Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.34690

Negligible hydrogen dissolution in FeS at high pressure and high temperature: implications for hydrogen storage during early core formation

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Iron monosulfide (FeS) is a major sulfide phase in planetary materials and a potential host of hydrogen in planetary interiors. However, the hydrogen solubility in FeS under high-pressure and high-temperature (*HPHT*) conditions remains controversial [1-4]. Here we experimentally and computationally reassess the origin of volume expansion in H-bearing NiAs-type phase of FeS (FeS V). X-ray absorption and in situ X-ray diffraction results demonstrate that the volume expansion observed under hydrogen-saturated conditions is primarily attributable to the reduction of Fe^{3+} to Fe^{2+} and a decrease in the δ value of Fe-deficient $Fe_{1-\delta}S$, rather than from incorporation of hydrogen into the crystal structure of FeS V. In H-bearing system, Rietveld refinements for the neutron diffraction pattern further show that a hydrogen-free structural model, incorporating preferred-orientation and extinction corrections, provides the best fit, while unrealistically large atomic displacement parameters are required to achieve a similar level of fitting using the hydride model. First-principles calculations predict that possible FeS V hydride configurations are energetically unstable and support that hydrogen is not reactive with FeS. The solubility limit of hydrogen content in the FeS V is estimated using the calculated formation-enthalpies. We estimated the upper limit of hydrogen content in FeS be only about 200 ppm up to 30 GPa, which is consistent with our experimental results. The negligible incorporation of hydrogen in FeS implies preferential partitioning of hydrogen into metallic Fe during the early stages of core formation. In addition to Fe_3C [5], FeS is an also hydrogen-incompatible phase whereas Fe–Ni and Fe–Si alloys can accommodate hydrogen, the influence of hydrogen during the early stages of core formation should be evaluated in terms of its effective concentration in the metallic phase (i.e., the hydrogen-to-metal ratio), rather than its abundance in the bulk core.

References

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