Atomistic Modeling of Thin Film Deposition

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Refreshments at 3:45 PM
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Abstract

Attempts to deposit uniform thin films often result in undesired morphologies, with facets, polycrystalline crystals, ripples in the surface, and even drastic shapes such as columnar microstructures and whiskers. In this talk we will discuss the modeling of several systems where the flux of material for growing the crystal is supplied by magnetron sputtering, and evaluate the ability to control the morphologies. We apply multi-scale atomistic models, including first principles calculations, molecular dynamics simulations, and kinetic Monte Carlo methods. Deposition of Al and Be films is simulated, with emphasis on the conditions that affect the shapes of the deposited material. Applications of the models to the metallization of silicon devices involve issues related to the filling of vias to connect the layers. The deposition models demonstrate breadloafing (the accumulation of deposited atoms close to the edge of the vias) that hinders the filling of the vias by the sputtered metal atoms. We also discuss the factors that lead to columnar grains, and grain coarsening with film thickness. The formation of voids and pinholes that extend through the thickness of the films is discussed. The elimination of such penetrating voids is critical for many applications of films for example, in high-pressure containers and in diffusion barriers. Also, we show that both the shadowing instability and the Schwoebel barrier instability are involved in the formation of these voids, and examine the effectiveness of increasing the kinetic energies of impinging atoms and changing the substrate temperature during growth. We briefly discuss models of the sputtering process and the properties of the sputtered material during transport through the plasma, conditions that also affect stress development in the films during deposition. We examined the influence of laser pulses on the structure of the surface of sputtered material to see if it can be improved by using laser pulses. Movies of the kinetic Monte Carlo models of film growth and of molecular dynamics simulations of femtosecond laser ablation will be shown.
Biographical Sketch

George H. Gilmer is a Research Professor at Colorado School of Mines, in the Mechanical Engineering department. Previously he worked at Lawrence Livermore National Laboratory, from 2001 to 2012 in the Computational Material Science group. He was a hired as a Physicist, and his research was mostly related to the National Ignitional Facility during this time. Before that, he was a Distinguished Member of the Technical Staff at Bell Laboratories, where he was employed from 1972 to 2001. He was a Professor in the Physics Department at Washington and Lee from 1964 to 1972, and during this time had a one year Sloan Fellowship to perform research at Delft Technical Institute in the Netherlands. He is a Fellow of the American Physical Society, and a member of the American Association for Crystal Growth and the Materials Research Society.