

Abstract Submitted
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Studying polymer films deposited on solid surfaces using generic microscopic and mesoscopic soft models JIANGUO ZHANG, DEBASHISH MUKHERJI, KURT KREMER, KOSTAS DAOULAS, Max Planck Institute for Polymer Research — Polymer films deposited on solid substrates are fundamentally interesting and have tremendous industrial applications. We develop a particle-based soft model where polymers are represented as worm-like chains, while non-bonded interactions are defined via a simple density functional[1]. The form of the functional and the values of involved parameters are specified taking into account certain thermodynamic properties known from experiments, e.g. phase-equilibria data. Films of poly(methyl methacrylate) adsorbed on silica are chosen as a test system. The soft model is validated by direct comparison with smaller scale simulations based on a generic microscopic model representing the same system. To compare the two models, we study chain-shape, structure of the adsorbed layer, as well as the statistics of loops, tails, and trains. The two models are found to be consistent with each other. Some deviations observed in polymer conformations and structure of adsorbed layer can be rationalized by the simplified description of polymer/surface interactions and local liquid packing in the soft model. [1] J. Zhang, D. Mukherji, and K. Daoulas, Eur. Phys. J. Special Topics 225, 1423 (2016)

Kostas Daoulas
Max Planck Institute for Polymer Research

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