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Key Points:

- We obtained the P-V-T equation of state of FeH based on volume measurements up to 142 GPa and 3660 K using a diamond-anvil cell
- ΔV_H, the volume increase of Fe by H atom, was determined as functions of P and T, enabling estimates of the H content in non-magnetic FeHx
- We estimate the maximum H content in the inner core and discuss the possible compositional range of the Fe-H-Si-S inner core

Supporting Information:

Supporting Information may be found in the online version of this article.

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High-Temperature Equation of State of FeH: Implications for Hydrogen in Earth's Inner Core

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Abstract While hydrogen is one of plausible major light elements in the core, the high-temperature equation of state (EoS) of Fe-H alloy has not been experimentally examined to the core pressure range. Here we measured the volume (V) of non-magnetic (NM) face-centered cubic (fcc) FeH at high pressure and temperature (P-T) to 142 GPa and 3660 K in a laser-heated diamond-anvil cell and obtained its P-V-T EoS. An increase in the lattice volume of Fe per H atom, ΔV_H, determined as functions of P and T is found to be substantially smaller than the volume of metallic H that has been used to estimate H concentration in Fe-H alloy. The ΔV_H is almost identical between fcc and double hexagonal close-packed phases in the NM state, suggesting that it may be applicable to hcp. The extrapolation of ΔV_H to inner core conditions indicates its maximum H content to be 0.8–0.9 wt%.

Plain Language Summary FeH is an important component in terrestrial planetary cores, and its equation of state (EoS) is useful to estimate their H concentrations from observed densities. The high-T EoS of FeH has not been examined experimentally to the Earth's core pressure range (>136 GPa) because of difficulties in high P-T experiments on H-bearing systems. The face-centered cubic (fcc) structure is known to be a stable form of FeH under a wide P-T range. Also, our first-principles calculations showed that fcc FeH loses the local spin moment above ~40 GPa. The present experiments determined the volume of fcc FeH to 142 GPa and 3660 K and obtained its EoS for the non-magnetic state. The lattice volume of Fe expands by incorporating H in its interstitial site. Our data show that ΔV_H, the volume increase per H atom, is similar between the fcc and double hexagonal close-packed phases in the absence of magnetism and may be applicable to hcp. Such ΔV_H obtained as functions of P and T predicts the density of FeHx under inner core conditions and gives the possible compositional range of the Fe-H-Si-S inner core.

1. Introduction

Hydrogen could be one of major light elements in planetary iron cores and has attracted much attention recently (see Hirose et al., 2021 for a review). Recent experimental and computational studies of metal-silicate partitioning of H showed that a large amount of H equivalent to that in 30–70 times Earth's ocean mass of water could have been distributed into the core during its formation (Li et al., 2020; Tagawa et al., 2021; Yuan & Steinle-Neumann, 2020). Indeed, the density and seismic velocity of both the outer and inner core can be reconciled with H-rich Fe alloys (Umemoto & Hirose, 2015, 2020; Wang et al., 2021). In addition, recent seismic observations of the Martian core indicate that its density is relatively low, possibly suggesting the presence of 1–2 wt% H (Stähler et al., 2021). Hydrogen in the cores of such terrestrial planets may have derived from water that was transported from an outer region of the solar system (Raymond & Morbidelli, 2020) and from proto-solar nebular gas (Ikoma & Genda, 2006; Olson & Sharp, 2019). The amount of H in the core is a key to better understanding the processes of planetary formation.

In order to constrain the H content in metallic cores, the EoS of Fe-H alloy is of great importance. While it has been reported by theory to inner core conditions (Caracas, 2015), its experimental determination has been challenging because (a) Fe has negligible solubility of H at 1 bar (e.g., Fukai & Suzuki, 1986) and (b) H concentration in Fe-H alloy therefore needs to be estimated under pressure. The EoS of stoichiometric FeH has been examined by X-ray diffraction (XRD) measurements under high pressure but only at room temperature (Badding et al., 1991; Hirao et al., 2004; Kato et al., 2020; Narygina et al., 2011; Pépin et al., 2014), except for multi-anvil experiments performed up to 21 GPa and 1573 K (Sakamaki et al., 2009). The EoSs obtained by these earlier

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studies differ from each other because of the differences in crystal structure (dhcp and fcc) and magnetic state (ferromagnetic, FM and NM).

