

High pressure behavior of iron alloys: insights into planetary cores. M. Mookherjee¹, ¹Department of Earth and Atmospheric Sciences, 2122 Snee Hall, Cornell University, Ithaca, NY 14853 (e-mail address: mainak.mookherjee@cornell.edu)

Understanding the chemistry physical properties of iron and its alloys is extremely important to understand the evolution and geodynamo of planetary interiors such as Mars [1-3]. Martian core is likely to contain volatile such as S [4-6], C, H [7]. However, owing to lack of seismological constraints, the size of the core is uncertain. It is likely that Mars has a liquid outer core and a solid inner core [2]. Experimental studies indicate that sulfur affects the physical parameters of liquid outer core quite significantly [8]. However, it is not known how volatiles such as hydrogen and carbon [8] dissolved in the iron liquid will affect the physical properties? Considerable research has been conducted on high-pressure behavior of iron alloys (**Figure 1**) including iron sulfides [9-11]. Pressure dependence of the elasticity of most of the volatile bearing iron alloys are limited to ambient temperatures except iron carbides [12-13]. For a better understanding of the thermal evolution of Mars it is important to constrain the elasticity, density, compressibility and thermal expansivity at conditions relevant to planetary cores. Using first principle simulations, we will report new results on energetics, equation of state, and elasticity of iron alloys at conditions relevant to planetary cores.

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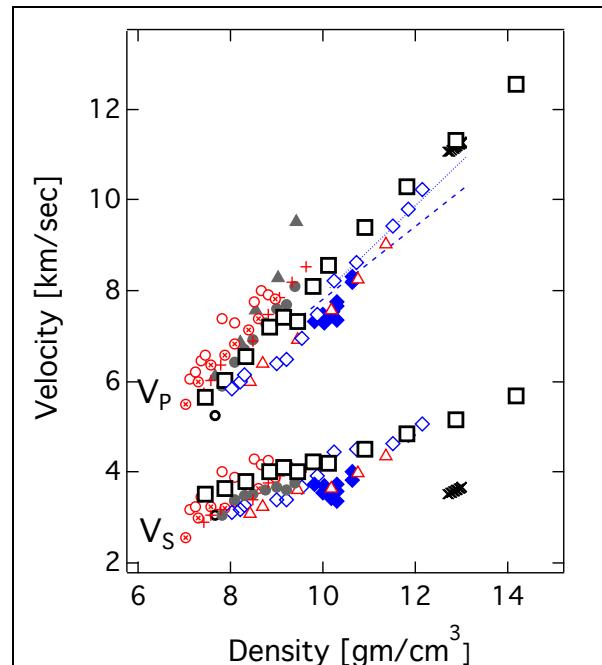


Figure 1. Velocity-density systematics for iron-rich alloys. Iron-alloys: Fe_3C [14] with grey filled circles, [15] in grey filled triangles and by [16] in grey open circles; Fe_7C_3 [17] in open grey squares); other volatile-bearing Fe-alloys are shown in red symbols FeH_x with open circles [18], $\text{Fe}_{0.85}\text{Si}_{0.15}$ with plus signs [19], $\text{Fe}_{0.92}\text{Ni}_{0.08}$ with open triangles [19], Fe_3S by open circles with a cross [10]; data on hcp-Fe at various temperature are shown in blue symbols: [20] (700-1700 K) with filled rhombs [21] (300 K) with open rhombs, [22] (298 K) with dashed lines, [23] (300 K) with a blue open square, and along the Hugoniot [24] with a dotted line.

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