Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Tying Polymer Knots to Find the Entanglement Length JIAN QIN, SCOTT MILNER, ChE at Penn State University — We propose two relations between the entanglement length and the probability distribution of topological states accessed by topologically equilibrated ring polymer melts. The first states that the rings are most likely entangled when the ring length exceeds the entanglement length. The second states that the topological entropy measuring the number of accessible topological states is about k_B per entanglement strand. To test these ideas, we simulated melts of ring polymers with hybrid MC/MD moves, and sampled their topological states by using various ring rebridging moves. Topological states are identified by mapping the molecular configurations to knots, and knots are distinguished by computing their invariant polynomials. We accumulated the state statistics, their ring length dependence, and extracted the entanglement length using these two approaches. The results are consistent with each other, and agree with those from the heuristic methods.

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Date submitted: 18 Nov 2010 Electronic form version 1.4