

Effect of light elements on the sound velocities in solid iron: Implications for the composition of Earth's core

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Abstract

We measured compressional sound velocities in light element alloys of iron (FeO, FeSi, FeS, and FeS₂) at high-pressure by inelastic X-ray scattering. This dataset provides new mineralogical constraints on the composition of Earth's core, and completes the previous sets formed by the pressure–density systematics for these compounds. Based on the combination of these datasets and their comparison with radial seismic models, we propose an average composition model of the Earth's core. We show that the incorporation of small amounts of silicon or oxygen is compatible with geophysical observations and geochemical abundances. The effect of nickel on the calculated light element contents is shown to be negligible. The preferred core model derived from our measurements is an inner core which contains 2.3 wt.% silicon and traces of oxygen, and an outer core containing 2.8 wt.% silicon and around 5.3 wt.% oxygen.

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The composition of the Earth's core is a standing problem in the field of Earth sciences [1–4]. Seismic wave propagation and normal mode oscillation are available probes to study the core, and their inversion yields a distribution of sound velocity, density, and compressibility profiles [5,6]. However, these models cannot directly constrain the chemical and structural properties of Earth materials. In order to understand and investigate the composition of the Earth, one has to use mineralogical and

geochemical models that in turn have to be in accord with these seismological models. Using shockwave measurements on iron, Birch [7] proposed that Earth's core was too light to be made of pure iron. Since then, multiple studies [8–10] have revealed that indeed iron is too dense to be the only constituent not only of Earth's core as a whole, but also more specifically of the solid inner core.

From a methodological viewpoint, high-pressure mineralogy provides sets of data that can be combined with seismic data in order to check the self-consistency of the models. In this sense, the study of Earth materials under extreme conditions (high-pressure and high temperature) in recent years unveiled information on the

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density and compressibility of minerals [11] in the conditions of the deep Earth from the *in situ* study of their crystal structure by X-ray diffraction. It was only very recently that probing static sound velocities in extreme conditions [9,12] became available, making it important to measure sound velocities of iron alloyed with lighter elements, among which sulphur [13–16], oxygen [14,16–18] and silicon [19–21] are the choice candidates. The question now is how to constrain the relative abundances of these light elements. Here, we report direct high-pressure measurements of sound velocities in iron compounds with elements supposedly entering in the composition of the Earth's core, i.e. iron oxide (FeO-wüstite), iron sulphide (FeS-troilite and FeS₂-pyrite) and iron silicide (FeSi), and address the question of the composition of the core. For modelling sound velocities in the combined composite mineral model within a first-order approximation, the compressional sound velocity in the $(1-\varepsilon_1-\varepsilon_2-\varepsilon_3)\text{Fe}+\varepsilon_1\text{O}+\varepsilon_2\text{Si}+\varepsilon_3\text{S}$ system is considered equal to that in the $(1-2.\varepsilon_1-2.\varepsilon_2-2.\varepsilon_3)\text{Fe}+\varepsilon_1\text{FeO}+\varepsilon_2\text{FeSi}+\varepsilon_3\text{FeS}$ system where $\varepsilon_1, \varepsilon_2, \varepsilon_3$ stand for the molar fractions of O, Si, and S in the inner core, respectively. This simplest expression for sound velocity in an ideal solid should hold for low light element contents.

