V-J Monte Carlo Simulation of Molecular Clusters

Monte Carlo simulation is a powerful method for studying soft matter such as polymer and gel. We performed the structure analysis of chemical gel and characterized gel with cross-linkers. For DNA in polymer solution, we simulated the linear-shaped and U-shaped motion, and studied the conditions for such motions. In both systems, we obtained qualitatively good agreement with experimental results.

V-J-1 Structure Analysis of Chemical Gel Using Monte Carlo Simulation

NOSAKA, Makoto; TAKASU, Masako

[*Trans. Mater. Res. Soc. Jpn.* **26**, 557 (2001)]

We studied the structure of gel using Monte Carlo simulation with modeled radical reactions. Simulation is performed using beads-spring model in three-dimensional continuous space. For the criterion of gel, we apply the concept of percolation to our clusters; we calculate the maximum size in all directions for each cluster, and sum up the number of percolated direction for all percolated clusters in a system. We call this the number of percolation. We obtained structure information of system from plotting the average number of percolation. We can determine whether the system has percolated clusters, and also whether the polymer network has inhomogeneous structure.

V-J-2 Characterization of Gel Using Modeled Radical Polymerization with Cross Linkers Performed by Monte Carlo Method

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[*J. Chem. Phys.* submitted]

In this study, some physical quantities for characterization of gel are proposed. Polymer networks (gel) are investigated by Monte Carlo simulation using modeled free-radical cross-linked polymerization in continuous system. The distributions of degree of polymerization for clusters obtained in this simulation show qualitatively good agreement with the experimental results. Linkers are classified to two types according to the roles in networks, and their ratios are discussed. The normal and weighted ratios of gel are defined using percolation theory. These ratios are compared with the changes in distribution.

V-J-3 Linear-Shaped Motion of DNA in Entangled Polymer Solutions under a Steady Field

NOGUCHI, Hiroshi; TAKASU, Masako

[*J. Phys. Soc. Jpn.* **69**, 3792 (2000)]

We studied the electrophoretic behavior of DNA chains in linear-polymer solutions using Brownian dynamics with an anisotropic friction tensor. We simulated the linear-shaped motion of DNA observed in highly entangled solutions (Ueda *et al.*) using a model with a chain segment equal to 1/4 of the persistence length. A linear conformation is seen for a chain with high segment-density regions, which remain at the same positions in space, with a high anisotropy of friction, while a U-shaped conformation is seen for a chain with a low anisotropy of friction.

V-J-4 Dynamics of DNA in Entangled Polymer Solutions: An Anisotropic Friction Model

NOGUCHI, Hiroshi; TAKASU, Masako

[*J. Chem. Phys.* **114**, 7260 (2001)]

We studied the electrophoretic behavior of DNA chains in linear-polymer solutions using Brownian dynamics with an anisotropic friction model in a three-dimensional space and projected on x-axis. For the three-dimensional model with a chain segment equal to 1/8 of the Kuhn length, a chain migrates with U-shaped conformation with low anisotropy of friction. With high anisotropy of friction, a chain always migrates with linear-shaped conformation with high segment-density regions, which remain at the same positions in space. This migration mode agrees with the observation of DNA in highly entangled solutions. [Ueda *et al.*] The projection model also reproduces the linear-shaped motion. We clarified that the essential conditions for linear shaped motion are the sufficient chain length of DNA, the small mesh size, and strong confinement by entanglement with solvent polymers.

V-J-5 Eelectrophoretic Behavior of Polyelectrolytes in Gel and Polymer Solutions

NOGUCHI, Hiroshi

[*Trans. Mater. Res. Soc. Jpn.* **26**, 687 (2001)]

Electrophoresis using gel and uncrosslinked polymer solutions is widely used to separate DNA chains by chain length. We studied the electrophoretic behavior of chains using Brownian dynamics with an anisotropic friction tensor. We show the anisotropic-friction model proposed by Curtiss and Bird is an effective method to describe dynamics of polyelectrolyte chains under an electric field in gel and polymer solutions. With a low anisotropy of friction (dilute polymer solutions), a chain fluctuates between elongated and compact states with no periodicity under a steady electric field. On the other hand,with a high anisotropy of friction (gel or entangled polymer solutions), a chain oscillates periodically: Polyelectrolyte chain is trapped by gel fibers with a U-

shaped conformation, stretches out, and re-acquires a compact conformation. The above results agree well with experiments on DNA electrophoresis.