4ay Solution-Phase Growth of Nanostructures

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Numerous nanostructures of technological importance are formed via solution-phase synthesis. Control of the formation of functional nanostructures is often difficult due to lack of understanding of the mechanistic details of their formation. For example, many materials formed from nanoparticles have size-dependent properties, so control of the size distribution of the nanoparticles is critical, but in order to control the size distribution, knowledge of the mechanism of formation is needed.

My PhD and postdoctoral research projects have focused on the development of coupled simulation and experimental studies to understand the mechanism of the solution-phase formation of nanostructures. In my PhD project, a coupled simulation and experimental methodology was used to understand the mechanism of formation of electrodeposited copper nanoclusters on a surface, from their nucleation[1] to their filling of on-chip interconnects in the presence of additives.[2] I was involved in the development of the electrodeposition procedure, including the use of Atomic Force Microscopy (AFM) for surface roughness measurement. I gained expertise in the development of Kinetic Monte Carlo (KMC) simulation models and I developed several simulation tools to analyze and use the KMC model. These tools include parameter sensitivity analysis[3] and estimation[2] techniques for stochastic simulation models and a coupled multiscale simulation model that consisted of an ODE model coupled to multiple instances of the KMC model to analyze surface roughness evolution of substrates under a potential gradient.[4]

In my postdoctoral research project, which will be featured in the presented poster, the mechanism of aging and coalescence of zeolite nanoparticles is investigated through a combined experimental and simulation study.[5] I developed an ODE population balance model that is used to investigate a candidate mechanism for zeolite nanoparticle aging and growth based on the oriented aggregation of nanoparticles in solution.[6] A KMC version of the population balance model[7] was also developed to analyze the aging and growth mechanism when more detailed particle interaction physics are considered, such as DLVO interactions. I have also developed a novel simulation tool to estimate the small-angle x-ray scattering (SAXS) curve and pair distance distribution function (PDDF) from a cluster population size distribution,[8] where the morphology of the particles that comprise the size distribution is simulated with an Eden model.[9] In this project, I also have gained experimental experience with SAXS, which has been used to gain information about the shapes and size distribution of the nanoparticles in solution.

I would like to build a research program that combines simulation and experimental studies to understand and control the solution-phase growth of functional nanostructures.

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