Compressional sound velocity of hexagonal close-packed iron up to 163 GPa and 3000 K

Seismological data reveal important physical properties of Earth's core, such as density and elasticity. Earth's core is mainly composed of iron (Fe), and the stable crystal structure of Fe under the inner core conditions is the hexagonal close-packed (hcp) structure. The density of the inner core based on the Preliminary Reference Earth Model (PREM) [1], which was proposed by using seismological data, is about 2–5% less than that of hcp-Fe (a core density deficit), and it is accepted that the inner core consists of iron and light elements, such as silicon, sulfur, oxygen, hydrogen, and carbon.

To constrain the sound velocity of the inner core and the abundances of light elements, the sound velocities of Fe and Fe alloys have been measured at high pressures by inelastic X-ray scattering (IXS) and nuclear resonant inelastic X-ray scattering (NRIXS). However, due to experimental difficulties, sound velocity measurements with static compression above 2000 K have never been reported. Some previous studies of IXS using external heated DAC showed a small temperature effect on the velocity; however, the maximum temperature range was limited to around 1100 K and the temperature dependence is still not sufficiently clear to discuss the Earth's core.

It is necessary to determine the sound velocity of hcp-Fe at high temperatures in order to quantitatively clarify the difference in the sound velocity between Earth's inner core and hcp-Fe. An important point is that the constituents of the Earth's inner core should fill the gap of both the density and the sound velocity between hcp-Fe and those in seismological models, such as PREM, under the inner core conditions. Here, we report the compressional sound velocity (V_P) of hcp-Fe up to 163 GPa and 3000 K (Fig. 1) based on a combination of laser-heated DAC [2] and IXS measurements at SPring-8 **BL35XU** [3].

V_P for hcp-Fe as a function of density is shown in Fig. 2, together with data obtained at 300 K [4] and shock compression data [5]. These data were fitted by allowing the coefficients in the linear ρ-V_P relation to vary with the temperature, so that Birch's law is preserved at any fixed temperature. A good fit to the data is possible by assuming a first order and linear temperature dependence of the coefficients. The dependence was parameterized as

$$V_P(\rho, T) = M\rho + B + A(T - T_0)(\rho - \rho^*) \quad (1).$$

We choose T_0 to be 300 K; thus, M and B are the coefficients of Birch's law at room temperature, while A and ρ^* indicate the temperature dependence. Fitting our data combined with room temperature data [3] and shock compression data along the Hugoniot [4] gives $M = 1.160 \pm 0.025$, $B = -3.43 \pm 0.29$, $A = 7.2 \pm 3.6 \times 10^{-5}$, and $\rho^* = 14.2 \pm 1.5$.

To demonstrate the difference in density and V_P between hcp-Fe and Earth's inner core, we compare the ρ-V_P characteristics under the conditions of the inner core boundary (ICB). The recent arguments on the thermal state of the outer core based on melting experiments of iron-light element systems suggest that the temperature at the ICB is around 5500 K. V_P at 330 GPa and 5500 K can be calculated by using the density of hcp-Fe and the temperature dependence of Birch's law given in Eq. 1. The obtained V_P for hcp-Fe at 5500 K is shown as a function of density in Fig. 3(a) and compared with PREM in the inner core [1]. The density and compressional velocity of hcp-Fe under the ICB conditions (330 GPa and 5500 K) are calculated to be 13.42 g/cm³ and 11.85 km/s, respectively. Thus, both the density and V_P for hcp-Fe are higher than those in PREM, which are 12.76 g/cm³ and 11.03 km/s at the ICB, respectively. The Earth's inner core has a 4–5% smaller density and 7% smaller V_P than hcp-Fe. Thus, we can conclude that the light elements or the combination of the light elements and nickel in the inner core decreases both the density and compressional velocity of hcp-Fe simultaneously under the inner core conditions.

The sound velocity and density of Fe and Fe alloys have been experimentally measured in order to demonstrate the effect of light elements on the properties of iron. Figure 3(b) shows the ρ-V_P plots of

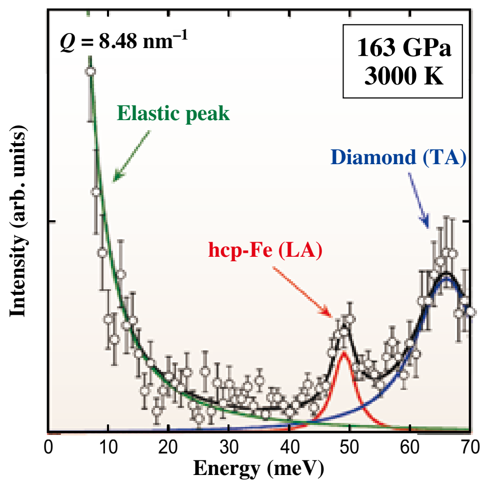

Fig. 1. IXS spectrum of hcp-Fe at 163 GPa and 3000 K. The peak at zero energy is from elastic scattering. Curves are individual contributions (green: elastic scattering, red: LA phonons of hcp-Fe, blue: TA phonons of diamond), with the experimental data fitted with Lorentzian functions.

