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Simulations of aging and plastic deformation in polymer glasses
MYA WARREN, JOERG ROTTLER, University of British Columbia — Experiments on a broad class of amorphous glassy materials show that their mechanical behavior strongly depends on the time since vitrification. The slow relaxation of configurational degrees of freedom, or aging, generally increases the material's resistance to applied stress. In this study, we investigate the interplay between aging and plastic deformation in a simple model for polymer glasses by means of molecular dynamics simulations. We determine the macroscopic creep compliance for different loading conditions and aging times and find excellent qualitative agreement with experiments: compliance curves can be shifted to form a universal master curve, and the applied stress can reduce the effective age of the glass (mechanical rejuvenation). We then measure microscopic, local relaxation times and show that they correlate well with the aging characteristics of the macroscopic creep response. In addition, we explore the evolution of several measures of local order during aging and discuss their role in the mechanical behavior.

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