Local structure analysis of iron phase transition from bcc to fcc using x-ray absorption spectroscopy

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Iron (Fe) is the most common element, present in many compounds of high practical importance like steels and alloys. In many real-life manufacturing processes, iron undergoes heat treatment. Three phases of iron are known to exist until its melting point at 1538 °C: body-centered cubic (bcc) form is stable up to 912 °C, face-centered cubic (fcc) phase exists from 912 °C till 1392 °C, and high-temperature bcc phase above 1390 °C. Besides, iron is ferromagnetic in low-temperature phase until the Curie point at 769 °C, and its lattice parameter shows small anomaly around the Curie point upon transition into paramagnetic phase associated with the disappearance of magnetostriction. At the same time, there are no many publications on temperature dependent X-ray absorption spectroscopy (XAS) of pure iron, which could shed more light on the behavior of its local atomic structure and lattice dynamics.

In this study, reverse Monte Carlo (RMC) method [1] was used as a tool to understand the bcc-to-fcc phase transition in pure iron from the analysis of the Fe K-edge extended X-ray absorption fine structure (EXAFS) measured in a wide range of temperatures (20-1000 °C). The RMC simulation results were used to obtain information on the atom-atom distribution functions and amplitudes of atom thermal vibrations. Besides, the regularization method [2] was used to reconstruct the radial distribution functions within the first two coordination shells, and thus obtained RDFs were compared with those determined by RMC calculations.

References

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