Sound velocities were measured at high-pressure by very high resolution inelastic X-ray scattering at the European Synchrotron Radiation Facility (ESRF) on beamline ID28, using the (8,8,8) reflection of a backscattering silicon monochromator at an energy of 15.618 keV (3.9 meV energy resolution, 5.5 meV total instrumental resolution). The details of the experimental setup have been reported elsewhere [22]. The samples were loaded in Mao-Bell type diamond anvil cells, except for the FeS experiment where the sample was loaded in a high temperature resistant membrane-driven cell. The dispersion of longitudinal acoustic (LA) phonons was measured for 5 values of the momentum transfers between 4 and 12 nm⁻¹. The sound velocity, which is equal to the slope of the dispersion curve at zone center, can thus be directly obtained from a sine fit to the dispersion. At each pressure (measured by ruby fluorescence), an angle-dispersive X-ray diffraction pattern was collected in order to obtain directly the molar volume and hence, the density (without using otherwise unreliable if not unavailable equations of state). The samples were allowed to relax at room temperature after each pressure increase. The measurements were performed to pressures of 90 GPa at room temperature for FeO, FeS₂ and FeSi. In the case of FeS, the measurements were performed at high-pressure and high temperature in the stability field of phase IV [23] which is the non-quenchable phase relevant to sulphur-rich planetary cores, between 4 GPa at 375 K and

13.5 GPa at 610 K. One has to note that the theoretically predicted phase of FeS relevant to planetary cores [24] with the CsCl structure could not be observed.

In the case of iron, we used a compilation of previously published experimental results, combining shockwave data [25] with static work [2,6], and limiting ourselves to pressures below 78 GPa for the static dataset (Fig. 1). This limitation is due to the fact that the measurements above that pressure need to be corrected for elastic anisotropy. Indeed, it was shown [26] that the angular dependence of the P-wave velocity (elastic anisotropy) could be measured with the IXS technique using differences in velocities measured in various geometries, thanks to the preferential alignment of grains of iron uniaxially compressed in a diamond anvil cell. The study [26] showed that there is no measurable anisotropy up to 78 GPa, because the P-wave velocities are independent of orientation. A measurable anisotropy then appeared at higher pressure. This anisotropy effect, although very useful for the comprehension of the anisotropic properties of Earth's inner core, impedes all use of such data for comparison with averaged radial models. So we only use the points measured below 78 GPa in our dataset.

The surprising correlation (Fig. 1) with the shockwave data (taken at high temperature) suggests that temperature effects at constant density on compressional

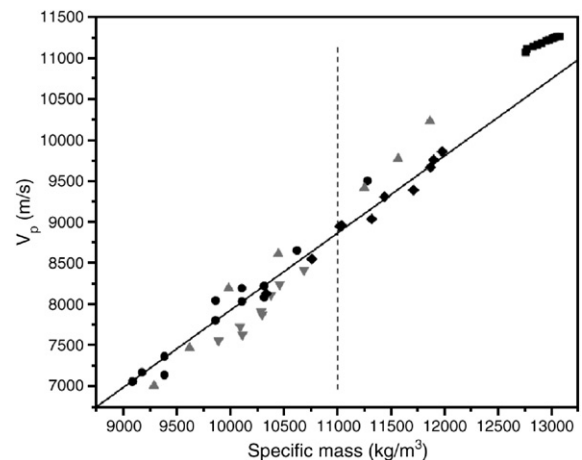


Fig. 1. Compressional (P-wave) sound velocities for ε -iron from static IXS work (black circles) [9,26], static NRIXS work [28] (gray up- and down-triangles), and shockwave measurements (black diamonds). The scatter in the NRIXS data is too large and can therefore not be used to obtain reliable velocity–density relationships. The IXS data was combined with the shockwave data, and the linear fit obtained is $V_p=0.94\rho-1466$. The dashed line shows the cut-off density above which the static data was not used, due to contributions of anisotropy to the measured sound velocity [26]. The black squares represent the inner core's velocity–density profile as obtained from PREM.

sound velocity are minimal, thus a linear relation with density (Birch’s law) can be assumed. The validity of the Birch’s Law has very recently been demonstrated theoretically for *hcp* and *bcc* iron [27]. Recent measurement of Debye sound velocities at high-pressure and high temperature [28], based on NRIXS, proposed that Birch’s law was violated at intermediate pressures and that temperature had an intrinsic effect on compressional sound velocities. However, the study also proposes that the Birch’s Law should be recovered at core pressures, where temperature effects should become marginal, in accord with our observation.

