Computer-aided Engineering Approach Towards Bottom-up and Top-Down Nanomanufacturing

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Presentation

Abstract: Practically, two options exist for production of materials and surfaces with controllable/tunable nanostructure: bottom-up processing with small, nanometer-scale building blocks (e.g. nanoparticle self- and directed-assembly) or top-down processing with nano-pattering from a prefabricated template (e.g. imprint lithography, mechanical embossing, contact printing, etc.). Although successful applications resulting in useful devices or materials using either approach are now common-place, new scientific breakthroughs in nanostructure control are still frequent and managing these processes over large areas and at throughputs practical for commercial or government applications can be very difficult. Empirical approaches (managed with careful experimental design methods) are currently the norm for industrial scale-up but are often prohibitively time-consuming and expensive. Modeling and simulation can decrease manufacturing process design cycle time enormously, as has been proved in many industry segments. Investment casting, high speed thin-film coating, specialty metals processing are but a few manufacturing processes in which Sandia has provided modeling support and accelerated process design. Nanomanufacturing processes are ripe for this type of support.

This presentation covers key elements of an ongoing research program at Sandia that seeks to develop and apply modeling and simulation tools to solve some of the outstanding challenges of nanopatterning by top-down and bottom up methods and to aid in the scale-up to large-area and/or high throughput. The nanopatterning processes using nanoparticle assembly or top-down methods can be broken down into simpler, underpinning physical rate processes and material phenomena. From a thermo-mechanical standpoint, material deformation, fluid-solid interactions (wetting, spreading, etc.), material rheology are but a few phenomena difficult to manage at high-speeds and over large areas. We will provide an overview of our ongoing modeling and simulation efforts across these areas. We also detail our activities specifically with regard to nanopatterning by detailed large-scale simulations of nanolithographical processes in which rigid molds are imprinted into polymer liquid that is subsequently hardened. We use a generic bead-spring polymer model that can be applied to both step-flash imprint lithography (SFIL), in which the polymer is either cross-linked by exposure to UV irradiationor nanoimprint lithography (NIL), in which the polymer liquid is hardened by lowering the temperature below its glass transition. Stamps are then either removed at constant velocity to study the effects of stress and adhesion on resulting features, or simply deleted to study the zero stress limit. We vary the size and pitch of the stamps in order to study the resolution limits of both methods.