The volume increase of Fe per H atom, ΔV_H, provides the density of an Fe-H alloy since the lattice volume of iron expands proportionally to the amount of H (Caracas, 2015). In addition, the ΔV_H has been widely used to estimate H concentration in Fe-H alloys (Fukai, 1992; Tagawa et al., 2021; Thompson et al., 2018). Originally Fukai (1992) employed ΔV_H from the volume of metallic H (Chakravarty et al., 1981). Recent neutron diffraction measurements directly gave ΔV_H at high *P-T* (Machida et al., 2014, 2019; Ikuta et al., 2019), but the pressure range for such neutron diffraction studies has been limited to 12 GPa, much lower than Earth's core conditions. The temperature effect on ΔV_H remains primarily unknown (Wang et al., 2021).

In this study, we examined fcc stoichiometric FeH at high *P-T* based on experiment and theory. The first-principles calculations were performed in order to confirm that the magnetic state of FeH is NM under conditions of the present volume measurements at high temperatures. The thermal EoS is obtained for the NM state by measuring the volume up to 146 GPa/300 K and 119 GPa/3720 K in a laser-heated DAC. By comparing its volume with that of pure Fe, we obtain ΔV_H (*P*, *T*) as functions of *P* and *T* and discuss H concentration in the Earth's inner core. Such ΔV_H (*P*, *T*) is also useful to estimate the H content in Fe-H alloys in-situ at high *P-T*.

2. Experimental Methods

High *P-T* experiments were performed in a laser-heated DAC (Figures 1a and 1b). Three separate runs were carried out using beveled anvils with 120 and 300 μm culet sizes. A Re gasket was preindented to about 25 μm thick. Sample configuration was similar to that in Tagawa et al. (2016). In order to prevent hydrogen loss to the Re gasket, we employed a NaCl inner gasket prepared with a Focused Ion Beam. The surface of the diamond anvils was coated with a thin layer of Ti by sputtering (Ohta et al., 2015). We loaded a ∼10 μm thick pure Fe foil (>99.999% purity, Toho Zinc) being sandwiched by thin NaCl plates that were used as a pressure marker. Only in run #3, a KCl pellet was placed between NaCl and Fe on one side as an additional pressure standard. After drying a whole DAC with the sample in it in an oven, we loaded liquid H using a liquid hydrogen-introducing system at temperatures below 20 K (Chi et al., 2011; Tagawa et al., 2016).

After compression to 15–30 GPa, dhcp FeH was synthesized by laser heating to ∼1000 K under hydrogen-saturated conditions in a DAC. High-temperature experiments above 60 GPa under such hydrogen-saturated conditions will form FeH_2 and FeH_3 from FeH and H_2 (Pépin et al., 2014). Therefore, after synthesizing FeH at such pressure range, we fully released pressure at liquid nitrogen temperature (∼85 K) in an N_2 atmosphere, removed excess hydrogen from a sample chamber while maintaining FeH, and repressurized the sample to >5 GPa under cryogenic temperature. It is known that metastable FeH is quenchable to 1 bar at low temperatures and begins to decompose and release hydrogen above ∼200 K (see Figure 2 in Antonov et al., 2019). No excess hydrogen remained in the sample chamber, which is supported by the fact that neither FeH_2 nor FeH_3 was formed upon heating in their stability fields (Pépin et al., 2014). During recompression, the volume of the dhcp phase was obtained at 300 K each time with thermal annealing to ∼1000–1400 K. We then heated the sample to >1500 K at ∼40–60 GPa and observed a complete transformation from dhcp to fcc FeH (Isaev et al., 2007; Kato et al., 2020; Thompson et al., 2018) (Figure 2).

