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## Liquid Crystals

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# Molecular dynamics simulation of polymer dispersed liquid crystal droplets under competing boundary conditions

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This paper is devoted to the molecular dynamics simulation of structural organization inside a polydispersed liquid crystal (LC) droplet under competing boundary conditions. The droplet is assumed to be placed at the liquid crystal interface between two different regions of the solid polymer matrix, which accordingly separates the droplet into two hemispheres: the first of these is under radial boundary conditions; the second hemisphere is under bipolar boundary conditions. The droplet is considered as a jagged sphere filled with LC molecules, modelled as classical spins (unit vectors), whose centres of mass are associated with sites of a cubic lattice inside the cavity. The orienting action of the polymer matrix, and hence the resulting boundary conditions, are modelled by the interaction between the internal LC molecules (possessing only orientational degrees of freedom), and those of a delimiting surface layer (a jagged spherical shell), whose orientations are fixed, radial or bipolar, respectively. All interactions are modelled by the short range McMillan pair potential. The molecular orientation inside the LC droplet has been determined for various anchoring strengths of the interaction between internal spins and boundary layers. We have investigated the structure of the spherical defect resulting in the central region of the droplet, as well as of the boojum - like defects existing near the poles of the droplet. It has been found that a change of relative radial and bipolar anchoring strengths can affect both central and boojum - like defects. The effect of an external field on the molecular orientation inside the droplet has also been investigated. It has been found that a sufficiently strong external field increases the radius of the spherical defect placed in the central region of the droplet.

## 1. Introduction

Over the last decade, polymer dispersed liquid crystals (PDLCs), which consist of a dispersion of low molecular mass liquid crystal microdroplets in a solid polymer matrix, have attracted great interest in connection with their possible use in advanced optical device applications, such as large flexible displays, switchable windows, or paper-like displays for electronic books [1–5]. These materials are also very interesting from a fundamental point of view, as mesophases in a restricted environment. In particular, topological defects inside the droplets can be studied for various kinds of orientation and anchoring strength of the LC/polymer interface, obtained with a suitable choice of the polymer and of the preparation method. The droplets are essentially independent of one another, and we can concentrate on just one, considered as a spherical or ellipsoidal cavity filled with LC.

Several different boundary conditions have been theoretically investigated for such droplets [6]: (i) radial, with the molecules at the polymer interface oriented normal to the local surface, pointing towards the center of the droplet; (ii) toroidal, where the molecules at the interface lie in planes perpendicular to a common direction (say, the  $z$ -axis), while having orientations tangential to the droplet surface; (iii) bipolar, where the molecules at the surface are tangential to the sphere and directed along the meridians towards the poles.

Radial and bipolar boundary conditions are particularly interesting for investigating topological defects. Actually, the radial case should produce a defect core at the centre of the droplet, called ‘hedge – hog’, while the bipolar case should present two defects (boojums) at the poles of the sphere [6]. These cases have been extensively investigated using both continuum theory [7–12] and Monte Carlo (MC) simulations [6, 13–16].

In addition to these simple cases, one can imagine a situation where the polymer matrix is in homogeneous

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and consists of regions producing different orienting actions on molecules inside LC droplets, and where some droplets are situated at an interface between two such regions. In the case under investigation, one hemisphere of the droplet shall be under, say, radial boundary conditions, and the second hemisphere under, say, bipolar, boundary conditions. In this case the molecular orientation in the droplet should be sufficiently complex and somehow intermediate between the two ‘pure’ radial and bipolar orientations. Hence, such a system should also demonstrate a set of topological defects very interesting from the fundamental point of view.

We have therefore performed a MD simulation of behaviour of the LC droplet under such mixed boundary conditions. The droplet is modelled as a ‘jagged’ sphere carved from a cubic lattice, and LC molecules are assumed to be classical spins (unit vectors), whose centres of mass are fixed at the lattice site inside the sphere. The orienting action of the polymeric matrix on the LC molecules is modelled by an interaction between these molecules and those of additional ‘surfactant’ (boundary surface) layers (or rather jagged spherical shell). The ‘surfactant’ molecules are also modelled as spins. Although centres of mass of the LC spins are fixed, these spins can rotate about their centres of mass under the action of torques from other LC and surfactant spins. At the same time, the surfactant spins are completely fixed, and their orientations are defined by the boundary conditions. Interaction between LC molecules and between them and molecules of the surfactant is described by the short range McMillan pair potential model [15].

The molecular orientation in this droplet has been investigated for various anchoring strengths at radial and bipolar LC/surfactant interfaces, and an analysis of a defect structure occurring in the droplet has been performed. It is shown that the orientational order in the interfacial regions of the droplet is almost purely radial for one of its hemispheres and almost purely bipolar for the other hemisphere. In contrast, in the central region of the droplet the orientational order is almost homogeneous, and this homogeneously oriented region borders with those with radial and bipolar order. Such a border can be considered as a spherical defect structure consisting of a homogeneous order/radial order interface and a homogeneous order/bipolar order interface.

