Geochemistry, Geophysics, Geosystems

Supporting Information for

High-pressure geophysical properties of *fcc* phase FeH_X

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Equation S1

$$V_S = a + b\rho + cX$$

V_S is in units of $km \cdot s^{-1}$, density (ρ) is in units of $kg \cdot m^{-3}$, and stoichiometry (X) is in formula units.

Figure S1. (a) Synchrotron Mössbauer spectra of non-stoichiometric (X~0.94) *fcc* FeH_X at 64 and 82 GPa, black dots are experimental SMS data and red lines are modeled spectra. (b) Energy spectra calculated from the modeled Mössbauer fits.

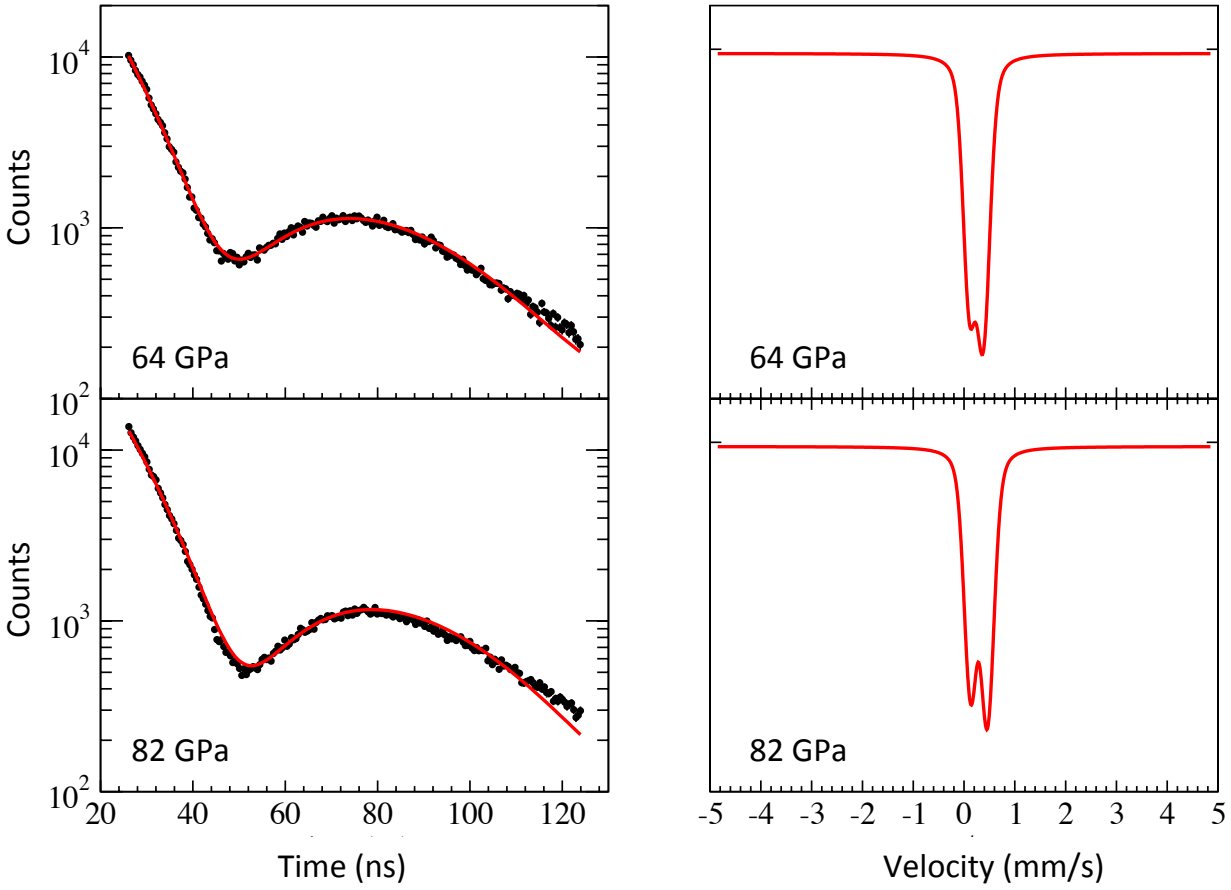

Figure S2. Birch's Law extrapolation of the influence of hydrogen stoichiometry on the shear velocity-density (V_s-ρ) relationship in iron hydrides. Dotted lines indicate Birch's law parameterization for varying FeH_X stoichiometries, including X=0 (blue), X=0.25 (green), X=0.5 (orange), X=0.75 (red), and X=1 (maroon). Experimental data includes *fcc* FeH_X (triangles), *dhcp* FeH_X (squares), and *hcp* iron (circles), with data points color coded to their approximate stoichiometry. Error are bars are smaller than symbols and excluded for clarity. This fit uses the hydrogen EoS based on *Caracas* [2015], sound velocities calculated using PHOENIX [*Sturhahn*, 2000], and Eq. S1. The PREM model for the inner core is represented by black crosses.

