

Supplementary Information

Sound velocity of hexagonal close-packed iron to the Earth's inner core pressure

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and Alfred Q. R. Baron*

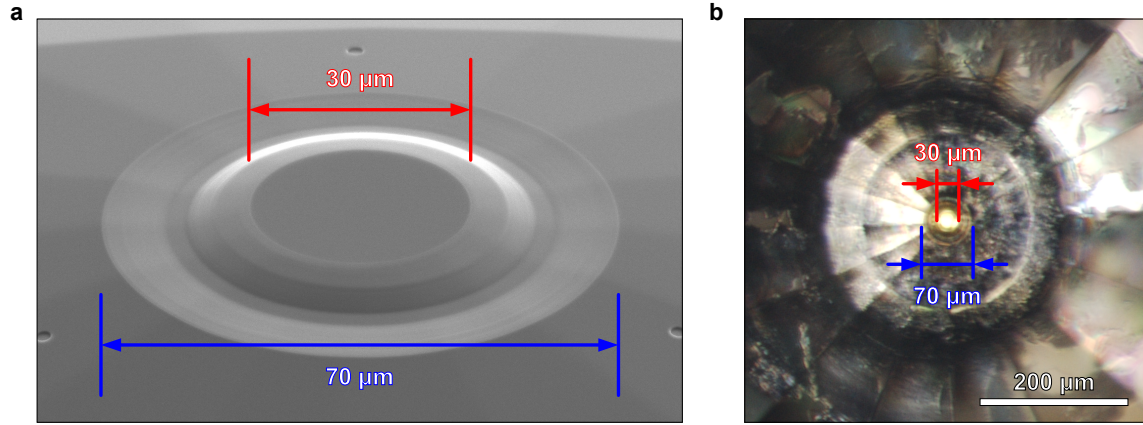
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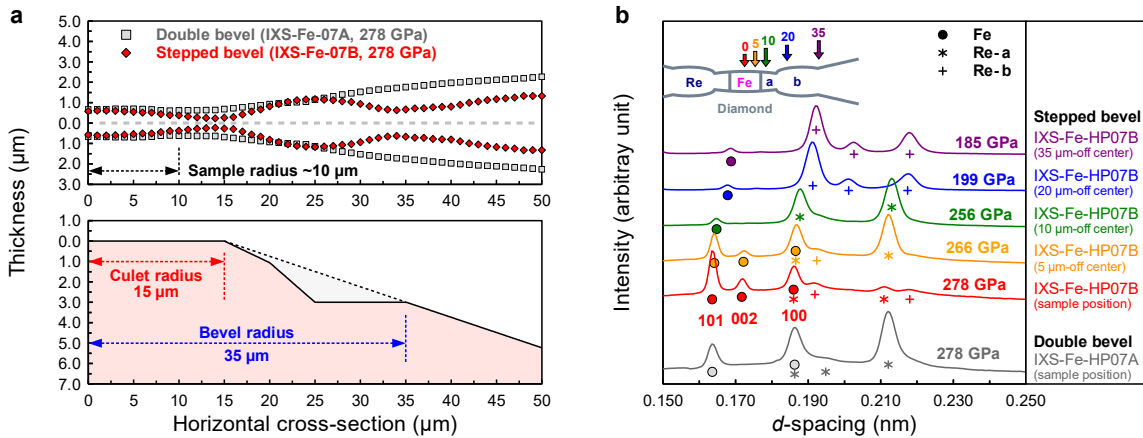
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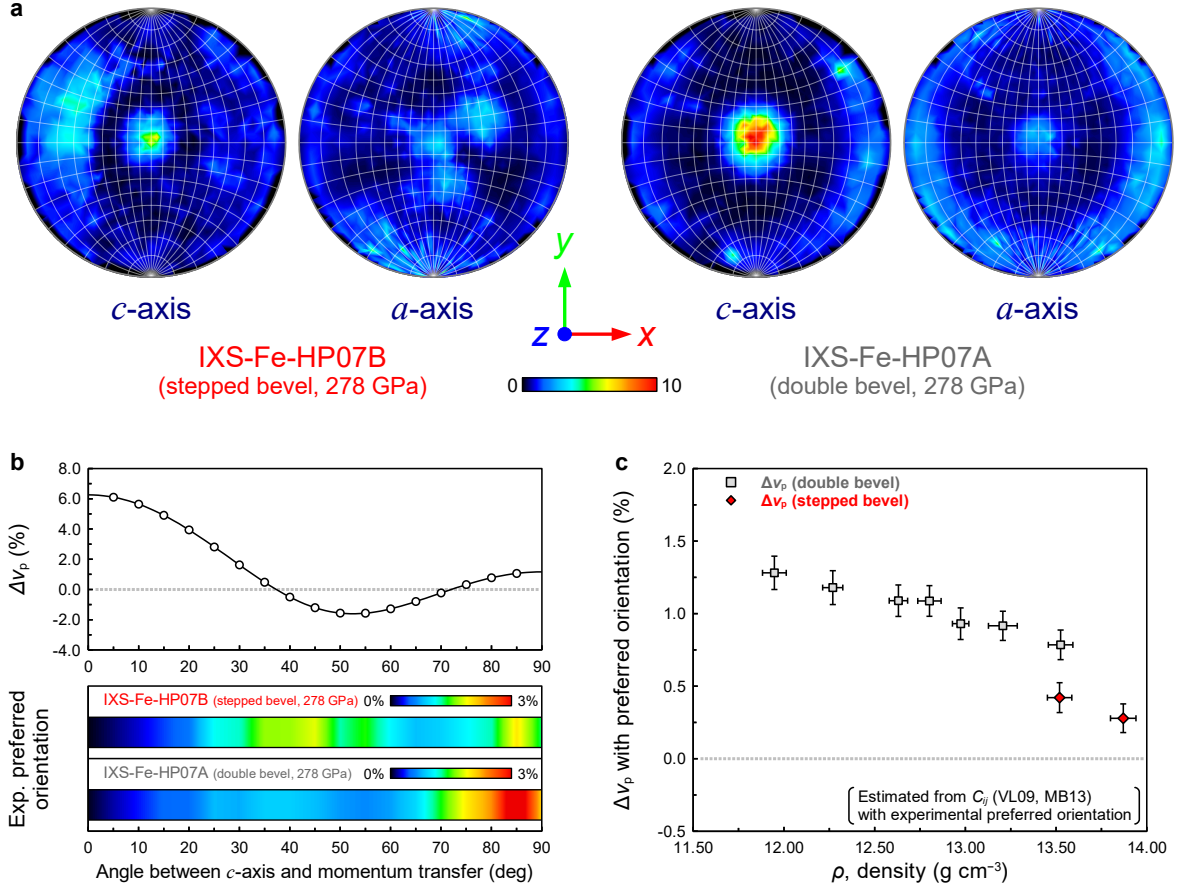




