Dynamics of Linear and Cyclic Chains in Two Dimensions

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Extensive and systematic simulation studies of two-dimensional polymer systems were performed. In contrast to other works we focused on cooperative phenomena that occurred where the motion of particles takes place in a dense system. Comparison studies of athermal cyclic and linear polymer chains systems on the two-dimensional triangular lattice are presented. We studied various polymers concentrations with respect to an explicitly considered solvent. We employed the Dynamic Lattice Liquid (DLL) model [1], which can work at the highest system density, where all lattice sites are occupied and it allows to take into account coincidences of elementary molecular motion attempts resulting in local cooperative structural transformations. Both static and dynamic properties of the model systems are characterized [2]. We showed the differences between the dynamic behavior of rings and linear chains in solution and how the structure of these objects influence the dynamics of the inert solvent. The simulation results reflect molecular packing and other properties of monomolecular polymer layers, which can be relevant for these, obtained in some thin film formation techniques.

References

[1] P. Polanowski and T. Pakula, *Studies of mobility, interdiffusion, and self-diffusion in two-component mixtures using the dynamic lattice liquid model*. J. Chem. Phys. **118**, 11139-11146 (2003).

[2] P. Polanowski, J. K. Jeszka and A. Sikorski, *Dynamic Properties of Linear and Cyclic Chains in Two Dimensions. Computer Simulation Studies*, Macromolecules **47**, 4830-4839 (2014).