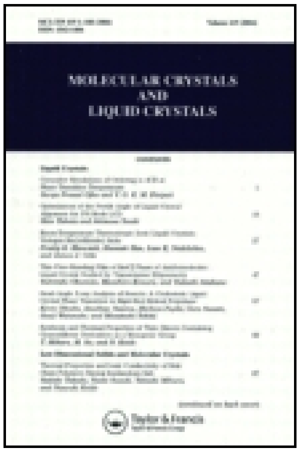

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# Computer Simulation on Liquid Crystal Order in Cell with Alignment Surfaces

Shoichi Kondo [a] & Isamu Ono [a]

[a] Department of Chemistry, Faculty of Science, Science University of Tokyo, Kagurazaka 1-3, Shinjuku-ku, Tokyo, 162 0825, JAPAN

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# Computer Simulation on Liquid Crystal Order in Cell with Alignment Surfaces

SHOICHI KONDO and ISAMU ONO
Department of Chemistry, Faculty of Science, Science University of Tokyo,
Kagurazaka 1-3, Shinjuku-ku, Tokyo 162 0825, JAPAN

Monte Carlo simulation based on the Luckhurst-Romano potential has been performed to evaluate the ordering property of liquid crystals in a cell with aligned surfaces. The transition temperature from the nematic to the isotropic phase is the same as that of the bulk system, but the high ordering state is induced near the surface around the transition. In addition, the direction of ordering can be regulated by the ordered particle on the surface. The effect of the alignment surface on the liquid crystal order in the nematic and isotropic phases is estimated by changing the number of alignment particles on the surface.

Keywords: Monte Carlo simulation; Luckhurst-Romano potential; surface; nematic phase; order parameter

## INTRODUCTION

Molecules in liquid crystal phases are aligned by their own anisotropy of the molecular shape or the intermolecular interaction. The direction of orientation is controlled by an external field or by rubbing surfaces of a cell. The effect of the rubbed surface on the ordering properties of liquid crystals is particularly important in the development of the liquid crystal display. In recent years, the alignment surface not only orients the liquid crystal molecules but also changes the direction of the liquid crystalline order. In the latter case, the photo-chromic molecules are bounded to the solid surface of a cell[1]. It has been known that the *trans-cis* photoisomerization or the reorientation of the photo-chromic molecules is induced by the irradiation of UV or linearly polarized light, and consequently the liquid crystal molecules are reoriented. Thus, the photo-chromic molecules regulate the direction of the liquid crystal order and their molecules on the surface contribute greatly to the ordering property of the liquid crystals. It is interesting to evaluate the effect of the alignment surface in the cell on the ordering properties of the liquid crystals and to evaluate the microscopic interaction between the surface of cell and liquid crystalline molecules.

Recently, computer simulations have been applied to the system including a solid surface. On these simulations, it is necessary to set enough thickness of the simulation cell in which the ordering property in the center is similar to that in the bulk with the three dimensional periodic boundary condition. But it is difficult to keep such thickness using the Gay-Berne potential or the atom based potential for lack of the ability of a computer. Therefore, simulations have merely been reported on a pore[2] or on the system neglected the bulk-like liquid crystals[3].

Our purpose of this work is to simulate the behavior of bulk-like liquid crystals in the cell with the alignment surface, and to evaluate the effect of the alignment surface on the liquid crystal order. We set a simple model based on a Luckhurst-Romano(LR) potential[4]. It is able to estimate the ordering of the bulk-like liquid crystal and the molecular order depending on the alignment surface using the LR potential with an anisotropic interaction.

However, the simulation using the potential without the molecular shape anisotropy is impossible to discuss directly the ordering behavior of the surface. The simulation model employed and the results of spatial order in the cell are described in this paper.

## SIMULATION MODEL

In the LR potential[4], the inter-particle energy between the particles $i$ and $j$,

$$U_{ij}(r_{ij},\theta_{ij}) = 4\varepsilon\left\{\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right\} - 4\varepsilon\lambda\left\{\left(\frac{\sigma}{r_{ij}}\right)^{12} + \left(\frac{\sigma}{r_{ij}}\right)^{6}\right\} P_2\left(\cos\theta_{ij}\right) \qquad (1)$$

is expressed as a function of a distance $r_{ij}$ and an angle $\theta_{ij}$. The first and second terms are the isotropic and anisotropic terms, respectively. The reported value of 0.15 is used for the constant $\lambda$[4]. Fig.1 shows the reduced temperature and density dependencies of the order parameter $S$ calculated by the Monte Carlo simulation using the LR potential for the bulk system with the three dimensional periodic boundary condition. For each density, the isotropic phase with the low value of $S$ is found at higher temperatures, and the nematic phase with the high order is formed at lower temperatures. The behavior of the order parameter exhibits a transition for all systems simulated.

