Prediction of Crystallization Behavior via Molecular Modeling and Simulation

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Crystallization behavior (CB), the key predictor for the resulting crystal phase or shape, is mostly influenced by thermodynamic and kinetic properties, temperature, reactant concentration, surfactant, shear rate, etc. Here, we systematically studied CB focusing on Ag nanocrystals (NCs) through multiscale molecular modeing and simulation under the effect of the properties. First, for Ag nanocube, it can be uniformly synthesized through heterogenous nucleation with AgCl particle mediation. The preferential growth of Ag on AgCl (100) surface, which reveal (100) facet, was explored by considering interfacial energy of the surfaces. Second, for Ag nanowire, we investigated its formation with surfactant control (i.e., alkyl ammonium halide). The halide types and alkyl chain length were found to be the determining factors of the nanowire thickness. Surfactants adsorption on each surface was essential to control exposed surface area and shape. Lastly, we investigated the early nucleation stage of Ag NCs, to which non-equilibrium process was applied, to predict the shape of the Ag clusters while considering reduction factor of Ag ions and shear rate.