Our simulation also shows that, for the hemisphere under radial boundary conditions, the regions close to the poles of the droplet exhibit a strong radial order. On the other hand, for the hemisphere under bipolar boundary conditions, in the regions close to the poles

of the droplet, one can observe boojum - like defects. It has been also found that by changing the relative radial and bipolar anchoring strengths, we can affect both central and boojum - like defects. The effect of an external field on the molecular orientation inside the droplet has been also investigated. It is shown that a sufficiently strong external field can give rise to a growth of the homogeneous central region of the droplet and to a shift of the spherical defect structure towards the LC/surfactant interface.

## 2. Basic equations and simulation details

As explained in the Introduction, the PDLC droplet can be modelled as a spherical cavity filled with LC molecules and surrounded by a layer of surfactant molecules. Such a droplet can be realized by a jagged sphere carved from a cubic lattice, and LC molecules are assumed to be unit spins with centres of mass fixed at sites of this lattice inside the sphere. These spins, however, possess orientational degrees of freedom, and their rotation is governed by the equations:

$$\dot{\vec{e}}_i = \vec{\omega}_i \times \vec{e}_i \quad (1)$$

$$\vec{\omega}_i = \vec{\tau}_i / I. \quad (2)$$

Here,  $\vec{e}_i$  denotes a unit vector, defining orientation of the long axis of the  $i$ -th molecule,  $\vec{\omega}_i$  is an angular velocity of rotation of this molecule about its centre of mass,  $\vec{\tau}_i$  is the total torque, acting on the  $i$ -th molecule and produced by other LC spins and surfactant molecules, and  $I$  is the molecular moment of inertia.

The LC molecules of the droplet are surrounded by an additional layer of molecules of surfactant which are also modelled as completely fixed unit spins. The orientation of these spins defines the boundary conditions through their interaction with the spins inside the droplet. To fix ideas and notation, the droplet is assumed to be separated into two hemispheres by a plane, taken to be the  $(y, z)$ -plane in a Cartesian reference frame whose origin coincides with the centre of the droplet. The molecules of surfactant in contact with molecules of one hemisphere of the droplet are aligned along normal to the droplet/surfactant interface, and the molecules of surfactant in contact with LC molecules of the other hemisphere are aligned parallel to tangents to the spherical droplet meridians passing through positions of their fixed centres of mass, and running to poles placed on the  $z$ -axis (the ‘vertical’ axis). Thus, the molecules of surfactant induce polar ordering in the first hemisphere and bipolar ordering in the second hemisphere. The interaction between LC molecules, and the LC/surfactant interaction, are

described by the anisotropic McMillan pair potential model [17], i.e.

$$V_{ij}^M(r_{ij}, \vartheta_{ij}) = -\varepsilon P_2(\cos \vartheta_{ij}) \exp\left(-r_{ij}^2/r_0^2\right) \quad (3)$$

Here  $P_2$  is the second order Legendre polynomial,  $r_{ij}$  is the distance between the centres of mass of the two interacting molecules,  $\vartheta_{ij}$  is the angle between their long molecular axes (i.e.  $\cos \vartheta_{ij} = \vec{e}_i \cdot \vec{e}_j$ ),  $\varepsilon$  is an interaction constant, and  $r_0$  is a characteristic length of this short range interaction which is of the order of the molecular size ( $\sim nm$ ).

It should be noted that in previous papers [6, 13, 14] dealing with MC simulations of PDLCs, the intermolecular interactions were modelled by the Lebwohl–Lasher (LL) potential model [18], having an angular form completely similar to the orientational part of the McMillan potential, see equation (3), but restricted to nearest neighbours. Although the pair potential (3) used in our simulations is very short-ranged, it describes not only interactions between nearest neighbours, but also takes into account interactions between other molecules of the system. So, it can be considered to be somewhat more realistic than the LL model. The total torque  $\vec{\tau}_i$ , acting on the  $i$ -th LC molecule is given by

$$\vec{\tau}_i = \sum_{j=1, j \neq i}^N \vec{\sigma}_{ij} \quad (4)$$

where  $N$  is the total number of molecules of the system, and

$$\vec{\sigma}_{ij} = -(\vec{e}_i \times \vec{e}_j) \left( \frac{\partial V_{ij}^M}{\partial \cos \vartheta_{ij}} \right). \quad (5)$$

