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Mechanisms, models and methods of vapor deposition

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Abstract

The condensation and assembly of atomic fluxes incident upon the surface of a thin film during its growth by vapor deposition is complex. Mediating the growth process by varying the flux, adjusting the film temperature, irradiating the growth surface with energetic (assisting) particles or making selective use of surfactants is essential to achieve the level of atomic scale perfection needed for high performance films. A multiscale modeling method for analyzing the growth of vapor deposited thin films and nanoparticles has begun to emerge and is reviewed. Ab-initio methods such as density functional theory are used to provide key insights about the basic mechanisms of atomic assembly. Recent work has explored the transition paths and kinetics of atomic hopping on defective surfaces and is investigating the role of surfactants to control surface atom mobility. New forms of interatomic potentials based upon the embedded atom method, Tersoff and bond order potentials can now be combined with molecular dynamics to investigate many aspects of vapor phase synthesis processes. For example, the energy distribution of atoms emitted from sputtering targets, the effects of hot atom impacts distribution of atoms emitted from sputtering targets, the effects of hot atom impacts upon the mechanisms of surface diffusion, and the role of assisting ions in controlling surface roughness can all be investigated by this approach. They also enable the many activation barriers present during atomic assembly to be efficiently evaluated and used as inputs in multipath kinetic Monte Carlo models or continuum models of film growth. This hierarchy of modeling techniques now allows many of the atomic assembly mechanisms to be incorporated in film growth simulations of increasing fidelity. We identify new opportunities, to extend this modeling approach to the growth of increasingly complicated material systems. Using the growth of metal multilayers that exhibit giant magnetoresistance as a case study, we show that the approach can also lead to the identification of novel growth processes that utilize adatom energy control, very low energy ion assistance, or highly mobile, low solubility chemical species (surfactants) to control surface diffusion controlled film growth. Such approaches appear capable of enabling the creation of multilayered materials with exceptionally smooth, unmixed interfaces, with significantly superior magnetoresistance.

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