

# Monte Carlo simulation of the interface between flexible polymers and low molecular liquid crystals

Junxiang Zhu<sup>a</sup>, Jiandong Ding<sup>a</sup>, Jianming Lu<sup>a</sup> and Yuliang Yang<sup>a,b,\*</sup>

<sup>a</sup>*Department of Macromolecular Science, Laboratory of Molecular Engineering of Polymers, Fudan University, Shanghai 200433, People's Republic of China*

<sup>b</sup>*Institute of Chemistry, Chinese Academy of Sciences, Beijing 100080, People's Republic of China*

(Received 15 October 1997; revised 18 November 1997; accepted 27 November 1997)

The lattice Monte Carlo (MC) simulation is performed to investigate the interface between flexible polymers and thermotropic low molecular liquid crystals (LCs), where the anisotropic attraction between nearest neighbour rods is described by the Lebwohl–Lasher nematogen model. The simulation outputs not only confirm some previous numerical calculations under mean-field assumptions, but can reveal some properties of the LC/polymer interface which are difficult to detect in experiment or predict in theory at the present time. The nematic ordering is found to enhance the driving force of the phase separation in the rod/coil mixture to a large extent, so that the LC/polymer interface is very narrow. The interface is sharpened and the interfacial tension is strengthened under one or some of the following conditions: enhancement of the anisotropic attraction between rods or of the isotropic repulsion between rods and coils, decrease of temperature and increase of chain length. © 1998 Published by Elsevier Science Ltd. All rights reserved.

(Keywords: interface; liquid crystal; lattice chain)

## INTRODUCTION

The interfaces existing widely in inhomogeneous materials influence the materials functions considerably. With the development of polymer alloys and other composite materials, it is much desired to establish the relationship between interfacial properties and macroscopic physical behaviours. Correspondingly, various composite systems have been investigated experimentally and theoretically during the last decades, such as the interface in the immiscible polymers<sup>1</sup>, microdomain structures in block copolymers<sup>2</sup>, the interface and interdiffusion between crystal and noncrystals<sup>3</sup>, the interface between saturated polymer solutions and solvents<sup>4</sup>, the interface between polymer melts and vacuum<sup>5</sup>. Most of the present studies touch on flexible molecules. In contrast, the studies on the interface in the mixture containing rigid molecules or a mesogenic component are rather scarce.

Polymer dispersed liquid crystal (PDLC), a prospective large-area electro-optical display materials is composed of flexible polymers and thermotropic low molecular liquid crystals (LCs)<sup>6–9</sup>. In PDLC films, nematic LCs are, in the form of microdroplets, embedded in a glass-state polymeric matrix. The droplet sizes are usually in the order of micron or submicron, which leads to a large amount of interfaces between anisotropic droplets and isotropic matrices. Those interfaces have strong effects on the director configurations of nematic droplets and then the properties of PDLC materials. For instance, they account for the faster electro-optical response of PDLC films compared to the conventional twisted nematic display devices<sup>6,7</sup>. Unfortunately,

the corresponding studies on LC/polymer interfaces are absolutely insufficient due to the difficulties in theoretical treatments and experimental observations. Kim *et al.*<sup>10</sup> carried out a wonderful paramagnetic resonance spin probe study on molecular motions and ordering of the interface in a PDLC film. The conclusion such as that the interface has little average order information is, however, rather limited, since this method is not straightforward to detect the interface. In fact, there is, at the present time, no experimental method to measure the concentration profile in the LC/polymer interface directly, mainly because the underlying interface is very sharp. In the previous paper of Fudan group<sup>11</sup>, the Helfand lattice theory about an inhomogeneous polymeric system<sup>4,12</sup> has been extended to deal with the LC/polymer interface, where the Lebwohl–Lasher (L–L) nematogen model<sup>13,14</sup> is employed to describe the nematic interaction between rods. The LC/polymer interface is found very narrow and the interfacial tension is increased with the decrease of temperature. However, the mean-field approximations are used and other assumptions such as infinitely long polymer chains are introduced in the theoretical treatment<sup>11</sup>. The validity of the mean-field theory about the LC/polymer interface remains to be checked. It is thus desired to perform a computer simulation, the third method between theory and experiment, to explore the LC/polymer interface. In this paper, a Monte Carlo (MC) simulation<sup>15,16</sup> is used to study the interface between flexible polymers and low molecular LCs on cubic lattices. The concentration profile of a polymer solution in anisotropic solvents can be obtained straightforwardly. Some fundamental properties of the LC/polymer interface are revealed qualitatively. To our knowledge, there is no other pertinent simulation research on the interface