When the LC droplet is placed into an external magnetic field  $\vec{H}$ , an additional term

$$\vec{\tau}_i^{ext} = \Delta\chi H^2 (\vec{e}_i \cdot \vec{h}) [\vec{e}_i \times \vec{h}] \quad (6)$$

should be added in equation (4); here  $\vec{h}$  is the unit vector parallel to  $\vec{H}$ , and  $\Delta\chi$  is the diamagnetic susceptibility anisotropy of the LC molecule. When the droplet is placed in an external electric field  $\vec{E}$ , equation (6) maintains the same structure, but now  $\vec{H}$  should be replaced by  $\vec{E}$ , and the diamagnetic susceptibility anisotropy  $\Delta\chi$  should be replaced by the molecular polarizability anisotropy  $\Delta\alpha$ . The interaction constant  $\varepsilon_M$  for interaction between LC molecules is assumed to be unit (in dimensionless MD units [19]), whereas the analogous constants for LC/surfactant interaction will be varied depending on the types of anchoring at the droplet/surfactant interface; to fix the notation,  $\varepsilon_1 = X\varepsilon_M$  will be

used for the hemisphere under radial boundary conditions, and  $\varepsilon_2 = Y\varepsilon_M$  for the hemisphere under bipolar conditions.

The interaction model contains a few adjustable parameters, and we have chosen to study here the cases:  $c1$ , defined by  $\varepsilon_1 = \varepsilon_2 = 10\varepsilon_M$ , i.e.  $X = Y = 10$ ;  $c2$ , defined by  $X = 10$ ,  $Y = 1$ ;  $c3$ , defined by  $X = 1$ ,  $Y = 10$ . In these three cases the external field is zero. We have also considered one case with a finite and rather strong field;  $c4$ , defined by  $X = Y = 10$ ,  $\Delta\chi H^2 = 5\varepsilon_M$ , and  $\vec{H}$  along the  $x$ -axis.

The droplet under consideration contains 1400 molecules (of variable orientations), surrounded by a surfactant layer composed of 988 molecules (of fixed orientations). The simulated sample is enclosed in a cubic simulation box which is  $16r_0 \times 16r_0 \times 16r_0$  in size and the characteristic length  $r_0$  is assumed to be 1 (in the same MD units) in all our simulations. MD simulations were performed at constant volume and reduced temperature  $T^* = k_B T / \varepsilon_M$ , where  $T$  is the temperature of the system, and  $k_B$  is the Boltzmann constant. In all these four cases the reduced temperature  $T^*$  was set to 1. All simulations were started from random initial particle orientations inside the droplet. The simulations were run for 100 000 time steps (one time step is equal to 0.001 in dimensionless MD units), and the molecular moment of inertia  $I$  is assumed to be unity (also in the MD units). At each time step, equations (1) and (2) were solved numerically by using the procedure described in [19], and the temperature of the system was kept constant by rescaling angular velocities.

Note that, when bulk simulations are carried out, the system is homogeneous; but here a significant heterogeneity occurs, so that orientational order must be defined on a smaller local scale (spherical shells, or plane layers). Moreover, and again in contrast to bulk simulations (where, in many cases, only the director frame matters), one has to consider here the average orientation of spins with respect to local frames, reflecting the boundary conditions. So, in order to describe the orientational order inside the droplet under consideration, the spherical cavity filled with LC molecules was separated into spherical layers of equal thickness, as well as into flat layers parallel to the  $(x, y)$ -plane; orientational order parameter  $S$  and an average director orientation were calculated for each layer on all steps of the simulation process. As in [6, 19, 20], for each layer we calculated and diagonalized the traceless ordering matrix  $\hat{Q}_k$  defined as

$$\hat{Q}_k = \frac{1}{2N_k} \left( \sum_{i=1}^{N_k} 3e_{i\alpha}e_{i\beta} \right) - \delta_{\alpha\beta}/2 \quad (7)$$

where  $e_{i\alpha}$  is the  $\alpha$ -th component of unit vector  $\vec{e}_i$ , and  $N_k$  is a number of molecules within  $k$ -th layer. The largest

eigenvalue of  $\hat{Q}$  was identified as the orientational order parameter  $S$  for the  $k$ -th layer, and the other two eigenvalues were used to calculate the polar angles  $\theta_k$  and  $\phi_k$  defining orientation of the director  $\vec{n}_k$  for this layer with respect to the axes of the above mentioned laboratory frame [19].

As in [6, 21], in addition to the order parameter  $S$ , we also calculated two additional order parameters, the radial order parameter  $\langle P_2 \rangle_R$ , and the meridian order parameter  $\langle P_2 \rangle_M$ , defined by

$$\langle P_2 \rangle_R = \frac{1}{N_k} \sum_{i=1}^{N_k} P_2 \left( \vec{e}_i \cdot \frac{\vec{r}_i}{r_i} \right) \quad (8)$$

$$\langle P_2 \rangle_M = \frac{1}{N_k} \sum_{i=1}^{N_k} P_2 \left( \vec{e}_i \cdot \vec{l}_i \right) \quad (9)$$

where  $\vec{r}_i$  and  $\vec{l}_i$  are the radial vector of the  $i$ -th molecule, and the unit vector tangent to the meridian of the sphere passing through its centre of mass, respectively. After running 100 000 time steps for equilibration, structural properties were averaged over some ( $v \times 5000$ ) time steps; averages obtained with different values of  $v$  ( $v=1, 2, 4, 10$ ) showed no significant differences. The set of averaged order parameters  $S$ ,  $\langle P_2 \rangle_R$ , and  $\langle P_2 \rangle_M$  is adequate for describing orientational ordering inside the droplet under consideration.

