nature portfolio

https://doi.org/10.1038/s41586-021-04361-x

Supplementary information

Superionic iron alloys and their seismic velocities in Earth's inner core

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Supplementary Information

Superionic iron alloys and their seismic velocities in Earth's inner core

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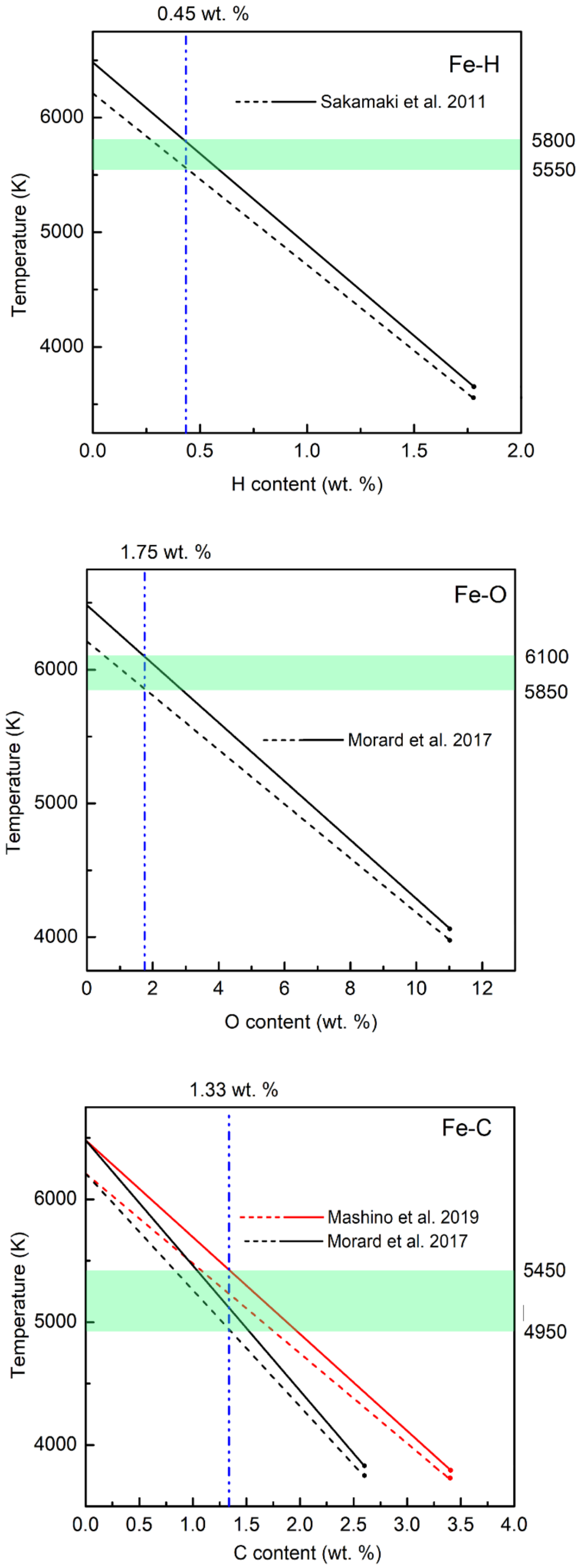
SI Guide

S1. The melting temperature of Fe alloys.

The melting behavior of Fe-H, Fe-C, and Fe-O binary systems has also been studied by previous high pressure experiments[1,2,3]. The presence of these light elements depresses the melting temperature. However, the eutectic melting experiments were conducted at relatively lower pressures. Thus, Simon–Glatzel equation was used to extrapolate the melting curve to the inner core conditions. The melting temperatures of Fe-rich side Fe binary alloys can be roughly estimated from eutectic temperature and composition as well as the melting point of pure Fe[4]. Based on the extrapolation of experimental data, the estimated melting temperatures are obtained (green regions in Supplementary Fig. 1), which are basically agree with our simulation results. Therefore, the elastic properties of the Fe alloys at 360 GPa are calculated at temperatures below 6000 K for $FeH_{0.25}$, and 5500 K for $FeO_{0.0625}$ and $FeC_{0.0625}$.



0.45 wt. %
Fe-H
Sakamaki et al. 2011
5800
5550
Temperature (K)
6000
5000
4000
0.0
0.5
1.0
1.5
2.0
H content (wt. %)
1.75 wt. %
Fe-O
6100
5850
Morard et al. 2017
Temperature (K)
6000
5000
4000
0
2
4
6
8
10
12
O content (wt. %)
1.33 wt. %
Fe-C
Mashino et al. 2019
Morard et al. 2017
5450
4950
Temperature (K)
6000
5000
4000
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
C content (wt. %)

