MAR08-2007-001696

Abstract for an Invited Paper
for the MAR08 Meeting of
the American Physical Society

Aging dynamics and the mechanical behavior of glassy solids

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Although aging is observed in most glassy materials, a molecular level understanding of the underlying microscopic processes is incomplete. The intrinsic slow relaxation dynamics in glasses can cause intriguing phenomena: aging changes the mechanical properties of the material, but deformation and yielding also modify aging. This talk will present a series of molecular simulations that provide new insight into the complex, microscopic origins of the elastoplastic behavior of amorphous matter and its relationship to the macroscopic material response. In particular, we investigate the interplay between aging and plastic deformation in coarse-grained models for polymeric and metallic glasses. Molecular dynamics simulations are used to determine the macroscopic shear yield stress as well as the compliance of the model glasses for different loading conditions, temperatures, strain rates and aging times, as well as reveal their relationship to the underlying microscopic distribution of relaxation times. As in experiments on polymer glasses, we find that large stresses can decrease relaxation times and cause mechanical rejuvenation. Furthermore, we find new behavior when the aging glass undergoes more involved thermal protocols such as a temperature step. Phenomenological models will be developed that describe the data over a wide range of temperature, stress and strain rates. We also discuss how continuum models such as energy landscape pictures and the recently formulated shear transformation zone (STZ) theory of amorphous plasticity can account for the aging effects observed in the molecular simulations.