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Monte Carlo Simulation of the Irreversible Adsorption of Polymers to Surfaces: Influence of Molecular Weight VIKRAM KUPPA, University of Cincinnati — Monte Carlo simulations using a coarse-grained, freely rotating chain model are employed to investigate the behavior of linear polymer chains whose constituent beads are attracted to flat, perfectly smooth surfaces by interactions much stronger than thermal energy, kT. We investigate the effect of chain molecular weights on such a system by conducting the simulations in an ensemble which provides control over the chain lengths by allowing the exchange of monomer beads between different chains. The structure of the adsorbed polymer layers is characterized by monomer density profiles, bond order parameters, fractions of adsorbed monomers per chain, and populations of tails, loops and trains. Systems in which polymer lengths are constrained to a narrow range show pronounced and structured density profiles as compared to those in which a distribution of chain molecular weights is permitted to exist. The adsorbed bead fraction shows a broad distribution only for the narrow molecular weight case, indicating that the competition amongst chains to make contact with the surface is modified by the population of chain lengths. Our results are derived in the context of varying interaction strengths, molecular weight distributions, segregation effects, and interacting monomer sequences.

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