Statistical Mechanics of Theta-shaped and Ring-shaped Polymer Chains

Erica Uehara (Ochanomizu University)

We evaluate the correlation function and gyration radius of a theta-shaped polymer and those of a ring polymer via the Monte-Carlo simulation and the Gaussian model. We generate random equilateral chains whose structure is given by either a theta-3 graph or a loop. The mean-square (MS) gyration radius of theta-shaped chains is given by 2/3 times gyration radius of ring-shaped chains of the same number of segments. It is similar that the ring polymer has half MS gyration radius compared with the linear polymer having the same number of segments. Therefore, the MS gyration radius of a linear chain with n segments, a ring chain with 2n segments and a theta-3 chain with 3n segments are equal. However, the correlation functions and Kratsky plots of a linear chain, those of a ring chain and those of a theta-shaped chain are different from each other. The Kratsky plots of the different polymers approach different asymptotic values in the limit of high frequency. It suggests that the correlation between short lengths depends on the topology of the structure of polymer chain.