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Monte Carlo Simulation of Ferronematic Suspensions with Three Elastic Constants

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We report the results of Monte Carlo simulations of the suspension of elongated magnetic particles in a nematic liquid crystal (LC) subjected to an external magnetic field. We deal with a model where the LC host is characterized by a set of directors on a spatially fixed three-dimensional lattice. For elastic free energy of the LC matrix, we use the expression based on the Gruhn-Hess lattice model. Ferroparticles are modeled as long line segments interacting with clusters of LC molecules within the unit cell of the lattice through pair potential similar to that in the Lebwohl-Lasher model.

Keywords: ferronematic; liquid crystal; magnetic field; monte carlo simulations

1. INTRODUCTION

In recent years there has been increasing interest in colloidal dispersions of magnetic particles in a liquid crystal (LC) host (ferronematics). The key property of such systems is the intrinsic high magnetic susceptibility as compared to pure LCs [1–4]. An essential feature in ferronematic (FN) systems is the macroscopic collective

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behavior, or the large-scale molecular reorientation of the entire LC matrix, in a varying magnetic field. Owing to these causes, such systems are very promising for ultra-sensitive magnetically controlled LC devices for information processing and storage.

Stable ferronematics were synthesized first employing the lyotropic LC (mixture of potassium laurate, 1-decanol, and water) and ferromagnetic quasi-spherical maghemite nanoparticles [5,6], and then using the thermotropic pentylcyanobiphenyl (5CB) LC and ultra-small elongated magnetite particles [7]. The first theory for a FN system was proposed by Brochard and de Gennes [1] and then generalized by Burylov and Raikher [8] to the case of a finite anchoring energy of the nematic at the ferroparticle surface. The mechanism of ferronematic reorientation in an external magnetic field for lyotropic FN systems was suggested by Morozov [9]. We note that existing continuum theories of FNs describe the nematic orientation profiles, induced by colloids, in two-dimensions assuming that the local director field distortion in the neighbourhood of the ferroparticle may be disregarded (this is true for many real systems).

One of the approaches for the investigation of ferronematics is computer simulation [10–13]. Monte Carlo (MC) simulation is an attractive technique to study 3D systems. This technique has been used in the papers on modeling a spherical colloid particle [10] or polymer fibrils [13] in a LC host.

In this work we report the results of MC simulations of the dilute suspension of elongated magnetic particles in a nematic host subjected to an external magnetic field. We assume that particles do not interact directly. To the best of our knowledge, we pioneered in applying MC simulations to study the behavior of the FN suspension in a varying magnetic field. A peculiarity of simulations is that we allow the free choice of the three elastic (Frank) constants of LC.

2. SIMULATION MODEL

We consider a nematic cell of thickness D confined between two parallel plates and filled with FN. We set the z-axis perpendicular to the plates. LC is characterized by a set of directors (three dimensional "headless spins") on a spatially fixed three-dimensional lattice. As in the Lebwohl-Lasher (LL) model [14], spins (clusters of nematic molecules) can freely rotate. Magnetic particles (rod-like micron-sized monodomain ferrite grains of length L) are modeled as long line segments (rods), which can move by translation in all directions and rotation. In this work we suppose strong homeotropic anchoring at the lower ($z = 0$) and upper ($z = D$) cell planes and periodic boundary

conditions with identical replicas surrounding the cell in the x- and y-directions. We also suppose a finite anchoring energy of the nematic at the ferroparticle surface. The cell is initially subject to a small bias magnetic field $(-H_b, 0, 0)$. The role of this field is to initially align particles in the x-direction [8]. An external magnetic field H normal to the cell planes rotates the ferroparticles, producing distortions within the LC matrix.

The discretized free energy of FN for our simulation:

$$F = \sum_{i,j,k} E_{el}^{(i,j,k)} l^3 - \sum_p M\left(\hat{\mathbf{m}}_p \cdot \mathbf{H}_s\right) + \sum_p \sum_{\langle i,j,k \rangle} f_p^{(i,j,k)}, \tag{1}$$

where $\langle i,j,k \rangle$ denotes a summation over all neighbors of the ferroparticle p within the potential cutoff, l is the distance of two neighboring lattice points, M is the absolute value of the particle magnetic moment, $\hat{\mathbf{m}}_p$ is the unit vector in the sample magnetization direction, and $\mathbf{H}_s = \mathbf{H} + \mathbf{H}_b$. For elastic (Frank) free energy of the LC matrix E_{el}, we use the expression based on asymmetric discretizations of the spatial derivatives in a free energy functional (Gruhn-Hess lattice model [15]). Note that in that way we correctly take into account three elastic constants (K_{11}, K_{22} and K_{33}) in the Frank free energy of the FN system. Spins, each represents the director within the cluster of LC molecules, interact with ferroparticles through pair potential f_p similar to that in the LL model. We suppose the anchoring of finite strength W_p of nematic molecules at the ferroparticle surfaces. The contribution from the nematic diamagnetic susceptibility to F is small in magnetic field under consideration ($H_s < 100\,\mathrm{Oe}$) and is disregarded here.