\* To whom correspondence should be addressed

between flexible polymers and low molecular LSCs up to now.

## MODEL AND SIMULATION ALGORITHM

### *Lebwohl–Lasher model and various interactions included in the model system*

The L–L model is very suitable for computer simulations of LCs on lattices. In that model, the uniaxial rod on the  $i$ th cubic lattice interacts with nearest neighbour (NN) sites with an anisotropic attractive potential of the form

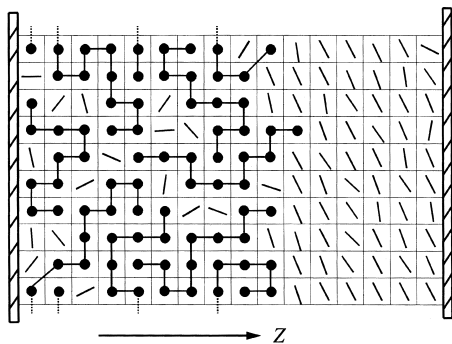
$$E = -\epsilon_{LL} \sum_{j \in NN} P_2(\cos \theta_{ij}) = -\epsilon_{LL} \sum_{j \in NN} \frac{1}{2}(3 \cos^2 \theta_{ij} - 1) \quad (1)$$

where  $\theta_{ij}$  is the angle between the two NN rods,  $\epsilon_{LL}$  is the maximum potential when the NN rods are oriented parallel with each other, reflecting the nematic interaction strength.

This model can be regarded as the discretized version of the Maier–Saupe model<sup>17</sup>. Nevertheless, the L–L model is free of mean-field approximations, since only the NN interaction is included in the L–L model and the thermal fluctuation is involved in the underlying sampling. The interaction between polymer segments and LCs,  $\epsilon_{PL}$  is assumed to be purely isotropic, which is equivalent to the assumption of completely flexible polymer chains.

### *Boundary conditions*

The simulation is carried out on cubic lattices in three dimensions. The schematic presentation of the model is shown in *Figure 1* in a simplified two-dimensional version. Each rod occupies one lattice, while each coil occupies  $x_p$  lattices. The size of the simulated system is with  $L_x \times L_y \times L_z = 10 \times 10 \times 60$ . Two impenetrable walls are set on the two sides of the  $Z$  dimension, whereas the periodic boundary condition is employed along the  $X$  and  $Y$  dimensions. The initial state is set as that the layers from  $Z = 1$  to 10 are full of polymer chains, while those from  $Z = 11$  to 60, full of rods. After sufficient MC micro-relaxation movements, an inhomogeneous equilibrium state can be achieved with an interface between the coil-rich phase and the rod-rich phase. The concentration profile along the  $Z$  dimension is then obtained directly by statistics layer by layer. Such an interface is extended along a plate rather than a curved plane as the binder of a nematic droplet. Nevertheless, the main characteristics of the interface between flexible polymers and low molecular LCs in PDLC films can be captured by a plane interface as simulated in this paper.



**Figure 1** Schematic presentation of the lattice model in the simulation of the interface between flexible polymers and low molecular nematic LCs. This figure is a simplified two-dimensional version of the model system

The two impenetrable walls must lead to two depletion layers. In order to deduce the depletion layers to avoid the interference of them to the LC/polymer interface, we introduce an imaginary adjustable surface potential near the two hard walls by virtually choosing rods and chain segments in the walls to interact with the NN layers. In every MC cycle, those virtual rods and segments at the 0th or 61th layers (two walls) are altered and selected randomly from the sites at the 1st or 60th layer respectively. Our simulation outputs demonstrate that such an artificial anchoring is reasonable and beneficial to our studies on the LC/polymer interface.