### 3. Results

Figure 1 shows a spin configuration for case  $c1$ , obtained after 100 000 time steps for equilibration,

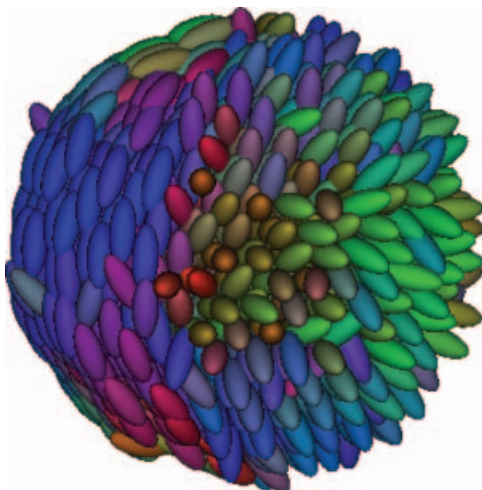


Figure 1. Spin configuration of the polydispersed LC droplet in case  $c1$ , obtained after running for 100 000 time steps and averaging structural properties over 5000 time steps; the elongated ellipsoids imitate molecules of the droplet.

and 5000 time steps for production. The elongated ellipsoids depicted in this figure imitate molecules of the droplet. It is easily seen that from the point of view of an external observer the droplet can be considered as a spherical defect with a topological charge  $s=1/2$  [6].

The internal orientational ordering of the droplet can be seen from figure 2 (also obtained for case  $c1$ ), which shows dependences of the radial  $\langle P_2 \rangle_R$ , meridian  $\langle P_2 \rangle_M$ , and ‘ordinary’  $S$  order parameters (determined for spherical layers of the droplet), on the distance  $r$  from the droplet center (in units of  $r_0$ ) under the same boundary conditions and at the same temperature  $T^*$ . In this figure, negative values of  $r$  correspond to the hemisphere under radial boundary conditions; positive values of  $r$  correspond to the hemisphere under bipolar boundary conditions. It is seen that both  $\langle P_2 \rangle_R$  and  $\langle P_2 \rangle_M$  order parameters have maximum and minimum values at the droplet/surfactant interface (see curves 1 and 2 in figure 2), where the orienting action of the surfactant molecules is strongest. Therefore, as expected, the orientational order in the interfacial regions is almost purely radial for the first hemisphere and almost purely bipolar for the second. It is also seen that, in the central region of the droplet, both  $\langle P_2 \rangle_R$  and  $\langle P_2 \rangle_M$  order parameters are nearly zero or even negative. Our simulation also shows that in this region the overall orientational order parameter  $S$  has a maximum value close to 1 (see curve 3 in the same figure).

This result can be illustrated by figure 3, which exhibits the orientation of the LC molecules inside a flat layer of the droplet parallel to  $(x, z)$ -plane. This layer has unit thickness (in units of  $r_0$ ) and contains the centre of the droplet. In this figure, the bold points denote the

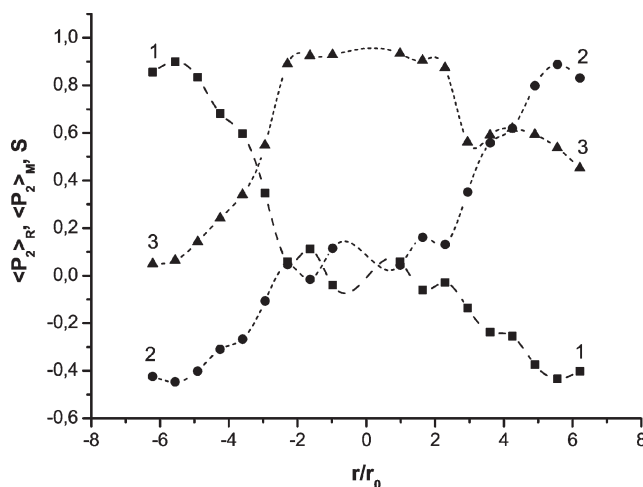


Figure 2. Case  $c1$ : dependences of the radial  $\langle P_2 \rangle_R$ , meridian  $\langle P_2 \rangle_M$ , and ‘ordinary’  $S$  order parameters, determined for spherical layers of the droplet, on the distance  $r$  from the droplet centre. 1 -  $\langle P_2 \rangle_R$ , 2 -  $\langle P_2 \rangle_M$ , 3 -  $S$ .