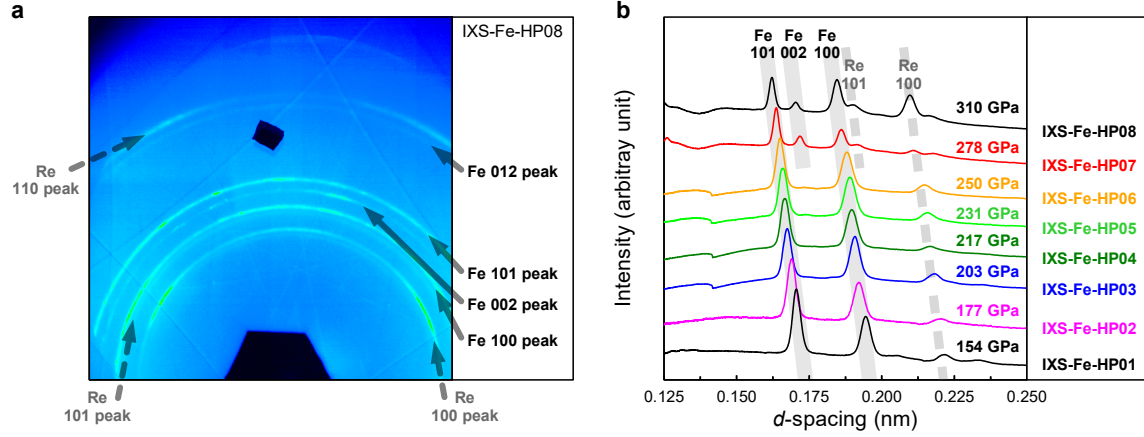
Supplementary Fig. 1. The stepped bevel diamond anvil. **a** Scanning electron microscope (SEM) image of the stepped bevel diamond anvil after machining by a dual focused ion beam (FIB). The red and blue arrows represent the 30 μm culet and a flat surface of 70 μm in diameter with a depth of ~ 3 μm outside the 30 μm culet of (100)-oriented double bevel anvils, respectively (see also Supplementary Fig. 2). **b** Optical microscope image at highest experimental pressure condition (310–327 GPa^{1-3}). The coloured arrows are the same as (a). The brightest area (~ 20 μm) inside the 30 μm culet is the iron sample.



