Superionic hcp-Fe alloys and their seismic velocities in Earth's inner core

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Abstract

Earth's inner core (IC) is less dense than pure iron, indicating the existence of light elements within it¹. Si, S, C, O, and H have been suggested to be the candidates^{2,3}, and the properties of Fe-light-element alloys were studied to constrain the IC composition⁴⁻¹⁹. Light elements have a significant influence on seismic velocities⁴⁻¹³, melting temperatures¹⁵⁻¹⁷, and thermal conductivities of Fe-alloys^{18,19}. However, the state of the light elements in the IC is rarely considered. Using *ab initio* molecular dynamics (AIMD) simulations, we found that H, O, and C in hexagonal close-packed (hcp) Fe transform to a superionic state under IC conditions, showing high diffusion coefficients like liquid. It suggests the IC can be in superionic state rather than normal solid state. The liquid-like light elements lead to a significant reduction in the seismic velocities approaching the seismological observation of the IC^{20,21}. The significant decrease in shear wave velocity (V_S) gives an explanation on the soft IC²¹. In addition, the light-element convection in the IC has potential influence on the IC seismological structure and magnetic field.

Full Text

Earth's inner core (IC), the central part of our planet, was formed and grown because of the solidification of liquid Fe alloys in the outer core. Seismological observations suggest that the structure of the IC is very complicated and difficult to understand. An unresolved problem is that the IC is soft with a low shear-wave velocity ($V_S = \sim 3.6$ km/s)^{20,21}, which cannot be matched by sound velocities in Fe and Fe alloys⁸⁻¹³. Theoretical prediction suggests that the premelting effect of Fe and Fe alloys can lead to strong nonlinear shear weakening at high temperatures²²⁻²⁴. However, a temperature close to the melting temperature with a small gradient is required. Alternatively, some fractions of melts need to be considered²⁵, but the mechanism of the stable presence of the melting fraction since the formation of the IC is unclear. Another long-standing controversy is the reason for the anisotropic seismic velocity structure. Generally, the compression wave velocities in the polar direction are ~ 3 % larger than those in the equatorial direction in the IC²⁶. This phenomenon is explained by the preferred orientation of hexagonal close-packed (hcp) Fe lattices with $\langle 001 \rangle$ directions²⁷ or body-centre-cubic (bcc) Fe lattices with $\langle 111 \rangle$ directions²⁸ along the spin axis. Moreover, earthquake doublets show that seismic waves present different travel times in the IC over the past few decades. This suggests that the IC structure changes with time, which is attributed to the super-rotation or oscillation of the IC²⁹⁻³¹. Investigations on the seismic properties of Fe and Fe alloys have improved the understanding of the IC structure. However, direct experimental measurements under the IC conditions are extremely challenging, while AIMD simulations have increased the knowledge on the properties of Fe alloys^{13,22-24,27,28}.

H, O, and C are, respectively, the first, second, and fourth abundant elements in our solar system³². They are also critical volatiles presenting in Earth's interior since its formation. In addition, they can be brought down to the core through mantle convection. In our simulations, H, O, and C atoms were placed at the interstitial sites of hcp-Fe to verify light-element effects on the properties of Fe alloys. AIMD simulations

were carried out at high P - T on $\text{FeH}_{0.25}$, $\text{FeO}_{0.0625}$, and $\text{FeC}_{0.0625}$ structures, which contained 0.45, 1.75, and 1.33 wt. % of light elements, respectively. The structures were constructed based on previous experimental studies, and the details are provided in the supplementary information S1. Solid-superionic-liquid phase transitions with increasing temperature are obtained and shown in Fig. 1. At low temperatures, light elements in hcp-Fe undergo small mean-square displacements (MSDs) and simply vibrate about their lattice positions demonstrating that the material is an ordinary solid. At temperatures above 3000 K, the light elements become highly diffusive like liquid as the MSDs increase monotonically during the simulation last over 100 ps indicating a superionic state (Supplementary Fig. 2). A further increase in temperature leads to the melting of the lattice. The melting temperatures of these structures were estimated using the two-phase method to exclude the superheating state in the calculations (Supplementary Information S2)³³. The estimated melting temperatures of $\text{FeH}_{0.25}$, $\text{FeO}_{0.0625}$, and $\text{FeC}_{0.0625}$ are approximately 5770 (± 200), 5595 (± 200), and 5413 (± 200) K at ~ 330 GPa, which are about 500-800 K lower than that of the pure hcp-Fe at the pressure of the inner core boundary (ICB)^{33,34} (Supplementary Fig. 5).