Structural determination and volume measurement were made on the basis of in-situ high *P-T* XRD spectra obtained at BL10XU, SPring-8 (Hirao et al., 2020). The incident X-ray beam was monochromatized to a wavelength of 0.41331–0.41463 Å (∼30 keV) and focused to 6 μm in diameter. We collected diffraction data on a flat panel X-ray detector (PerkinElmer). The sample was heated from both sides with a couple of 100 W single-mode Yb fiber lasers. A laser beam was converted to one with a flat energy distribution by beam-shaping optics, and the laser-heated spot was 30–40 μm across. Sample temperature, T_{sample}, is an average for both sides of the sample. The temperature at each side is also averaged over 6–8 μm area at a laser-heated hot spot, which corresponds to the X-ray beam size. We consider the temperature uncertainty to be ±5% according to Mori et al. (2017). Pressure was determined from the unit-cell volume of NaCl (pressure medium) using its thermal EoS (Dorogokupets & Dewaele, 2007). We followed Campbell et al. (2009) to estimate the effective temperature of the pressure medium; $T_{NaCl} = (3 \times T_{sample} + 300)/4 \pm (T_{sample} - 300)/4$. Such pressure at high temperature has been validated by estimates using both NaCl and KCl pressure standards in run #3. KCl may give pressures more accurately in particular when a pressure marker plays also as a pressure medium and thus its temperature variation is relatively

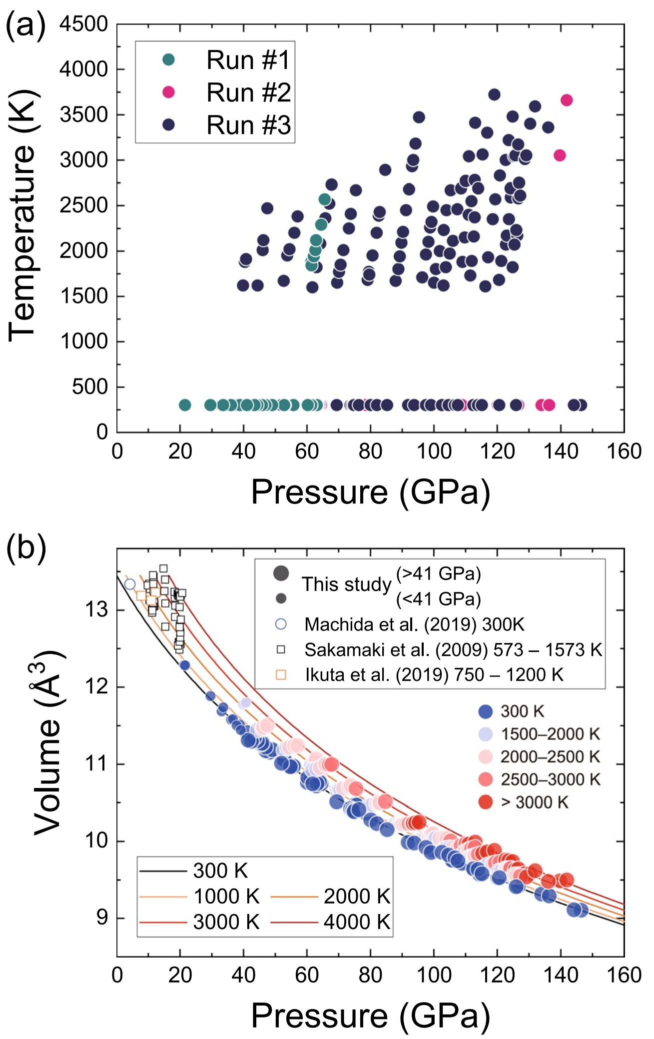

Figure 1. (a) *P-T* conditions for measuring the volume of FeH in runs #1–3. (b) *P-V* data for face-centered cubic FeH at 300 K and high temperatures. Closed large circles, this study; small open circle, Machida et al. (2019) at 300 K; black squares, Sakamaki et al. (2009) at 573–1573 K; yellow squares, Ikuta et al. (2019) at 750–1200 K. Errors in pressure and volume are presented in Dataset S1. Isothermal compression curves are for the non-magnetic state stable above ~40 GPa. They deviate from previous low-pressure measurements on the ferromagnetic and paramagnetic (with local spin moment) states.

large, because the thermal expansivity of KCl is much smaller than that of NaCl. We found that the pressures from NaCl are almost identical with those calculated by using the EoS of KCl proposed by Tateno et al. (2019) (Figure S1 in Supporting Information S1).