On account of the exclusion of the shape anisotropy in the LR potential, it is appropriate to regard a particle not as a single molecule but as an ordered cluster consisted of some liquid crystal molecules. As shown in Fig.2A, clusters (particles) of 64 were placed to the down side of the cell, and their directions were fixed. These were assumed to fix on the alignment surface, and named aligned clusters (AC). The AC of 64 was also placed on the upside surface. For the inner part of the cell, liquid crystal clusters (LC), whose positions and angles were not fixed in the simulation, were arranged with face-centered cubic and in random direction for the initial configuration as shown in Fig.2B. The number of the LC was decided to be 1152 from the result of preliminary calculations[5]. The value of density $\rho^*$ ($=N/V^*$) used was 0.9 where $N$ is the number of clusters and $V^*$ is the scaled volume. The Monte Carlo simulation was carried out with the two dimensional (x and y) periodic boundary condition.

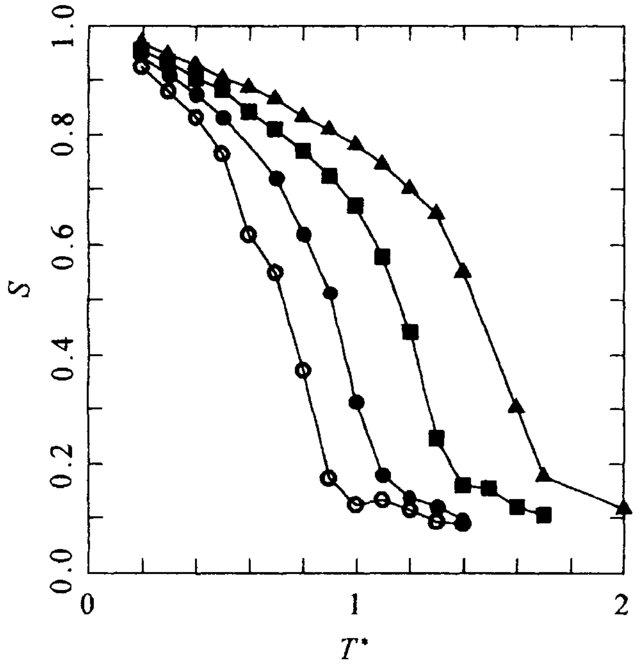

FIGURE 1 Plots of the order parameter $S$ vs. the reduced temperature $T^*$. ▲: $\rho^*$=1.0, ■: $\rho^*$=0.9, ●: $\rho^*$=0.8, ○:$\rho^*$=0.7.

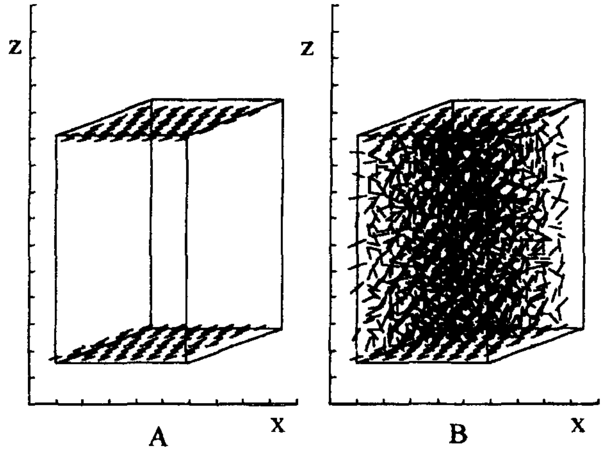

FIGURE 2 (A) Two AC layers and (B) the initial configuration.

## RESULTS AND DISCUSSION

The order correlation parameter $\eta$ is defined to evaluate the correlation between the direction of the LC and that of the AC.

$$\eta = \frac{1}{2}\left\langle 3(\vec{u}_{\mathrm{AC}} \cdot \vec{u}_{\mathrm{LC}})^2 - 1 \right\rangle \tag{2}$$

Fig.3 shows the plots of $\eta$ for the LC vs. the vertical distance, $z^*$ between the LC and the AC layer. At a reduced temperature $T^*$of 1.0 (nematic phase), the value of $\eta$ is kept constant ca. 0.65 corresponding to the order parameter for the bulk and is independent of $z^*$. Such an orientation is also induced by changing the direction of AC from z axis to x or y axis. The findings confirm that the orientation of the LC can be controlled by the direction of the AC, but the AC is unable to produce higher an order state than the bulk.

