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Approaching the Glass Transition from Various Directions[1]

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In recent years a significant amount of experimental work has appeared on glassy systems, both polymeric and small molecule. However, this rich explosion in data has not been met with a concomitant leap in fundamental understanding. We have developed a number of approaches to elucidate some of the underlying mechanisms of behaviour in bulk and confined glassy systems. Using our Limited Mobility (LM) coarse-grained simulation model we have characterized the dynamic heterogeneity associated with approaching the glass transition, explored interfacial behaviour when layering materials of differing mobility, and analyzed the effect of a free surface on a supported thin film. Approaching related problems from a different direction we have modified a simple thermodynamic description of the bulk to account for missing interactions at a film surface, and substrate interactions in the case of supported films. Characterizing the systems via bulk data alone, we find our film-averaged predictions for the effects of confinement agree well with experimental data on several freestanding and supported polymer films. That work deals with confined systems; a fundamental understanding of bulk glass transitions also remains incomplete. Most recently we have been applying our Locally Correlated Lattice (LCL) equation of state model, which has met with success in modeling polymer melt and mixture behaviour, to reveal hints of the underlying glassy nature of a bulk polymer sample, even while above its transition temperature (Tg). Correlations between Tg and a variety of equilibrium bulk quantities have lead us to make connections not only with a substantive amount of experimental data on a wide range of polymers, but also with other models of glassy polymeric systems. This talk will comprise an efficient summary of past progress from these different directions, and will then focus on our most recent results and current understanding.

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