3. Results

The *P-V-T* data of fcc FeH were collected in a wide *P-T* range up to 146 GPa in *P* and 3720 K in *T* (Figure 1a and Dataset S1). Melting was not observed even at such high temperatures. It is possible that the melting temperature of stoichiometric FeH is much higher than that of FeHx ($1 < x < 2$; Hirose et al., 2019) above 40 GPa, which is supported by the recent experiments performed by Piet et al. (2021). Also, it is most unlikely that hydrogen escaped from the sample during heating because its lattice volumes obtained after heating at 300 K are always plotted on a single compression curve (Figure 1b). We employ volume data obtained only at high temperatures or at 300 K after heating, in order to avoid the effect of deviatoric stress on a sample. The fcc phase observed here was formed from dhcp FeH (Figure 2). Both phases should be stoichiometric FeH because their volumes are consistent with those of what were synthesized under hydrogen-saturated conditions (Kato et al., 2020; Pépin et al., 2014; Figure S2 in Supporting Information S1). The fcc phase being stoichiometric FeH in this study is also supported by the fact that its volume agrees with that formed in the presence of excess H_2 in Kato et al. (2020). The volume of dhcp FeH was measured in run #1 at 22–61 GPa (Dataset S1).

Our total energy calculations demonstrate that the FM state is stable for fcc FeH at ambient pressure and the FM-NM transition occurs at 47 GPa and 0 K (see text in the, Figure S3b in Supporting Information S1). The FM state changes to PM above the Curie temperature, which rapidly decreases with compression (Figure S3c in Supporting Information S1). The local spin moment of the PM state will be quenched at the volume larger than that for FM (Figure S3a in Supporting Information S1), indicating that the PM fcc FeH is also expected to lose its local spin moment at pressure lower than 47 GPa.

The present *P-V* data of fcc FeH obtained at 300 K are compared with the compression curves previously reported by experiments for the dhcp and fcc phases (Badding et al., 1991; Hirao et al., 2004; Kato et al., 2020; Narygina et al., 2011; Pépin et al., 2014; Figure S2 in Supporting Information S1). Deviations among these studies including the present one may be attributed to the difference in the magnetic state, resulting from different crystal structure, as well as thermal annealing during compression. The extrapolated compression curves reported by Hirao et al. (2004) and Narygina et al. (2011) disagree with ours because volumes were measured in limited pressure ranges in these two earlier experiments.

Here we obtain the room-temperature Vinet *P-V* EoS for the NM state by using the present 300 K data collected only above 41 GPa considering the pressure uncertainty in our first-principles calculations;

$$P = 3K_{0,300\,\mathrm{K}}\left(\frac{V}{V_{0,300\,\mathrm{K}}}\right)^{-2/3}\left[1-\left(\frac{V}{V_{0,300\,\mathrm{K}}}\right)^{1/3}\right]\exp\left\{\frac{3}{2}\left(K'_{0,300\,\mathrm{K}}-1\right)\left[1-\left(\frac{V}{V_{0,300\,\mathrm{K}}}\right)^{1/3}\right]\right\} \tag{1}$$

High-temperature (>1600 K) FeH data were acquired for the NM state above 41 GPa in this study (Figure 1a). These data are fitted by the Mie-Grüneisen-Debye model (e.g., Dewaele et al., 2006);

$$P_{th}(V,T) = \frac{\gamma(V)}{V}\left\{E_{th}(T,V) - E_{th}(300\,\mathrm{K},V)\right\} \tag{2}$$

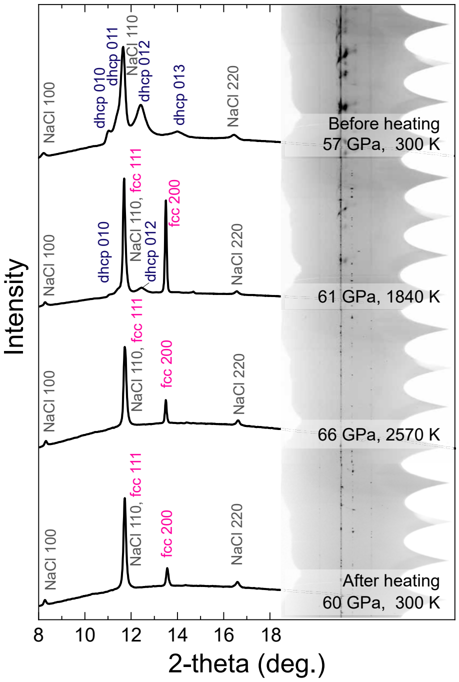

Figure 2. X-ray diffraction data collected in run #1 before heating for double hexagonal close-packed FeH and during/after heating for the face-centered cubic phase.

