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Monte Carlo Simulation of Interacting Liquid Crystal and Substrate using Rigid Model Molecules

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Abstract

In the present study, we propose Monte Carlo simulation that takes into consideration the interface phenomena between liquid crystal and substrate. We use rigid model molecules of liquid crystal and substrate. Interface is generated using potential field that induces decomposition of molecules. We use hard spherocylinders as model liquid crystal molecules. Substrate is modeled as region composed of shorter spherocylinders. Our results show that there is a case in which nematic order is reinforced in the vicinity of rubbed substrate.

Keywords : Monte Carlo simulation, Nematic phase, Interface, Substrate

1. Introduction

Base structure of liquid crystal display (LCD) consists of liquid crystal material between rubbed substrates. Alignment of liquid crystal molecules around the substrate is hence an important consideration in the development of LCD. However, the molecular mechanism in connection with the alignment of liquid crystal on substrate is not well understood. There are cases of both 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]. There has not been sufficient examination on these phenomena, from either a theoretical and simulation point of view.

In this study, we propose a 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[4,5], hard cutspheres show nematic and columnar phases, and hard spherocylinders show nematic and smectic phases[6,7].

We used hard spherocylinders as model liquid crystal molecules. The substrate was modeled as region composed of shorter spherocylinders. Using square well, spacial potential, interface of substrate and liquid crystal was generated in a simulation box.

2. Simulation

Fig. 1 shows the shapes of the present model molecules. These are categorized as spherocylinders. Spherocylinder is a cylnder each end of which is capped with a hemisphere. It is characterized by diameter D and aspect ratio L/D where L is length of cylinder part. We denote the length of substrate spherocylinders as L_s and liquid crystal spherocylinders as L_c. The diameter of each and every molecule is the same, and denoted by D for the present case. We set $L_c/D=5$ for liquid crystal molecule and $L_s/D = 3$ for substrate molecules. Alignment of cylinder shape of substrate molecules was considered to examine in-plane anisotropy that could be imposed for substrate by alignment method such as rubbing process.

We set total energy H of the system to be

$$H = \sum_{j<k} \phi_{jk} + \sum_{j} \left[\psi_j - \frac{3}{2} h_j (\mathbf{u} \cdot \mathbf{n}_j)^2 \right], \quad (1)$$

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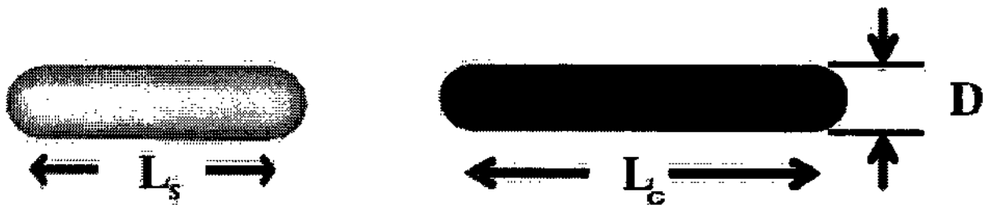

Fig. 1. Model molecules of substrate molecule (a) and liquid crystal molecule (b).

where ϕ_{jk} is the repulsive hard core potential between j-th and k-th molecules, u is a unit vector indicating direction of alignment field, n_j is direction of j-th molecule, h_j is strength of alignment field, and ψ_j is position dependent potential for j-th molecule. The repulsive hard core potential is defined by

$$\phi_{jk}\begin{cases}\infty, & \text{if j-th and k-th molecules intersect,}\\ 0, & \text{otherwise.}\end{cases} \tag{2}$$

This eliminates the intersection of molecules from molecular configuration. The role of the aspect ratios of two molecules appears in Hamiltonian through Eq. (2). In the simulation, we have coordinates that describe molecular positions and orientations. Update of these coordinates are performed by random number generation. A configuration that contains molecular overlapping expressed by infinite energy in Eq. (2) is cancelled in the update process.

