and Planetary Science Letters 593 (2022): 117650.

[3] Man, L., et al., Nature Communications 16 (2025): 1710.