Superionic state is an intermediate state between solid and liquid. Superionic ice has been widely investigated and is suggested to exist in the interior of ice giants such as Neptune and Uranus³⁵⁻³⁹. Liquid-like protons in superionic ice may have a significant influence on the magnetic field of these exoplanets³⁹. In this study, it is shown that Fe alloys (H, O, and C) also transform to the superionic state under the IC conditions. In this case, H, O, and C behave like liquid diffusing within the hcp-Fe lattice. The diffusion coefficients of H, O, and C in solid and liquid iron were calculated (Fig. 2). The diffusion coefficients increase dramatically with temperature, while the effect of pressure is insignificant. Intriguingly, the diffusion coefficients of H, O, and C in solid and liquid Fe alloys are nearly identical under the ICB conditions. Although a significant phase transition from liquid to solid in Fe takes place at ICB, some light elements such as H, O, and C still maintain high mobility as fluids in the IC. Therefore, Earth's IC may be composed of solid-like iron and liquid-like light elements, and the convection of light elements continues in it.

The electric conductivities of Fe alloys are very important in understanding the energy budget of geodynamo and the heat flux of Earth's core^{18,19}. For superionic Fe alloys, the electric conductivity is composed of ionic conductivity and electronic conductivity. The ionic conductivities were calculated by Nernst-Einstein equation, and the values are in the range 10^2 – 10^3 S m⁻¹ (Supplementary Fig. 7). We also estimated the electronic conductivities using the combination of density functional theory with dynamical mean field theory (DFT+DMFT) method (Supplementary Information S4). Although the presence of light elements decreases the electronic conductivity of pure Fe, it is still over 2-3 orders of magnitude higher than the ionic conductivity, and therefore the conductivity contribution due to the ionic diffusion is negligible.

The liquid-like light elements in the Fe lattice also affect the seismic velocities. AIMD simulations with the NVT ensemble were conducted on $\text{FeH}_{0.25}$, $\text{FeO}_{0.0625}$, and $\text{FeC}_{0.0625}$ at 2000–6000 K and 360 GPa. In

order to exclude the effect of the superheating state, the simulation temperatures are lower than the predicted melting temperatures. The structures and cell parameters were carefully determined to maintain hydrostatic stress. The independent elastic constants for C_{11} , C_{12} , C_{13} , C_{33} , and C_{44} were calculated by distorting the equilibrium structure and solving the stress-strain relations (Supplementary information S5). The compression (V_P) and shear (V_S) wave velocities of these structures at high P - T were deduced from the elastic constants and are plotted in Fig. 3. The V_P of the alloys decrease almost linearly with temperature, while V_S show an accelerated decline upon the solid-superionic transition (Fig. 3c). It suggests that the diffusion of light elements may introduce anharmonic vibration in the lattice resulting in significant effect on V_S . Owing to this effect, a small amount of diffusive light elements lead to a decrease in seismic velocities and densities approaching the geophysical observations at the IC conditions. H, O, and C superionic light elements have different effects on seismic velocities and densities. A content of 0.45 wt. % superionic H in hcp-Fe causes the expected decrease in density. The density of $\text{FeH}_{0.25}$ at 6000 K is 13.12 g/cm^3 , which is very close to that of the Preliminary Reference Earth Model (PREM), while the presence of superionic O and C elements has an inconspicuous effect on the density. On the other hand, the V_S of $\text{FeO}_{0.0625}$ and $\text{FeC}_{0.0625}$ is lower than that of $\text{FeH}_{0.25}$ at approximately 5500 K. Although the V_S of the Fe alloys are slight higher than that of the PREM, they may be further reduced considering the presence of nickel⁸. Poisson's ratio is also an important probe to constrain the composition and structure of the IC. The presence of superionic light elements also increases Poisson's ratio to 0.41 for H, and 0.43 for C and O, which is quite close to that of the PREM (Supplementary Table 1 and Supplementary Fig. 9). Therefore, the superionic Fe alloys at 5500–6000 K show quite similar seismic characteristics as that of the IC. Previous theoretical simulations show a decrease in V_P and V_S of Fe and Fe alloys with increasing temperature because of the premelting effect^{22–24}. However, the calculated velocities can be consistent with the PREM at approximately 7200 K for Fe and 6700 K for Fe-Si-C alloy^{22,24}, which are higher than the most computationally and experimentally predicted temperatures of IC^{15–19}. Here we provide a new mechanism by which highly diffusive light elements bring strong anharmonic vibration to Fe alloys and lead to significant reductions of V_P and V_S close to the PREM model at 5500–6000 K. Elastic softening caused by its superionic effect was also reported in Li_2O when it is used as a nuclear fusion material at high temperatures⁴⁰.