$$E_{th} = 9nk_B\left(\frac{\Theta_D}{8} + T\left(\frac{T}{\Theta_D}\right)^3\int_0^{\Theta_D/T}\frac{x^3}{\exp(x)-1}dx\right) \tag{3}$$

$$\Theta_D = \Theta_0 x^{-\gamma_\infty}\exp\left[\frac{\gamma_0-\gamma_\infty}{\beta}\left(1-x^\beta\right)\right] \tag{4}$$

$$\beta = \frac{\gamma_0}{\gamma_0-\gamma_\infty} \tag{5a}$$

$$\gamma(V) = \gamma_\infty + (\gamma_0-\gamma_\infty)x^\beta \tag{5b}$$

where E_{th} is thermal energy, γ is Grüneisen parameter (subscript 0 and ∞ denote values at ambient and infinitely compressed conditions, respectively), Θ_D is Debye temperature, n is the number of atoms per formula unit ($n = 2$ for FeH), k_B is Boltzmann's constant in GPa·Å^3·K^{-1} unit, and β is a fitted parameter. Θ_D is also formulated from the Debye sound velocity as;

$$\Theta_D = \frac{h}{2\pi k_B}\left(\frac{6\pi^2 N}{V}\right)^{\frac{1}{3}} \upsilon_D \tag{6}$$

where h is Planck's constant and υ_D is Debye sound speed. We estimated Θ_0, γ_0, and γ_∞ to be consistent with both our P-V-T data and υ_D reported by Thompson et al. (2018) from NRIXS measurements above 41 GPa. These fittings provide V_0 = 13.45(15) Å^3 for a formula unit, K_0 = 183(20) GPa, K' = 3.84(37), Θ_0 = 758 K (fixed), n = 2, γ_0 = 0.738(40), and γ_∞ = 0.547(83). These parameters are compared with those for fcc pure Fe (Tsujino et al., 2013) and for dhcp FeH based on data collected below 20 GPa (Sakamaki et al., 2009) in Table S1 in Supporting Information S1. The present EoS for the NM state predicts smaller volumes than observed by Sakamaki et al. (2009) for the FM and possibly PM (with local spin moment) states at <21 GPa and high temperatures to 1573 K (Figure 1b).

4. Discussion

4.1. ΔV_H at High P and T

We obtain ΔV_H from the difference in volume between FeH and Fe. Here we employ the EoSs of fcc and hcp Fe for the NM state reported by Dorogokupets et al. (2017), in which pressure was calibrated to be consistent with the NaCl scale by Dorogokupets and Dewaele (2007) that is employed in this study. The room-temperature ΔV_H for both fcc and dhcp FeH is shown as a function of pressure in Figure 3a. The volume of dhcp FeH was obtained in run #1 between 22 and 57 GPa, and ΔV_{H_dhcp} is calculated by using the volume of hcp Fe which is similar in structure to dhcp. ΔV_{H_dhcp} is larger than ΔV_{H_fcc} for the fcc phase at relatively low pressures, which is also evident from neutron diffraction experiments at <5 GPa (Machida et al., 2014; Ikuta et al., 2019; Antonov et al., 1998). Nevertheless, ΔV_{H_dhcp} decreases more rapidly than ΔV_{H_fcc} with compression, and both become similar above 45 GPa. Such behavior of ΔV_{H_dhcp} is likely attributed to the FM to NM transition in dhcp FeH (Ying et al., 2020). Also, ΔV_{H_fcc} data below 40 GPa including neutron diffraction data at 4.2 GPa are for the FM and possibly PM (with local spin moment) states and larger than that for its NM state (Figure 3a). It is noted that once Fe loses its local spin moment, ΔV_{H_fcc} and ΔV_{H_dhcp} are found to be almost identical with each other, suggesting that ΔV_H determined for the fcc NM state may be applicable to hcp Fe-H alloys.

