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Formation of Surface Stabilised Smectic Phases Driven by Electric Field under Homogeneous Anchoring

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By constant temperature molecular dynamics simulation of the Gay-Berne system sandwiched by homogeneous anchoring walls, formation of surface stabilised order with homeotropically anchored layers (SmAII) driven by the electric field is studied. The phase SmAII is shown to be stabilised even in the anisotropic homogeneous anchoring condition where SmAII is never observed without the field, while in case dipole-dipole is not neglected the layer of SmAII is destabilised and eventually a sort of smectic C phase appears.

Keywords: Gay-Berne model; electric field-dipole coupling; dipole-dipole interaction; homogeneous texture; surface stabilised smectic phase; symmetry breaking field for positional order

INTRODUCTION

Response of liquid crystalline phases to an electric field is not only quite important problem in the application fields to control the systems[1] but also interesting from fundamental point of view to understand the stability of the phases and order formation.[2] Recently, we have found a new phase at quite thin system by molecular dynamics simulation of Gay-Berne system,[3] which has homeotropically anchored layers in spite of homogeneous wall condition.[4,5] This phase (SmAII), appearing at the low temperature side of the homogeneously anchored smectic A phase (SmAI), is a surface stabilised one due to the symmetry breaking effect of the walls to the layer ordering.[4-6] Here, we study the order formation

of SmAII from SmAI driven by an electric field applied in the direction to stabilise SmAII under the condition where SmAI is stable without the field.

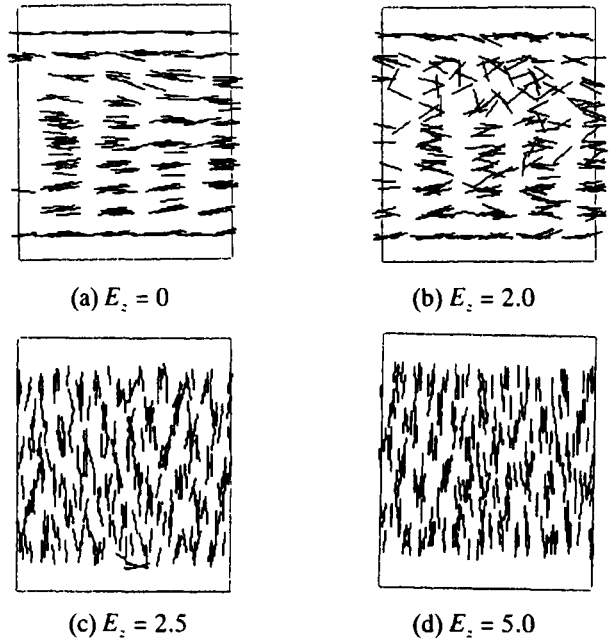
The system is composed of Gay-Berne molecules[7-10] with an electric dipole (unit strength) attached at the centre of mass in the direction of molecular long axis, put into a cell sandwiched by homogeneous anchoring walls. Two types of anchoring conditions, anisotropic in one case (y-anisotropic wall) and isotropic in the another (isotropic wall),[4,5] are tested, because SmAII is observed only under the latter type of anchoring condition.[4] In order to study the effect of the dipole-dipole interaction[11] to the ordering of the surface stabilised smectic phases, typical two cases, where such interaction is switched on/off, are simulated and the results for each wall condition are compared.

MODEL AND CONDITIONS OF SIMULATION

The system is composed of 256 Gay-Berne molecules with length of 3 times of diameter[7,8], and the simulation box is $9\times 9\times 9$ in the unit of molecular diameter with some additional space to take account of the excluded volume effect of walls in z-direction.[4] The walls are replaced by the imaged particles with which molecules interact with the same Gay-Berne potential. The centre of mass of the imaged particle is put on the wall, and the long axis of each particle is in y-direction (y-anisotropic wall), and in parallel direction to the projection of the accompanied molecule onto the wall (isotropic wall), respectively. Both of these walls correspond to the homogeneous anchoring. The periodic boundary condition is imposed at the xz- and yz-boundaries. In addition to Gay-Berne potential,[7,8] the dipole-dipole interaction V_{dd} (the parameter is taken to be 1.0 in the unit of energy parameter of Gay-Berne potential, ε_{GB}) and a coupling of the dipole to the external electric field in the z-axis, E_z, are taken into account. Because of the smallness of the size of the system, the interaction range of V_{dd} is so small effectively that we need no technique such as cut off. The parameters in the model are chosen after the work by Luckhurst *et al.*,[8] and values in the previous works[4,5] for anisotropic and well-depth parameters are utilised.

