Dynamical heterogeneity and structural relaxation in periodically deformed polymer glasses

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The dynamics of structural relaxation in a model polymer glass subject to spatially-homogeneous, time-periodic shear deformation is investigated using molecular dynamics simulations. We consider a coarse-grained bead-spring model of short polymer chains below the glass transition temperature. It is found that at small strain amplitudes, the segmental dynamics is nearly reversible over about 10,000 cycles, while at strain amplitudes above a few percent, polymer chains become fully relaxed after a hundred cycles. At the critical strain amplitude, the transition from slow to fast relaxation dynamics is associated with the largest number of dynamically correlated monomers as indicated by the peak value of the dynamical susceptibility. The analysis of individual monomer trajectories indicated that mobile monomers tend to assist their neighbors to become mobile and aggregate into relatively compact transient clusters.