NANOSYSTEMS: PHYSICS, CHEMISTRY, MATHEMATICS, 2015, 6 (4), P. 513–523

Entropic sampling of star-shaped polymers with different number of arms: temperature dependencies of structural properties

I. A. Silanteva[1], P. N. Vorontsov-Velyaminov[1]

[1]Saint Petersburg State University, Dept. of molecular biophysics and polymer physics, Faculty of Physics, 198504, Saint Petersburg, Russia

sila3@yandex.ru, voron.wgroup@gmail.com

PACS 02.70.-c, 02.70.Uu, 05.10.Ln, 05.70.-a, 05.70.Fh, 07.05.Tp, 36.20.-r, 36.20.Hb, 64.60.-i, 64.70.Nd, 64.70.km, 64.70.pj, 65.40.Ba, 65.80.+n, 81.07.Nb, 82.20.Wt, 82.35.Lr, 87.10.Rt, 87.15.ak, 87.16.aj, 87.53.Wz, 87.55.K

DOI 10.17586/2220-8054-2015-6-4-513-523

The lattice model for a star-shaped polymer with a total number of up to 72 segments is considered. The number of arms varied, ranging from 2 to 6. Entropic sampling Monte Carlo simulation is used to obtain the equilibrium, thermal and structural properties of the considered systems over a wide range of temperatures. The coil-globule transition is observed and the transition temperature is shown to shift toward lower temperatures with an increase in the number of arms. This study demonstrates how the structure of the star-shaped polymer affects its equilibrium properties.

Keywords: star-shape polymer, lattice model, entropic sampling, Wang-Landau algorithm, phase transition.

Received: 20 June 2015

1. Introduction

Over the last couple of decades, there has been an increased interest in studying nano-objects of various types including the polymer molecules. Modern facilities are now able to synthesize macromolecules with complicated architecture, such as stars, brushes, nets or dendrimers. In this paper, we restrict ourselves to the simulation study of star-shaped molecules. Due to their specific structural features, these polymers have essentially new characteristics in comparison to linear chains. As a result, their average size is considerably smaller than that of the linear polymers with the same number of segments. Consequently, they have greater concentration of monomers that leads to greater volume effects. Star-like molecules can be considered as unique objects, combining properties of linear polymers and colloid particles as was also pointed out in [1, 2]. It was correctly mentioned in [3] that the star polymer with a small number of arms is close in its behavior and properties to that of a linear polymer, while with an increased number of arms, it becomes closer to a rigid spherical particle. The main aim of this paper is to observe how initial structural characteristics, such as the number of its arms, influence its equilibrium structural properties, including features of the coil-globule transition. This problem is also discussed in a number of papers [4, 5] so it would be desirable to compare our data with that of [4]. It is known that in the star-like polymers, there can be observed transitions of two types: liquid-crystal (1st order) and the coil-globule (2nd order), wherein the second order transition is very sensitive to the polymer's topology.