Computer simulation study of defects near a colloid droplet dispersed in a nematic host

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Abstract

We use molecular dynamics to study a large spherical particle suspended in a nematic liquid crystal matrix modeled with a soft ellipsoid potential. Homeotropic boundary conditions and strong anchoring create a hedgehog director configuration on the particle surface. The topological mismatch with the uniform director at large distances leads to the formation of two possible defect structures: a quadrupolar one with a ring defect or a dipolar one with a satellite defect. We examine the stability of these defects as a function of the droplet size in systems with up to one million particles using a domain decomposition MD program on a massively parallel computer. We are able to observe density and order parameter variations near the particle surface and in the disclination core region that are not taken into account by elastic theory.

1 Introduction

Macroparticles introduced into liquid crystals considerably influence their electro-optical properties. The physical mechanism is long-range interaction of the macrodroplets. A macrodroplet distorts the director distribution and thus provides an effective long-range interaction with another similar droplet. This leads to the formation of new supermolecular structures, e.g. threadlike structures consisting of colloid particles [1]. The complexity of such emulsions is caused by the presence of defects. Due to the topological mismatch between the local director on the particle surface and the uniform director at large distances, a droplet with homeotropic boundary conditions will create a hedgehog director configuration in its immediate vicinity.
Phenomenological theories predict that two defect structures can result in the case of strong anchoring [1, 2]: a quadrupolar structure with a ring defect; a dipolar structure with a satellite defect (Fig. 1). There are no defects in the case of weak anchoring.
The main disadvantages of the existing theories are:

- The core region is treated as an isotropic inclusion with some unknown free energy [2, 3].
- The phase is treated as uniaxial (which is not true near the disclination core), and the order parameter is considered constant (which is not true either near the particle surface) [1, 2, 3].

Computer simulation allows one to resolve the nematic orientational ordering near the particle taking into account density and order parameter variations as well as possible biaxiality of the nematic phase close to the particle in the disclination core region [4, 5].

2 Molecular model and simulation methods

We chose the repulsive part of the soft ellipsoid potential, a variant of the Gay-Berne potential [6] with exponents $\mu = 0, \nu = 0$:

$$U_{ij}(\mathbf{r}_{ij}, \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j) = 4\varepsilon_0 \left[\varrho_{ij}^{12}(\mathbf{r}_{ij}, \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j) - \varrho_{ij}^{6}(\mathbf{r}_{ij}, \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j)\right] + \varepsilon_0$$

$$\varrho_{ij}(\mathbf{r}_{ij}, \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j) = \frac{\sigma_0}{r_{ij} - \sigma(\hat{\mathbf{r}}_{ij}, \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j) + \sigma_0}, \qquad \varrho_{ij}^{-1} < \sqrt[6]{2}$$

$$\sigma = \sigma_0 \left\{1 - \frac{\chi}{2}\left[\frac{(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{e}}_i + \hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{e}}_j)^2}{1 + \chi\,\hat{\mathbf{e}}_i\cdot\hat{\mathbf{e}}_j} + \frac{(\hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{e}}_i - \hat{\mathbf{r}}_{ij}\cdot\hat{\mathbf{e}}_j)^2}{1 - \chi\,\hat{\mathbf{e}}_i\cdot\hat{\mathbf{e}}_j}\right]\right\}^{-1/2}$$

$$\chi = (\kappa^2 - 1)/(\kappa^2 + 1), \qquad \kappa = \sigma_{end-end}/\sigma_{side-side} = 3.$$

The macroparticle has a radius R and exerts a shifted Lennard-Jones repulsion on the centers of the mesogens, resulting in homeotropic anchoring of the latter on the macroparticle surface, $\sigma_c = (\kappa - \sigma_0)/2$:

$$U_i(\mathbf{r}_i) = 4\varepsilon_0 \left[\left(\frac{\sigma_0}{r_i - \sigma_c}\right)^{12} - \left(\frac{\sigma_0}{r_i - \sigma_c}\right)^{6}\right] + \varepsilon_0, \qquad \frac{r_i - \sigma_c}{\sigma_0} < \sqrt[6]{2}.$$

The systems consist of 8,000-1,000,000 mesogens. A molecular dynamics program was run on a Cray T3E using a domain decomposition algorithm. The colloid particle was fixed in the center of the box. The director was constrained along the z axis.