The present experiments give not only the pressure effect but also the temperature dependence of ΔV_H (P, T) for the NM state (Figure 3b), which has not been demonstrated previously except for the recent calculations by Wang et al. (2021) performed only at 360 GPa and 2000–6500 K (Figure 3c). It is different from that with the local spin moment, which was previously reported at pressures less than 12 GPa (Ikuta et al., 2019). As demonstrated in these figures, ΔV_H diminishes with increasing temperature likely because the interstitial sites for H around

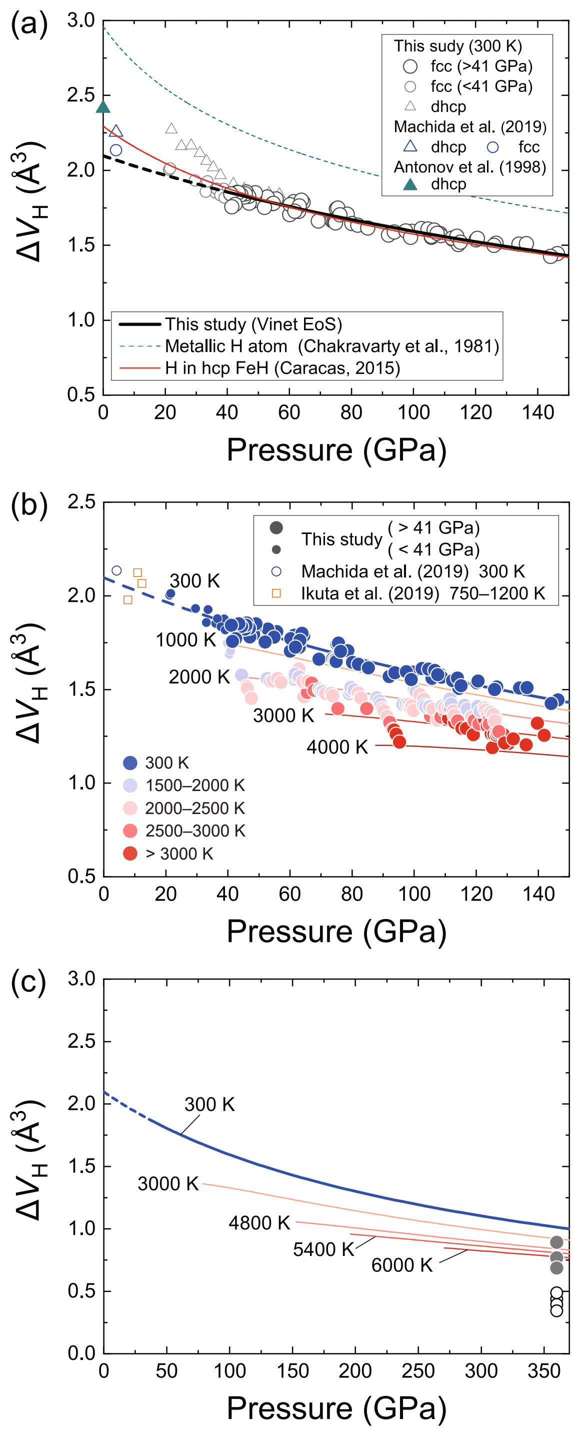

Figure 3. ΔV_H obtained in the present experiments. (a) ΔV_H at 300 K and high pressures found for face-centered cubic (fcc) (circles) and double hexagonal close-packed (triangles) FeH (black solid line). Data by neutron diffraction measurements at low pressures are from Machida et al. (2019) (blue) and Antonov et al. (1998) (green). Large and small symbols represent the data for non-magnetic (NM) and ferromagnetic (FM) (or paramagnetic (PM) with local spin moment) states, respectively. They are much smaller than the calculated volume of metallic H (Chakravarty et al., 1981) (green broken line), which was employed by Fukai (1992) to estimate H concentration in Fe-H alloys. The present data for NM fcc FeH is consistent with the ΔV_H theoretically calculated for hcp FeH at 0 K by Caracas (2015) (red line). (b) Changes in ΔV_H for NM (large circles) and FM (or PM with local spin moment) (small circles and squares) fcc FeH at high pressures with increasing temperature. Neutron diffraction data (open symbols) are given for 300 K (Machida et al., 2019) and 750–1200 K (Ikuta et al., 2019). Colored curves indicate the effect of temperature from 300 to 4000 (K) (c) ΔV_H extrapolated to inner core *P-T* (colored curves). Data for hcp $Fe_{60}Si_4H_8$ (gray circles) and $Fe_{64}H_4$ (open circles) by first-principles calculations (Wang et al., 2021) are also plotted.