### *Monte Carlo algorithm*

The dynamic MC algorithm is employed to achieve an inhomogeneous equilibrium state. The MC evolution is carried out by the position exchange between rods and chain segments. As the LC is concerned, the reorientation of the rods should be taken into consideration. Since the rotational friction of a low molecular LC is very weak<sup>18</sup>, we reasonably assume that in each MC step (every lattice is tried once on average), the rods have sufficient time to alter their orientation. So, if a randomly selected lattice site is occupied by a nematogen, its orientation is tried to change; otherwise, if the chosen lattice is occupied by a chain segment and a randomly selected NN site is occupied by a rod, the position exchange is tried whereas the rod retains its old orientation. The lattice chain is self-avoided. Their micro-relaxations follow the chain-twisting and reptation modes<sup>19</sup>, which is very useful to deal with a multiple-chain system. The reptation mode is especially efficient for use to achieve an equilibrium state. The Metropolis importance sampling<sup>15,16</sup> is employed to determine every reorientation of a rod or position exchange between a rod and a segment with the acceptance probability  $\min[1, \exp(-\Delta E/kT)]$ , where  $\Delta E$  is the energy difference between the new state and the old state.

### *Statistics of order parameter and interfacial tension*

The simulation is performed on an IBM586 personal computer. The NDP FORTRAN is used as the language code. The strength of the anisotropic interaction between rods and that of the isotropic interaction between polymer segments and rods are inputted as two reduced parameters  $\chi_{LL}$  and  $\chi_{PL}$  written as

$$\chi_{LL} = \frac{z\epsilon_{LL}}{kT}, \quad \chi_{PL} = \frac{z\epsilon_{PL}}{kT} \quad (2)$$

where  $k$  is the Boltzman constant,  $T$  is the absolute temperature, and  $z$  is the coordination number ( $z = 6$  for cubic lattices).

The statistics are performed layer by layer along the  $Z$  direction. Besides the LC concentration  $\phi_{LC}$ , the orientation order parameter  $S$  is obtained as

$$S = \langle P_2(\cos \theta_i) \rangle = \langle \frac{1}{2}(3 \cos^2 \theta_i - 1) \rangle \quad (3)$$

where  $\cos \theta_i = \mathbf{n}_i \cdot \mathbf{n}$ ;  $\mathbf{n}_i$  and  $\mathbf{n}$  refer to the unit vectors describing the orientation of the  $i$ th rod and the LC director, respectively.

On the molecular level, the interface is structured and with a depth albeit the LC/polymer interface is very sharp. Especially at the critical point of the phase separation, the interface must be broad enough to make the concentration of one component change continuously from one phase to another. The change of the concentration through the

interface is determined by the so-called interfacial tension  $\gamma$ , the interfacial free energy in a unit area of the interface. According to the relation between the interfacial tension and the concentration profile as revealed by the Cahn–Hilliard phenomenological theory<sup>20</sup>, the free energy of an inhomogeneous system is composed of two parts: one is  $f(\varphi)$  associated with the local concentration itself, the other is the interfacial energy  $g(\nabla\varphi)$  induced by the concentration gradient. For a plate interface, the minimization of the free energy of the system (the equilibrium condition) leads to the interfacial tension being proportional to the square of the concentration gradient

$$\gamma = \text{const} \cdot \int \left( \frac{d\varphi}{dZ} \right)^2 dZ \quad (4)$$