The molecules were first generated randomly in the simulation box and

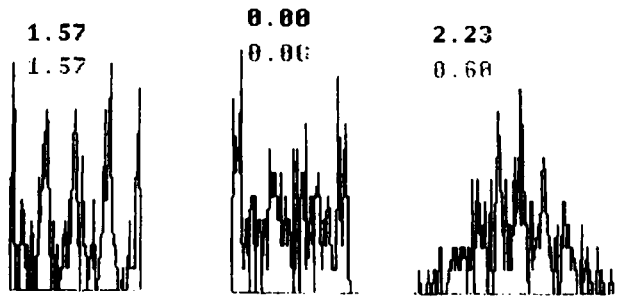
the temperature was lowered and the equation of motion was solved successively using Verlet algorithm[8] by 100000 time step, at which the system is assumed to reach the thermal equilibrium at that temperature.



(a) $E_z = 0$ (b) $E_z = 2.0$

(c) $E_z = 2.5$ (d) $E_z = 5.0$

FIGURE 1 Snapshot projected on yz plane (y-anisotropy).



(a) $E_z = 2.0$ (y) (b) $E_z = 5.0$ (z) (c) $E_z = 5.0$ (ln)

FIGURE 2 Positional distribution of molecules (y-anisotropy).

Next, the external field E_z (in the unit, ε_{GB}) was applied and the simulation was carried out up to 40000 time step and the data during the last 5000 step were picked up at that field strength. Then, E_z was raised and the same procedure was continued up to the field $E_z = 5.0$.

RESULTS OF SIMULATION

Y-Anisotropic Wall System

First, we show the results of the system with y-anisotropic wall. The simulations are carried out at the temperature $T = 0.2$, at which the system is in the smectic A phase (SmAI) with director in the y-axis as shown in Fig. 1(a). The highly ordered layer is due to the dipole-dipole interaction.[11-15] In this case the distribution of the sense of dipole is even in y-direction. The electric field is applied in the z-direction, and changes of the profiles of molecular configurations are shown in Fig. 1 for several values of the field strength E_z, in which we see the field induced phase transition between the fields 2.0 (b) and 2.5 (c) from SmAI to a phase with director in z-axis. The phases shown in (c) and (d) are qualitatively same, where we perceive a layer structure in a oblique direction. In Fig.2 the distributions of the centre of mass of molecules are shown along y-axis at $E_z = 2.0$ for (a), along z-axis (b) and along the direction of layer normal (ln) at $E_z = 5.0$ (the numbers shown at the top denote the polar and azimuthal angles of the layer normal, respectively), where four layers are observed distinctly in (a) while in (b) four layers are barely recognised. This means that SmAII is destabilised by the longitudinal displacement of molecules due to the aligned dipoles and eventually the ordering like smectic C phase (SmC) appears as shown clearly in (c), which agrees with the general observation that the longitudinal dipole stabilises SmC.[16] The layer spacing of (c) is about 3/5 times of the order of SmAII shown in (b) and layer tilts from the wall about 50 degree. Here, in Fig. 3 we show the result of the system without wall at $E_z = 5.0$, where two domains are observed to coexist, one of which similar to Fig. 1(d) remains because of the insufficiency of the simulation time. The layer spacing is common to both domains and same to the one in Fig. 1(d). Thus, the effect of walls as the symmetry breaking field to the layer ordering is shown in the high field region,

though the order observed in Fig. 1(d) and Fig. 2(b) is disturbed thoroughly. On the other hand in the bulk system, SmC is stabilised by V_{dd} as shown at the left domain in Fig. 3.

As V_{dd} destabilises SmAII, we study here the y-anisotropic wall system without V_{dd} to see precisely the effect of the symmetry breaking field of walls. This system corresponds to the one with quite small value of dipole moment, or the one with no dipole moment but with positive dielectric anisotropy in which the value of E_z used here is proportional to the square of the field in such system. The initial phase projected on yz-plane without E_z is shown in Fig. 4, which is considered to be SmAI, though it looks like some highly ordered smectic phase such as SmB.[8] The projection on xy-plane shows diverged profile with short range ordering. In general it is not easy to identify such highly ordered smectic phase at a small system like the present one. At the weak field region (E_z = 0.5, 1.0), the degree of layer order of SmAI is observed to be rather enhanced, because of probably the steric effect originated from the inclination of molecules (effectively the diameter is increased). The transition from SmAI to SmAII observed at E_z = 2.0, where the temporal change of molecular configuration is shown in Fig. 5. The final state within our computation step is SmAII with layer misconnection as shown in Fig. 5(d). Such misconnection is pinned by the periodic boundary condition.[5] If we carry out the simulation for sufficient time step, then SmAII free from the misconnection will be achieved. Here, we obtain such phase at larger field strength (E_z = 5) for the sake of saving the

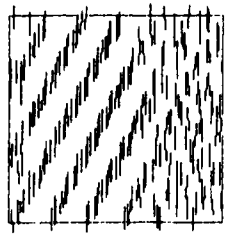


FIGURE 3 Snapshot on yz-plane (without wall, E_z = 5.0).

