174e Molecular Dynamics Simulation of the Coalescence Kinetics of Bare and Coated Nanoparticles

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One of the significant challenges in the use of nanoparticles, is the control of primary particle size and extent of agglomeration when grown from the gas–phase. In this paper we consider the role of surface passivation of the rate of nanoparticle coalescence. We have studied the coalescence of bare and H-coated silicon nanoparticles of sizes between 2-6 nm using molecular dynamics simulation at 1000 and 1500 K. We found that coalescence of coated particles consists of two steps. First chemical reaction between particles, and relocations of surface atoms near the reacting region occurs, which comprise an induction period. The second step consists of the nominal coalescence event, which depends on the surface tension and solid-state diffusion in the particle. The hydrogen passivation layer was found to remain on the surface during the entire coalescence event. We also develop a mathematical model to describe the dynamics of coalescence of coated particles. The model is able to describe both the initial induction period, and the coalescence period, and the role of extent of surface coverage on the coalescence rate. In general, the entire coalescence time of coated particles is about 3 to 5 times that of bare particles, and the exothermicity from coalescence is about half that for the unpassivated particles.

We will also present results for other coated systems including LJ and polymeric coatings.