3 Simulation results

Simulation results were analysed to give director, density, order parameter, and biaxiality maps.
Typical director profiles are shown in Fig. 1. The ring defect does not have long-range director distortions. In contrast, the satellite defect has a wide area of director distortion (therefore, the simulation box for the satellite defect has to be large enough).

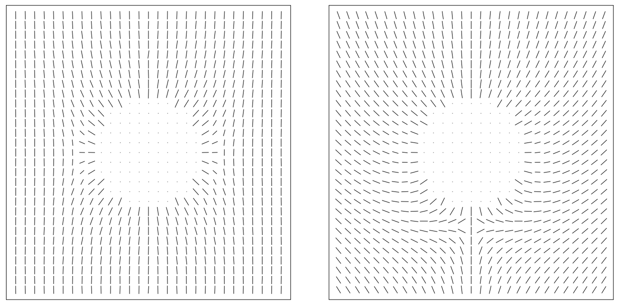

Figure 1 Director profiles of the *ring* (left) and *satellite* (right) defects. Slice through a 3d configuration (zy-plane)

4 Ring defect

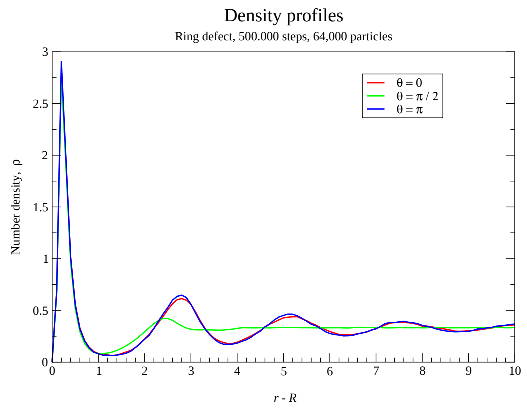

Figure 2 Density profiles. The following directions are shown: $\theta = \pi/2$ (across the disclination ring) and $\theta = 0, \pi$ (no defect). The profiles without the disclination have oscillating structure near the particle surface which is typical for a *liquid-wall* interface. The profiles with the disclination ring do not have oscillations and are similar to those of a *gas-wall* interface. The difference may be due to melting of the liquid crystal in the disclination core region. This melting damps the influence of the droplet surface on the interface region.

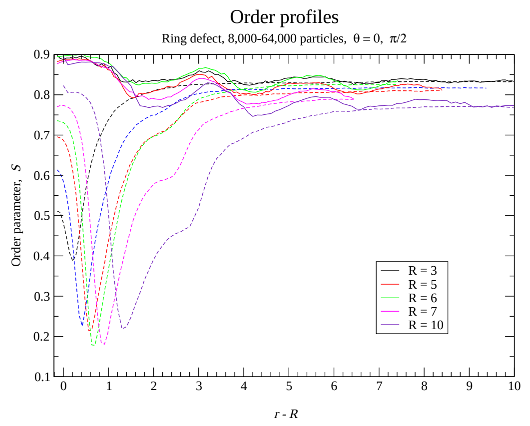

Figure 3 Order parameter profiles for $\theta = 0, \pi/2$. The disclination ring position is given by the minimum of the order parameter. For large enough R a second mimimum appears pointing out that the disclination ring defect has a complex structure.

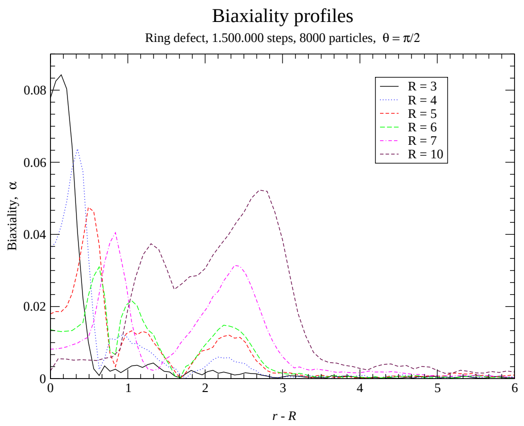

Figure 4 Biaxiality profiles. It is clearly seen that the disclination ring has a complex structure. The main biaxial ring has a lower order parameter than the bulk value. This ring is accompanied by one biaxial ring for large R or even two for some R (e.g. $R = 5, 6$).