Seismologic observations suggest that Earth's core is composed of the liquid outer core with V_S equal to zero, and the solid inner core with V_S equal to $\sim 3.6 \text{ km/s}$. At the ICB, solidification of the IC generates latent heat and leads to the separation and buoyancy of light-element phases, which promote the convection flows of the outer core, producing and powering the geomagnetic field (black dashed arrows in Fig. 4). Based on our simulations, some light elements such as H, O, and C can present in the IC in the superionic state. Owing to the high diffusion coefficients, light elements continue their circulation in the IC (red dashed arrows in Fig. 4). In this case, the IC is not conventionally known normal solid Fe alloy, but a mixture of solid Fe and light-element fluids. The convection of the ionic light elements may generate magnetic field in the IC. However, quantitative modelling is needed to study if this magnetic field is sufficient to influence Earth's magnetic field.

The liquid-like light elements also bring significant influence on the elastic properties of the IC, and the long-standing seismic puzzles in the IC, as mentioned above, can be rationalized within the superionic IC model. First, the liquid-like light elements have a profound effect on the seismic velocities, presenting the V_S quite close to that of the PREM at 5500–6000 K, which explains why the IC is quite soft. In addition, superionic Fe alloys show 8–11 % lower V_p than that of pure Fe. If the distribution of superionic light elements in the IC is inhomogeneous with a higher concentration in the equatorial direction than in the polar direction, seismic velocities along the equatorial direction will be lower, which gives a simple reason for the anisotropic seismological structure. Also, the enrichment of liquid-like light elements may enhance seismic wave attenuation, which has been widely observed in the IC²¹. Moreover, the light-elements convection changes the distribution of light element in the IC leading to the evolution of the seismological structure with time. This phenomenon may provide an alternative interpretation of the differential travel time of similar earthquakes²⁹⁻³¹. Generally, the seismic properties of superionic Fe alloys are consistent with the seismology characteristics of the IC.

Suggested by some geodynamo models, geomagnetic field also has influence on the IC^{41,42}. In this case, the diffusion of ionic light element can be affected by the inner-core magnetic field under Lorentz force, and the convection and distribution of light elements may related with geometry and strength of the magnetic field. Besides, both seismic velocity in the IC and the geomagnetic field show observable change in last few decades²⁹⁻³¹. Then, it is important to study if there is a certain relation between the inner core seismic structure and geomagnetic field, which might be a clue for understanding the structure and evolution of the IC.

