## Iron phases at high pressures and temperatures: Phase transition and melting

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## ABSTRACT

Based on an in situ X-ray study of Fe and a review of the available data, we propose the following triple-points in the Fe phase diagram—the hexagonal closest packed (HCP), face-centered cubic (FCC), and the  $\beta$  phase: P = 40 (4) GPa at T = 1550 (100) K, the  $\beta$ -phase-FCC-melt; P = 60 (10) GPa at T = 2600 (100) K. We define the stability of  $\beta$  phase from a combination of new X-ray results on externally heated Fe between pressures of 37 to 300 GPa, as well as the previous data on externally heated and laser-heated samples. X-ray data on externally heated Fe, without any pressure medium, confirms the double hexagonal closest packed (DHCP) structure for the  $\beta$  phase. The HCP- $\beta$  phase boundary has a very small negative dP/dT indicating the similarity of physical properties (molar volume, thermal expansion, and bulk modulus) between the two phrases, but a higher entropy and enthalpy for the  $\beta$  phase.