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Molecular simulations of polymer glasses under active deformation

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Many of the technologically important mechanical properties of polymers depend crucially on their properties in the glass state. Despite their tremendous importance, our understanding of many of the commonly-observed phenomena in the glass state (e.g. aging and the changes in mobility with deformation) remains primitive. In this talk, I will describe recent molecular simulations examining how the segmental dynamic properties evolve during aging and deformation of polymer glasses. When a constant stress is applied to our materials, we find that the mobility is immediately enhanced by a substantial amount and continues to increase until the material begins to strain harden. After strain hardening begins, the mobility gradually decreases. However, when we deform at a constant strain rate, we find that the mobility is essentially constant after the yield point even when strain hardening occurs. Although comparable experimental measurements of the mobility in polymer glasses examine time scales many orders of magnitude longer than those observable from our simulations, the trends in the changes in mobility agree very well between the experiments and the simulations. In addition, we will explore how the dynamic heterogeneity can be tuned with various additives such as antiplasticizers, which render our polymer a stronger glass former with more homogeneous dynamics, and how this dynamic heterogeneity evolves with deformation.