Intrinsic Stability Limits for Glassy Nanoscale Films: Insights from the Energy Landscape

Pooja Shah[1] and Thomas M. Truskett[1,2]
[1]Department of Chemical Engineering and [2]Institute for Theoretical Chemistry
The University of Texas at Austin,
Austin, TX 78712

Introduction

The ability to predict the behavior of materials near interfaces and in confinement is important for understanding many problems of scientific and technological interest. Applications include protective coatings for magnetic hard disks, multiple-layer nanocomposites, and intermediate layers for controlling adhesion, bonding, or wetting in printing or patterning technologies. Interfacial interactions and finite-size effects can strongly influence material properties at these length scales, introducing structural and dynamic inhomogeneities that modify both the glass transition temperature and the phase diagram of the sample. Understanding the factors that determine the stability of solid (glassy or crystalline) nanostructures is of particular interest because many applications require components that exhibit mechanical integrity over a broad range of conditions. Unfortunately, the mechanisms that control molecular-scale ordering and relaxation processes in nano-confined systems are still poorly understood, making property modifications difficult to predict a priori.

Discussion

One powerful tool for understanding the relationship between the properties, the structure, and the molecular interactions of materials is the energy landscape [1], i.e., the hypersurface that the total potential energy forms as a function of the configurational degrees of freedom. Recently, the energy landscape formalism has been invoked using statistical mechanical theory [2] and molecular simulation [3] to gain insights into how confinement impacts liquid-state dynamics and the glass transition in thin films. In this talk, we explore the "equation of state of the energy landscape" of an ultrathin Lennard-Jones film confined between solid substrates (sampled via molecular simulation). We discuss how it can be used to construct a failure diagram, which quantifies how film-substrate interactions and thickness determine the film's intrinsic vulnerability to adhesive, cohesive, or transverse cavitation modes of failure [4].

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