

Monte Carlo simulation of interacting liquid crystal and substrate using rigid model molecules

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Abstract

In the present study, we propose MC simulation that takes interface phenomena between liquid crystal and substrate into consideration. We use rigid model molecules of liquid crystal and substrate. Interface is generated using potential field that induces decomposition of molecules.

1. Introduction

Alignment of liquid crystal molecules around substrate is a key factor for development of liquid crystal display. However molecular mechanism of alignment of liquid crystal on substrate is not well understood. Experimentally there are both cases of increase and decrease of nematic order around substrate[1,2]. Preferential alignment of molecules was examined by using near-edge X-ray absorption analysis[3]. These phenomena have not been yet examined by theory and simulation.

In this study we propose Monte Carlo simulation to examine interface phenomena between liquid crystal and substrate using hard repulsive model molecules. There are several types of hard repulsive molecules that express liquid crystal phases. Hard ellipsoids of revolution shows nematic phase, hard cut-spheres show nematic and columnar phases, and hard spherocylinders show nematic and smectic phases.

We use two types of hard spherocylinders of different length as liquid crystal molecules and substrate molecules. Longer spherocylinders are liquid crystal molecules and shorter substrate molecules.

2. Simulation

Our models for liquid crystal molecules and substrate molecules are hard spherocylinders. Spherocylinder is a cylinder each end of which is capped with a hemisphere. Fig. 1 shows present model molecules.

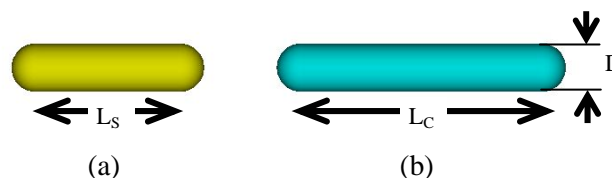


Fig.1 (a) Model molecule for substrate. (b) Model molecule for liquid crystal.

Diameters of substrate molecules and liquid crystal molecules are the same as indicated by D in Fig. 1. Lengths L_s and L_c , respectively, of substrate molecule and liquid crystal molecule are set as $L_s/D=3$ and $L_c/D=5$ for the present study. We assume that the substrate molecules to be rod-like for that they have molecular force to align liquid crystal molecules.

Hard repulsive molecules of different shapes show spontaneous decomposition depending on their shapes[4,5]. However it is not realistic to consider that such decomposition automatically forms substrate desired for simulation study. In this study, in order to form interface between substrate and liquid crystal, we introduce potential field that prefer to separate different molecules.

We consider rectangular simulation box that obeys

periodic boundary conditions along x-, y- and z-direction. Size of the box fluctuates in isobaric Monte Carlo simulation.

We introduce two potential boundary planes that are perpendicular to z-direction. Position of one of the planes are set as $z=0$. Position of the other plane is adjustable in the simulation and we demote it as $z=B$. The planes divides the simulation box into two regions a and b . The a is region of $0 < z < B$ and b of the other case for $B > 0$. There are two regions due to the periodic boundary conditions. For the case of $B < 0$, on the other hand, the region b is of $B < z < 0$, and the region a for the other case. We denote positional potential energy of each substrate molecule in the region a (b) by ϵ_{aS} (ϵ_{bS}). For liquid crystal molecules we denote them by ϵ_{aC} (ϵ_{bC}). In order to decompose substrate molecules into region a and liquid crystal molecules into region b , we set $\epsilon_{aS} < \epsilon_{bS}$ and $\epsilon_{aC} > \epsilon_{bC}$.

3. Results and discussion

The values for positional potential we used in the present calculation was $\epsilon_{aS} = 0$, $\epsilon_{bS} = 100k_B T$, $\epsilon_{aC} = 100k_B T$ and $\epsilon_{bC} = 0$, where T is temperature, and k_B the Boltzman constant. Equilibration was made at pressure p giving normalized value $pD^3/(k_B T) = 1.3$. Fig. 2 is an obtained snapshot of the simulation for 600 substrate and 1200 liquid crystal molecules. Fig. 3 shows distribution of nematic order parameter S of liquid crystal molecules.

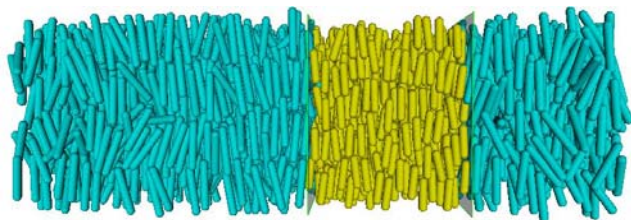


Fig. 2. Snapshot of simulation.

Fig. 3 shows a region in which order parameter disappear around $z=0$. This region corresponds to region a where liquid crystal molecules are excluded by the decomposition potential. Our present results do not show significant difference between bulk order parameter and surface order parameter. We expect that this is because bulk order parameter is about 0.8 which is remarkably higher than typical value of actual liquid crystal.

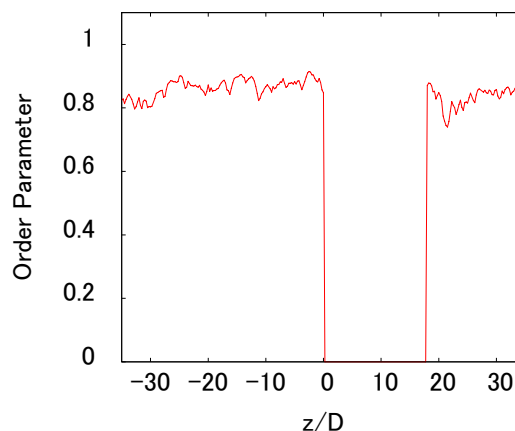


Fig. 3 Distribution of nematic order parameter along z direction.

4. Summary

We have proposed a simulation that construct artificial interface in Monte Carlo simulation scheme. The work have been just started. Examination with various simulation conditions are now going on.

5. References

1. S.-K. Hong, H. Kikuchi and T. Kajiyama, *Polym. J.* **31**(1999)160.
2. L. Xuan, T. Tohyama, T. Miyashita and T. Uchida, *J. Appl. Phys.* **96**(2004)1953.
3. J. Stohr, M. G. Samant, A. Cossy-Favre, J. Daiz, Y. Momoi, S. Odahara and T. Nagata, *Macromolecules*, **31**(1998)1942.
4. T. Koda, M. Numajiri and S. Ikeda, *J. Phys. Soc. Jpn.* **65**(1996)3551.
5. T. Koda and H. Kimura, *J. Phys. Soc. Jpn.* **63**(1994)984.