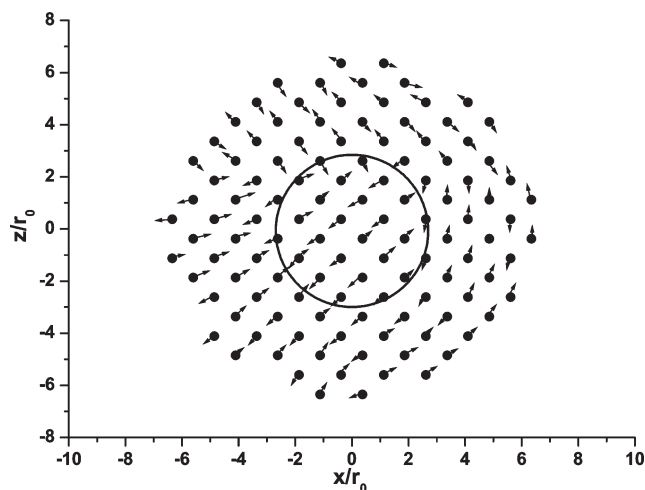


Figure 3. Orientations of the LC molecules within the central  $(x, z)$  layer of the droplet. The bold points denote the sites of LC spins and the arrows denote their projections on the  $(x, z)$ -planes.

sites of the lattice within such a layer, and the arrows denote projections of corresponding spins on the  $(x, z)$ -plane. One can see that all spins within a certain circle have the corresponding projections very similar to each other.

Thus, in the central spherical region of the droplet, orientational order is nearly homogeneous, and this homogeneously oriented region borders with regions possessing dominant radial and bipolar order. These two borders, homogeneous order/radial order interface, and homogeneous order/bipolar order interface, can be regarded as comprising a defect. From figure 2 one can determine its radius to be about  $3r_0$ , which is in good agreement with the result of MC simulation [6, 19] of the LC droplet under 'pure' radial boundary conditions performed using the LL potential model.

We also investigated the dependences of all order parameters, determined for flat  $(x, y)$  layers of the droplet, on the vertical coordinate  $z$ . The  $z$ -axis has a special importance because, as noted earlier, the molecules of one of the droplet hemispheres are under an orienting action of the surfactant aligned along the droplet meridians running to the poles placed on this vertical axis. These dependences for radial and bipolar hemispheres of the droplet are shown in figures 4 and 5, respectively. It can be seen that in the hemisphere under radial boundary conditions all layers possess well developed radial order; and near the poles this order is even stronger than that in the central part of the droplet. On the other hand, in the hemisphere under bipolar boundary conditions (see figure 5), the radial order parameter  $\langle P_2 \rangle_R$  is negative for all flat  $(x, y)$  layers, and  $\langle P_2 \rangle_M$  and  $S$  order parameters are

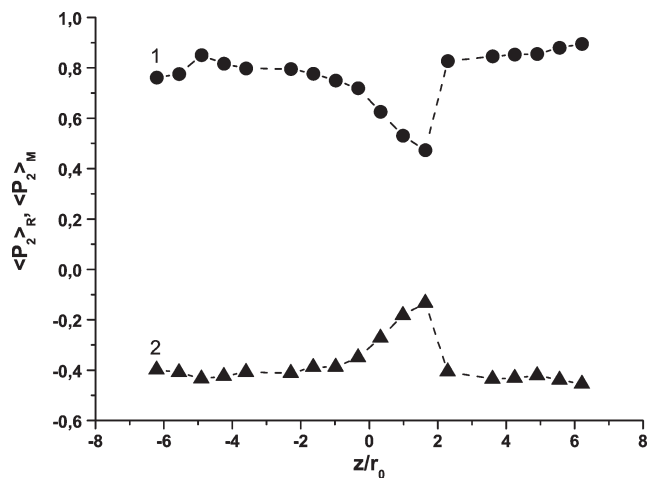


Figure 4. Case  $c1$ : dependences of  $\langle P_2 \rangle_R$  and  $\langle P_2 \rangle_M$ , determined for flat  $(x, y)$  layers of the radial hemisphere of the droplet, on the vertical coordinate  $z$ . 1 -  $\langle P_2 \rangle_R$ , 2 -  $\langle P_2 \rangle_M$ .

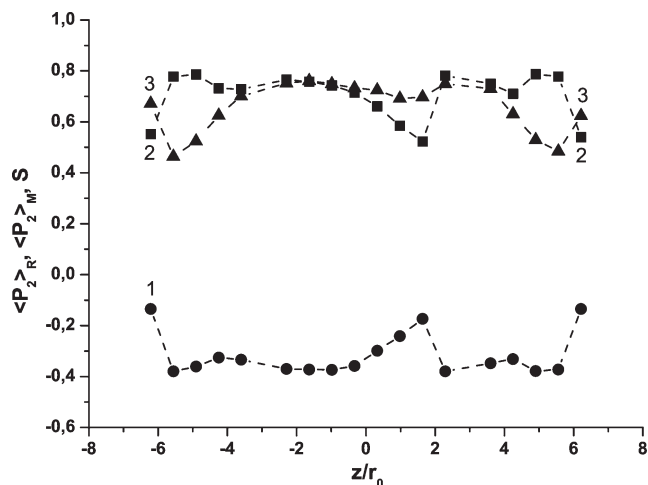


Figure 5. Case  $c1$ : same dependences as in figure 3, for  $\langle P_2 \rangle_R$ ,  $\langle P_2 \rangle_M$  and  $S$ , but for the bipolar hemisphere of the droplet. 1 -  $\langle P_2 \rangle_R$ , 2 -  $\langle P_2 \rangle_M$ , 3 -  $S$ .

