Light elements in iron-hydrous silicate system: Searching for core formation process using in-situ high-pressure and high-temperature neutron and X-ray observations

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The Earth's core is considered to consist of Fe alloy with some light elements (H, C, O, Si, S). Hydrogen (H) is the most abundant element in the universe and one of the promising candidates for light elements in the Earth's core. However, its amount in the core and the process/contribution are still unknown because H cannot be experimentally detected using X-ray and it easily escapes from iron by the release of pressure. Recently, H contents in face-centered cubic (*fcc*)-Fe at high pressure and high temperature (high-PT) have been determined using in-situ neutron diffraction measurements [1–3]. Our previous study [2] suggested that H had preferentially dissolved into iron before the other light elements have dissolved in the early stage of Earth's evolution. Our final goal is to clarify the behaviors of multi light elements during the formation of Earth and other planetary cores. We have focused on sulfur (S) and investigated its effect on hydrogenation of iron (iron hydride) in Fe-hydrous silicate system using *in-situ* high-PT neutron and X-ray observations.

A starting material simulates an ideal composition of the primitive Earth, iron-enstatite ($MgSiO_3$) system with water. An Fe powder was pelletized and placed in the center of the capsule. Powder mixture of quartz (SiO_2), brucite $Mg(OD)_2$ (or MgO for comparison of water existence) surrounds the Fe pellet to avoid the contamination of carbon from the capsule into Fe. High-PT neutron diffraction experiments up to 6.5–11.5 GPa, 750 ˚C were performed using our original multi-anvil 6-6 type assembly [2] and a six-axis multi-anvil press "Atsuhime" installed at PLANET (BL11), J-PARC. The diffraction data obtained were refined using the Rietveld method to determine structural and atomic parameters of Fe polymorphs. *In-situ* X-ray imaging and diffraction measurements were also conducted at NE7A, PF-AR, KEK in order to identify the products and reaction process. A camera system with a high spatial resolution was newly developed to clearly observe the formation and motion of iron droplets in the silicate melts within the area of ~1 mm square. All the recovered samples were analyzed using an X-ray diffractometer and a SEM-EDS to more precisely identify the products, their compositions, and the elements partition.

A series of reactions (phase transitions of Fe, dehydration of $Mg(OD)_2$, and formation of FeS-V and silicates) were observed with temperature increase. X-ray radiography successfully visualized that Fe droplets coalesce together, migrate by thermal convection, and then sink to the core. The solubility of D in *fcc*-Fe increased with temperature (i.e., endothermic reaction) and also had positive correlation with pressure. The maximum D content *x* in *fcc*-FeD_x was about 0.25 at 11.5 GPa, 750 ˚C for the sample without sulfur, accompanied with a slow hydrogenation process through the redox reaction. On the other hand, the cell volume of FeS-V did not increase regardless of time, although sulfur seemed to inhibit the hydrogen dissolution into iron. Recovered samples exhibited that S and Fe were not mobile and could not react with each other without water, suggesting that the formation of FeS was promoted in the presence of water. Sulfur seemed to be a siderophile element and selectively concentrated at the Fe surface to reduce the interfacial energy. Both H and S can be preferentially incorporated into solid Fe and lower the melting point. It suggests that the other light elements (C, O, Si) could have dissolved into molten iron hydride and/or FeS in the later process of Earth's core-mantle differentiation at much higher-PT condition.

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[1] A. Machida, H. Saitoh, H. Sugimoto, T. Hattori, A. Sano-Furukawa, N. Endo, Y. Katayama, R. Iizuka *et al*, *Nature Commun.*, 5:5063 (2014).
[2] R. Iizuka-Oku, T. Yagi, H. Gotou, T. Okuchi, T. Hattori and A. Sano-Furukawa, *Nature Commun.*, **8**, 14096 (2017).
[3] D. Ikuta, E, Ohtani, A. Sano-Furukawa, Y. Shibazaki, H. Terasaki, L.Yuan and T. Hattori, *Scientific Reports*, 9:7108 (2019).

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