Experimental confirmation of the predicted high-PT Fe body-centered cubic phase

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Iron is the major element of the Earth and Earth–like exoplanets cores. The crystal structure of iron, the major component of the Earth's inner core (IC), is unknown under the IC high pressure (P) (3.3–3.6 Mbar) and temperature (T) (5000–7000 K) and conditions of the exoplanets cores. Experimental and theoretical data on the phase diagram of iron at these extreme PT conditions are contradictory. Though most comprehensive large scale *ab initio* molecular dynamics (AIMD) points to the stability of the body-centered cubic (*bcc*) phase, the latest experimental data are often interpreted as the evidence for the stability of the hexagonal close-packed (*hcp*) phase. At the same time, small scale AIMD studies also point to the stability of the *hcp* phase. Applying large scale AIMD we computed properties of iron phases that allow us to suggest that the experimentalists have observed the *bcc* phase, however, mistakenly assigned its signature to either *hcp* or liquid phase. Large scale 2-phase AIMD determination of the *hcp* melting T at the pressure of 360 GPa (7000 K) dismiss most of the previous MD iron melting curves and support the iron phase diagram with the broad PT field of the *bcc* stability. The best estimate for the Fe melting T at the pressure of 360 GPa is 7100 K. Recent experiments have observed the *bcc* phase up to P≈550 GPa below melting curve, prooving the *bcc* stability in the cores of the Earth and exoplanets.