



~~Special Polymer Physics Seminar ~~

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301 Steidle Bldg.

Entanglements in Ring Polymers: Visualization and Topological Analysis

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Polymer entanglements originate from the molecular uncrossability, which are responsible for various mechanical properties of polymeric materials. The effects of entanglements may be understood by considering the test chains as being confined inside a tube like region. The goal of this work is to develop a molecular understanding of the tube and entanglements by studying ring polymers. Ring polymers are selected because the entanglements are permanent, due to the absence of end effects. We approached the problem from two complementary points of view: one based on direct visualization of confining tubes at the monomer scale, and the other based on statistical analyses of entanglement topologies. In the first part, we visualize the confining tubes by running multiple (up to 500) MD simulations or replicas, all starting from the same initial configuration, and average the ring trajectories recorded at different time delays. The statistics of monomer positions from different replicas around the mean trajectories are then studied, from which the strength of the confining effects or the tube diameter can be estimated. We studied the inhomogeneity of tube diameters along the mean trajectories, and the effects of free surfaces on the tube diameter. In the second part, we simulated topologically equilibrated ring polymers by implementing various ring rebridging Monte Carlo moves. We identified entanglement topology by mapping ring configurations onto knots and computing knot invariant polynomials, which are uniquely defined for each knot type. We accumulated the probability distribution of entanglement topologies for rings confined under both aperiodic and periodic (1D and 2D) boundary conditions, and for varying ring lengths. The length at which the behavior of rings change from most likely disentangled to most likely entangled is a good approximant to the entanglement length. We then computed the topological entropy from the distribution of entanglement states. The dependence of this entropy on the ring length for big rings are used to estimate the entanglement length. The value is consistent with that from more heuristic methods.