For the MC simulation in this paper, this relation can be simplified as

$$\gamma = \sum_{z=2}^{60} (\varphi_z - \varphi_{z-1})^2 \quad (5)$$

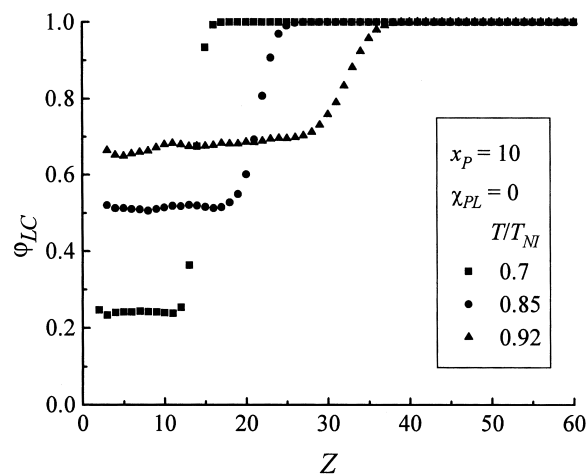
The constant in equation (4) is omitted in equation (5). So, the interfacial tension  $\gamma$  given in the paper is a reduced quantity.

## RESULTS AND DISCUSSION

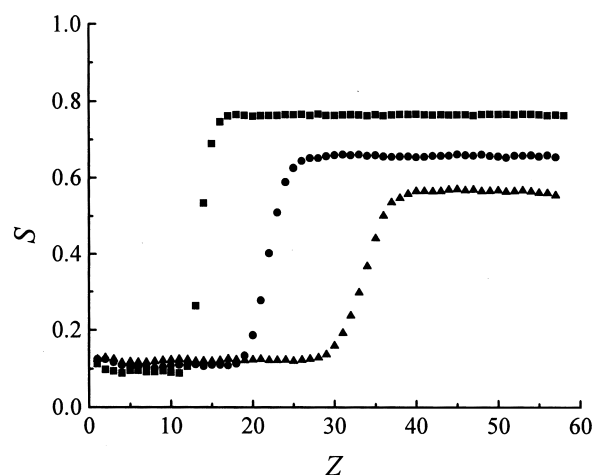
The order parameter of a bulk LC as a function of the anisotropic interaction parameter  $\chi_{LL}$  or the temperature  $T$  is examined before studies on the LC/polymer interface. Similar to the reports in the literature<sup>13–15</sup>, an isotropic–anisotropic transition takes place with increasing  $\chi_{LL}$  or decreasing  $T$  across the critical point  $\chi_{LL}^* = 5.2$ . That value is higher than 4.54 predicted by the Maier–Saupe theory<sup>17</sup>, mainly due to the neglect of the thermal fluctuation in the mean-field theory. In the following discussion, we set  $\chi_{LL} > \chi_{LL}^*$  or  $T < T_{NI}$  in most cases, since the ordered state is in our interest. For convenience, we take the reduced parameter  $T/T_{NI}$  or  $\chi_{LL}/\chi_{LL}^*$  ( $=T_{NI}/T$ ) to describe the strength of the anisotropic interaction between rods. The phase diagram for the mixture of flexible polymers and low molecular rods is very complicated. The corresponding numerical calculation based on the mean-field theory has been published by the Fudan group for the first time and partly confirmed by the MC simulation<sup>21</sup>. In the present simulation of the LC/polymer interface, most of state points are reasonably set to locate in the phase-separation regime. Some fundamental properties of the LC/polymer interface as a function of the temperature, chain length and the interaction between coils and rods are revealed in this paper.

### Dependence of the LC/polymer interface upon temperature

Figure 2 corresponds to the LC/polymer system without any net interaction between coils and rods ( $\chi_{PL} = 0$ ) but with a certain anisotropic attraction between rods. The counterpart without the anisotropic interaction between low molecular solvents is an athermal polymer solution and must lead to a homogeneous polymer solution at the equilibrium state. In contrast, phase separation takes place in the ordered polymer solution immersed in an anisotropic solvents. There are three regions in this inhomogeneous system (Figure 2): a rod-rich phase, a saturated solution of flexible polymers, and a sharp LC/polymer interface. Since the rod-rich phase is composed of almost pure rods, the phase diagram for the binary mixture of rods and coils must be seriously asymmetric, which confirms the calculation



(a)

