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Contrasting Polymer Behavior Under Nanoconfinement using Thermomechanically Consistent Coarse-Grained Models SINAN KETEN, WENJIE XIA, DAVID HSU, Northwestern University — We present a systematic, two-bead per monomer coarse graining strategy that simulates the thermomechanical behavior of polymers several hundred times faster than all-atom MD (Hsu et al. JCTC, 2014). The predictive capability of the technique is illustrated here for 5 different methacrylate monomers and polystyrene stereoisomers. The approach involves optimization of analytical bonded potentials from atomistic bonded distributions to emulate local structure, as validated by chain end-to-end length and the radius of gyration comparisons with experiments and random coil theory. Nonbonded Lennard-Jones potentials are tuned to reproduce the elastic modulus (E) and glass transition temperature (T_g) at a single thermodynamic state. Density-corrected parameters capture temperature-modulus dependence in the 150-600 K range. Flory-Fox constants of the CG models are commensurate with all atomistic and experimental results, even though all calibrations are done at a single molecular weight. Finally, we further demonstrate the predictive capabilities of the models by examining thin film nanoconfinement effects for different polymers, film thicknesses, interfacial energies, and molecular weights. Our technique, called thermomechanically consistent coarse graining (TCCG), is demonstrated, using polystyrene and poly(methylmethacrylate) as universal benchmarks, to be a robust and effective technique to understand the thermomechanical behavior of polymers thin films and nanocomposites.

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