Monte Carlo Simulation of Gelation under External Field

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We are promoting crystal growths using a gel prepared under a magnetic field as a medium. Whereas nano crystallites did not oriented if the gel was prepared without magnetic field, crystallites are aligned in the gel prepared under a magnetic field. This may reflect the anisotropic structure of the gel network.

We performed Monte Carlo simulations of geltaion under an external field using a model described in ref. 1). The system consists of radicals, monomers, and linkers. Interparticle interactions are the Lennard-Jones (LJ) potential $\varepsilon\left[\left(l_0/r\right)^{12}-2\left(l_0/r\right)^{6}\right]$, harmonic spring potential $C_s\varepsilon\left(r-l_0\right)^2/l_0^2-J$, and inverse twelfth power potential $\varepsilon\left(l_0/r\right)^{12}$ for, respectively, between active pairs, bonded pairs, and others. An active particle is a radical, active monomer, or active one of particles forming a linker. Bond can form between active particles; change of particle species is accompanied. For simplicity, we consider the interaction between the external field (*z* direction) and a bond of the form $-H\cos^2\theta$, where H is the strength of the field and θ indicates the angle between the field and the bond.

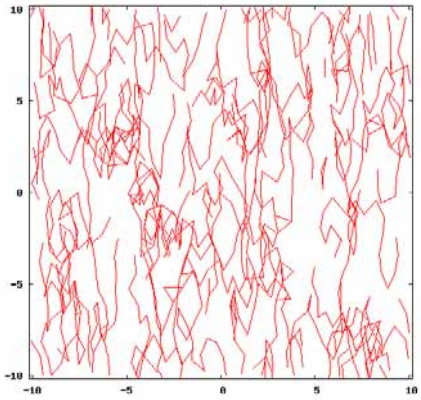

Fig. 1: Snapshot projected on to *xz* plane for $H=9\varepsilon$.

Figure 1 is a side view (*xz* view) for $H=9\varepsilon$. Initially $N_r=63$ radicals, $N_m=86$ monomers, and $N_l=87$ linkers were placed in a cubic box of the side length $L=20l_0$ with the periodic boundary condition. We set $\varepsilon/k_BT=0.3$, $C_s=2000$, and $J=9k_BT$. This figure shows that the bonds prefer to align parallel to the field. We performed box counting for bonds using boxes of right-angle parallelepiped with square cross section. The results depend on the box shape, indicating the anisotropy of the gel network. Corresponding to the decrease of the number of bonds perpendicular to the field due to energy cost the pore size also increase with the increase of H.

1) M. Nosaka, M. Takasu, and K. Katoh, J. Chem. Phys. **115** (2001) 11333.

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