Triple point hcp-fcc-liquid in pure Fe phase diagram determined by in-situ XANES diagnostic

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Abstract

Iron is the main constituent of planetary cores. Studying its phase diagram under high pressure is mandatory in order to constrain properties of planetary interiors, and to model key parameters such as the generation of magnetic field.

Strong controversy is still large regarding the melting curve of pure Fe. In contrast, throughout the literature, we can observe an overall agreement on the melting temperature of many iron alloys under extreme conditions, with results within mutual uncertainties, irrespectively of the melting diagnostics. However, a controversy has been recently pointed out on the case of pure iron, with XANES measurements (Aquilanti et al, PNAS, 2015) in open disagreement with previous results by x-ray diffraction (Anzellini et al, Science, 2013).

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We performed in situ XANES experiments on the beamline ID24, using the available experimental setup combining dispersive absorption set up and laser heated diamond anvil cell. Samples recovered from high temperature-high pressure experiments were probed by XRD and FIB techniques, to assess the melting criterion derived by XANES change. Low melting temperatures, corresponding to the ones described in Aquilanti et al, 2015, are systematically related to the presence of Fe3C, that is to say carbon contamination from the diamonds, evidenced by XRD and XANES.
Triple point in the Fe phase diagram is located at 105 ($\pm$10) GPa and 3600 ($\pm$200) K. This seems to be related to a small kink in the melting curve around the triple point. Over the triple point, melting seems to be in relative agreement with previously published XRD melting curve (Anzellini et al, 2013). The refinement of the Fe phase diagram could be used to compute thermodynamic model for planetary cores.