COLLISIONAL MOLECULAR DYNAMICS TECHNIQUE FOR MODELING OF COMPLEX POLYMER SYSTEMS

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Molecular dynamics (MD) simulations are considered today as an important source of information on molecular nano-scale level. When simulating a system of particles, for a variety of reasons, some of them are treated explicitly whereas others are represented only by their stochastic influence on the former subsystem. Various methods have been proposed for the stochastic coupling of a system under simulation to an external heat bath. In the collisional dynamics (CD), the coupling of the subsystem to a solvent is simulated by stochastic collisions with virtual solvent atoms, which takes into account an atomistic feature of a solvent. In CD method, there are two parameters, m_0 (the mass of the virtual solvent particle), and λ (the number of collisions per atom in a unit time), which control energy and momentum exchange between the subsystem and the bath. Velocities of virtual particles are taken in each time moment from normal distribution that corresponds to prescribed temperature of the bath and given flow conditions. The result of each collision is an instantaneous change in the atom velocities of the subsystem. Between the stochastic collisions, the system evolves in accordance with the equations of motion as in the usual molecular dynamics. In comparison with other approaches CD method seems to be more accurate in mimicking the dynamical coupling to the solvent, and yields more realistic dynamical behavior of the simulated molecular system.

Effective computer codes were elaborated for CD simulation of different complex polymer systems. We use this method to simulate the solvent, to maintain the temperature of the system, and to incorporate shear and elongational flows.

Initial structure of a complex polymer system (coordinates and velocities of all atoms) plays the key role for successful modeling of its behavior. The preparation of representative structure of the system is usually complex and expensive procedure. The more complex is polymer system, the slower is its equilibration. The modeling technique developed on the base of CD method makes possible to realize the flexible control of the process of initial data preparation.

Collisional dynamics technique for simulation of different polymer systems will be presented. A comparison with Brownian dynamics will be conducted. Some results for linear polymers in dilute solution under shear flow will be submitted. A modification of the method is proposed by taking into account an accessibility of polymer atoms to virtual particles of the solvent.

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