

DETERMINATION OF THE MECHANICAL PROPERTIES OF AMORPHOUS COLUMNAR THIN FILMS FROM MD SIMULATIONS

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The optical, electromagnetic and mechanical properties of thin films (TFs) are directly correlated to their morphology at the nanoscale. This, in concert with the fact that

- new deposition techniques are enabling the growth of thin films with very complex morphologies,
- there is an increasing interest in model-based simulation (MBS) for the design of engineering structures (including nanostructures), and
- increasing computer speeds are beginning to make MBS an effective design tool capable of bridging the nanoscale with the continuum scale,

has made it increasingly important to understand how the nanostructure of a thin film impacts its properties at all length scales. The authors are developing the capability to determine the mechanical properties of thin films with amorphous nanostructure by combining molecular dynamics, *i.e.*, position of particles (*e.g.*, atoms or molecules) and their interatomic potential(s), with the principles of continuum mechanics. This work concerns the application of this capability in order to determine mechanical properties, such as stability and distributions of elastic moduli and residual stresses. We are interested in thin films grown via physical vapor deposition (PVD) under conditions in which the deposition angle of the incident species is *not* normal to the substrate. Deposition in this manner results in an amorphous thin film with a porous, columnar nanostructure, whose morphology depends primarily on the deposition angle.

In this presentation, we will focus on translation, via the principles of continuum mechanics, of the discrete MD simulation results into mechanical properties. In addition, we hope to present the relationship between the deposition angle in PVD and the resulting mechanical properties of the film for important species such as MgF₂ and GaN. The films are created via molecular dynamics simulations using potentials available in the literature.