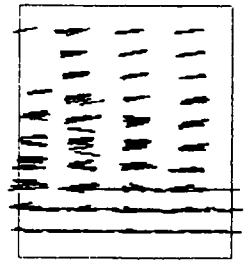
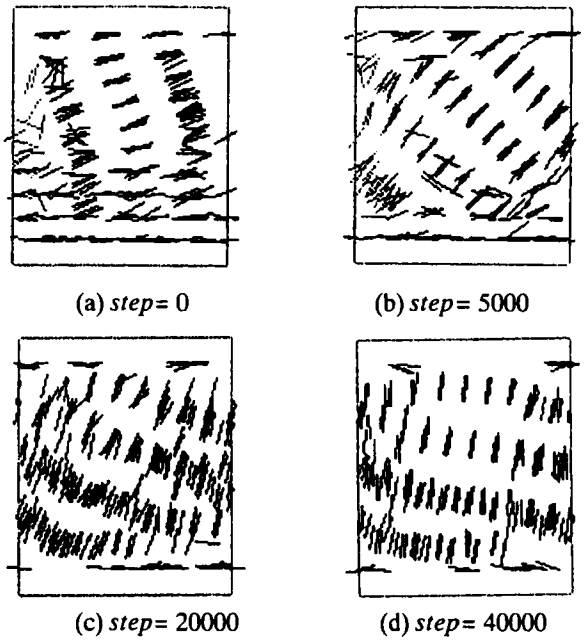


FIGURE 4 SmAI (y-anisotropy).

computation step, as shown in Fig. 6. From the above studies, SmAII stabilised by the walls is shown to be induced by the electric field even in the y-anisotropic wall system, where SmAII is not observed so far



(a) *step*= 0 (b) *step*= 5000

(c) *step*= 20000 (d) *step*= 40000

FIGURE 5 Order formation of SmAII from SmAI at $E_z = 2$. (y-anisotropic wall system with $V_{dd} = 0$).

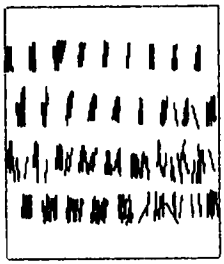


FIGURE 6 SmAII at $E_z = 5$ (y-anisotropic, $V_{dd} = 0$).

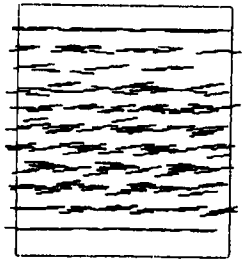
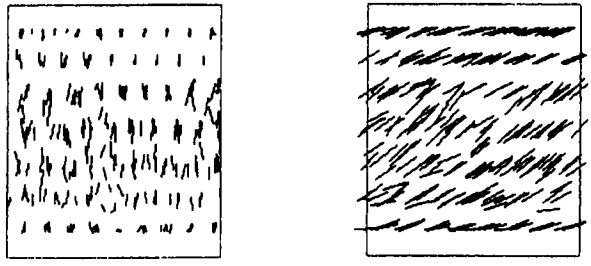


FIGURE 7 Initial state on yz plane (y-anisotropy).

without the field. Here it is noticed that the transition between SmAI and SmAII is the first order, because the directions of the layer normal of these phases make an right angle and one state is not possible to change continuously to the another one, even if the difference of the degree of ordering is neglected.

The transition from SmAI to SmAII is first order and the critical field is considered to be less than that obtained in the above. In the first place taking into account V_{dd}, the critical field is estimated about 2.3 which is fairly large, eventually the layer order is strongly disturbed due to the high alignment of dipole as shown in Fig. 1(c). Here we apply the strong electric field in the y-axis (E_y = 4) to destabilise the layer ordering of SmAI of the initial state as shown in Fig. 7, in which we see the strongly disturbed state not only with eleven layers in z-direction but also with something like a layer in oblique direction similar to the case of Fig. 1(d). Then, the field E_z is applied in place of E_y, and the simulation is carried out. A the field E_z = 1.0, a phase transition occurs as shown in Fig. 8 in which seven layers are found, and at E_z = 1.5 a phase with six layers is observed while the layers are more dispersed than those at E_z = 1.0. These phases are interpreted as the surface stabilised smectic C phase (SmCII), that is, at SmAII shown in Fig. 6 molecules tilt from layer normal due to V_{dd}. Because of the thinness of the system, these phases appear successively in a *quantized* manner. As E_z is increased, the tilt from z-axis decreases and the ordering of layer is lowered, and finally at strong field (E_z = 2.5 and 5.0) the phases similar to those in



(a) xz plane (b) yz plane

FIGURE 8 Projection of snapshot at E_z = 1.0 (y-anisotropy).

