Some Properties of Polymer Chains in Confinement. Monte Carlo Simulations

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The main goal of this study was to investigate the dynamic properties of branched polymer chains located in a slit. The idealized models of polymers were built of united atoms (segments) restricted to vertices of a simple cubic lattice. The macromolecules were star-branched and consisted of there branches of equal length. The chains were at good solvent conditions and the only interaction between the segments was the excluded volume. The polymers were located in a slit formed by a pair of parallel and impenetrable surfaces which were attractive for polymer segments. The confining surfaces contained also some repulsive points. The properties of the model chains were determined by means of dynamic Monte Carlo method using a sampling algorithm based on chain's local changes of conformation. It was shown that at certain temperature and the size of the slit the chains were adsorbed at one of the confining surfaces and after a certain period of time they were detached from this surface and approached the opposite one. The conditions necessary for these jumps were determined. The influence of the repulsive patterns at the confining surfaces on the properties of the system was also studied.

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