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General model for the aqueous precipitation of rough-surface nanocrystals and application to ferrihydrite genesis

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Abstract

Ferrihydrite is a key reactive nanoparticle in the Earth surface environment that regulates nutrient and metal cycling in marine, lacustrine, and groundwater settings; yet its genesis is unknown and there is no mechanistic explanation of its nanostructural nature. We develop a model, based on established aqueous precipitation theory, for rough-surface phases growing by accretion of monomers under fast diffusion conditions. The model is entirely defined in terms of a minimal set of necessary microscopic (molecular-scale) characteristic parameters. It is applied to ferrihydrite where the needed microscopic parameters are constrained by some of the mineral's known physico-chemical properties. Our model qualitatively reproduces the main nanostructural properties and known precipitation kinetics of ferrihydrite, predicting that ferrihydrite will be nanometric in size, will have a narrow particle size distribution (standard deviation width equal to a fraction of the average particle size), and will typically precipitate from supersaturated conditions within times ranging from a fraction of a second to several days, under normal environmental-proxy conditions. The model also suggests that different metastable structures of ferrihydrite having similar rough surfaces would kinetically compete during nucleation and growth to coexist in the final product, as observed by Janney et al. (2000a, 2001).

Keywords: Ferrihydrite, precipitation, nucleation, oxyhydroxide, nanoparticle