Liquid properties in the Fe-FeS system under moderate pressure: Tool box to model small planetary cores

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ABSTRACT

Physical properties of liquid Fe-S alloys (from 10 to 50 at%S) under high pressure were investigated by in situ X-ray diffraction (up to 5 GPa and 1900 K) and by ab initio calculations. The local structure of Fe-S liquid alloys clearly shows how S modifies the local arrangement of the Fe atoms. Density has been extracted from the diffuse scattering by minimization of the oscillation in the short distance of the radial distribution function g(r). Two different formalisms for the P-V-T-X equation of state are presented to model density and sound velocity as a function of pressure, temperature, and sulfur content. Based on these results, Moon’s core composition is discussed. This coherent data set will serve as a thermodynamically consistent ground for modeling the core of small telluric planets and large icy satellites.

Keywords: Iron alloys, liquid, Fe-S liquid, planetary cores

INTRODUCTION

Elements lighter than iron are expected to be present in planetary cores, due to their abundance in iron meteorites and their affinity with the metallic phase. Among the potential light elements (Poirier 1994), sulfur is likely the most abundant in the cores of iron meteorites parent bodies (Chabot 2004). From tungsten isotopes data (Kleine et al. 2009) and experimental studies of percolation processes (Yoshino et al. 2003), core formation is expected to occur within a few million years of the solar system formation, even in small planetesimals (Greenwood et al. 2006). It is therefore important to constrain the physical properties of Fe-S liquid alloys to better understand core formation in the early stage of the solar system.

Melting properties in the Fe-FeS system under high pressure have been intensively investigated by in situ (Campbell et al. 2007; Morard et al. 2007b, 2008a, 2008b; Chen et al. 2008a; Andrault et al. 2009) or ex-situ methods (Chudinovskikh and Boehler 2007; Stewart et al. 2007; Chen et al. 2008b; Kamada et al. 2012). However, although the Fe-rich side of the phase diagram begins to be relatively well described, we still lack precise knowledge of important physical properties, especially in the liquid state such as density or viscosity (LeBlanc and Secco 1996; Sanloup et al. 2000; Vočadlo et al. 2000; Balog et al. 2003; Nishida et al. 2008).

As today, the inner structures and in particular the cores of planetary bodies in the solar system are not well known, mostly because of the absence of seismological data, with the clear exception for the Earth and, to some extent, for the Moon.

Inferences about planetary cores can be obtained from geodesy, electrical, and magnetic data and size, density, and composition have been estimated (e.g., Yoder et al. 2003; Margot et al. 2007; Rivoldini et al. 2009; Zhang and Pommier 2017). However, those inferences require detailed modeling of the interior structure, and the precision of the estimates, in particular core composition, calls for extensive knowledge about core material properties. In this study, we investigated the density of liquid Fe-S alloys up to 5 GPa and 1900 K and assessed how it affects the lunar interior.

Simultaneous measurements of density and liquid structure have been performed to emphasize the strong link between the evolution of the local atomic arrangement and changes in the liquid density. This experimental study has been complemented by ab initio calculations of the liquid structure in similar P-T conditions. We present two models describing thermoelastic properties of liquid Fe-S as a function of pressure, temperature, and S content based on our data and results published in the literature. These models are finally applied to estimate S content in Moon’s core.

EXPERIMENTAL PROCEDURES

Paris-Edinburgh Press experiments

X-ray diffraction experiments were carried out at the High Pressure Beamline ID27 at ESRF in Grenoble, France (Mezouar et al. 2005) using a large volume VXS type Paris-Edinburgh Press (PEP) (Besson et al. 1992; Klotz et al. 2005). This press allows large opening angle in the equatorial plane. The very high brilliance X-ray beam delivered by two in-vacuum undulators was collimated down to 50×50 μm (typical values). The X-ray wavelength was fixed to λ = 0.24678 Å (gadolinium K-edge) using a Si(111) channel-cut monochromator. A multichannel collimator (Mezouar et al. 2002; Morard et al. 2011) was used to minimize the X-ray background coming from sample environment materials. The data were collected using a MAR345 imaging plate system (X-ray research company GmbH,