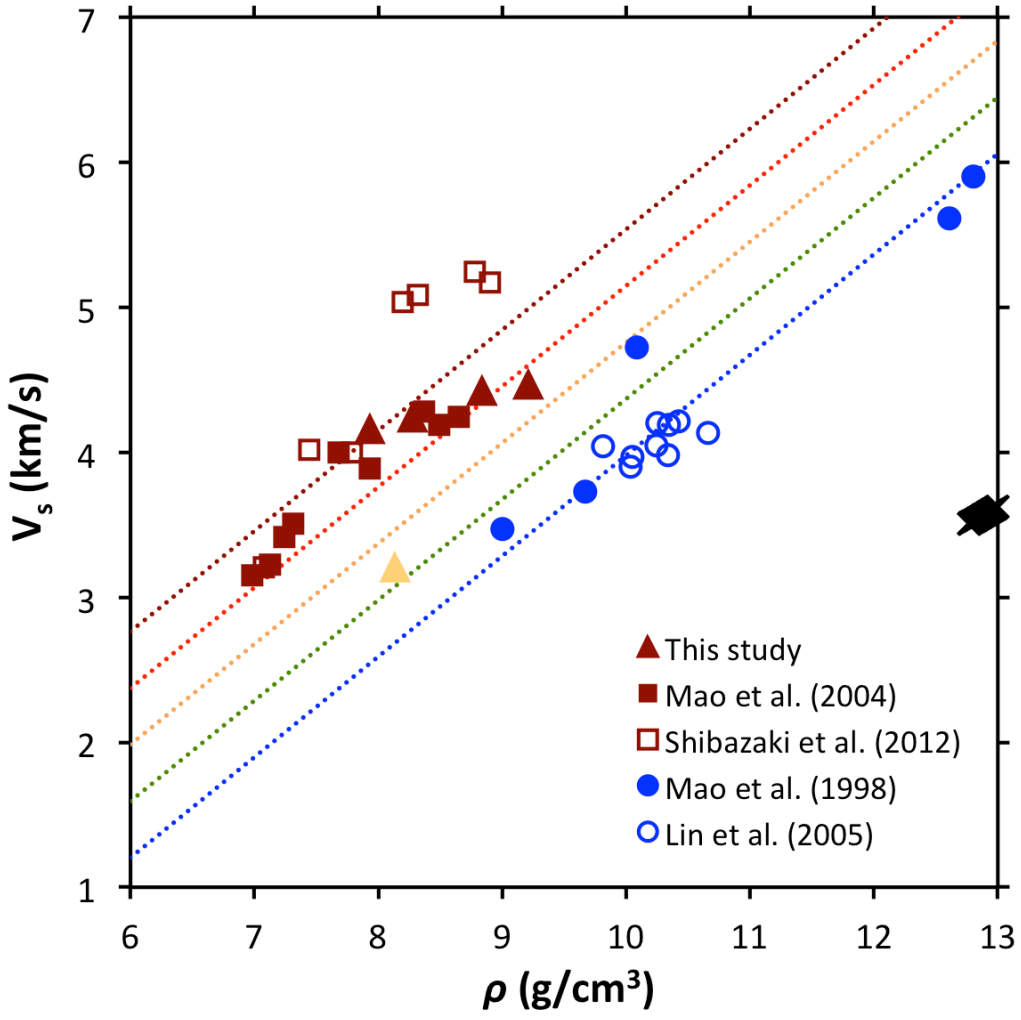

Table S1. Details of sample synthesis including primary pressure standard, percent isotopic enrichment, gasket material, pre-heating pressure, *hcp* iron unit volume, peak temperature and total duration of laser heating, quench pressure (300 K), lattice parameter of the resultant *fcc* FeH_X, and observed quenched phases. Values in parenthesis reflect uncertainties in final digit. Samples primarily laser heated at the University of Chicago are denoted with a (*) symbol. In some instances preheating pressures or *hcp* iron unit volumes are unavailable, which is denoted as (—).

