MONTE CARLO COMPUTER SIMULATION OF LIQUID-CRYSTALLINE ORDERING IN SOLUTION OF STIFF-CHAIN MACROMOLECULES

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We use a coarse-grained model of semiflexible macromolecules to study the phase diagram of solution of these macromolecules varying both the temperature and the density.

We have applied Monte Carlo techniques using the bond fluctuation model with local and "slithering-snake" moves as well as grand canonical (GC) moves by means of configurational bias scheme (CBMC) [1]. Two different types of interactions were taken into account: a purely intramolecular potential depending on the angle between successive bonds along the chain and on the bond length to control the chain stiffness, and an attractive interaction between effective monomer units to model variable solvent quality. Chain length was equal to $N = 20$ effective monomer units. Volume fraction of macromolecules was varied in a very broad interval from 0 up to 0.98.

The phase diagram (temperature-density) has been obtained for some particular value of stiffness parameter, and comparison with theoretical results [2] has been performed. For this goal, we have implemented the hard wall algorithm for measuring pressure [3] and developed it for the case of semiflexible chains. In the case of nematically ordered solution of stiff macromolecules we have used the histograms of orientational order parameter to determine the transition lines.

The polymer-solvent critical point for the case of flexible chains was studied in [1], while the lyotropic first-order isotropic-nematic phase transition in the purely steric solution of stiff macromolecules was reported in [4]. In the present work the interplay between the liquid-vapor transition and isotropic-nematic transition has been investigated in detail. The liquid-vapor critical point at low polymer densities can be found for moderate values of stiffness parameter. At high values of polymer density the isotropic-nematic phase transition takes place. At higher values of stiffness parameter the liquid-vapor critical point cannot be observed anymore at low densities.

References

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