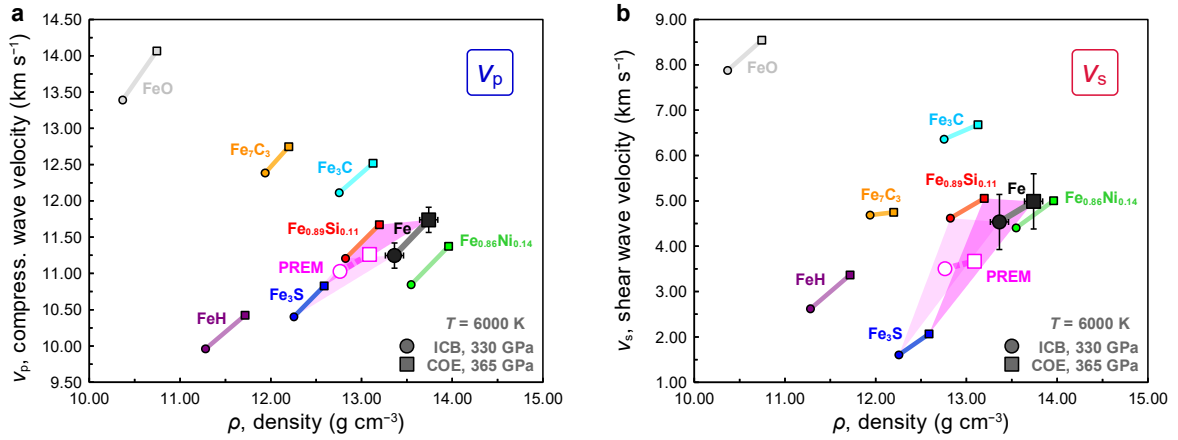
Supplementary Fig. 2. High-pressure generation in a stepped bevel anvil. **a** Upper column shows that sample/rhenium gasket thickness distribution with a stepped bevel anvil (red diamonds) and a double bevel anvil (grey squares) at 278 GPa^1 derived from x-ray absorption measurements. The grey dashed line represents the centre of the sample/rhenium gasket. The bottom column shows the schematic diagram representing the initial shape of both stepped and double bevel anvils. The red shaded area represents the stepped bevel anvil and grey shaded area indicates the part machined by FIB from the initial double bevel anvil. **b** Integrated x-ray diffraction (XRD) profiles at 278 GPa^1 with a stepped bevel anvil in sample position (red), and 5 (yellow), 10 (green), 20 (blue), and 35 (purple) μm off-centred positions. The position of each XRD pattern is shown schematically in the upper left. The grey line shows the integrated XRD patterns at a sample position at 278 GPa^1 with a double bevel anvil. The pressures in each position derived from the hexagonal close-packed (hcp) iron peaks based on Dewaele-EoS¹ are also shown. The circle and asterisk symbols represent the peaks of hcp-iron and rhenium, respectively. Re-a and Re-b are inferred to be the peaks from the rhenium gasket contacted with the diamond culet and the gasket outside the diamond culet, respectively. Those positions are also indicated in the upper left.



