An Energy Landscape Based Mean-Field Theory for the Thermal and Mechanical Behavior of Confined Amorphous Materials

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Introduction

Understanding the behavior of amorphous materials confined to nanoscale dimensions is becoming important in a host of scientific and technological applications including communication, data storage, protective coatings, adhesives, and optical electronics. One of the most pressing issues is that the density variations and large surface-to-volume ratios characteristic of nanostructures can lead to thermodynamic, chemical, and mechanical limits of stability that are quite different than the corresponding bulk materials. The physical reasons for these differences are incompletely understood, which impacts negatively on the development of new materials and innovative processes for high-resolution applications.

Discussion

In this talk, we will discuss how the potential energy landscape [1] of a material can provide insights into how it will perform when it is confined to small spaces. In particular, we will present an energy landscape based mean-field theory [2, 3] that relates the inherent anisotropic stresses in confined glassy materials to sample dimensions and geometry, the chemical nature of the confining substrates, and the balance between molecular packing and cohesive forces. We will use the theory to predict some potential thermal and mechanical limits for forming glassy nanostructures. Finally, we will discuss how some of the approximations of the landscape based mean-field theory (identified through recent molecular simulations [4]) can be improved.

[1] F. H. Stillinger, Science **267**, 1935 (1995)

[2] T. M. Truskett and V. Ganesan, J. Chem. Phys. **119**, 1897 (2003).

[3] J. Mittal, P. Shah, and T. M. Truskett, J. Phys. Chem. B. (in press)

[4] P. Shah and T. M. Truskett, in preparation.