The ψ_j of Eq. (1) is introduced to generate substrate region and liquid crystal region in the simulation system of hard core molecules. It is a square well potential depending on molecular type and position. In order to set the normal of interface plane along the z-direction in a Cartesian coordinate system, as expressed by Fig. 2, we divide the simulation box into two regions along the z-direction, regions **S** and **B** as shown in Fig. 2. The j-th molecule is in region **S** when z_j the z-component of center of j-th molecule satisfies $0 \le z_j < Z_B$, where z=0 is a fixed boundary and $z=Z_B$ is an adjustable boundary between regions **S** and **B**. Two regions denoted by **B** in Fig. 2 are connected by the periodic boundary condition of the simulation box. We denote the temperature and Boltzmann constant, respectively, as T and k_B the in order to construct the substrate in region **S**, the square well potential is set as

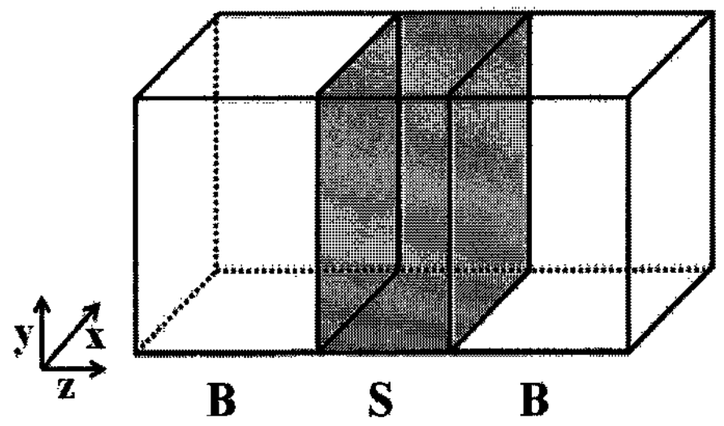

Fig. 2. Division of system into substrate region **S** and liquid crystal region **B**.

$$\Psi_j=\begin{cases}-100k_BT, & \text{for } 0 \le z_j < Z_B\\ 0, & \text{otherwise,}\end{cases} \tag{3}$$

if j-th molecule is a substrate molecule, and

$$\Psi_j=\begin{cases}0, & \text{for } 0 \le z_j < Z_B,\\ -100k_BT, & \text{otherwise,}\end{cases} \tag{4}$$

if j-th molecule is a liquid crystal molecule. The Z_B fluctuates during simulation due to the Metropolis trial scheme.

The h_j of Eq. (1) is introduced to control the alignment of substrate molecules and initial direction of liquid crystal molecules. The Monte Carlo simulation scheme use is an isobaric Metropolis method with normalized pressure p^* which is defined as $p^* = p/(k_BT)$, where p is actual pressure.

The effect of aligned substrate molecules on interfacing liquid crystal molecules in homogeneous alignment was examined with 400 substrate molecule of $L_s/D = 3$ and 1400 liquid crystal molecules of $L_c/D = 5$. The pressure was set as p^*=1.3. A previous study done on the bulk system of hard spherocylinder of $L_c/D = 5$ by Jackson's group indicates that $p^* = 1.3$ is in the nematic phase[6]. Initial alignment was generated by setting $h_j/(k_BT)$ =10 for all the molecules with **u** along y-direction which is along the interface plane. Relaxation of the molecular configuration was performed with $h_j/(k_BT)$ =10 for substrate molecules and $h_j/(k_BT) = 0$ for liquid crystal molecules.

Aspect ratio of liquid crystal molecules $L_c/D = 5$ is selected, because it is one of the most widely studied cases[6,7,8]. Sphecocylinders longer than $L_c/D = 5$ take similar phase sequence as that of $L_c/D = 5$.

The other parameters for the present preliminal study were tentatively determined. We consider that intrinsic ability of substrate molecules to align molecules is weaker than that of liquid crystal molecules themselvs. However it should be anisotropic in order to induce anisotropy of substrate. Hence we use modeling of substrate by spherocylinders by setting $L_s/D = 3$ which is smaller than $L_c/D = 5$ of liquid crystal molecules. We set ψ_j=-100k_BT in order to obtain well defined decomposition between substrate molecules and liquid crystal molecules. The value $h_j/(k_BT)$ =10 is given tentatively to induce alignment of substrate molecules.