positive. From figure 4 it can be seen that the meridian order parameter is dominant in all flat  $(x, y)$  layer, except for regions close to the poles of the droplet, where the parameter  $S$  exceeds parameter  $\langle P_2 \rangle_M$ , which has a minimum value in these regions. So, the polar regions in the hemisphere under bipolar boundary conditions exhibit a higher orientational order than that under bipolar conditions; and one can consider boundaries between these regions and regions with the bipolar order as boojum-like defects, which exist only in the bipolar hemisphere of the droplet.

In cases  $c2$  and  $c3$ , we have also investigated the effect of varying  $X$  and  $Y$  on the resulting structural

organization inside the droplet. Our simulation shows that, in case *c2* (see figure 6), the part of the spherical defect disposed inside the hemisphere under radial boundary conditions is very similar to that depicted in figure 2; whereas, inside the hemisphere under bipolar boundary conditions, the homogeneous order/bipolar order interface disappears. In case *c3* (see figure 7), inside the hemisphere under bipolar boundary conditions, the homogeneous order/bipolar order interface is very similar to that depicted in figure 2; and the homogeneous order/radial order interface, which is disposed inside the hemisphere under radial boundary conditions, does not disappear but undergoes a small displacement towards the LC/surfactant interface.

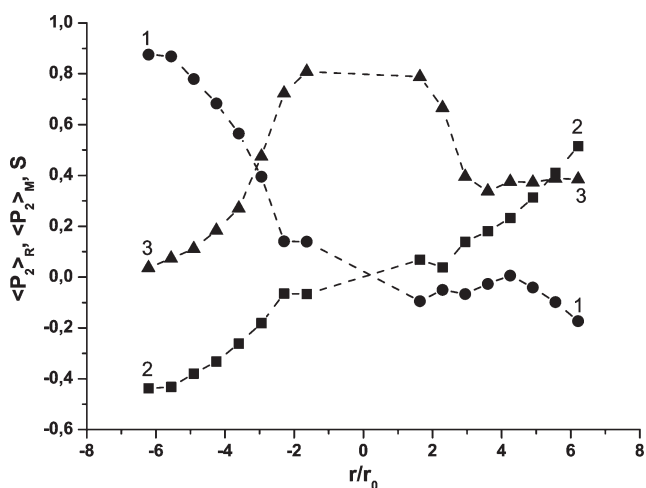


Figure 6. Case *c2*: same observables as in figure 2. 1 -  $\langle P_2 \rangle_R$ , 2 -  $\langle P_2 \rangle_M$ , 3 -  $S$ .

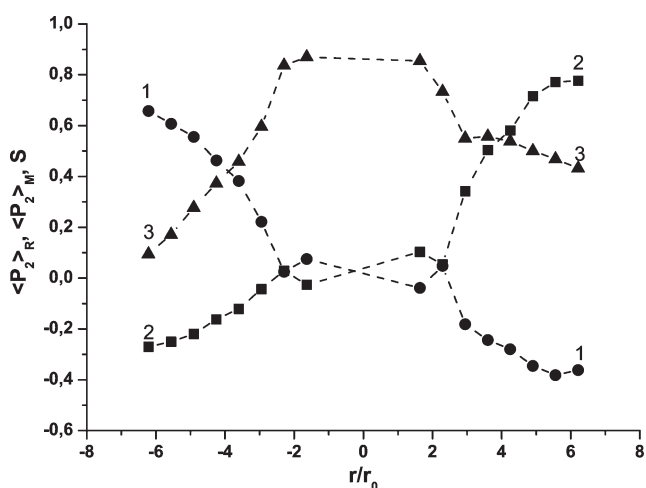


Figure 7. Case *c3*: same observables as in figures 2 and 5. 1 -  $\langle P_2 \rangle_R$ , 2 -  $\langle P_2 \rangle_M$ , 3 -  $S$ .

Thus, in case *c2* one can observe only a half of the spherical defect surface, whereas in case *c3* only a small deformation of this defect surface occurs.