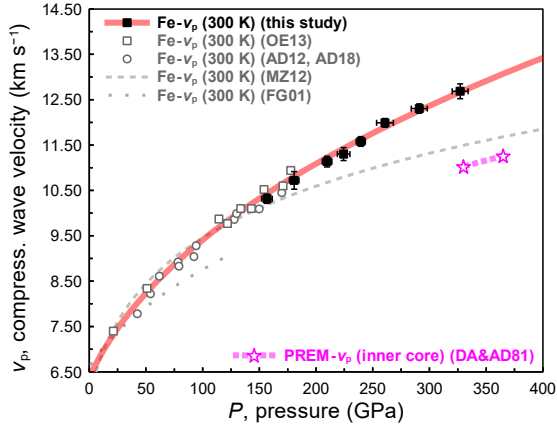
Supplementary Fig. 3. Estimation of the anisotropy of the velocity in the experimental conditions. **a** The experimental probability densities for c - and a -axis concentrations of hcp-iron in both stepped and double bevel anvil experiments at 278 GPa¹ with stereographic projections, derived from the XRD patterns. The x - y - z arrows represent each direction of the experimental apparatus; x : horizontal, y : vertical, and z : compression directions of a diamond anvil cell (DAC), respectively. The colour scale bar represents the multiple of uniform density. For stepped bevel anvil experiment, we observed the preferred orientation that the c -axis in all crystals grains has been concentrated about six times around the compression direction compared with a random orientation. On the other hand, for double bevel anvil experiment, the c -axis has been much more concentrated, about ten times. Although the a -axis was also unevenly distributed, but the concentration was weak compared to the c -axis. **b** Upper panel shows $\Delta v_p(\psi) \{= [v(\psi) - v_{\text{VRH}}] / v_{\text{VRH}}\}$ as a function of angle ψ (where ψ is the angle between c -axis and the lattice vibration direction due to inelastic x-ray scattering) at 13.52 g cm^{-3} (corresponding to 278 GPa¹), calculated using the elastic constants, C_{ij} , from theoretical calculations (VL09, MB13)^{4,5}. The v_{VRH} is the average velocity of Voigt–Reuss–Hill average (VRH) obtained from C_{ij} . (e.g., ref. 6). The open circles with curves represent velocity anisotropies compared with the v_p of VRH. The lower panel shows the probability density of the grains with the preferred orientation as a function of ψ for both stepped bevel anvil and double bevel anvil experiments at 278 GPa¹. The probability densities were shown as one-dimension as a function of ψ by integrating (a). The colour contour represents the concentrations of crystal directions in the experimental grains. While the stepped bevel anvil experiment had widely distributed preferred orientation at 30–90 degrees, the double bevel anvil experiment has strong preferred orientation concentrated at ~85 degrees. **c** Δv_p for both stepped bevel and double bevel diamond anvil experiments as a function of density. Δv_p is the integrated velocity difference weighted by the preferred orientation, which is derived from the integration, $\frac{1}{\pi} \int_0^\pi x(\psi) \Delta v_p(\psi) d\psi$, where $x(\psi)$ is the weight derived from the preferred orientation [here, $x(\psi)$ is normalised as $\frac{1}{\pi} \int_0^\pi x(\psi) d\psi = 1$. Red diamonds are the anisotropies in stepped bevel anvil experiments and grey squares are those in double bevel anvil experiments. The magnitudes of anisotropy on v_p are <0.5% and <1.3% for stepped bevel anvil and double bevel anvil experiments, respectively. The error bars represent 1 σ uncertainties. The effect of anisotropy on v_p is within the uncertainty of the present v_p measurement shown in Table 1.



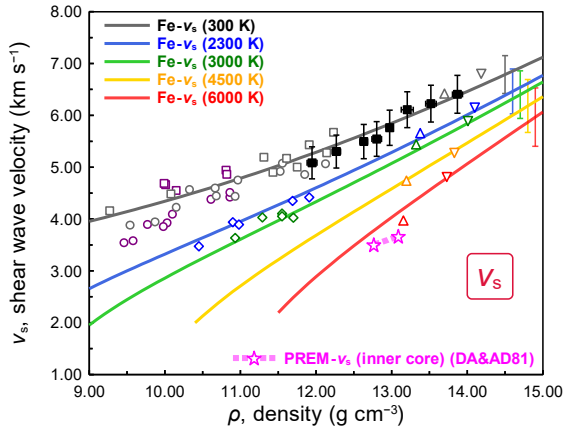
Supplementary Fig. 4. XRD image and integrated patterns. **a** XRD image at 13.87 g cm^{-3} (corresponding to 310 GPa). Typical hcp-iron (sample) and rhenium (gasket) peaks are indicated by arrows. The black areas are lead shadows for detector protection. **b** Integrated XRD patterns at all experimental pressures. The pressures in each experiment derived from the hcp-iron peaks based on Dewaele-EoS¹ are also shown. Bold and dashed lines represent the change of hcp-iron and rhenium peak positions, respectively.