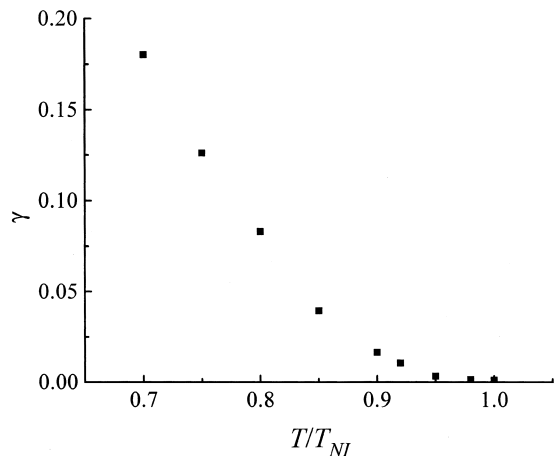


(b)

**Figure 2** Distribution of the LC concentration  $\varphi_{LC}$  and the orientation order parameter  $S$  at different layers along the  $Z$  direction obtained from the MC simulation with the indicated simulation parameters. The temperature is gradually raised from a completely demixing state in the simulation. The inhomogeneous equilibrium state at one temperature is taken as the initial state at the subsequent temperature. For each temperature, the evolution for 50 000 MC steps is performed to achieve the equilibrium state, and then the time average over 15 000 MC steps is made

based on the combination of the Flory–Huggins and Maier–Saupe mean-field theories<sup>21</sup>. The ordered rod-rich phase excludes flexible coils so strongly that the interface acts as a hard wall to bounce coils, which leads to very narrow LC/polymer interface. That argument confirms the similar viewpoint put forward in the previous paper using the Helfant lattice theory of polymer interface and the L–L nematogen model<sup>11</sup>.

Some other properties of the LC/polymer interface can be concluded from Figure 2 that with the anisotropic attraction between rods reduced or the temperature raised, the rod-rich phase is less ordered, the saturated rod concentration in the coil-rich phase is increased and the LC/polymer interface is broadened. It should be noted that the non-zero order parameter in the coil-rich phase (Figure 2b) is purely artificial. Similar phenomenon can be found in any other simulations of LCs such as Brownian dynamics simulation<sup>22</sup>. That arises from the thermal fluctuation relevant to the finite size effect. The apparent value of  $S$



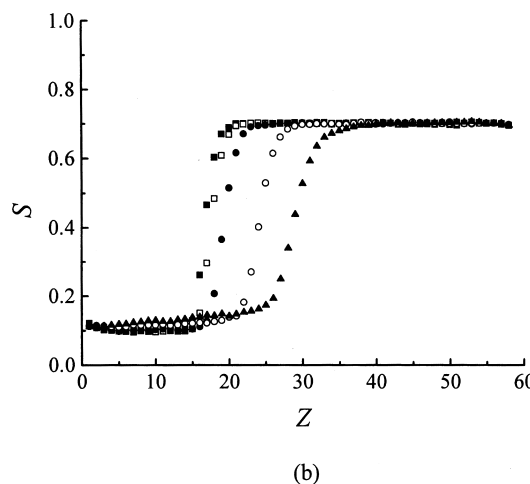
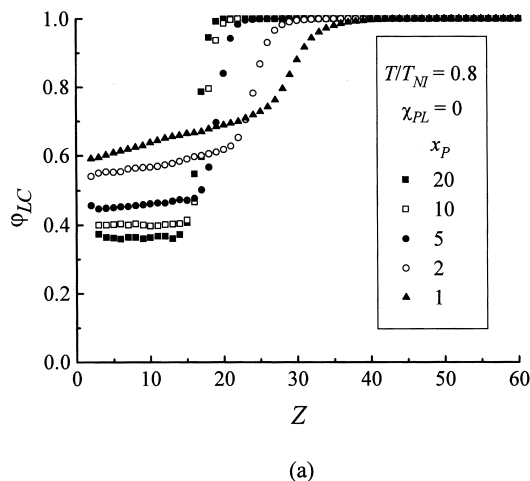
**Figure 3** Dependence of the reduced interfacial tension  $\gamma$  upon the reduced temperature  $T/T_{NI}$ . The simulation parameters are the same as those in Figure 2

in the exact isotropic state obtained from a simulation is decreased with increasing the simulated system size. Nevertheless, this does not change any conclusion in the simulation. The detailed discussion has been given in the literature<sup>23–25</sup>. It is thus very reasonable that the so-called orientation order parameter in the isotropic coil-rich phase seems not to change, whereas the ordering in the rod-rich phase is weakened with the increase of temperature (Figure 2b).

