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# Properties of iron alloys under the Earth's core conditions



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#### ABSTRACT

The Earth's core is constituted of iron and nickel alloyed with lighter elements. In view of their affinity with the metallic phase, their relative high abundance in the solar system and their moderate volatility, a list of potential light elements have been established, including sulfur, silicon and oxygen. We will review the effects of these elements on different aspects of Fe–X high pressure phase diagrams under Earth's core conditions, such as melting temperature depression, solid–liquid partitioning during crystallization, and crystalline structure of the solid phases. Once extrapolated to the inner–outer core boundary, these petrological properties can be used to constrain the Earth's core properties.

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### 1. Introduction

In the absence of direct sampling, the study of Earth's interior is largely based on indirect approaches. The comparison between seismic observations and minerals properties at extreme conditions of pressure and temperature is arguably one of the most successful ways. The accurate determination of physical properties (density, sound speed, etc.) is a longstanding problem in the mineral physics community. At first, Earth's differentiation models argued that iron should be the main constituent of the Earth's core, as the direct consequence of the comparison between chondrites compositions and bulk silicate Earth. This notion was confirmed on the basis of the good match between shock measurements performed on Fe and the seismological profiles of the Earth's core. However, the addition of elements lighter than iron is required to account for the density difference between pure Fe and seismic models. For the liquid outer core, the classically estimated amount is about 10 wt% (Birch, 1964).

Internal geophysics (Physics of Earth's interior)

The list of potential light elements in the Earth's outer core includes S, Si, O, C, and H (Poirier, 1994). Here we focus on the potential role of S, Si, and O. High volatilities of H and C make them unlikely to incorporate the core at the early stages of the Earth's differentiation. Metal-silicate partitioning experiments under high pressure agree on carbon content in the Earth's core lower than 1 wt% (Dasgupta et al., 2013; Zhang and Yin, 2012). Higher C content in the Earth's core would require unrealistic C contents in the Earth's mantle. Concerning hydrogen, the Earth's internal composition is strongly depleted in volatile elements (McDonough, 2003). It is therefore difficult to introduce large amount of hydrogen in the Earth's core, as the main part of the volatile elements present in the Earth were gained during a late veneer, when the Earth's core was already completely formed (Albarède, 2009). Altogether, taking into account the facts that (i) S is the major light element in planetesimal cores (Chabot, 2004), and (ii) core material has certainly been equilibrated with molten silicates at the bottom of a magma ocean (Siebert et al., 2012), it seems appropriate to consider Si, O and S as the major potential light elements of the Earth's core.

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Fig. 1. Phase diagrams at ambient pressure on the Fe-rich side of Fe-S, Fe-Si, and Fe-O systems (Kubaschewski, 1982; Meco and Napolitano, 2005).

Temperature profile in the Earth's core is controlled by the melting curve of iron alloys under high pressure. Accurate determination of the temperature jump across the Core-Mantle Boundary is required to constrain the heat flow from the core, with strong implications for the geodynamo (Lay et al., 2008) Furthermore, thermochemical flows in the liquid outer core are sustained by the slow crystallization of the inner core. The different forces driving this flow are therefore strongly related with the composition and the partitioning of light elements during inner core crystallization (Aubert et al., 2008). Finally, Earth's core composition is strongly related with its scenario of differentiation and its building blocks (Corgne et al., 2009; Siebert et al., 2013). Determination of light element content from a geophysical point of view should help to understand the geochemical context of Earth's formation.

Properties of Fe–X (X = S, Si or O) systems differ very much upon the nature of the light element, as known from ambient pressure metallurgy (Fig. 1; Kubaschewski, 1982). The Fe–FeS system exhibits a simple eutectic system, with strong incompatibility of S in solid Fe, and no intermediate compounds between Fe and FeS. Concerning the Fe–FeSi system, the solubility of Si reaches 10 wt% in bcc Fe (A2 structure). Finally, the Fe–FeO phase diagram presents a large immiscible gap between a metallic Fe-rich liquid and

an ionic FeO-rich liquid. However, these phase diagrams drastically evolve at high pressure, especially at the P-T conditions of the inner core boundary (ICB), as the direct consequence of the significant modifications in the physical properties of all solid and liquid phases.

Different characteristics of phase diagrams control ICB properties (Fig. 2). Defining accurately the different phase diagrams of iron alloys under high pressure thus provides important constraints on the Earth's core composition based on mineral physics arguments. In particular, the temperature at the ICB is directly related to the melting curve of the Fe-X alloys, specifically to the liquidus temperature at 330 GPa, which represents the anchoring point for temperature profiles in the outer and inner core (Fig. 2a). This liquidus temperature is primarily controlled by the melting temperature depression ( $\Delta T = T_m - T$ , where  $T_m$  is the melting temperature of pure iron) associated with the addition of light elements in pure Fe. Furthermore, the density jump between the liquid outer core and the solid inner core is largely due to the compositional difference ( $\Delta X$ ) between solid and liquid Fe alloys in equilibrium with each other at the ICB. Indeed, the volume change in pure Fe at melting cannot account alone for the density difference between inner and outer core  $\Delta \rho = 0.6 - 0.9 \,\mathrm{g \cdot cm^{-3}}$  obtained by seismology (Cao and Romanowicz, 2004). Therefore, parti-



Fig. 2. (Color online.) Schematic phase diagram of a hypothetic binary Fe–X system. The parameters having major implications for the properties of the Earth's inner–outer core boundary are the melting temperature depression compared to pure Fe ( $\Delta$ T), the compositional difference between solid and liquid phases in equilibrium with each other ( $\Delta$ X), and the crystallographic structure of the solid phase.

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