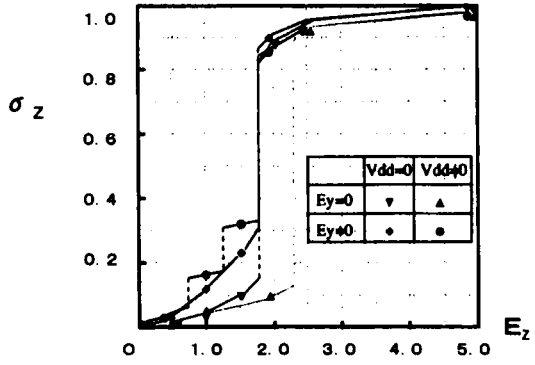


FIGURE 9 Response of the z-component of director to E_z at the y-anisotropic wall system.

Figs. 1(c) and (d) are achieved, which means that these are irrespective of initial states.

In case V_{dd} is vanishing, strong longitudinal field E_y stabilises SmAl. The simulation is also carried out from this initial condition. The response to E_z is similar to those starting from the state shown in Fig. 4, and no phenomenon essentially new is observed. In Fig. 9 dependences of zz-component of order parameter tensor on E_z are shown.

Isotropic Wall System

The simulation is carried out at the temperature $T = 1.0$, because SmAII isstable at $T = 0.2$ at this wall condition in the absence of V_{dd}.[4] Up to the field strength $E_z = 2.0$, SmAI looks like stable and any remarkable change is not observed due to the rather dispersed layer ordering of SmAI[4]. At the field $E_z = 2.5$, the phase transition occurs and SmAII appears, and at $E_z = 5.0$ the degree of the layer order is quite similar to the one in Fig. 6, showing the insensitivity to the order to wall property at this field strength.

In the system with non vanishing V_{dd}, the response of the system to E_z is similar to the case without V_{dd}, where the layer ordering is more dispersed than the former up to the field $E_z = 2.0$.

In the range of the present data, we can not find any qualitative differences between both systems with each walls because mainly of the strong layer fluctuation at the system with isotropic wall. In this respect the system with y-anisotropic wall is suitable for the present purpose.

SUMMARY

By constant temperature molecular dynamics simulations of polar Gay-Berne system, the formation of the surface stabilised smectic phase driven by the electric field is studied to clarify again the wall effect as the symmetry breaking field to the positional order of smectic layer. In the system without the dipole-dipole interaction, such phase (SmAII) is induced from homogeneously anchored smectic A phase (SmAI) by the electric field at the homogeneous anchoring walls, even in the y-anisotropic wall system in which SmAII is not observed without the field. Due to the effect of the dipole-dipole interaction the director tilts from the layer normal of SmAII and eventually the surface stabilised smectic C phase (SmCII) appear instead of SmAII. The tilt angle decreases as the field strength increases, and in the extremely thin system the number of layer changes quantized manner. At the strong field the layer of SmCII is destabilised and another kind of smectic C phase stabilised by the dipole-dipole interaction appears.

In the present study, systems with various conditions are tested, and by comparing data the above results are derived. Such method is considered to be effective to the study of phenomena accompanied by drastic changes such as the phase transitions, though the conclusions are qualitative as a matter of course. For quantitative study it is crucial to check whether the simulation time step is sufficient or not to get the thermal equilibrium. In the present simulation the electric field is elevated stepwise. If the phase at the final time step for some value of the field is metastable, the development to the stable phase is accerlated by elevated value of the field at the next step. In this respect, the shortness of the time step is compensated by the present method and the results are considered to be correct qualitaitively. As to the size of the system, we have studied the system with the same size to the present one[4] and with triple one,[5] where stability of SmAI and SmAII are certified in both

system. From these results, we can expect that the present results are no harmed by the smallness of the present system.

In the y-anisotropic system without the dipole-dipole interaction, the layer order of SmAI is observed to be slightly enhanced by the weak transverse field. While this phenomenon is conceptually quite interesting, final conclusion should be carried over into the following study, because quantitative study is required in nature.

The stability of phases anchored homeotropically is also interesting problem, which will be reported elsewhere in a near future.

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