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Structure analysis and stability field of β-iron at high *P* and *T*

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ABSTRACT

New synchrotron X-ray diffraction data confirm our previous report of the transformation of the hexagonal close-packed (hcp) phase of iron to the *Pbcm* orthorhombic lattice (β-iron) at high *P* and *T*. The volume differences between the ε and β, and the β and γ polymorphs are determined as 1.4 and 1.8%, respectively, indicating positive Clapeyron slopes between these polymorphs in the *P*-*T* phase diagram. All three polymorphs have a similar bulk modulus between 30 and 60 GPa.

The *Pbcm*-polymorph can be observed in a metastable state as quenched from high *T* at high *P* and also at high *T* for *P* lower than 35 GPa where β-iron is not a stable phase. Metastability is possible because the gliding of the same dense atomic layers is involved in both *T*-induced ε-hcp to γ-fcc and ε-hcp to β-*Pbcm* transformations. These observations explain why a controversy exists on the structure and *P*-*T* stability field of β-iron. From our set of experiments, we estimate that *Pbcm*-iron is stable above 35 GPa and 1500 K, and that the (γ, β, liquid-iron) triple point is located at about 55 GPa and 2400 K.