On the other hand, at $T^*$ of 1.6 corresponding to the isotropic phase of bulk a high order state is induced within $z^* \leq 3$. The increased order correlation parameter $\eta$ near the layer is apparently caused by the AC. But the averaged order parameter in the whole cell is ca. 0.1 to be the same value in the isotropic phase of the bulk, in keeping with the finite size of the system.

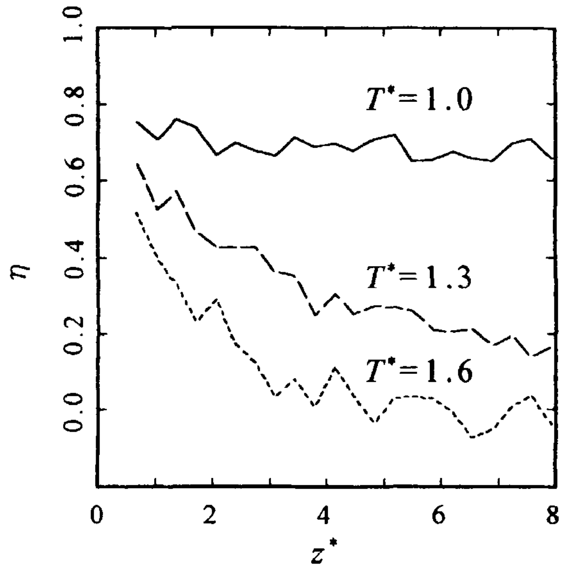

FIGURE 3 Plots of the order correlation parameter $\eta$ vs. the vertical distance $z^*$. (AC-layer corresponds to $z^*=0$.)

Fig.4 shows temperature dependencies of the order parameter $S$ (closed circles) and the averaged order correlation parameter $<\eta>$ in $z^* \leq 3$ for the AC/LC system (triangles), and also the order parameter for the bulk system (open circles). At all temperatures, the order parameter of the AC/LC system agrees closely with that of the bulk. The results imply that the system has a sufficient thickness to estimate the order parameter in the center part. At the temperatures just above the transition, values of $<\eta>$ are much larger than the order parameters for the bulk and then the difference between $<\eta>$ and $S$ tends to decrease with increasing temperature in the isotropic phase. This phenomenon is not found in the nematic phase. The results indicate that the high order of the LC near the AC layer is induced along the direction of the AC alignment especially after the transition from the nematic to the isotropic phase.

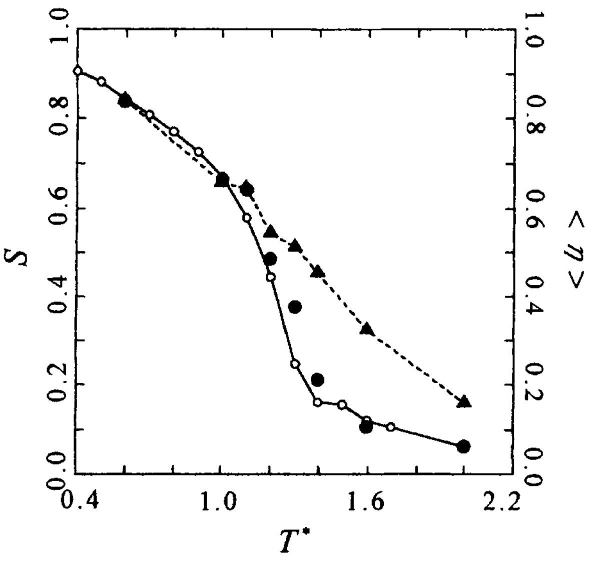

FIGURE 4 Temperature dependence of $S$ (closed circles) and $<\eta>$ ($z* \leq 3$, triangles) for the AC/LC system, and $S$ for the bulk system (open circles).

The induction of the highly ordered nature just after the transition in the isotropic phase would be depended on ordering states of the AC layer. Next, we performed the simulation with decreasing the number of the AC, in order to evaluate the influence of AC-number on the ordering property of the LC. The layer of a surface was composed of two kinds of particles; the AC to be fixed in both position and direction, the other particles to be fixed in position only. The number of the AC, $N_{\mathrm{AC}}$ in a layer was changed from 1 to 64.

