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Constraints on structural models of ferrihydrite as a nanocrystalline material

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Abstract

Recently, Michel et al. (2007a) have presented a structure for ferrihydrite that we show to be incorrect. We do this by comparing (1) the sample form factor without adjustable parameters from powder X-ray diffraction data using a recently developed method with (2) exactly simulated (Debye-sum method) theoretical sample form factors for the recently proposed structure (including vacancy, particle size and shape, and positional disorder effects). Michel et al. (2007a) used pair distribution functions (PDFs) extracted from synchrotron diffraction data fitted with calculated PDFs using adjustable scale and peak shape parameters. The PDF method gives consistent short-range (coordination sphere) correlations but under-emphasizes intermediate-range correlations that represent more stringent constraints on the structure. Main characteristic diffraction peaks of six-line ferrihydrite (lines 2, 3, and 4) are not reproduced by the proposed structural model. We expect our method to offer rigorous tests of proposed structures of any nanocrystalline materials.

Keywords: Ferrihydrite, X-ray diffraction, structure, oxyhydroxide, nanoparticle