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Effects of sulfur on the hydrogenation of iron in early Earth's evolution

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Hydrogen (H) is considered to be one of the light elements in the Earth's core. However, the amount and timing of its delivery have remained unclear partly because of experimental difficulties in detecting hydrogen in iron (Fe) under high pressure and high temperature. We determined hydrogen solubility in fcc iron using in-situ neutron diffraction observations at high pressure and high temperature by estimating the site occupancies of hydrogen in the crystal structure of iron [1]. Our previous study on the iron–hydrous silicate system revealed that H preferentially dissolved into iron over other light elements in the very early stage of Earth's evolution.

In this study, we further investigated the effects of sulfur (S) on the hydrogenation of iron up to 6–12 GPa, ~1200 K [2]. The initial samples contained saturated water as brucite in the ideal composition (Fe–$MgSiO_3$–water) simulating the primitive Earth. Deuterated substitutes were used for avoiding incoherent scattering in neutron diffraction measurements. Anhydrous samples and samples without sulfur were also investigated for comparison. Phase transitions of Fe, dehydration of the hydrous mineral, and the formation of iron sulfide (FeS) and silicates (olivine, enstatite) sequentially occurred with increasing temperature. The deuterium (D) solubility (x) in iron deuterides (FeD_x) increased with both temperature and pressure, resulting in a maximum of x~0.33 in fcc iron for the hydrous sample without S. The unit cell volume of FeS was unchanged, suggesting that FeS is hardly hydrogenated until iron hydrogenation has completed. Such lower H(D) concentrations in sulfur-containing system do not exceed the miscibility gap ($x < \sim 0.4$). This is likely due to low H pressure and slow kinetics of hydrogenation caused by redox reaction via water. Elemental mappings in the recovered samples showed that both H and S can be incorporated into solid Fe. The other light elements (C, O, Si) could have dissolved into molten iron hydrides and/or FeS at much higher pressure and temperature during the later process of the Earth's core–mantle differentiation.

[1] Iizuka-Oku et al. (2017), *Nature Communications* 8, 14096.

[2] Iizuka-Oku et al. (2021), *Scientific Reports* 11, 12632.