Multiscale Computer Simulation of Nanoparticle Formation and Growth in Vapor Phase Condensation Process

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There is significant progress in nanotechnology in recent years, and methods for producing metal nanoparticles are quite diverse. One of the most efficient methods is inert-gas consolidation (IGC) method. In this method, a metal is evaporated in a cooled chamber containing a low density inert gas. The metal vapour flows from a heat source to a cooler gas by convective diffusion. A decrease in temperature leads to a rapid decrease in the equilibrium vapour pressure and to attainment of high degrees of supersaturating. This favours fast formation of critical nuclei and growth of clusters, which then reach the chamber walls and deposit on them. We are investigating the "bottom-up" formation of metal nanoclusters via a multiscale computer simulation method that includes quantum mechanical calculations of the inter-particle forces, classical molecular dynamics simulations of atomic structure and macro-scale simulations of turbulent mixing to form nucleus of crystal that grow rapidly due to coalescence and coagulation. Multiscale simulation propose not only simulation in different scales, but also a possibility of application of results of the simulation obtained at one level as input data for simulation at a following level of scaling. Such combination allows discovering associations between various physical properties and processes of nanoparticles formation, to investigate requirements at which metal nano-powders formation is possible, having demanded sizes and structures. We use computer simulation to understand the fundamental principles of how nano-scale systems, such as metal nanoparticles, self assemble, and to discover how to control the assembly process.

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