Dragging a polymer chain into a nanotube: theory and simulation

H.-P. Hsu[1], K. Binder[1], L. I. Klushin[2], and A. M. Skvortsov[3]
[1] *Institut für Physik, Johannes Gutenberg-Universität Mainz, D-55099 Mainz, Staudinger Weg 7, Germany*
[2] *American University of Beirut, Department of Physics, Beirut, Lebanon*
[3] *Chemical-Pharmaceutical Academy, Prof. Popova 14, 197022 St. Petersburg, Russia.*

We present a scaling theory and Monte Carlo (MC) simulation results for a flexible polymer chain slowly dragged by one end into a nanotube. MC simulations were performed for a coarse grained model, self-avoiding walks on a simple cubic lattice with finite cylindrical confinement, using a biased sequential sampling algorithm with re-sampling, similar to the pruned-enriched Rosenbluth method (PERM) [1,2]. The nanotube is considered as a long channel opened at one end and its diameter D is much smaller than the size of the polymer coil in solution. We analyze the following characteristics as functions of the chain end position x inside the tube: the free energy, the average end-to-end distance, the average number of imprisoned monomers, and the average stretching of the confined part of the chain for various values of D and for the number of monomers in the chain, N. When the chain end is dragged by a certain critical distance x^* into the tube, we see that the polymer undergoes a first-order phase transition whereby the remaining free tail is abruptly sucked into the tube. This is accompanied by jumps in the average size, the number of imprisoned monomers, and in the average stretching parameter. The critical distance scales as $x* \sim ND^{1-1/\nu}$. The transition takes place when approximately 3/4 of the chain units are dragged into the tube. The theory presented is based on constructing the Landau free energy as a function of an order parameter that provides a complete description of equilibrium and metastable states. All simulation results are in perfect agreement with the analytical theory. Finally, we apply the theory to estimate the lifetime of confined DNA in metastable states in nanotubes [3].

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