

Abstract Submitted
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Dynamics of a polymer nanocomposite under stress ROBERT RIGGLEMAN, JUAN DE PABLO, University of Wisconsin - Madison — The response of polymer glasses to deformation has received much attention in recent years. Previous simulation studies have shown that strain applied to a polymer glass can destroy energy barriers that impede relaxation on the potential energy landscape. However, less attention has been placed on the response of a polymer glass to an applied stress, as in a creep experiment. We have performed molecular simulations of the non-linear creep of a coarse-grained polymer glass and a polymer nanocomposite in shear, compression, and extension. We study the effects of the applied stress on the dynamics of our system and find dynamic enhancement up to a factor of 100 compared to the quiescent polymer glass below its glass transition temperature, T_g . We find that the free volume changes induced by the stress are not indicative of the changes in dynamics; however, the strainrate is strongly correlated with the dynamics.

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