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Microscopic Theory of Entangled Polymer Melt Dynamics: Flexible Chains as Primitive-Path Random Walks and Super Coarse-Grained Needles KEN SCHWEIZER, University of Illinois at Urbana-Champaign, DANIEL SUSSMAN, University of Pennsylvania — We qualitatively extend our recent microscopic dynamical theory for the transverse confinement potential and diffusion of infinitely thin rigid rods (PRL, 107, 078102 (2011)) to construct a first-principles theory of topologically entangled melts of flexible polymer chains (PRL, 109, 168306 (2012)). Polymer coils are treated as ideal random walks of self-consistently determined primitive-path (PP) steps, and chain uncrossability is included exactly at the binary collision level. A strongly anharmonic (tube) confinement potential for a primitive path segment is derived and favorably compared with recent simulations. A fundamental basis is derived for the Lin-Noolandi conjecture that relates the tube diameter to the invariant packing length, along with the reptation scaling laws for the diffusion constant and terminal relaxation time, including numerical prefactors. The relationship of the PP-level theory to two simpler models, the melt as a disconnected fluid of primitive-path steps, and a super coarse-graining that replaces the entire chain by a needle corresponding to its end-to-end vector, is examined. Remarkable connections between the different levels of coarse graining are discovered.

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