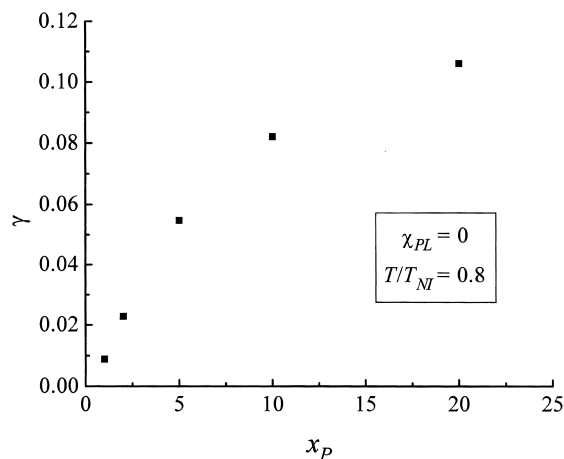
It is not difficult to understand why the interface-broadening with the increase of the temperature might coincide with the decrease of the interfacial tension, as shown in Figure 3. When the temperature is over the critical point of the phase separation ( $T/T_{NI} \sim 0.95$  for  $\chi_{PL} = 0$  and  $\chi_P = 10$ ), the width of the interface is infinite in theory, or equivalent to say, the interface disappears in a homogeneous state. In this case, the interfacial tension is ideally zero. The very small residue interfacial tension shown in Figure 3 with  $T/T_{NI} > 0.95$  comes merely from the data fluctuation in statistics of the layered rod concentrations. Figure 3 also exhibits a thermodynamic transition for the interfacial tension from none to being with the decrease of temperature, which is basically in accord with the calculation from the mean-field theory<sup>11</sup>. The difference between theory and simulation is that a weak-first-order transition is predicted in the mean-field theory (Figure 5 in reference 11), while an apparent continuous transition is shown in the simulation (Figure 3 in this paper). Since it is difficult to observe a first-order thermodynamic transition in a MC simulation with strong thermal fluctuation in a finite-size system and the predicted transition is rather weak, the simulation and theory is not contradictory with each other in essence.

*Dependence of the LC/polymer interface upon chain length*

The mean-field theory<sup>21,26</sup> demonstrates that the driving force of the phase separation in a mixture of flexible polymers and low molecular LCs is enhanced with chain length, which might originate from the more serious entropy loss when a longer chain is immersed in an LC. This predicted phenomenon is observed in our MC simulation and the trend is especially pronounced when the chain length is relatively short (Figures 4 and 5). In fact, this mechanism affords the theoretical basis to prepare PDLC films by the polymerization induced phase separation<sup>6–8</sup>. Our simulation implies that it is crucial to control the



**Figure 4** Distribution of the LC concentration  $\phi_{LC}$  and the orientation order parameter  $S$  at different layers along the  $Z$  direction obtained from the MC simulation with different lengths  $\chi_P$  as marked in the Figure. In the simulation, the evolution for 80 000 MC steps is performed to achieve the equilibrium state, and then the time average over 15 000 MC steps is made



