Collapse transitions in thermosensitive multi-block copolymers: A Monte Carlo study

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The focus of the present study is to investigate the self-assembly behavior of a single linear multiblock copolymer chain of various lengths (N), via Monte Carlo simulations.[1] More specifically, the chain is of type $(A_n B_n)_m$ and consists of alternating A and B blocks, where A are solvophilic (i.e., extended conformations are preferred) and B are solvophobic (i.e., condensed conformations are preferred "globules") and $N = 2nm$. We explore the conformational transitions of the chain and their dependence of the chain length and the number of blocks. In order to achieve this we classify the chain transitions in five cases based on the globules formed by the solvophobic B-blocks (Figure 1). We study systems with relatively high molecular weights i.e., N in the range of [*500 – 5000*] units. Energy parameters have values which correspond to good - almost athermal solvent for A-blocks and very poor solvent for B-blocks. A rich phase behavior is observed as a result of the alternating architecture of the multiblock copolymer chain. Furthermore the combination of all parameters of the phase space plays a key role in the preferred conformations. We trust that thermodynamic equilibrium has been reached for chains of N up to *2000* units, while the results for longer chains indicate kinetic issues. Finally, we compare the globules formed by the copolymer chains with their homopolymer analogs.[2] This comparison underlines the substantial influence of solvophilic B-blocks on the chain configurations.

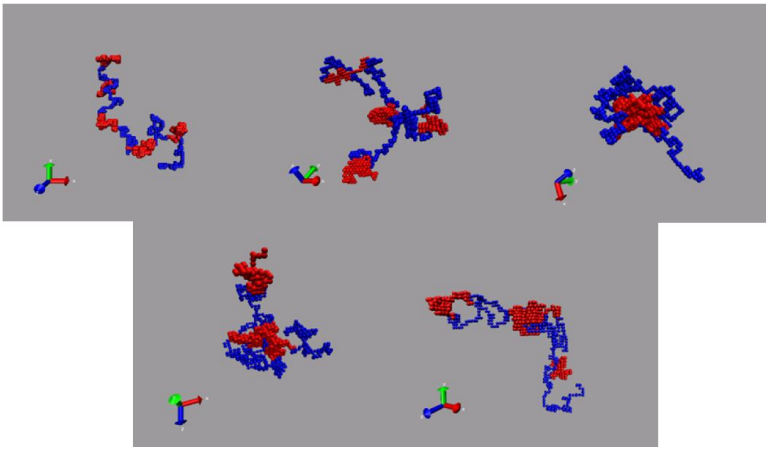

Figure 1: Snapshots of configurations of a single multiblock copolymer chain.

References

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[2] A. N. Rissanou, S.H Anastasiadis, and I.A. Bitsanis "A Monte Carlo Study of the Coil-to-Globule Transition of a Model Polymeric System", Journal of Polymer Science: Part B: Polym. Phys. **44**, 3651-3666 (2006).

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