

Simulation of statistical and kinetics characteristics of polymer melt using the cooperative motion algorithm.

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Mobility of the polymer chains in the melt is drastically limited and correlation of their movement with the movement of other surrounding particles is required. Thus, simulations of the changes in the polymer structure require algorithms working with the density ratio of unity what means that each cell of the model lattice is occupied by a single kinetic element. In the cooperative motion algorithm [1,2] movement of the kinetic elements is carried out by local transfer of a number of elements in closed loops. During such transfer operations, conformations of the macromolecules also undergo transformations, while maintaining their identity, i.e. the number and order of the elements in the chain backbone and the topology of the bonds in each polymer macromolecule are fixed [3]. Present simulations are performed on 2D triangular lattice.

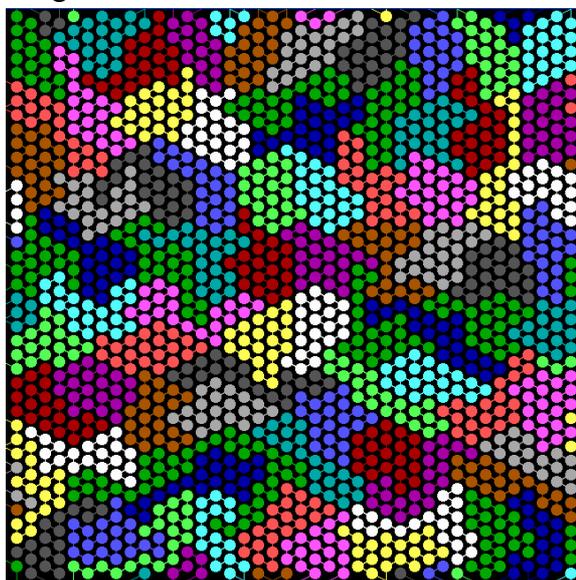


Fig.1. Chain macromolecules in the simulated polymer melt with periodic boundary (colors indicate individual chains).

Values of relaxation time of the polymer chain segments which correspond to local mobility are used to determine global relaxation time of the chains in the system and the autocorrelation function of the chain end-to-end vector. The dependence of the chain relaxation time on the polymer molecular weight obtained in the simulations is linear.

The collected data enable us to determine statistical dimensions of the polymer random coil and the diffusion constant of the center of mass of the chain macromolecule. The chain mean square end-to-end distance and the radius of gyration increase with increasing the molecular weight. Stability of the radius of gyration during the simulation indicates that the system is ergodic [4]. Lack of low-molecular weight substances and absence of vacancies in the lattice limit local mobility of the kinetic elements in the system. The local mobility weakly depends on the chain length and is influenced by the contribution coming from the elements at the chain ends.

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