

# Single-Chain Dynamics in a Homogeneous Melt and a Lamellar Microphase: A Comparison Between Smart-Monte-Carlo Dynamics, Slithering-Snake Dynamics, and Slip-Link Dynamics

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We investigate the ability of Monte-Carlo algorithms to describe the single-chain dynamics in a dense homogeneous melt and a lamellar phase of a symmetric diblock copolymer. A minimal, coarse-grained model is employed that describes connectivity of effective segments by harmonic springs and where segments interact via soft potentials, which do not enforce non-crossability of the chain molecules. Studying the mean-square displacements, the dynamic structure factor and the stress relaxation, we show that local, unconstrained displacements of segments via a Smart-Monte-Carlo algorithm give rise to Rouse dynamics for all but the first Monte-Carlo steps. Using the slithering-snake algorithm, we observe a dynamics that is compatible with the predictions of the tube model of entangled melts for long times, but the dynamics inside the tube cannot be resolved. Using a slip-link model, we can describe the effect of entanglements and follow the different regimes of the single-chain dynamics over seven decades in time. Applications of this simulation scheme to spatially inhomogeneous systems are illustrated by studying the lamellar phase of a symmetric diblock copolymer. For the local, unconstrained dynamics, the single-chain motion parallel and perpendicular to the interfaces decouples; the perpendicular dynamics is slowed down but the parallel dynamics is identical to that in a homogeneous melt. Both, the slithering-snake dynamics and the slip-link dynamics, give rise to a coupling of parallel and perpendicular directions and a significant slowing-down of the dynamics in the lamellar phase.

[1] M. Müller and K.Ch. Daoulas, *J. Chem. Phys.* **129**, 164906 (2008)