THERMOELASTIC PROPERTIES OF LIQUID IRON-RICH ALLOYS UNDER PLANETARY CORE CONDITIONS.

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Introduction: As commonly found in rocky planets, liquid Fe-rich metallic cores play a key role, by vigorous convection, in generating a magnetic field that is necessary to known forms of life to exist; consequently, their thermoelastic properties at high pressures, that determine the convecting fashion, are vital parameters for constructing planetary models. Here, we perform ab initio molecular dynamics (AIMD) calculations on liquid Fe-X (X = Ni, S, C, O and H) mixtures at moderate P-T conditions (up to 35 gigapascal and 2400 kelvin), in order to construct a reliable mineral physics toolbox for modelling physical properties of mid-sized planetary cores.

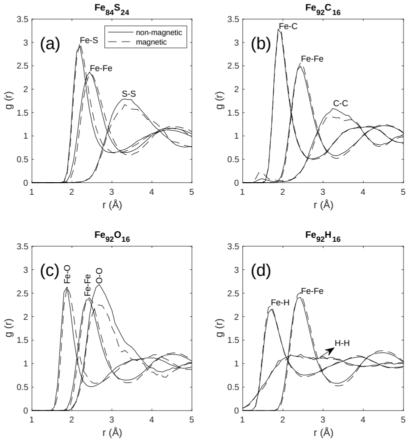

Figure 1: *Partial radial distribution functions of Fe-S, Fe-C, Fe-O and Fe-H liquids based on spin- and non-spin-polarised AIMD simulations at 19 GPa / 2100 K.*

Non-magnetic vs. Magnetic Fe-X mixtures: Liquid Fe at low pressures is found to be paramagnetic [1]. To test the effect of magnetism on the AIMD equation of state, we run parallel simulations on both non-spin-polarised (non-magnetic) and spin-polarised (magnetic) liquid Fe-X mixtures. The partial radial distribution functions for the spin- and non-spin-polarised simulations are shown in Fig. 1 and illustrate structural similarities across the binary systems studied here. In general, at the same density, the spin-polarised treatment increases bond length, i.e. the position of the first peak for each species in the partial radial distribution functions, and therefore yields higher pressures relative to the non-magnetic simulations. After applying a pressure correction derived from comparison between AIMD with recent experimental data [2], density changes between non-magnetic and magnetic systems are summarised in Table 1.

Table 1. Comparison of calculated density (ρ, in g/cm) and density difference ($\Delta\rho$) between non-spin-polarised (NSP) and spin-polarised (SP) simulations of liquid Fe-X (X = S, C, O and H) at 19 GPa / 2100 K.

	$Fe_{84}S_{24}$	$Fe_{92}C_{16}$	$Fe_{92}O_{16}$	$Fe_{92}H_{16}$
NSP ρ	6.72	7.68	7.32	7.68
SP ρ	6.88	7.59	7.24	7.52
$\Delta\rho$	-2%	1%	1%	2%

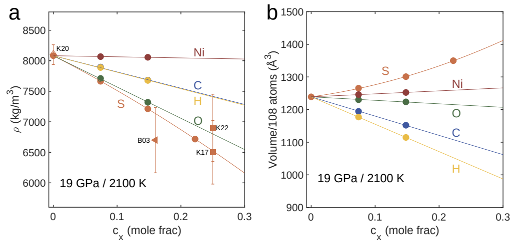

Figure 2: *Density and volume of liquid Fe-X (X = Ni, S, O, C and H) as a function of X's concentration at 19 GPa / 2100 K. Results from our AIMD simulations are shown as solid circles. Experimental data for liquid Fe (K20 [2]), Fe-S (B03 [3], K17 [4] and K22 [5]) are shown as angular markers.*

Non-ideality of Liquid Fe-S Alloy: The addition of light elements invariably decreases the density of liquid Fe (Fig. 2a), with (i) S and O affecting density more than C and H on a molar basis, and (ii) the negligible influence of Ni. This is consistent with previous simulations at the conditions of Earth's core in which the magnitude of the density reduction of iron diminishes following the sequence Si, S, O, C and H [6–9]. Unlike S, the volumes (Fig. 2b) of Ni, C, O and H mix ideally with liquid Fe at the investigated pressures, in agreement with observations at 1 bar [10] and melting experiments at higher pressures [11–13] that suggest non-ideality for the Fe-S system.

Implications for Mars' Core Composition: The Martian core is large and therefore light, as found by the InSight mission [14]. This means that its liquid iron-nickel core has to be enriched in light elements. The calculated elastic properties of various Fe-Ni-rich-light element mixtures will be compared with those obtained from e.g. InSight to place further constraints on Mars' core composition, but can also be used for studying metallic cores of other planets such as Mercury and mid-sized exoplanets.

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