P-V-T equation-of-state of liquid Fe from *ab-initio* simulations to the TPa regime

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The pressure-volume-temperature (*P-V-T*) equation-of-state (EoS) of liquid iron provides important information (reference adiabat, density ρ, and higher order thermodynamic parameters) in the modelling of the internal structure of planetary bodies with Fe-based cores. Relevant P-conditions range from a few GPa (Moon, Mercury) through the Mbar range (Earth) to several TPa (super-Earth exoplanets). Experimental data on ρ in the liquid stability field are scarce and a thermodynamic assessment of ρ depends on matching Gibbs energy along the melting line which remains controversial to this day. The alternative determination of a *P-V-T* EoS based on ab-initio simulations, on the other hand, suffer from the fact that ρ at ambient P is predicted too large by as much as 20% in the simulations [e.g., 1]. Here, we have fitted *P-V-T* triplets from *ab-initio* molecular dynamics simulations with an EoS formulation that is thermodynamically self-consistent [2] and combined it with a correction formalism that accounts for the known ρ-mismatch at ambient P [3]. As the correction is additive to the Helmholtz potential and shows the correct limiting behavior at high and low ρ, the thermodynamic self-consistency of the results is not affected. Using this combination, the EoS we have developed reproduces ρ from shock-wave experiments as well as previous models, but shows a significantly improved agreement at ambient P, the critical point and the sole low ρ measurement at 4.3 GPa [4] (T11 in Figure). We explore the performance of our thermodynamic potential and various previously published models [1,5,6] for liquid iron over a wide range of conditions: (i) at ambient pressure as a function of temperature, (ii) along the melting curve of Fe to 40 GPa, relevant for the cores of smaller terrestrial bodies in our solar system (Figure), (iii) along isentropes in the Earth's outer core and (iv) for the core of super-Earth Kepler-36b. The correction term significantly improves the agreement of computed properties with experiments and other thermodynamic models that are based on an assessment of the phase diagram at ambient and moderate pressure, showing how *ab-initio* molecular dynamics simulations can be used at par with other thermodynamic techniques. For the Earth's core, densities from the various models are similar, but higher-order derivatives (acoustic velocities and Grüneisen parameter) show significant differences. Evaluated along a core-temperature profile in Kepler-36b, differences in density from various models are negligible, for core mass they do not exceed 2%, showing robust extrapolation of all equation of state models.

[1] Ichikawa et al., JGR 119, 240 (2014) (I14); [2] Vlček et al., PRB 85, 184201 (2012); [3] French & Mattsson, JAP 116, 013510 (2014); [4] Tateyama et al., PCM 38, 801 (2011) (T11); [5] Komabayashi, JGR 119, 4164 (2014) (K14); [6] Dorogokupets et al., SciRep 7, 41,863 (2017) (D17); [7] Nishida et al., PEPI 257, 230 (2016) (N16); [8] Jing et al., EPSL 396, 78 (2014) (J14); [9] Assael et al., JPCRD 35, 285 (2006) (A06); [10] Morard et al., AmMin 103, 1770 (2018) (M18); [11] Tsu et al., BRIMDM 41, 1 (1985) (T85).

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