

609c Computational Fluid Dynamics (CFD) Modeling of a Laser-Driven Aerosol Reactor

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Fundamental understanding of the thermally driven nucleation and growth of silicon nanoparticles is of great importance in the microelectronics and nanotechnology industries. Computational modeling can enable us to understand the details of the particle formation process and to gain valuable insight into the various interconnected mechanisms by which particle size and morphology evolves, as well as to optimize reactor systems to produce particles of controlled size and morphology. The overall goal of the present work is to couple a chemical reaction mechanism for silicon particle nucleation and growth to an aerosol dynamics model to predict particle size and morphology. The temperature and flow fields in which this chemistry and aerosol dynamics occur are the focus of the CFD modeling of our aerosol synthesis reactor presented here. Thus, we present a detailed 3D model of a laser-driven (photothermal) reactor system used in our laboratory to produce nanoparticles of silicon and other materials. This model includes detailed descriptions of the fluid flow, heat and mass transfer, and chemical reactions leading to silane decomposition in the gas phase. A three-dimensional CFD model was developed using MPSalsa, a finite element reacting flow code developed by Sandia National Laboratories. Preliminary results show that the reaction zone is centered in the middle of the reactor, as observed in our experiments. The overall characteristics of the photothermal reactor system were captured. Velocity contours show no major re-circulations in the reactor system under conditions investigated. These simulations show that there is significant radial diffusion of silane outward from the inlet nozzle, limiting the conversion of the silane to silicon particles. Preliminary results are encouraging and work is underway to obtain more realistic and accurate three-dimensional simulations of the reactor and to use temperature, velocity, and silane concentration profiles from these as the basis for coupled aerosol dynamics and detailed chemical kinetics simulations that cannot be carried out in simulations using the detailed 3-dimensional geometry of the reactor system.