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Increase of hydrogen-induced volume expansion of hcp-Fe by Si dissolution – Constraint to hydrogen content in the core

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Seismic observations indicated that the density of the Earth's core is notably lower than that predicted for pure iron [1] though the main component of the Earth's core is iron. The reason for this density deficit is believed to be the dissolution of light elements in the core. Hydrogen is one of the plausible light elements in the core [2] because it becomes highly sirerophile under *HPHT* conditions [3]. The volume expansion of iron caused by the dissolution of one hydrogen atom is called the "*hydrogen-induced volume expansion coefficient*" (v_H). To date, some researches estimated hydrogen content in the core by using the value (v_H). Especially, neutron diffraction under high-pressure conditions has been used to refine the crystal structure of iron hydrides to date because neutron diffraction is the unique method to determine the hydrogen occupancy [4, 5].

On the other hand, there are several candidates for light elements in the Earth's core, and there have been very few direct studies on the effects of other light elements on hydrogenation of iron. Here, we focused on Si, one of the most promising candidates for light elements in the inner core, and performed neutron diffraction experiments on hcp-$Fe_{0.95}Si_{0.05}$ deuterides under high temperature and high pressure. Also, we conducted X-ray diffraction experiments of hcp-$Fe_{0.95}Si_{0.05}$ and determine the value (v_H) of hcp-$Fe_{0.95}Si_{0.05}$. The obtained v_H was notably larger than that of pure iron. This result indicates that silicon may enhance the effect of density reduction caused by hydrogenation. If the results are adaptable to much higher-pressure environments such as the Earth's inner core, the amount of hydrogen in the core has to be reconsidered when assuming that silicon is a major light element. This implies that the effect of the presence of other light elements in addition to hydrogen cannot be ignored when hydrogen dissolves into the Earth's core.

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