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Shear elasticity and shear relaxation in glass-forming polymer melts and films

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The shear modulus G can be thought of as an order parameter distinguishing the liquid ($G = 0$) from the glass (solid, $G > 0$). Here we present results from molecular dynamics simulations for the temperature (T) dependence of G . Our simulations examine a coarse-grained polymer model for bulk polymer melts and free-standing films of various thicknesses. For the bulk we apply two methods to calculate $G(T)$: a method based on the fluctuations of the wave-vector dependent strain and the “stress-fluctuation formalism” which determines G from the fluctuations of the shear stress (in different thermodynamic ensembles). We discuss both methods, show that they give consistent results, and also compare the resulting G with estimates of the nonergodicity parameter from the shear-stress auto-correlation function and the monomer mean-square displacement. The analysis is then extended to free-standing films. We find that the presence of the free interfaces weakens the shear rigidity of the polymer glass relative to the bulk. We discuss the dependence of this effect on film thickness and on the distance to the free interface and compare our results to similar findings in the literature.

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