Pre-heating sample					Laser-heating		Quenched sample		
Pressure Standard	**% ^{57}Fe**	**gasket**	**P (GPa)**	***hcp* Fe V (Å^3)**	**T (K)**	**Time (mins)**	**P (GPa)**	***fcc* FeH_X *a* (Å)**	**Observed quench phases**
ruby	95%	Be/CBN	19.3(1)	—	*1800(400)	8	18.4(2)	3.607(2)	Iron hydride
ruby	0%	Re	19.3(1)	20.47(1)	1810(101)	3	18.7(3)	3.691(9)	Iron hydride, diamond
MgO	0%	Re	22.6(1)	20.22(1)	2070(103)	20	22.3(1)	3.666(1)	Iron hydride, MgO
ruby	0%	Re	24.4(2)	—	*1800(400)	10	24.0(3)	3.602 (1)	Iron hydride
ruby	0%	Re	25.7(1)	20.00(1)	1550(106)	15	25.0(4)	3.673(3)	Iron hydride, diamond
MgO	0%	Re	27.0(1)	19.91(1)	2004(100)	21	26.4(1)	3.651(6)	Iron hydride, MgO
ruby	95%	Be/CBN	—	—	*1800(400)	8	29.0(4)	3.628(1)	Iron hydride
MgO	0%	Re	30.6(1)	19.67(1)	2000(101)	16	29.8(2)	3.628(1)	Iron hydride, MgO
ruby	0%	Re	30.9(1)	19.65(1)	1500(100)	4	30.4(5)	3.579(3)	Iron hydride, diamond
MgO	0%	Re	32.1(1)	19.57(1)	1730(146)	13	31.2(2)	3.580(2)	Iron hydride, MgO
ruby	0%	Re	33.6(1)	19.48(1)	1700(103)	16	33.1(5)	3.618 (1)	Iron hydride, diamond
ruby	20%	Be/CBN	40.0(2)	—	*1800(400)	10	39.5(6)	3.577(2)	Iron hydride
ruby	0%	Re	40.4(1)	19.09(1)	1540(101)	4	40.1(6)	3.587(7)	Iron hydride, diamond
ruby	95%	Be/CBN	—	—	*1800(400)	8	41.0(6)	3.577(2)	Iron hydride
ruby	0%	Re	41.8(1)	19.01(1)	1570(105)	6	41.5(6)	3.613 (1)	Iron hydride, diamond
ruby	0%	Re	42.7(1)	18.96(1)	1500(100)	4	41.9(6)	3.602(3)	Iron hydride, diamond
ruby	0%	Re	44.0(1)	18.90(1)	1650(124)	2	43.7(7)	3.602(2)	Iron hydride
ruby	0%	Re	47.8(1)	18.70(1)	1590(100)	3	47.3(7)	3.562(1)	Iron hydride, diamond
MgO	0%	Re	48.4(1)	18.67(1)	1890(138)	18	47.9(2)	3.553(1)	Iron hydride, MgO
ruby	0%	Re	49.2(1)	18.63(1)	1590(108)	3	48.5(7)	3.577(4)	Iron hydride
ruby	0%	Re	50.5(2)	18.57(1)	1520(101)	3	50.1(8)	3.578 (2)	Iron hydride
ruby	0%	Re	50.7(2)	18.57(1)	1520(109)	3	50.2(8)	3.551(3)	Iron hydride
MgO	0%	Re	53.1(2)	18.45(1)	1860(111)	18	52.7(2)	3.552(1)	Iron hydride, MgO
MgO	0%	Re	55.3(2)	18.35(1)	1948(103)	28	55.1(3)	3.532(2)	Iron hydride, MgO
ruby	0%	Re	55.6(2)	18.34(1)	1590(108)	4	55.2(8)	3.533(1)	Iron hydride
MgO	0%	Re	60.0(2)	18.15(1)	1660(101)	7	59.7(2)	3.541(1)	Iron hydride, MgO
ruby	0%	Re	60.3(3)	18.14(1)	1560(101)	2	60.0(9)	3.554(1)	Iron hydride
ruby	0%	Re	60.5(3)	18.13(1)	1740(140)	3	60.0(9)	3.540(2)	Iron hydride
ruby	0%	Re	60.6(3)	18.13(1)	1570(100)	4	60.3(9)	3.543(3)	Iron hydride
ruby	0%	Re	62.2(3)	18.07(1)	1750(124)	4	62(1)	3.530(4)	Iron hydride
ruby	95%	Be/CBN	65(1)	—	*1880(100)	9	64(1)	3.519(4)	Iron hydride
ruby	0%	Re	66.2(3)	17.91(1)	1560(100)	3	66 (1)	3.499(1)	Iron hydride, diamond
ruby	0%	Re	68.4(3)	17.81(1)	1700(121)	3	68(1)	3.531(4)	Iron hydride, diamond
ruby	95%	Be/boron	—	—	*1800(400)	9	82(1)	3.470(5)	Iron hydride