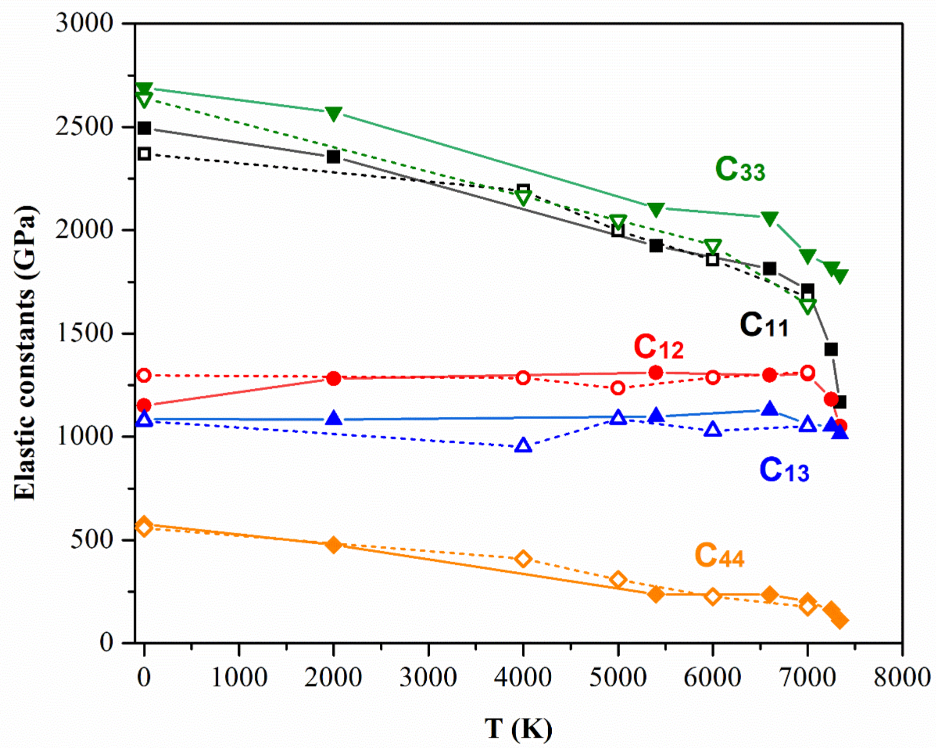
Supplementary Fig. 1 | Estimated melting temperatures of Fe-H, Fe-O, and Fe-C alloys with different light element contents at 330 and 360 GPa. The melting temperatures are estimated from the extrapolated melting curves of Fe-H, Fe-O, and Fe-C systems measured by high pressure experiments[1,2,3]. The solid and dash lines represent the melting temperatures at 360 and 330 GPa. The dot-dash lines exhibit the light element content in our simulation modes, with corresponding melting temperatures shown by green regions.

S2. Simulation and convergence tests

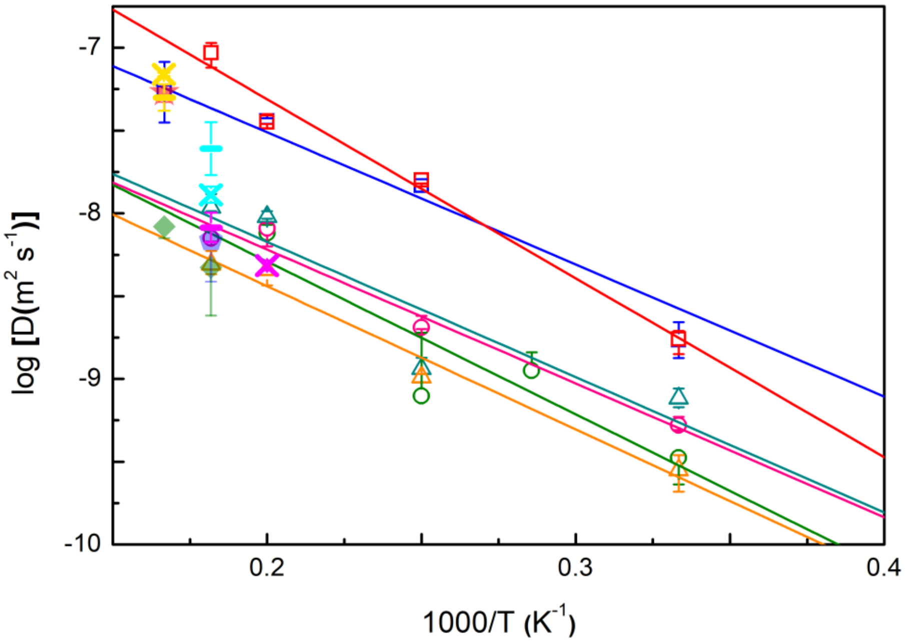
The elastic constants for pure hcp-Fe at 360 GPa were also calculated and compared with the results of the previous report (Supplementary Fig. 2)[5]. Our results show good consistence with the previous report at temperatures below 7000 K.

Convergence tests were performed on $FeH_{0.25}$, $FeO_{0.0625}$, and $FeC_{0.0625}$ at 360 GPa and 5000-6000 K with supercells containing over 200 atoms and simulation time above 100 ps. 4 × 4 × 6 supercells containing 240, 204, and 204 atoms for $FeH_{0.25}$, $FeO_{0.0625}$, and $FeC_{0.0625}$ are used for AIMD simulations. The simulations clearly confirm the superionic state of these Fe alloys. Also, the calculated diffusion coefficients and ionic conductivities are well converged (Supplementary Fig. 3).