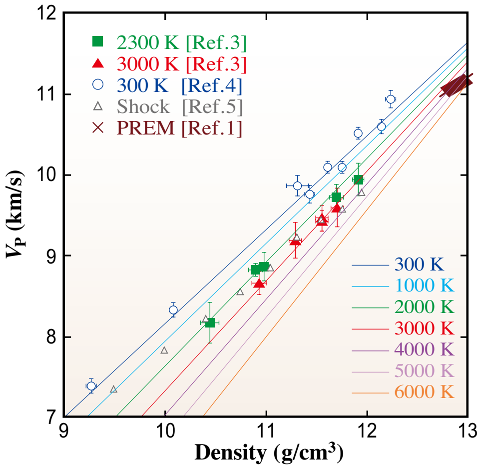

Fig. 2. Compressional velocity of hcp-Fe at several temperatures as a function of density along with high-temperature data [3] and room-temperature data [4] based on IXS and shock compression experiments [5]. Isothermal ρ-V_P fitting lines are expressed as $V_P = [1.160\rho - 3.43] + [7.2\times10^{-5}\times(T-300)\times(\rho-14.2)]$.

hcp-Fe, hcp-$Fe_{92}Ni_8$, dhcp-Fe, hcp-$Fe_{85}Si_{15}$, Fe_3S, FeO (B1/rhombohedral phase), Fe_3C, and Fe_7C_3. Each ρ-V_P plot of iron alloys and iron-light element compounds is shown from the center of the Earth (364 GPa) to the ICB (330 GPa). Star symbols indicate the ρ-V_P points at 330 GPa and 5500 K, obtained by extrapolating to the ICB conditions assuming that the temperature effect on these compounds is the same as that for hcp-Fe. In order to account for the composition of Earth's inner core, the triangles (Fe, Fe-Ni alloy, Fe-light element compounds) need to overlap with the star of PREM. Assuming the ideal mixing of hcp-Fe, hcp-Fe-Ni, and Fe-light element alloys, we obtain the average ρ-V_P for Fe alloy with light elements. As a result, we demonstrate that oxygen and carbon may not be major light elements in the inner core. On the other hand, silicon, sulfur, and hydrogen are potential candidates because they can decrease both the density and velocity. In particular, hydrogen is a good candidate because the mixing of hcp-Fe, hcp-$Fe_{92}Ni_8$, and dhcp-FeH can account for the ρ-V_P plot of PREM. Thus, there is a possibility that the inner core is a hidden hydrogen reservoir in the Earth. In addition, silicon and sulfur can also be major light elements if their temperature effects on V_P are larger than that of hcp-Fe.

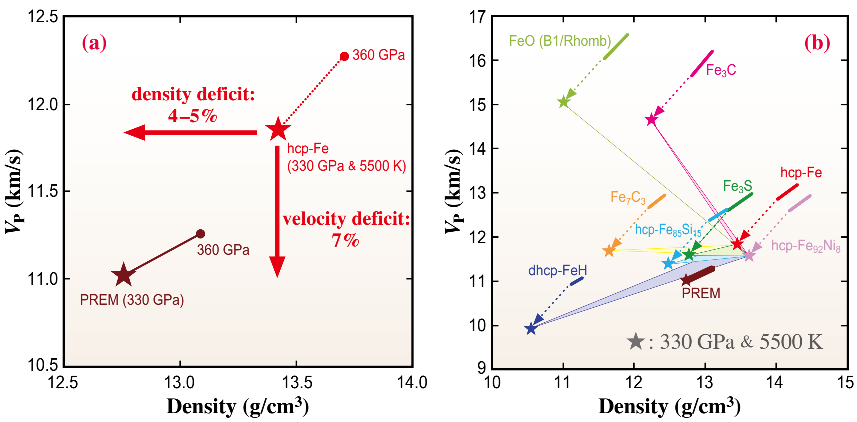

Fig. 3. ρ-V_P plot of hcp-Fe under inner core conditions. **(a)** Comparison of the ρ-V_P plot between hcp-Fe and PREM [1]. Stars indicate V_P and ρ for hcp-Fe and PREM at 330 GPa. The difference in the ρ-V_P plot between PREM and hcp-Fe at 5500 K shows a 4–5% core density deficit and a 7% core velocity deficit. **(b)** Comparison of the ρ-V_P plot between hcp-Fe and Fe-light element compounds. The values for hcp-Fe and the Fe-light element compounds (hcp-$Fe_{92}Ni_8$: purple, dhcp-FeH: blue, hcp-$Fe_{85}Si_{15}$: aqua, Fe_3S: green, FeO [B1/rhombohedral phase]: yellow-green, Fe_3C: pink, Fe_7C_3: orange) show distributions from the inner core boundary (ICB) to the center of the earth. The obtained ρ-V_P for hcp-Fe at 5500 K is indicated by red and star represents the expected ICB conditions. The other stars denote ρ-V_P for Fe-light element compounds under ICB conditions assuming the temperature effects of these compounds are the same as those of hcp-Fe (the dashed arrows are the temperature effects). Triangles connecting the three stars (Fe, Fe-Ni alloy, Fe-light element compounds) indicate the potential ρ-V_P region obtained by mixing the three components.

T. Sakamaki[a]*, E. Ohtani[a], H. Fukui[b,c] and A. Q. R. Baron[c]

[a] Department of Earth and Planetary Materials Science, Tohoku University
[b] Center for Novel Material Science under Multi-Extreme Conditions, University of Hyogo
[c] RIKEN SPring-8 Center

*Email: sakamaki@m.tohoku.ac.jp

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