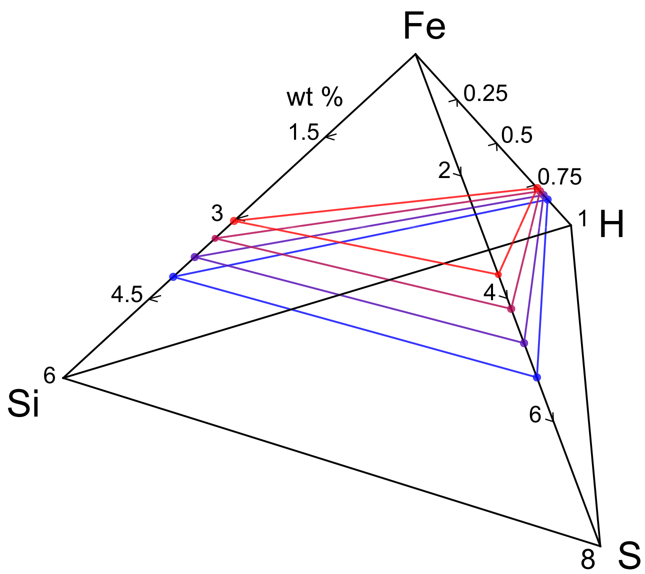

Figure 4. Possible ranges of the Fe-H-Si-S inner composition illustrated by each triangle plane depending on inner core boundary temperature (blue, 4800 K; purple, 5400 K; magenta, 6000 K; red, 6600 K).

Fe atoms expand at high temperature; the ΔV_H decreases by about 10% at 2000 K in a wide pressure range and by 16%–20% at inner core boundary (ICB) conditions of 330 GPa and 5400–6000 K.

Fitting Vinet EoS (Equation 1) to ΔV_{H_fcc} data at 300 K for NM FeH gives V_0 = 2.097(1) Å^3, K_0 = 301.2(9) GPa, and K' = 1.404(6). And, the temperature effect can be approximated as; ΔV_{H_fcc} (P, T) = −0.00241(1) × P − 1.338(13) × 10^{-4} × T + 2.724(46) × 10^{-7} × P × T + 1.872(3) (Figure 3b). This equation predicts ΔV_H that deviates by less than 0.1 Å from our experimental data at >60 GPa and 300–6600 K.

At 0–300 K, both ΔV_{H_dhcp} and ΔV_{H_fcc} observed here are remarkably smaller than the volume of metallic hydrogen, $\Delta V_{metal\text{-}H}$ (Figure 3a), which was calculated considering a close-packed structure and vibrational contributions by Chakravarty et al. (1981). The $\Delta V_{metal\text{-}H}$ was originally employed by Fukai (1992) and has been used to calculate H concentration in Fe-H alloys (e.g., Shibazaki et al., 2011; Terasaki et al., 2012). However, they were always underestimated by several tens % since $\Delta V_{metal\text{-}H}$ is substantially larger than ΔV_H in FeH. In contrast, the ΔV_{H_fcc} at room temperature is approximately consistent with that previously calculated at 0 K by Caracas (2015). When our ΔV_{H_fcc} is extrapolated to high P-T conditions for the Earth's inner core (330–364 GPa, >4800 K), it is broadly consistent with ΔV_{H_hcp} obtained for hcp $Fe_{60}Si_4H_8$ by first-principles calculations (Wang et al., 2021), although their calculations for $Fe_{64}H_4$ gave smaller values (Figure 3c).