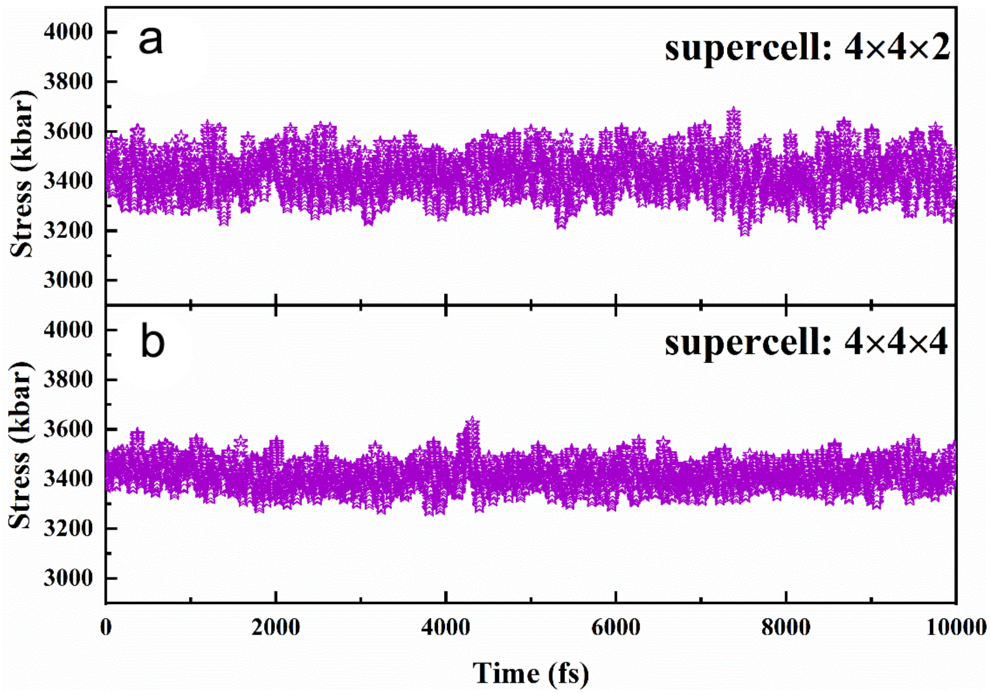
As the calculation results of the elastic constants are also very important in this work, we carried out convergence tests on the stresses of $FeH_{0.25}$ with different supercells. For each test, we made a gird of calculations to ensure the hydrostatic state. Then, we tested the stress with 1% (δ=0.01) strain in the [001] direction and all the simulations lasted ~10000 time steps. Our convergence tests are shown in Supplementary Fig. 4 and Supplementary Table 1. It suggests a larger supercell does not change our results on elastic constants.



Supplementary Fig. 2 | Calculated elastic constants for hcp-Fe as the function of simulation temperature at 360 GPa. Our data represented by open symbols is compared with the results of a previous report[5] represented by solid symbols. The elastic constants C_{11}, C_{12}, C_{13}, C_{33} and C_{44} are shown with black, red, blue, green and orange symbols, respectively.



Supplementary Fig. 3 | Comparison of calculated diffusion coefficients with different supercells and simulation time. Diffusion coefficients calculated using 4 × 4 × 2 supercells and 10 ps simulation time are shown with different open symbols: $FeH_{0.25}$ at ~260 GPa; red squares: $FeH_{0.25}$ at ~360 GPa; cyan triangles: $FeO_{0.0625}$ at ~260 GPa; orange triangles: $FeO_{0.0625}$ at ~360 GPa; green circles: $FeC_{0.0625}$ at ~260 GPa; pink circles: $FeC_{0.0625}$ at ~360 GPa. The convergence test results using 4 × 4 × 6 supercell and 100 ps simulation time are labelled by crosses and bars. The results of convergence test are presented with yellow, magenta, and cyan symbols for $FeH_{0.25}$, $FeO_{0.0625}$, and $FeC_{0.0625}$, respectively. The solid red star, green diamonds and blue pentagon represent the diffusion coefficients of H, O and C in liquid Fe at ~330 GPa.



Supplementary Fig. 4 | Convergence tests of supercell size on $FeH_{0.25}$. (a), (b) exhibited the simulated stress, induced by 0.01 strain in ε_{zz}, of [001] direction changed with time of a 4×4×2 supercell and 4×4×4 supercell, respectively.

Supplementary Table 1 | Convergence tests on supercell size.

Phase	*P* (GPa)	*T*	*Supercell*	*N* (*atom*)	*Strain* (%)	*Stress* (*GPa*)
hcp	360 *GPa*	5000 *K*	4 × 4 × 2	80	0.01	342.582
hcp	360 *GPa*	5000 *K*	4 × 4 × 4	160	0.01	341.360

S7. References

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