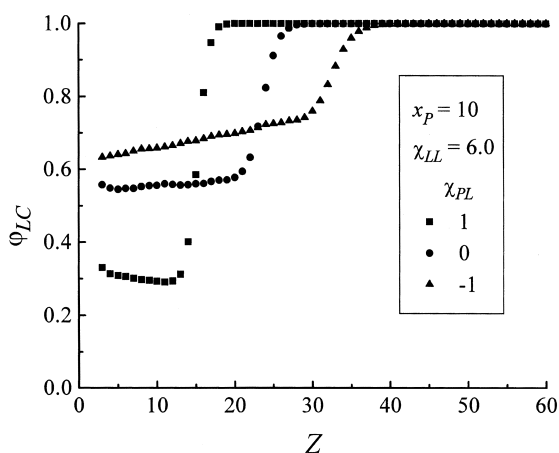
**Figure 5** Dependence of the reduced interfacial tension  $\gamma$  upon the chain length  $\chi_P$ . The simulation parameters are the same as those in Figure 4

reaction kinetics and therefore the average molecular weight and molecular weight distribution at the initial stage of polymerization in the preparation of PDLC films.

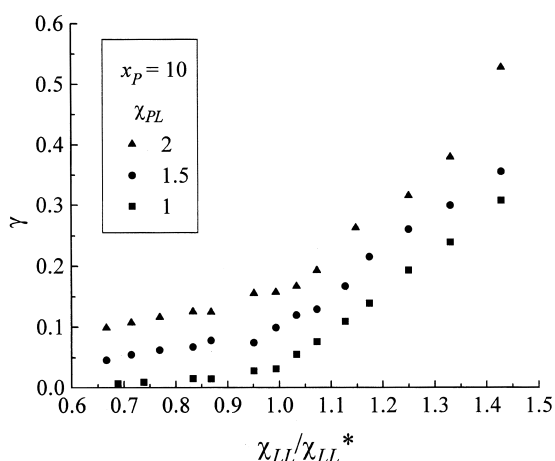
According to Figure 4, the orientation order parameters in both rod-rich phase and coil-rich phase do not obviously change with chain length at a fixed strength of anisotropic

interaction between rods ( $T/T_{NI}=0.8$ ), although the saturated rod concentration in the coil-rich phase is decreased with chain length increased. It can be understood easily from the following arguments: the coil-rich phase is isotropic and so the orientation order parameter is always nearly zero; on the other hand, the ordered phase is composed of almost pure rods similar to the bulk LC, thus the order parameter is only a function of the reduced temperature.

It is worth pointing out that some conclusions about the LC/polymer interface made from our MC simulation, such as the chain length dependence of the interfacial width (Figure 4) and of the interfacial tension (Figure 5), have been unobtainable from both theory and experiment up to now. Figure 5 indicates that the interfacial tension is not proportional to the chain length and implies an asymptotic interfacial tension associated with infinitely long



**Figure 6** Distribution of the LC concentration  $\phi_{LC}$  at different layers along the  $Z$  direction obtained from the MC simulation with different isotropic interactions between rods and chain segments  $\chi_{PL}$  as marked in the Figure. In the simulation, the evolution for 80 000 MC steps is performed to achieve the equilibrium state, and then the time average over 15 000 MC steps is made



**Figure 7** Dependence of the reduced interfacial tension  $\gamma$  upon the reduced anisotropic interaction strength between  $NN$  rods  $\chi_{LL}/\chi_{LL}^*$ . For each series of data with a fixed isotropic interaction strength between polymer segments and rods  $\chi_{PL}$  as indicated in the figure, the simulation is started from the highest  $\chi_{LL}/\chi_{LL}^*$  with 80 000 MC steps for relaxation followed by 15 000 MC steps for time average. The  $\chi_{LL}/\chi_{LL}^*$  is then gradually lowered. At every subsequent  $\chi_{LL}/\chi_{LL}^*$ , the evolution for 50 000 MC steps is performed to achieve the equilibrium state, and then the time average over 15 000 MC steps is made

chains, which actually serves as the basis to the calculation of  $\gamma$  under the assumption of the very high molecular weight of the polymer chain in the previous study on the LC/polymer interface in the formalism of the mean-field theory<sup>11</sup>.

#### Dependence of the LC/polymer interface upon the rod/coil interaction

It is obvious that the interaction between coils and rods must influence the phase equilibrium and then the interface in a mixture of flexible polymers and rigid rods (Figure 6). For instance, when the isotropic interaction between rods and coils is altered from attraction ( $\chi_{PL} < 0$ ) to repulsion ( $\chi_{PL} > 0$ ), the saturated rod concentration in the coil-rich phase is lowered, whereas the LC/polymer interface is narrower.