As for the influence of the anchoring strength at the LC/surfactant interface for radial and bipolar hemispheres of the droplet on the behaviour of boojum-like defects, our simulations show that, in case *c2* radial order dominates in all  $(x, y)$  layers of the hemisphere under radial boundary conditions, and boojum-like defects do not occur in this hemisphere. On the other hand, one can easily observe such defects (see figure 8) near the poles of the hemisphere under bipolar boundary conditions. However, in this case, the polar regions of the bipolar hemisphere exhibit a molecular ordering which is rather radial than homogeneous. So, such boojum-like defects can be considered as boundaries between polar regions with radial order and other regions of the hemisphere with bipolar order. In case *c3*, bipolar order dominates in all  $(x, y)$  layers in the hemisphere under the bipolar boundary conditions and, hence, boojum-like defects do not occur in this hemisphere. In this case, our simulation also reveals absence of boojum-like defects in the hemisphere under radial boundary conditions (see figure 9). It can be seen that homogeneous order dominates in all  $(x, y)$  layers of this hemisphere, except for a few central layers, where the radial  $\langle P_2 \rangle_R$  and ordinary  $S$  order parameters are practically equal. So, a sharp decrease of the radial order parameter  $\langle P_2 \rangle_R$  in the polar regions of the radial hemisphere could not be considered as an attribute of occurrence of the boojum-like defects.

Finally, in case *c4* (field along the  $x$ -axis), we have also investigated the effect of an external field on molecular orientation inside the droplet, in particular on the

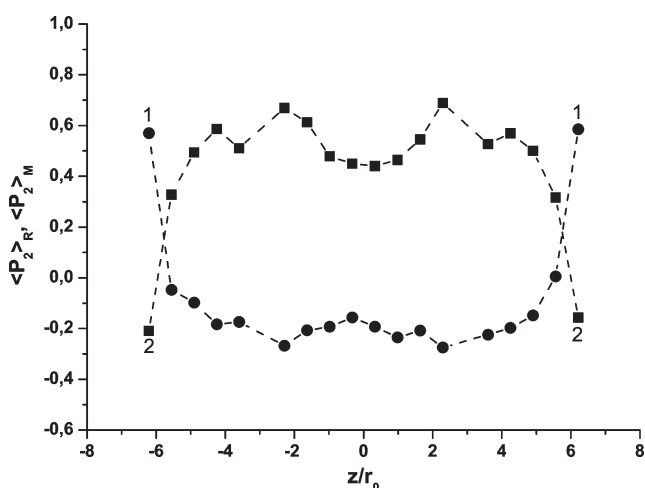


Figure 8. Case *c2*: same observables as in figure 4, but now for 1 -  $\langle P_2 \rangle_R$ , 2 -  $\langle P_2 \rangle_M$ .

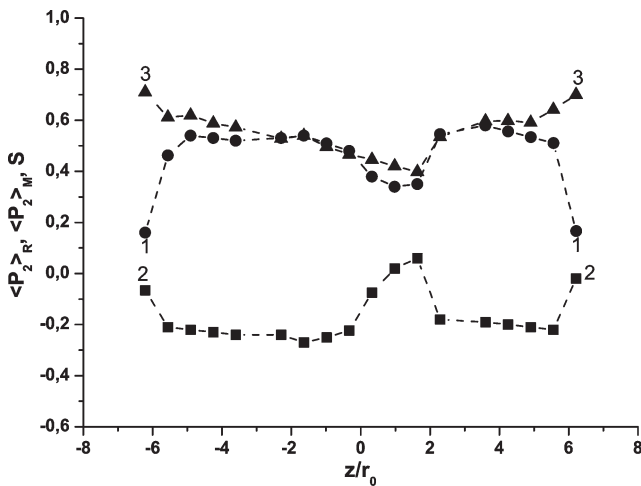


Figure 9. Case *c3*: dependences of  $\langle P_2 \rangle_R$ ,  $\langle P_2 \rangle_M$  and  $S$ , determined for flat  $(x, y)$  layers of the radial hemisphere of the droplet, on the vertical coordinate  $z$ . 1 -  $\langle P_2 \rangle_R$ , 2 -  $\langle P_2 \rangle_M$ , 3 -  $S$ .

spherical defect in its central region and boojum - like defects. One influence of the external field on the central spherical defect is illustrated by figure 10, which demonstrates dependences of the radial  $\langle P_2 \rangle_R$ , meridian  $\langle P_2 \rangle_M$ , and ‘ordinary’  $S$  order parameters, determined for spherical layers of the droplet, on the distance  $r$  from the droplet centre. It should be noted that the ordinary order parameter  $S$  profile depicted in this figure is very similar to those obtained in [22]. We see that the spherical defect in the central part of the droplet placed in the external field is qualitatively the same as when the field is absent. We also see a homogeneously oriented central part of the droplet which borders with regions with dominant radial and bipolar

