Quantitative Model for β-FeOOH Nucleation and Growth Determined Using Small Angle X-Ray Scattering

BENJAMIN A. LEGG[1], MENGQIANG ZHU[2],
BENJAMIN GILBERT[3] AND JILLIAN F. BANFIELD[4]

[1]Pacific Northwest National Laboratory, Richland, WA (benjamin.legg@pnnl.gov)
[2]University of Wyoming, Laramie, WY (mzhu6@uwyo.edu)
[3]Lawrence Berkeley National Laboratory, Berkeley, CA (bgilbert@lbl.gov)
[4]University of California, Berkeley, CA (jbanfield@berkeley.edu)

Although classical theories of nucleation and growth are well established, there remain important cases where quantitative models of mineral precipitation have remained elusive. The precipitation of sparingly soluble iron oxyhydroxides has been one such system, in which precipitation may be a complex process involving the formation of poorly crystalline precursors, nanoparticle aggregation, and secondary phase transformations.

In this work, we track the nucleation and growth of β-FeOOH (akaganeite) nanoparticles from acidic (pH 1.5-3) $FeCl_3$ solutions using *in situ* small angle x-ray scattering (SAXS). This process generates highly monodisperse nanoparticles. Variations in temperature and solution chemistry provide fine control over nucleation and growth rates. Subsequent precipitation modeling shows that the system is well-modeled by classical nucleation theory, and the critical parameters controlling nucleation rates are determined.

The interfacial tension of the β-FeOOH nucleus is shown to range from 0.06 to 0.12 J/m^2, with a strong pH dependence that is consistent with a protonated surface. The size of the critical nucleus ranges from 4-30 iron atoms at the onset of precipitation. These values should prove useful for developing models of more complex iron oxyhydroxide precipitation processes.