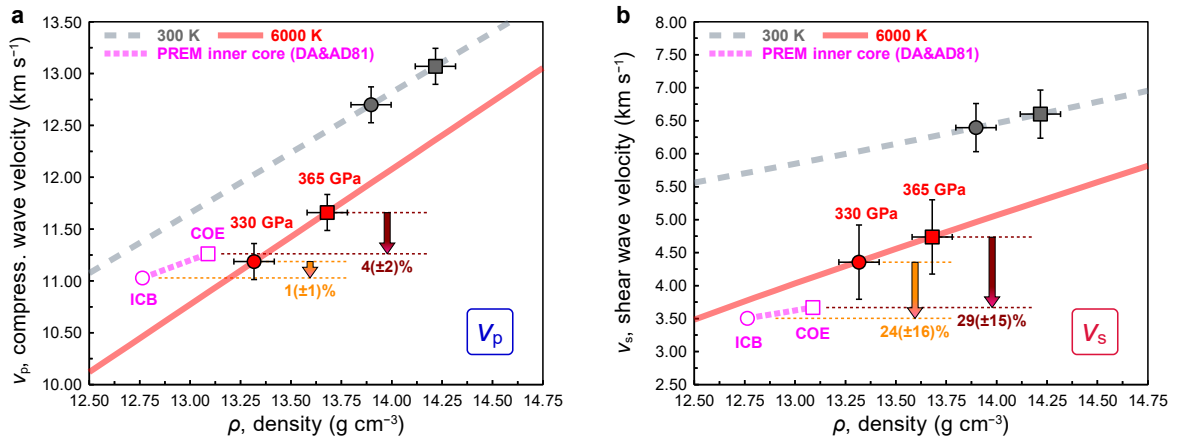
Supplementary Fig. 5. Comparison of v - ρ relations of hcp-iron, iron alloys, and iron compounds with Preliminary reference Earth model (PREM) at the inner core boundary (ICB, 330 GPa, and 6000 K) and centre of the Earth/core (COE, 365 GPa, and 6000 K) conditions, **(a)** v_p - ρ relations of each material, **(b)** v_s - ρ relations of each material. The circle and square symbols indicate ICB and COE conditions, respectively. The coloured symbols are as follows: black is hcp-iron by this study (pressure is evaluated by the Dewaele et al.¹), red is $\text{Fe}_{0.89}\text{Si}_{0.11}$ (6 wt% silicon, hcp)^{7,8}, green is $\text{Fe}_{0.86}\text{Ni}_{0.14}$ (15 wt% nickel, hcp)^{9,10}, blue is Fe_3S (tetragonal)^{11,12}, orange is Fe_7C_3 (orthorhombic)¹³, cyan is Fe_3C (non-magnetic, orthorhombic)¹⁴, purple is FeH (dhcp)¹⁵⁻¹⁷, grey is FeO (cubic B1)¹⁸, and magenta (open symbol) is PREM¹⁹. The v - ρ relations for hcp-iron at the ICB and COE conditions are determined by this work (see text and Methods). The v - ρ relations of other iron alloys and iron compounds are calculated from previous studies on sound velocity and EoSs⁷⁻¹⁸, and the present temperature dependence of hcp-iron (details are in Methods) except for $\text{Fe}_{0.89}\text{Si}_{0.11}$, Fe_7C_3 , Fe_3C , and FeO in which the temperature dependencies were experimentally determined^{7,13,14,18}. The magenta triangles represent the potential v - ρ relations of the iron compound consisting of three endmembers (hcp-iron, $\text{Fe}_{0.89}\text{Si}_{0.11}$, and Fe_3S) (lighter and darker colours indicate ICB and COE conditions, respectively). The error bars represent 1σ uncertainties for hcp-iron.



Supplementary Fig. 6. The pressure dependence of v_p of hcp-iron at ambient temperature. The pressure was evaluated by the isothermal EoS of hcp-iron ($\rho_0 = 8.45 \text{ g cm}^{-3}$, $K_{T0} = 177.5 \text{ GPa}$, $K'_{T0} = 5.66$) derived from the isentrope of hcp iron by Smith-EoS³. Solid squares are the results of this work; open squares from Ohtani et al. (OE13)²⁰; circles from Antonangeli et al. (AD12, AD18)^{21,22}; a dashed curve extrapolated by a power-law relation from Mao et al. (MZ12)²³; and a dotted curve from Fiquet et al. (FG01)^{24,25}. The magenta dashed curve with stars is the PREM inner core (DA&AD81)¹⁹. The symbols are the same as those in Fig. 2. The error bars represent 1σ uncertainties.



Supplementary Fig. 7. v_s - ρ relations using Smith-EoS³. We used the same experimental and theoretical data as those given in Fig. 3. The error bars represent 1σ uncertainties.



Supplementary Fig. 8. Comparison of density-velocity relations of hcp-iron based on Smith-EoS³ at inner core conditions with PREM. The v_p deficit (a) and the v_s deficit (b) in the inner core. The symbols are the same as those in Fig. 4. The v_p deficit and the v_s deficit are $1(\pm 1)\%$ and $24(\pm 16)\%$ at ICB, and $4(\pm 2)\%$ and $29(\pm 15)\%$ at COE, respectively. The error bars represent 1σ uncertainties.

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