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Fast Lattice Monte Carlo Simulations of Grafted Homopolymers under Compression PENGFEI ZHANG, QIANG WANG, Colorado State University — Fast lattice Monte Carlo (FLMC) simulations [Q. Wang, Soft Matter 5, 4564 (2009); 6, 6206 (2010)] with multiple occupancy of lattice sites and Kronecker δ-function interactions give orders of magnitude faster/better sampling of configuration space for many-chain systems than conventional lattice MC simulations with the self- and mutual- avoiding walk and nearest-neighbor interactions. Using FLMC simulations with the novel Wang-Landau-Optimized-Ensemble sampling, we have studied homopolymers end-grafted on an impenetrable and flat substrate under the compression by another impenetrable and flat surface. Comparing various quantities (including chain dimensions, internal energy, Helmholtz free energy, and pressure) obtained from FLMC simulations with predictions from the corresponding lattice self-consistent field (LSCF) calculations, both using the same model system (Hamiltonian) and thus without any parameter-fitting, we unambiguously quantify the effects of system fluctuations and correlations neglected in LSCF theory. In particular, we find LSCF theory underestimates the pressure for compression of mushrooms in the athermal and θ-solvents and for compression of brushes in the θ-solvent, but overestimates it for compression of brushes in the athermal solvent.

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