The sound velocities measured as a function of density are reported in Fig. 2 (the data in Table 1), along with the linear regressions and their parameters. For the reasons pointed out above, the linear regression for iron was calculated only taking into account the IXS datasets up to 78 GPa grouped with the shockwave data. It is worthy to note that the densities were not obtained using previously published equations of state, but rather by direct measurement of the molar volumes by X-ray diffraction at each pressure point and for each compound, hence reducing all systematic errors transferred from the equations of state. It can be seen from Fig. 2 that all compounds follow the empirical “Birch’s Law” in the investigated pressure and temperature range. This behaviour is well-suited for our modelling because it allows combining datasets obtained at different pressures and temperatures (static and shockwave measurements). More importantly, this allows the interpolation of the value of sound velocity of any such material to any given pressure or temperature inside the

Earth, as long as we know its equation of state in order to calculate density.

Unfortunately, P–V–T equations of state of iron alloys are not readily available, and very little data are present in order to calculate their densities at the P–T conditions of Earth’s core. Nevertheless, knowing the P–V–T equation of state of the major compound, namely ϵ -iron in the present case [29], it is possible based on our measurements, to reconstruct the composition–velocity–density profiles of terrestrial solid core models constituted of iron and one light element. Indeed, the average density ρ and compressional sound velocity V of a two-component ideal solid is given in first approximation by

$$\rho = x\rho_1 + (1-x)\rho_2$$

and

$$V = \frac{V_1 \cdot V_2}{(1-x)V_1 + xV_2},$$

respectively, where x is the volume fraction of component 1. Forcing $\rho = \rho_{\text{PREM}}$ and $V = V_{\text{PREM}}$, and knowing ρ_1 (density of iron) from thermal equation of state measurements [29], and V_1 and V_2 being linear functions of ρ_1 and ρ_2 (Birch’s Law for iron and the light element), we are left with two equations and two unknowns that can be analytically solved to give a unique solution for x (the volume fraction of the alloying compound) and ρ_2 (density of the light element). Unlike most previous studies, we did not attempt to extrapolate measurements made on solid state phases to the liquid outer core, but used partitioning and solubility data in the literature to estimate the composition of the outer core from that constrained for the inner core with the method described above. The results are summarised in Table 2.

The most striking observation is that a very high concentration of sulphur (in the FeS form) would be needed to account for the density and velocity profile of Earth’s inner core, significantly above typical values inferred from geochemistry [2–4,30,31]. If sulphur were to be the only light element entering in the composition of the inner core, the latter would have to contain around 10 wt.% sulphur in order to exhibit the density and compressional sound velocity profiles obtained by PREM, and would also require a very low bulk modulus for FeS, since the compression (V_0/V) needs to be 2.49, which is unrealistic for any core-forming material under such pressures. From geochemical models, a value of more than 1.7 wt.% in the core is highly unlikely [30]. Moreover, the very low bulk modulus of FeS would dramatically soften the inner core, similarly to what was already shown for the outer core in a structural study of

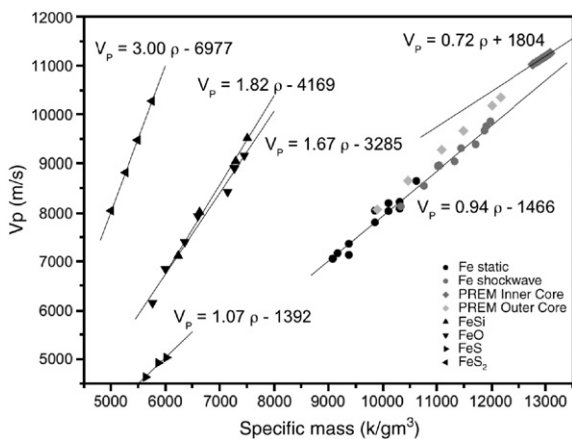


Fig. 2. Compressional (P-wave) wave velocities in Fe, FeS, FeO, FeS₂ and FeSi as a function of density. Seismic velocity profiles from the radial PREM model for the inner and outer core are also reported, along with the parameters of the linear regressions used for each compound.

