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Polymer twists: entanglement and packing ansatz

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Polymer motions in dense liquids (molten plastics) are severely constrained by surrounding chains, due to the fact that chains cannot cut through each other. Effectively, polymers may be considered as being confined inside a tube-like region. The tube diameter is the key parameter needed by the modern molecular theory for polymer rheology. But a molecular understanding of the tube diameter is missing. We summarize our recent attempts at estimating the tube diameter from simulated topologically equilibrated ring polymers, which have well–defined topological states and are free from the complication caused by chain end relaxation dynamics. We consider two non–invasive methods for estimating the tube diameter, one based on the extent of bead position spreading over an ensemble of short dynamic trajectories, and another based on statistics of topologically distinct states collected with the help of a generalized knot invariant polynomial. For simulated polymer melts, we get a tube diameter value that agrees with values obtained by more heuristic methods. We then present results on the effects of chain stretching and neutral solvent dilution on the tube diameter, and examine the three possible variants of the Lin-Noolandi packing arguments for the tube diameter, which all yield the same prediction for unperturbed polymer melts, but each gives different prediction when applied to stretched and diluted systems. The analyses are in favor of a binary view of polymer entanglement.