We further examine the curves of the interfacial tension  $\gamma$  versus the reduced anisotropic interaction between rods  $\chi_{LL}/\chi_{LL}^*$  obtained at different strengths of the isotropic interaction between coils and rods  $\chi_{PL}$  as shown in Figure 7. The simulation outputs agree with the corresponding calculation based upon the Helfand lattice theory (Figure 5 in reference 11) quite well. Both the theory and simulation indicate that the more repulsive the interaction between rods and coils, the higher the interfacial tension. Due to the very strong repulsion between rods and coils (Figure 7), the rod-coil mixture is inhomogeneous even under a weak anisotropic interaction between rods. Consequently, the interface and thus the interfacial tension do not vanish when  $\chi_{LL}/\chi_{LL}^* < 1$ . Nevertheless, a striking transition takes place in the curve of  $\gamma$  versus  $\chi_{LL}/\chi_{LL}^*$ , along with an isotropic–anisotropic transition at  $\chi_{LL}/\chi_{LL}^* = 1$ . It reveals that the nematic ordering, which leads to the exclusion of the flexible coils from the ordered LC phase, has very strong effects on the LC/polymer interface and is responsible for the considerable differences between the phase behaviours in a binary rod/coil mixture and a polymer solution or a polymer blend.

#### SUMMARY

The LC/polymer interface in an inhomogeneous binary mixture of flexible polymers and thermotropic low molecular LCs is studied in this paper by the dynamic MC simulation on cubic lattices in three dimensions. The isotropic interaction between coils and rods is introduced, whereas the anisotropic attraction between  $NN$  rods is described by the  $L-L$  nematogen model. Our simulation confirms the previous numerical calculation under the mean-field assumption and affords some information about the LC/polymer interface which is very difficult, if not impossible, to be obtained by the present experimental and theoretical approaches. Some fundamental properties of the LC/polymer interface are revealed as follows:

- (1) The driving force of the phase separation in an LC/polymer mixture is very strong, mainly due to the exclusion of the ordered phase to the flexible coils. The inhomogeneous rod/coil mixture can be divided into three parts: an anisotropic LC phase with almost pure rods, an isotropic saturated polymer solution immersed in rod-like low molecular solvents, and a sharp LC/polymer interface.
- (2) With the increase of the anisotropic attraction between rods (the decrease of the temperature), the increase of the chain length and/or that of the isotropic repulsion

between coils and rods, the driving force of the phase separation in the rod/coil mixture is enhanced, the LC/polymer interface becomes narrower and the interfacial tension gets higher.

- (3) Some physical quantities associated with the LC/polymer interface such as the interfacial tension take on a thermodynamic transition in the processes such as lowering temperature. This thermodynamic transition is closely related to the isotropic–anisotropic transition. Hence, the orientation ordering plays a central role in determining the interface in the mixture of flexible and rigid molecules.

The LC/polymer interface is a challenging topic and many questions are still open for discussion. Since the LC/polymer interface is very narrow, it is difficult for us to accurately measure the width of the interface on lattices. The scaling relations of the interfacial width and tension with the temperature etc. have not been established yet. The anisotropic interaction between polymers and LCs might have complicated effects on the phase equilibrium and the underlying interface. The surface anchoring considerably influences the director configurations of the nematic droplets and their restructuring in external electric or magnetic fields<sup>9,27</sup>. The electro-optical response in PDLC films must be determined by the LC/polymer interface to a large extent. Further investigation is thus required.

#### ACKNOWLEDGEMENTS

This research was supported by NSF of China, The Doctoral Programme Foundation of Institution High Education from the State Education Commission (SEDC) of China, The Foundation for Young Scientists from The State Science and Technology Commission of China (STCC), and

The National Key Projects for Fundamental Research ‘Macromolecular Condensed State’ from STCC.

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