Characterizing Particle Mediated Crystal Formation

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Crystal growth often occurs by a combination of mechanisms. For example, oriented attachment is a particle mediated crystal growth mechanism, but experimental data consistently demonstrate that crystals concomitantly grow by dissolution and reprecipitation. Predicting the nature and rate of nucleation of fundamental building block particles as well as predicting how a system will evolve once precipitation occurs is an ongoing challenge in understanding particle mediated crystal formation and growth. Initial and/or intermediate phases form on the basis of more favorable kinetics, while the trajectory of stages is governed by thermodynamics. An important consideration is that nanoparticle structure is not static; it changes in response to the environment. Thus, the dominant growth mechanisms are expected to be exquisitely sensitive to conditions such as pH; ionic strength; solubility; the presence of passivating agents, chelating agents, or macromolecules; and more. Particle-particle interactions will be sensitive to both the nature of the precursor phases as well as their environment. For example, surface charge may be homogeneously distributed over an amorphous precursor particle but heterogeneously distributed over a nanocrystal. A wholistic suite of characterization techniques is essential to elucidating the dominant mechanisms by which crystals form. There is a critical need to identify which physical characteristics could indicate whether crystals formed predominantly by monomer-by-monomer or by particle mediated mechanisms. Direct imaging, scattering, spectroscopy, and data tracking the kinetics of crystal growth can be combined to provide robust datasets that enable elucidation of the dominant crystal growth mechanisms.