3. Results and discussion

Fig. 3 shows the equilibrium snapshot of the present simulation. The snapshot shows the position potential field h_j works effectively in decomposing the substrate molecules and liquid crystal molecules. Region of aligned substrate cylinders are centered in simulation box. It is put between regions of liquid crystal molecules. Liquid crystal regions are connected with the periodic boundary condition along z-direction of the simulation box. Fig. 3 shows a typical snapshot of unit cell of periodic boundary. Fig. 3 shows the typical size of the present simulation box that is divided into liquid crystal region and substrate region.

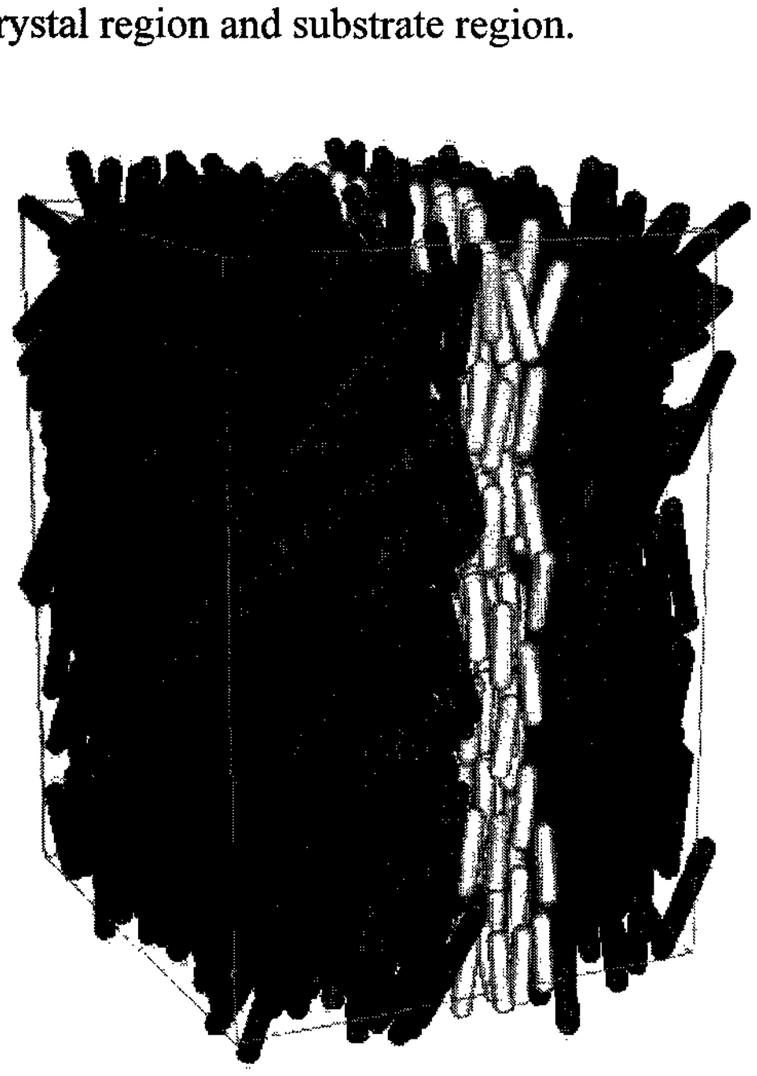

Fig. 3. A snapshot of an equilibrium structure obtained by present simulation. Upper direction is y-direction. Shaded molecules are liquid crystal molecules. White molecules are substrate molecules. Interface plane is along xy-plane and perpendicular to z-axis.

In Fig. 4, we show the averaged distribution of order parameter and density in terms of z-component of position. The unit of position in Fig. 4 is diameter D of cylinders. We can estimate D to be ~ 0.5 nm for real liquid crystal molecules.

Fig. 4 shows that, for the present case, the nematic order parameter increases near the interface, while the experimental results show cases of both increase[1] and decrease[1, 2]. The effect of the condition of substrate anisotropy that is controlled by parameters L_s/D and h_j on the interfacial phenomena should be examined in the future in order to make sure whether our model can also express the decreasing case or not.

