Simulation Study of the Structure and Dynamics of Jungle-gym type Gel

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Abstract in Japanese: 化学ゲルのモデルを作成し、ブラウニアンダイナミクスを用いたシミュレーションを行った。角度ポテンシャルの大きさの異なる2種類のゲルの構造とダイナミクスを比較して議論した。

1. Introduction

Chemical gels[1] are important material, used, for example, in contact glass and artificial muscle.[2] Furukawa et al. studied jungle-gym type gels by scanning microscopic light scattering method (SMILS) [3,4]. We perform simulation to investigate the structure and dynamical properties of jungle-gym type gels. We define order parameters and compare two types of gels, hard gels and soft gels.

2. Model and Method

To construct gel structure, we started with two types of units, D and T, representing dimmer and triangular units. The Lennard-Jones type potential is assumed between D and T, and the repulsive potential is assumed between D and D, or T and T. We compare two types of gel: one with strong angle potential (hard gel) and the other without angle potential (soft gel).

We performed Brownian dynamics simulation[5,6,7] with these models. The crosslinking occurs when the units D and T are within certain distance.

3. Results and Discussion

We define two local parameters χ_1 and χ_2. χ_1 is the average of the inner products of normal vectors of two triangular units T. χ_2 is the average of the inner products of the normal vector of T and the bond vector of D.

The time dependence of the number of units of the largest cluster is shown in Fig. 1, (a) and (b). The soft gel shows faster clustering than the hard gel. The fluctuation of quantities χ_1 and χ_2 is much larger for hard gel than for soft gel.

In Fig. 2, the radial distribution for two types of gel is shown. The soft gel shows more compact structure. The void structure was also analyzed for the two types of gels.

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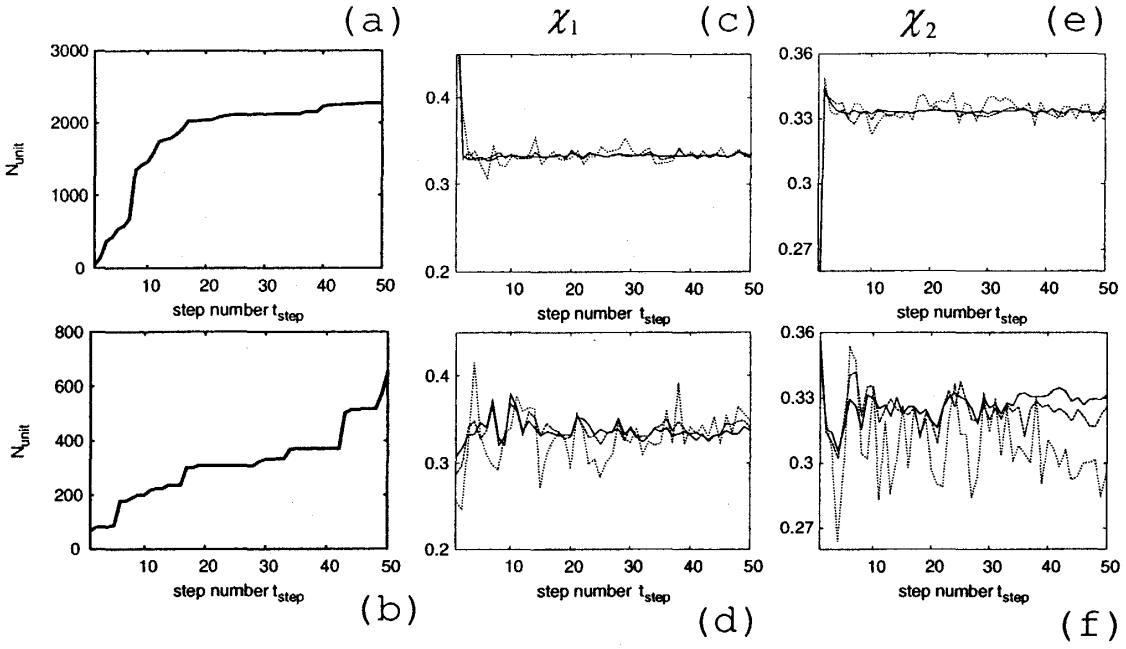

Fig. 1 The time dependence of number of units in the largest cluster (a, b), χ_1 (c,d) and χ_2 (e,f). (a), (c), (e) are for soft gel, and (b), (d) and (f) are for hard gel. In (c), (d), (e) and (f), the solid line is calculated for all pairs of monomers, and the dotted line is for pairs of monomers which are within the distance L/5, where L is the system size.

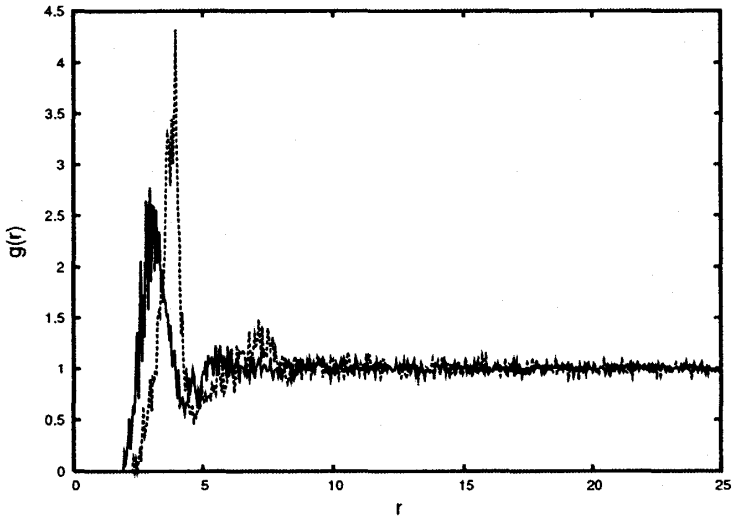

Fig. 2 Radial distribution function of crosslinking points for soft gel (solid line) and hard gel (dotted line).

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