Intramolecular structures in a single copolymer chain consisting of flexible and semiflexible blocks: Monte Carlo simulation of a lattice model

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We study the conformational properties of a single multiblock copolymer chain consisting of flexible and semiflexible blocks. Monomer units of different blocks are equivalent in the sense of the volume interaction potential, but the intramolecular bending potential between successive bonds along the chain is different. We consider a single flexible-semiflexible regular multiblock copolymer chain with equal content of flexible and semiflexible units and vary the length of the blocks and the stiffness parameter. We perform flat histogram type Monte Carlo simulations based on the Wang-Landau approach [1] and employ the bond fluctuation lattice model, for which the phase diagram for flexible chains has been determined [2] using the Wang-Landau simulation method and for which the state diagram of semiflexible chains has been determined by use of expanded ensemble simulation techniques [3].

We present our data on different non-trivial globular morphologies which we have obtained in our model for different values of the block length and the stiffness parameter. We demonstrate that the collapse can occur in one or in two stages depending on the values of both these parameters and discuss the role of the inhomogeneity of intraglobular distributions of monomer units of both flexible and semiflexible blocks. For short block length and/or large stiffness the collapse occurs in two stages, because it goes through intermediate metastable structures, like a dumb-bell shaped conformation. In such conformations the semiflexible blocks form a cylinder-like core, and the flexible blocks form two domains at both ends of such a cylinder. For long block length and/or small stiffness the collapse occurs in one stage, and in typical conformations the flexible blocks form a spherical core of a globule while the semiflexible blocks are located on the surface and wrap around this core.

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