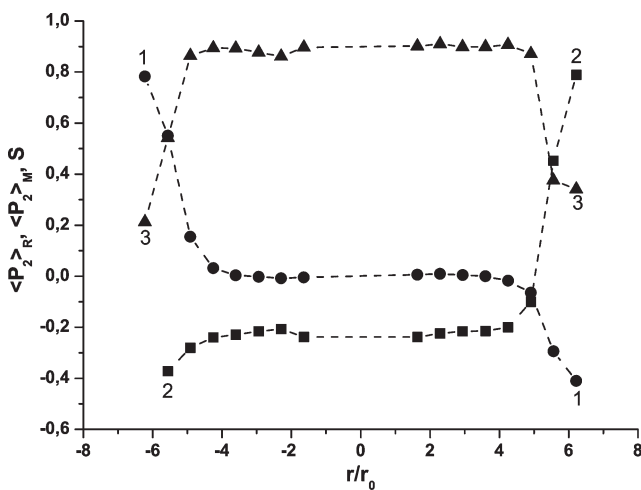


Figure 10. Case *c4*: same observables as in figure 2. 1 -  $\langle P_2 \rangle_R$ , 2 -  $\langle P_2 \rangle_M$ , 3 -  $S$ .

order. However, the radius of this spherical defect is about twice as large as that in the droplet not subjected to an external field (case *c1*). Thus, one can conclude that an external field increases the size of the spherical defect in the central region of the droplet. Our simulations also show that, under the above-mentioned external field, the radial order dominates in all flat  $(x, y)$  layers of the radial hemisphere of the droplet. As for the influence of the external field on the orientational order inside the bipolar hemisphere, from figure 11 one can conclude that the ordering close to homogeneous dominates in the central flat  $(x, y)$  layers of this hemisphere; whereas in layers adjacent to the poles the bipolar order parameter  $\langle P_2 \rangle_M$  exceeds the ordinary order parameter  $S$ , and just in the poles the order parameter  $S$  is dominant again. So, at each pole of the bipolar hemisphere one can observe two boundaries between regions with dominant homogeneous and bipolar orientational order, and these boundaries can be considered as boojum - like defects.

#### 4. Conclusions

We have performed a molecular dynamics simulation of the structural organization inside a polydispersed LC droplet disposed at the interface between two different regions of a solid polymer matrix. The interface separates the droplet into two hemispheres, the first of which is under radial boundary conditions induced by one region of the polymer matrix, while the second hemisphere is under bipolar boundary conditions induced by another region of the polymer matrix. The orienting action of the polymer matrix on the LC molecules is modelled by the McMillan - like interaction between these molecules and completely fixed molecules

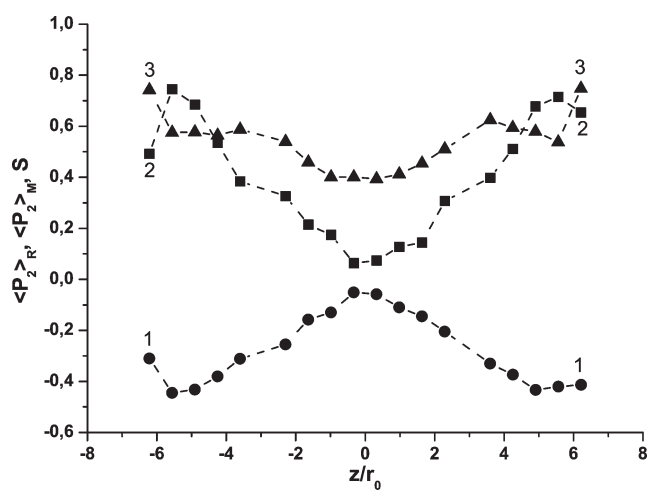


Figure 11. Case *c4*: same observables as in figure 4. 1 -  $\langle P_2 \rangle_R$ , 2 -  $\langle P_2 \rangle_M$ , 3 -  $S$ .



of 'surfactant' layers surrounding the droplet. The centres of mass of the LC spins are fixed, but these spins can rotate about their centres of mass under the action of torques from other LC and surfactant spins.

The interaction between LC molecules is also described by the McMillan model pair potential. The molecular orientation inside the LC droplet has been investigated for various anchoring strengths at radial and bipolar LC/surfactant interfaces. It has been shown that orientational order in the interfacial regions of the droplet is almost purely radial for one of its hemispheres and almost purely bipolar for the other. However, its central region is almost homogeneously oriented, and this central region borders with those with radial and bipolar order. Such a border can be considered as a spherical defect structure which consists of a homogeneous order/radial order interface and a homogeneous order/bipolar order interface.

Our simulation also shows that, in the hemisphere under radial boundary conditions, the polar regions of the droplet exhibit a strong radial order, whereas in the hemisphere under bipolar boundary conditions, homogeneous order dominates in the polar regions of droplet. The boundaries between these regions and other parts of the bipolar hemisphere, where the bipolar order is dominant, can be considered as boojum-like defects. It has been also found that by changing relative radial and bipolar anchoring strengths, one can affect both central and boojum-like defects.

We have also investigated the effect of an external field on the molecular orientation inside the droplet. It was shown that a sufficiently strong external field increases the homogeneous central region of the droplet and shifts the spherical defect structure towards the LC/surfactant interface.

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