Abstract Submitted
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Structure and dynamics of highly adsorbed semiflexible polymer melts[1] JAN-MICHAEL CARRILLO, SHIWANG CHENG, RAJEEV KUMAR, MONOJOY GOSWAMI, ALEXIE SOKOLOV, BOBBY SUMPTER, Oak Ridge National Lab — We present a detailed analysis of coarse-grained molecular dynamics simulations of melts of semi-flexible polymer chains in the presence of an adsorbing substrate. For polymer chains located far from the substrate the chain conformations follow the worm-like chain model, in contrast to the reflected Gaussian conformation near the substrate. This is demonstrated in the chain center-of-mass distribution normal to the substrate and the probability of a polymer chain ends to be the closest to the substrate. Both quantities agree with Silberberg's derivation for an ideal chain in the presence of a reflecting wall. We characterized the adsorbed chains and counted the number of loops and tails. For stiff chains, a tail and an adsorbed segment dominate the chain conformation of the adsorbed layer. Also, the mean-square end-to-end distance normal to the substrate is proportional to the normal component of the mean-square end-to-end distance of the tails. The tails do not follow the worm-like chain model and exhibit a stretched conformation. This picture for the adsorbed layer is akin to the "polydisperse pseudobrush" envisioned by Guiselin. We probe the dynamics of the segments by calculating the layer (z-)resolved intermediate coherent collective dynamics structure factor, S(q,t,z), for q values equivalent to the bond length. The segment dynamics is slower for stiffer chains. In the adsorbed layer, dynamics is slowed down and can be described by two relaxation times.

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