Method

The calculations were performed using the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional and projector augmented wave (PAW) method⁴³ as implemented in the Vienna Ab Initio Simulation Package (VASP)⁴⁴. A plane wave representation for the wave function with a cutoff energy of 800 eV was adopted. In AIMD simulations, the cutoff energy was set to 400 eV with Γ point for k-space sampling. AIMD simulations within canonical ensemble (NVT) were conducted to study the solid-superionic-liquid phase transition and diffusion coefficients of superionic light elements. The simulations lasted ~10-100 ps at temperatures from ~2000 to ~7000 K and pressure from ~250 to ~400 GPa with a time step of 1fs. The two-phase method³³ was adopted to predict the melting temperatures for $\text{FeH}_{0.25}$, $\text{FeO}_{0.0625}$ and $\text{FeC}_{0.0625}$. The simulations within NVE ensemble were conducted on the solid-liquid coexistence system containing 256 Fe atoms and 64, 16, and 16 of H, O, and C atoms, respectively (Supplementary Information S2). Our calculations on ionic transport and elastic properties of superionic phases were constrained at the temperatures below the melting temperature. Structures for Fe-hcp with C, H and O atoms at the interstitial sites of $4 \times 4 \times 2$ supercells at 2000–6000 K and 360 GPa were constructed to investigate elastic properties. We determined the equilibrium volumes and cell parameters at different temperatures by conducting a grid of NVT ensemble simulations over volumes and temperatures using a Nosé thermostat⁴⁵. For each equilibrium structure, a 10,000 time-steps (10 ps)

simulation was conducted to check for sure that the stress field is hydrostatic. The elastic constant C_{ij} was calculated by distorting the equilibrium structure and solving the stress-strain relations. Details for the calculation methods and convergence tests with large supercells and long simulation time are provided in Supplementary Information.

Declarations

Data availability

The data that support this study are available from the corresponding author upon reasonable request.

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Author contributions:

Y.H. and S.S. contributed equally to this work, conducted the calculations, analysed the data, and wrote the manuscript. Y.H., D.Y.K., and H.K.M initiated and designed the project. S.S. performed simulations on elastic properties. B.G.J. performed electronic conductivity calculations. All authors discussed the data analysis and interpretation and commented on the manuscript.

Competing interests

The authors declare no competing interest

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Figures

Figure 1

Phase diagrams of FeH_{0.25}, FeO_{0.0625} and FeC_{0.0625} at temperatures and pressures in the range ~2000–7000 K and ~250–400 GPa. The green, blue and red squares show the solid, superionic and liquid states sampling in our simulations. The orange star represents estimated melting temperature calculated by the two-phase method (Supplementary S2). Estimated melting curve is shown by the thick grey curve between the red and blue regions. Blue squares above the melting curves indicate the superheating state. The dashed black curve represents the melting temperatures of pure hcp-Fe by high P-T experiments⁴⁰. The dashed grey lines show the pressures of the ICB and the central IC.

Figure 2

Diffusion coefficients of light elements (H, O, C) in solid and liquid Fe alloys under the IC conditions. Different diffusion coefficients are labeled by different symbols. Blue squares: FeH0.25 at ~260 GPa; red squares: FeH0.25 at ~360 GPa; cyan triangles: FeO0.0625 at ~260 GPa; orange triangles: FeO0.0625 at ~360 GPa; green circles: FeC0.0625 at ~260 GPa; pink circles: FeC0.0625 at ~360 GPa. The diffusion coefficients are linearly fitted and shown with colour lines. The solid red star, green diamonds and blue pentagon represent the diffusion coefficients of H, O and C in liquid Fe at ~330 GPa.

Figure 3

Seismic velocities of FeH_{0.25}, FeO_{0.0625} and FeC_{0.0625} as the function of density and temperature at 360 GPa. a. calculated compressional wave velocities (V_P) and b. shear wave velocities (V_S) of hcp-Fe alloys comparing with the velocities of the PREM in IC (red stars)²⁰. The seismic velocities are compared with the results of previous simulations by different symbols: red open squares: FeH_{0.25}; orange open triangles: FeO_{0.0625}; green open circles: FeC_{0.0625}; purple solid diamonds: hcp-Fe₂₂; magenta solid triangles: hcp-Fe_{0.9375}Si_{0.0625}23; cyan solid circles: Fe₆₀Si₂C₂₂24. The maximum simulation temperatures for different models are labeled. c. The evolution of V_P and V_S upon the transition from solid to superionic state with increasing temperature.

Figure 4

Schematic of the outer core fluid convection and the IC light-elements convection. Black and red dashed arrow curves represent the outer core convection generating the geomagnetic field (blue solid curves) and superionic light-element (H, O and C ions) convection in the IC, respectively.

Supplementary Files

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