Ferrihydrite: Surface Structure and its Effects on Phase Transformation

Zhao Jianmin, Frank E. Huggins, Feng Zhen and Gerald P. Huffman

The Consortium for Fossil Fuel Liquefaction Science, 341 Bowman Hall, University of Kentucky Lexington, Kentucky 40506

Abstract: X-ray absorption fine structure (XAFS) spectra were collected on a series of ferrihydrite samples prepared over a range of precipitation and drying conditions. Analysis of the XAFS pre-edge structures shows clear evidence of the presence of lower coordination sites in the material. These sites, which are most likely tetrahedral, are believed to be at the surface and become coordination unsaturated (CUS) after dehydroxylation. With chemisorbed water molecules, the CUS sites become the crystal growth sites responsible for the phase transformation of ferrihydrite to hematite at low temperatures. On the other hand, when impurity anions such as SiO_4^{-4} are present in the precipitation solution, the CUS sites may instead absorb the impurity anions, thereby blocking the crystal growth sites and inhibiting the formation of hematite.

Key Words: Ferrihydrite • Mössbauer spectroscopy • Phase transformation • Surface structure • X-ray absorption fine structure (XAFS)

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