Table 1
Measured densities and velocities for Fe, FeO, FeSi, FeS, and FeS₂

ρ (kg/m ³)	+/-	V_P (m/s)	+/-
<i>Fe</i>			
9084	33	7055	49
9382	34	7363	52
9861	32	7802	62
10107	54	8032	72
10315	58	8222	90
9084	35	7059	49
9175	35	7169	57
9382	30	7137	57
9861	35	8042	72
10107	46	8197	82
10315	60	8085	89
10621	58	8654	121
<i>FeO</i>			
5770	39	6150	49
6000	40	6850	58
6360	34	7400	66
6600	48	7930	73
7270	56	8910	88
7147	62	8430	93
7450	54	9160	110
<i>FeSi</i>			
6239	28	7121	70
6630	28	8013	96
7293	34	9043	127
7507	33	9515	152
<i>FeS</i>			
5640	46	4630	79
5870	54	4920	113
6020	66	5030	126
<i>FeS₂</i>			
5010	11	8042	88
5277	14	8824	124
5492	21	9476	133
5757	32	10278	144

the Fe–S liquid system [32]. The case of FeS₂ was also considered, mainly because of the different bonding properties of sulphur in this compound (different oxidation state, low-spin compound). Although the abundances of FeS₂ in a binary assemblage may sound

reasonable (Table 2), the inferred compression is unacceptable, because it would require FeS₂ to have the same density at core pressures and temperatures than at normal room conditions.

On these bases, one could consider that sulphur in the FeS form can represent a maximum of 1.7 wt.% of the composition of the Earth's inner core, but we further note that when condensation/volatilisation temperatures of sulphur are taken into account, it is indeed rather likely that values of less than 1 wt.% of S in the inner core are even more realistic. In any case, other elements need to be used for explaining the core velocity–density characteristics.

The abundances obtained for silicon and oxygen in binary assemblages, namely 2.3 wt.% and 1.6 wt.% respectively (see Table 2), are in the range given by various geochemical models. Moreover, the compression ratios given by our model are in reasonable accord with existing equations of state. Therefore, both silicon and oxygen are good candidates for a light alloying element in Earth's inner core.

The Earth's core contains 5 wt.% of nickel, alloyed with iron. Lin et al. [21] have shown that the effect of nickel alloying on the sound velocities in iron is very small, and that the slope of $V_P(\rho)$ is parallel to that of Fe. This linear relation can therefore be calculated for any Ni concentration from that of pure Fe by adjusting the density of Fe to that of the Fe–Ni alloy. The effect of Ni (up to 15 wt.%) is negligible both in terms of the amount of light elements that can be incorporated in the inner core as well as for determining the valid candidates. Indeed, the amount of Si changes from 2.3 wt.% in pure Fe to 2.4 wt.% in a Fe–Ni alloy containing 15 wt.% Ni. Similarly, the amount of O changes from 1.6 wt.% in pure Fe to 1.7 wt.% in a Fe–Ni alloy containing 15 wt.% Ni.

Theoretical calculations [33] show that the (weight-converted) partition coefficient for silicon, sulphur and oxygen between the liquid and solid phases of iron is

Table 2
Results from our model for the major element composition of the core

Element / mineral	Fraction for one element (wt%)	Compression (V_Q/V)	Model fraction inner core (wt%)	Model fraction outer core (wt%)
Si FeSi	2.3	1.28	2.3	2.8
O FeO	1.6	1.33	0.1	5.3
S FeS	9.7	2.51	0	0
S FeS ₂	3.6	1.0	0	0

The first two columns give the weight fraction and compressions obtained by resolving our doubly-constrained sound velocity and density model for the inner core according to PREM. It shows that both forms of sulphur cannot reasonably fit the model, either because of extreme values of the compression ratios (huge compression for FeS, no compression for FeS₂), or because of the unrealistic content (9.7 wt.% sulphur). Silicon and oxygen on the other hand can both satisfy the double-constraints for the inner core. Our final preferred model is given in the shaded columns, and satisfies high-pressure Si and O solubility measurements in iron and theoretically calculated solid–liquid partition coefficients.