Table S2. Properties of synthesized samples including sample pressure at time of NRIXS measurement (*P*), composition in terms of FeH_X (X), compressional wave velocity (V_P), Debye velocity (V_D), and shear wave velocity (V_S), Lamb-Mössbauer factor (f_{LM}), and mean interatomic force constant (Φ) as extracted using Sciphon software. Hyperfine parameters quadrupole splitting (QS) and isomer shift relative to α-Fe (CS) as determined from CONUSS software. Parameters are shown as calculated using both *fcc* FeH_X equations of state rooted in the Caracas (2015) hydrogen values (denoted as 'C' below) and the Pépin et al. (2014) hydrogen volumes (denoted 'P'). Values in parentheses are uncertainties.

***P* (GPa)**	**EoS**	**X**	V_P **(km·s^{-1})**	V_D **(km·s^{-1})**	V_S **(km·s^{-1})**	f_{LM}	Φ **(N/m)**	**QS**	***CS* (mm/s)**
18.4(2)	C	0.63(4)	6.5(3)	3.6(5)	3.2(5)	0.785(3)	116	-	-
18.4(2)	P	0.59(3)	6.3(3)	3.6(5)	3.2(5)	0.785(3)	116	-	-
29.0(3)	C	0.98(4)	7.6(1)	4.6(2)	4.2(2)	0.860(3)	294	-	-
29.0(3)	P	0.94(4)	7.5(1)	4.8(1)	4.3(1)	0.860(3)	294	-	-
41.0(4)	C	0.97(5)	8.1(1)	4.9(1)	4.4(1)	0.862(2)	246	-	-
41.0(4)	P	0.95(5)	7.7(1)	4.7(1)	4.2(1)	0.860(2)	246	-	-
64.0(6)	C	1.05(5)	8.6(1)	4.9(2)	4.4(2)	0.873(3)	279	0.26	0.21
64.0(6)	P	1.06(5)	8.4(1)	4.9(2)	4.4(2)	0.873(3)	279	0.26	0.21
82.0(8)	C	1.04(6)	8.9(1)	5.1(1)	4.5(1)	0.880(3)	305	0.32	0.26
82.0(8)	P	1.04(6)	8.8(1)	5.1(1)	4.6(1)	0.880(3)	305	0.32	0.26

Table S3. Birch's law parameters calculated using both *fcc* FeH_X equations of state rooted in the Caracas (2015) hydrogen volumes (denoted as 'C' below) and the Pépin et al. (2014) hydrogen volumes (denoted 'P'). Input sound velocities (V_P) have been calculated from NRIXS data using Sciphon software [*Dauphas et al.*, 2014]. Values in parentheses are uncertainties in last digit.

EoS	*a* (k·ms^{-1})	*b* (m^4·kg^{-1}·s^{-1})	*c (dimensionless)*	Data included in fit
C	-4 (fixed)	1.206 (fixed)	1.72(8)	This study; Shibazaki et al. 2012; Mao et al. 2004
C	-4 (fixed)	1.206 (fixed)	1.9(1)	This study
C	-5.1(8)	1.32(7)	2.0(2)	This study; Shibazaki et al. 2012; Mao et al. 2004; Antonangeli et al. 2012; Ohtani et al. 2013
P	-4 (fixed)	1.206 (fixed)	1.79(7)	This study; Shibazaki et al. 2012; Mao et al. 2004
P	-4 (fixed)	1.206 (fixed)	1.7(2)	This study
P	-4.7(6)	1.27(6)	1.9(2)	This study; Shibazaki et al. 2012; Mao et al. 2004; Antonangeli et al. 2012; Ohtani et al. 2013

Table S4. Birch's law parameters calculated using both *fcc* FeH_X equations of state rooted in the Caracas (2015) hydrogen volumes (denoted as 'C' below) and the Pépin et al. (2014) hydrogen volumes (denoted 'P'). Experimental shear wave velocities from this study (V_S) were calculated using both Phoenix [Sturhahn, 2000] and Sciphon [*Dauphas et al*., 2014] software packages as denoted below. Values in parentheses are uncertainties in last digit.

EoS	**NRIXS**	***a*** **(k·ms^{-1})**	***b*** **(m^4·kg^{-1}·s^{-1})**	***c (dimensionless)***
C	Phoenix	-3.0(8)	1.6(2)	0.69(7)
C	Sciphon	-3.1(8)	1.6(2)	0.71(7)
P	Phoenix	-3.0(8)	1.6(2)	0.69(7)
P	Sciphon	-3.0(8)	1.6(2)	0.70(7)