Another AC layer was set in a similar manner as above.

Fig.5 shows the plots of $\eta$ vs. $z^*$ at $T^*$of 1.6 (isotropic phase). The high ordering near the AC layer depends on the number of the AC, and the $\eta$ of the LC nearest to the AC layer increases in proportion to $N_{AC}$.

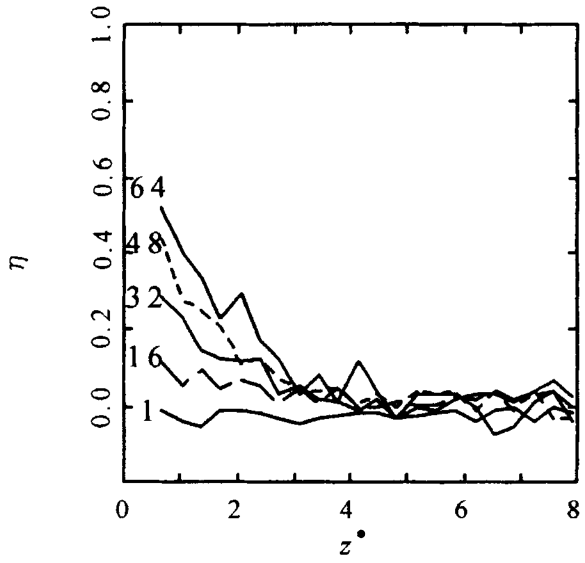

FIGURE 5 Plots of the order correlation parameter $\eta$ vs. the vertical distance $z^*$ at $T^*$=1.6 ($N_{AC}$=1-64).

In the nematic phase of $T^*$ of 1.2, the value of the order parameter in the whole cell are found to be ca.0.5 despite of the value of $N_{AC}$ as shown in Fig.6. In the case of $N_{AC}< 8$, the value of $< \eta >$ is significantly smaller than the order parameter. This is indeed, as we can see, that the direction of the LC is independent of that of the AC. In contrast, the direction of the LC is regulated by that of the AC in the case of $N_{AC} \geq 8$.

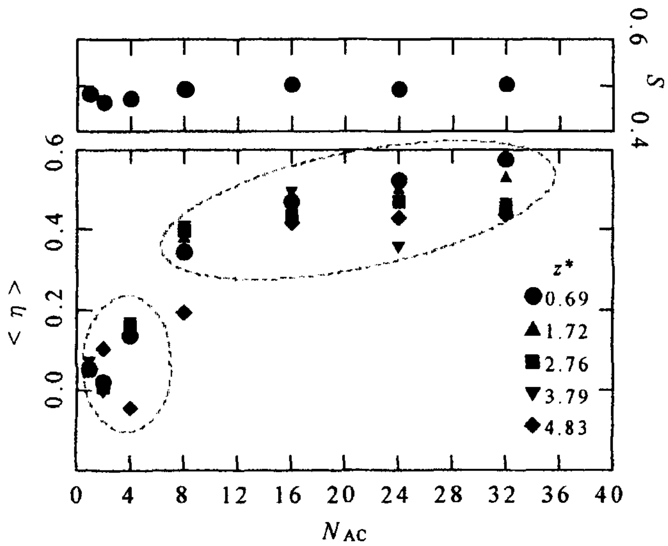

FIGURE 6 Plots of $S$ and $<\eta>$ vs. $N_{\mathrm{AC}}$ at $T^{*}=1.2$.

## CONCLUSIONS

The Monte Carlo simulations using Luckhurst-Romano(LR) potential have allowed us to evaluate the ordering properties in the cell with aligned surfaces, though the part of surface is highly approximated as a model. The order of liquid crystal molecules is governed by the aligned clusters on the surface. No influence of the AC on the transition temperature of the LC is found, but the director of the LC is regulated parallel to the direction of the AC. At the temperatures around the transition point, the AC induces the high ordering state for the LC near the AC layers. This induction in the orientational order increases proportionately with the number of the AC in the isotropic phase. The direction of the LC in the nematic phase depends on that of the AC in the case of $N_{\mathrm{AC}} \geq 8$ in a layer.

Consequently, we can not directly discuss the surface ordering, but the results are in qualitative agreement with the experimental results of so-called command surface system etc.

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