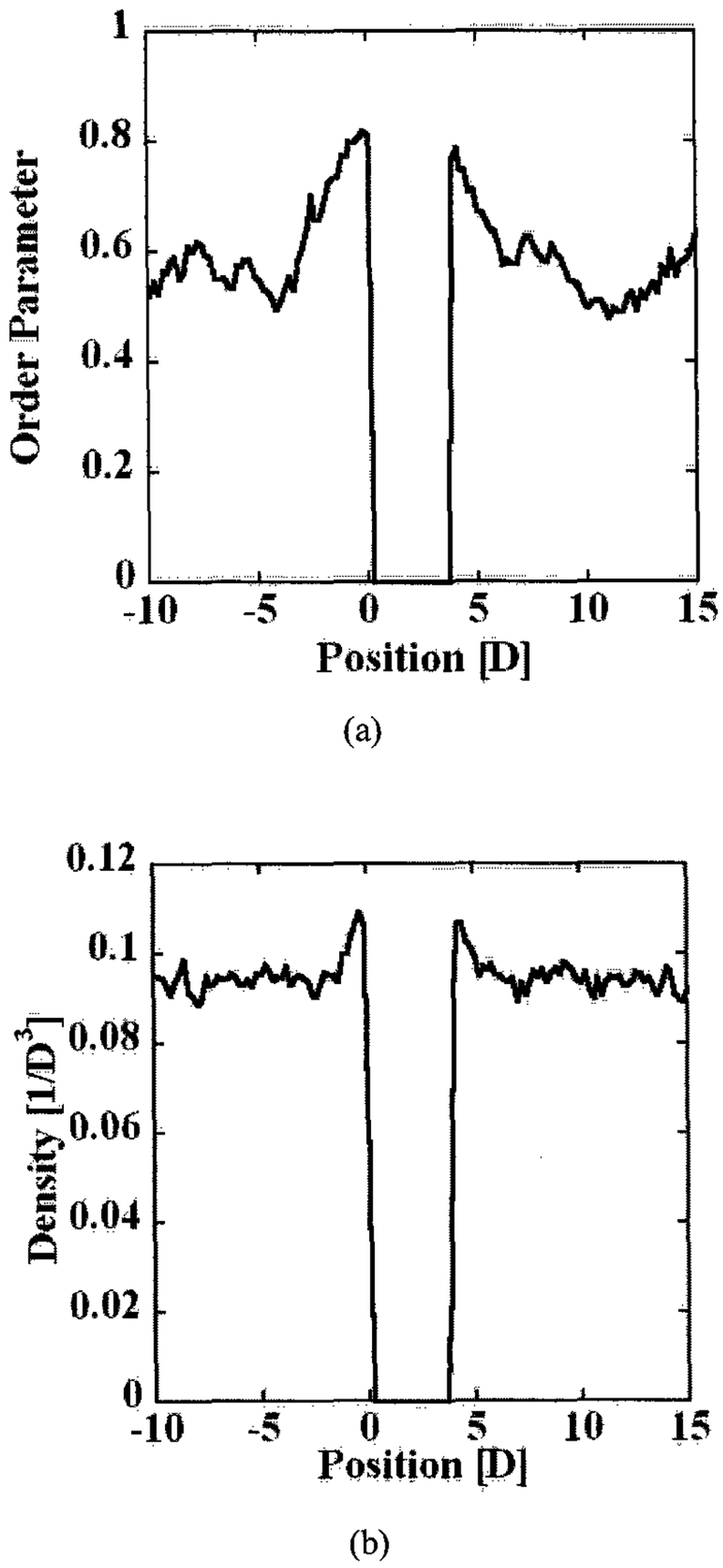

Fig. 4. Average of (a) nematic order parameter and (b) number density of centers of liquid crystal molecules as a function of position along z-direction which is perpendicular to interface plane. Resion with zero values corresponds to the substrate region.

4. Summary

We proposed a molecular simulation method to examine interfacial phenomena of liquid crystal molecules around a rubbed substrate. This method uses simplified model molecules with an artificial potential for generating interface. It is important to note that by using this potential, we can examine interfacial phenomena of liquid crystals. Our simulation has just begun and thus the results are still preliminary results. More detailed simulation is needed and now on progress for further discussions.

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