Liquid properties in the Fe-FeS system in the 0 to 5 GPa range: a tool box to model small planetary cores

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Properties of liquid Fe-S alloys under high pressure were investigated by both in situ X-ray diffraction, and ab initio calculations. The partial radial distribution function g(r) obtained by ab initio calculations clearly emphasizes how S modifies the liquid structure. Density has been extracted from the diffuse scattering following previously described protocol (Morard et al. 2013), based on the minimization of the oscillation in the short distance of the g(r) (Eggert et al. 2002), and compared with data from the litetrature. A thermodynamic model, anchored on ambient pressure measurements, well fits our dataset and allow to model density and sound velocity as a function of pressure, temperature and sulfur content. The so-validated model could be applied in the future to parametrize the properties of small planetary cores, such as those of the Moon or Ganymede.