4.2. Implications for Hydrogen in Earth's Inner Core

Hydrogen can be an important light impurity element in the Earth's outer core to explain its density and seismic velocity (Umemoto & Hirose, 2015, 2020). Previous multi-anvil experiments performed at 15–20 GPa demonstrated the solid-Fe/liquid-Fe partition coefficient of H, D_H (solid/liquid) to be ∼0.7 by weight (Imai, 2013), indicating that hydrogen could be a major light element in the solid inner core as well. Indeed, the recent calculations by Wang et al. (2021) demonstrated that the inner core may include up to 0.23 wt% H together with Si, depending on its temperature, to explain the observed density and velocities simultaneously.

Independently from earlier estimates, we can constrain H concentration in the inner core based on ΔV_H (P, T) obtained above. If hydrogen is a sole light element, the inner core density is explained with 0.8–0.9 wt% H (0.78–0.85 wt% H at the ICB) considering its temperatures to be 4800–6600 K (Figure 4). We note that such estimate of the H content is almost independent on temperature, because the higher the inner core temperature is, the smaller the density deficit with respect to pure Fe is, but ΔV_H also becomes smaller (Figure 3c). It is not the case for silicon nor sulfur, another plausible light elements in the inner core. With the thermal EoSs of hcp Fe-9wt%Si alloy (Fischer et al., 2014) and Fe (Dorogokupets et al., 2017), the amount of Si required to explain the inner core density deficit as a single light element is estimated to be 4.1 wt% at the ICB pressure of 330 GPa and 4800 K, which decreases to 3.1 wt% with increasing temperature to 6600 K (Figure 4). Also, the experiments performed by Sakai et al. (2012) on an Fe-Ni-S alloy demonstrated that 5.3 to 3.6 wt% S explains the density at the inner core side of the ICB when the effect of nickel is not considered, depending on its temperature ranging from 4800 to 6600 K.

The Earth's inner core should be an Fe-H-Si-S (-Ni) alloy with least amounts of C and O because their solid-Fe/liquid-Fe partition coefficients are limited to 0–0.1 (Alfè et al., 2002; Hasegawa et al., 2021; Li et al., 2019; Ozawa et al., 2010). If the excess volume of mixing is negligible, the inner core composition may be represented by a mixture among Fe-0.85 wt% H, Fe-4.1 wt% Si, and Fe-5.3 wt% S when the ICB temperature is 4800 K. The possible ranges of the Fe-H-Si-S inner core composition are illustrated in Figure 4, depending on the ICB temperature ranging from 4800 to 6600 K. Furthermore, such possible ranges of the inner core composition can constrain the possible liquid outer core composition, once the partitioning of light elements between the outer and inner core is better understood including their interactions (e.g., Hirose et al., 2021; Tao & Fei, 2021; Tateno et al., 2018).

5. Conclusions

We constructed the high-temperature EoS of fcc FeH in the NM state based on its volume measurements of fcc FeH were carried out to 142 GPa and 3660 K in a laser-heated DAC, in which we avoided the formation of FeH_2 and FeH_3 by releasing excess H_2 from a sample chamber after the synthesis of stoichiometric FeH. According to our first-principles calculations, we employed data only above 41 GPa that represent the NM state. The EoS of FeH provides ΔV_H (P, T), the volume increase per H atom, for Fe-H alloys as functions of P and T, which we found is similar between fcc and dhcp at NM conditions and may therefore be applicable to hcp as well. Such ΔV_H (P, T) is remarkably smaller than the volume of metallic H at equivalent conditions and will be useful for in-situ quantification of H contents in Fe-H alloys under P-T. When extrapolated to inner core conditions, our ΔV_H (P, T) is in broad agreement with that by recent theoretical predictions (Wang et al., 2021). It gives the maximum H content in the inner core to be 0.8–0.9 wt%, which is almost independent of temperature because the higher the inner core temperature is, the smaller the density deficit is, but ΔV_H (P, T) also decreases. We also estimated the possible compositional range of the Fe-H-Si-S inner core.

Data Availability Statement

Datasets for this research are found in Dataset S1 available online (from https://doi.org/10.5281/zenodo.5513718).

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