$D^{\text{Liq/Sol}}(\text{Si or S})=1.2$ and $D^{\text{Liq/Sol}}(\text{O})=400$. Thus, one has to rule out the possibility that oxygen be a major light element component of the inner core. Therefore, we conclude that the light element in the inner core should be silicon, amounting to 2.3% of its weight.

We can also constrain the composition of the outer core. With an inner core containing 2.3 wt.% Si, and using the partition coefficient given above, the outer core should contain 2.8 wt.% Si. This value is in perfect agreement with recent measurements of Si solubility in iron in equilibrium with perovskite at 97 GPa [34]; in these experiments, Takafuji et al. [34] found 2.8 wt.% Si quenched in the liquid metal, along with 5.3 wt.% O. Therefore, the light element in the inner core is mainly silicon, amounting to 2.3 wt.%, with traces of oxygen. According to the partition coefficients proposed in Ref. [33], the outer core should contain 2.7 wt.% silicon and about 5.3 wt.% oxygen.

Sulphur, if any is present, might be at levels of 1.4 wt.% in the inner core and 1.7 wt.% in the outer core. Considering the low condensation/volatilisation temperatures of sulphur, we even propose that sulphur concentrations might be well below 1 wt.% and indeed do not consider it in our final preferred core model given in Table 2. Sulphur is probably necessary to explain some partitioning data between core and mantle but levels of much less than 1 wt.% might be sufficient. Hydrogen [35] was proposed as another light element in the core but due to its large volatility, we also prefer to rule it out from our core model.

This final model is synthesised in Table 2. Based on our data, we propose that the light alloying element in Earth's inner core is silicon, constituting 2.3 wt.% of its weight, along with traces of (0.1 wt.%) oxygen. The outer core would then bear 2.7 wt.% silicon along with 5.3 wt.% oxygen. This satisfies the chemical equilibrium given by experimental petrology [34], and the elastic properties of the core given by seismic models, while remaining geochemically and cosmochemically plausible. Sulphur does not belong to our preferred core model in agreement with recent theoretical [36] studies and experimental work on the compressibility [32] and wetting properties of the Fe–S liquid. We note that the most recent geochemical studies [37] do not favour large amounts of sulphur in the core, in accord with cosmochemical models of the core. We still acknowledge that up to 1.7 wt.% of sulphur in the core would still be compatible with current data. On the other hand, recent results from experimental petrology [34,38] show that significant amount of oxygen and silicon can be dissolved in iron. The total light element content of the inner core is about 2.5 wt.%, that of the outer core is around 8 wt.%.

This study reveals the need for further experimental (whether in the static or dynamic domain) and theoretical data, in order to constrain such composite models; most importantly, P–V–T equations of state [29] and compressional sound velocities [9] in iron need to be measured with increased accuracy to very high-pressures and temperatures, since this is the dataset that plays the most significant role in the inversion of the sound velocity and density data, iron being the major element in the core. Secondly, similar measurements need to be performed on light element alloys. Thirdly, solubility experiments in extreme conditions [38] and state-of-the-art solid–liquid elemental partitioning data in iron are required to infer the composition of the outer core, on the basis of an inverted composition model of the inner core. Such measurements can be combined with structural (density) and dynamic (sound velocities) information on liquid iron. Obtaining such a model for the composition of the core would help address many standing issues in Earth sciences, ranging for the conditions (pressure, temperature, oxygen fugacity) and processes that occurred during core formation [39], to the nature of the material that formed the Earth during the early and late stages of planetary accretion [2,4].

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