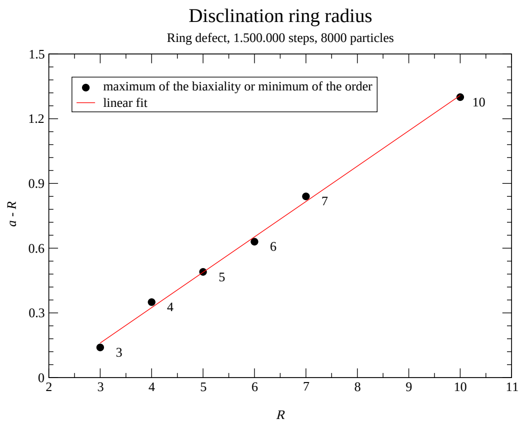

Figure 5 Distance of the core of the disclination ring from the particle surface. There is a correlation between the phenomenological theory predicting $a \approx 1.25R$ and simulation results giving $a - R = -0.33 + (0.164 \pm 0.004)R$.

5 Satellite defect

The satellite defect is not stable for small droplets. We observed a transition of the satellite defect in to the ring defect for $R < 15$. At the same time, the director distortion occupies a larger area than for the ring defect. Therefore, to simulate the satellite defect, one needs very large systems. We used 1.000.000 particles with droplet radius $R = 15$. The original configuration was prepared with a satellite defect embedded in it: we used approximate analytical solutions for the director field [1] to do this.

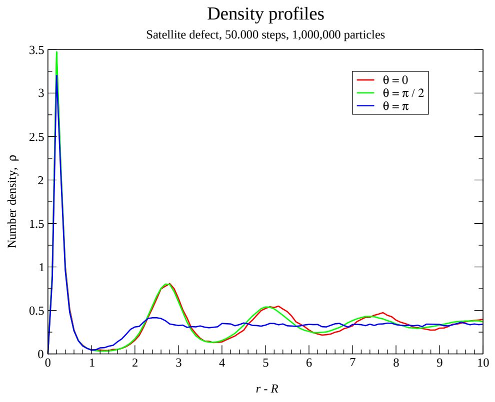

Figure 6 Density profiles. Two directions are shown: $\theta = \pi$ (through the disclination) and $\theta = 0, \pi/2$ (no defect). Since the satellite defect is at $\theta = \pi$ the density profile along this direction does *not* have oscillating structure.

Figure 7 Order parameter profiles for $\theta = 0, \pi/2, \pi$. It is difficult to judge the position of the satellite defect from the order parameter profiles: the region occupied by the disclination core is rather big (of the order of the particle size).

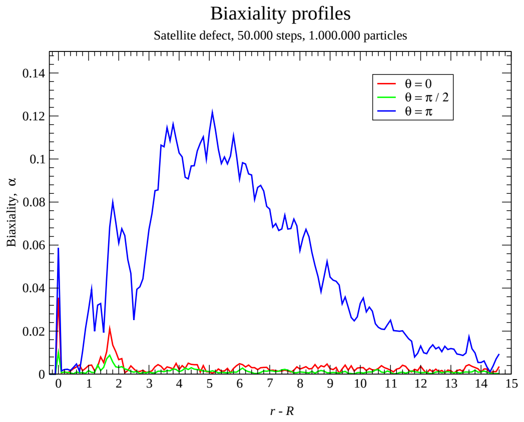

Figure 8 Biaxiality profiles for $\theta = 0, \pi/2, \pi$. From these profiles one can see that the center of the defect core is located at a distance $\approx 1.4R$. The value predicted by theory is about $1.2R$.

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