MAR17-2016-009516

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Deformation and Recovery of Polymer Glasses: Insights from Molecular Simulations

JOERG ROTTLER, University of British Columbia

This presentation will explore the atomistic level processes in quiescent and actively deformed polymer glasses with molecular simulations. Generic polymer models capture the macroscopic phenomenology of thermal creep or deformation at constant strain rate remarkably well. Monomer trajectories obtained from molecular dynamics simulations allow us to track the evolution of relaxation time distributions under different deformation protocols and thermal histories, and to relate spatially heterogeneous relaxation dynamics with local structure. Molecular simulations successfully reproduce experimentally observed phenomena such as accelerated segmental motion and narrowing of the relaxation time spectrum, and suggest a common framework in which to understand them. Polymer glasses are also ideal materials to study the interplay between physical aging (structural recovery) and erasure of memory (rejuvenation) due to mechanical driving, which is important in other structural glasses (amorphous metals or dense colloidal suspensions) as well. We conclude by testing the predictions of recently proposed theories for the behavior of the relaxation time during plastic flow against simulations, and thus identify the relevant deformation variables that control mechanical rejuvenation.