In our simulations we used the dimensionless quantities $F^* = 2F/l\,K_{33},\ h = MH/k_BT,\ h_b = MH_b/k_BT,\ T^* = 2k_BT/l\,K_{33}$ and $f_p^* = 2f_p/l\,K_{33};\ T$ is the temperature and k_B is the Boltzmann constant. From here on, we shall use the dimensionless distance of two neighboring lattice points (set equal to unity) as a unit for measurement of distance.

Potential f_p^* was modeled as $f_p^{*(i,j,k)} = -f(s)\,P_2(\hat{\mathbf{s}} \cdot \hat{\mathbf{e}}_{i\,j\,k})$, where P_2 denotes the second Legendre polynomial, s is the shortest distance between the spin $\hat{\mathbf{e}}_{ijk}$ and the rod (ferroparticle), and $\hat{\mathbf{s}} = \mathbf{s}/s$ We have chosen to write $f(s)$ as $U_p \exp(-Bs)$, where U_p equals $U_p = U > 0$ for $s \le s_c$ and is zero otherwise; B and U are constants and s_c is a cutoff distance. Simulations for thin rod-like particles (with length-to-radius ratio $L_p/r_p \to \infty$) resulted in physically improper equilibrium configuration of the system. We therefore simulated a hard surface of the ferroparticle at a finite effective distance r_p from the rod (r_p close to $1/\sqrt{2}$ in the dimensionless units). For this purpose, it was assumed that U_p is nonzero and equals to U over the range $r_p \le s \le s_c$.

3. NUMERICAL RESULTS AND DISCUSSION

We have performed simulations of FN cell for various lattice sizes and numbers of ferroparticles. In this paper, we show the results for lattice of $N_s = 8 \times 8 \times 64$ spins plus two additional layers of fixed spins at the top and two at the bottom of the cell and $N_p = 7$ ferroparticles. To find the state of the lowest energy and avoid local energy minima in the process, we used the method of simulated annealing [10].

We started at the lowest field strength H from the state where the spins have random orientation but the ferroparticles are distributed uniformly in the cell volume and their long axes are aligned along the x-axis. For subsequent values of H we started from a configuration equilibrated at the previous field strength H. The system was cooled gradually down from the dimensionless temperature $T_0^* \sim 0.2$ to T_R^* corresponding to the temperature $T \approx 298\,\mathrm{K}$.

Each MC sweep consisted of attempted particle rotations, translations, and spin rotations. The total run length was at least 7.5×10^5 MC sweeps. After equilibration of the system at $T^* = T_R^*$, a set of further $\sim 1.9 \times 10^5$ MC sweeps was used to accumulate averages. The acceptance rate was about 50% for particle and spin moves to obtain the best results.

To compare the results of MC simulations and continuum theory, we accepted $l = 83\,\mathrm{nm}$ and used the following plausible FN parameters: $L = 0.332\,\mu\mathrm{m}$, $L_p/(2r_p) = 2.83$, $K_{33} = 7.5 \times 10^{-7}\,\mathrm{dyn}$, $K_{11}/K_{33} = 0.8$, $K_{22}/K_{33} = 0.53$ (MBBA) [8] and $M_s \sim 40\,\mathrm{G}$ (the saturation magnetization of the particle substance). In these parameters we find $v \approx 4.4 \times 10^{-15}\,\mathrm{cm}^3$ (the volume of the particle) and $D = (N_z + 1)l = 5.4\,\mu\mathrm{m}$ (the thickness of the cell), where $N_z = 64$ is the number of spins in the z-direction. We set $B = 4$ and $U_p = \frac{1}{3} W_p l C / K_{33}$, where $C = 20.1$.

It is well known that the individual particles distort the orientational structure of the LC matrix within the distance $\xi \approx \sqrt{K_{33}/(W_p c S)}$ [16], where $S = \pi d(L + d)$ is the surface area of the particle and c is the volume number concentration. For long distances from the individual particle a distortion is screened out due to the presence of the other particles. When the regions of distortions are overlapped, the interactions between the ferroparticles arise. This effect is called macroscopic collective behavior [1,16].

Our simulations were performed for the intermediate (Figs. 1, 2) and weak nematic-director anchoring strengths (Fig. 3(a)). The volume number concentration of ferroparticles $c = N_p/l^2 D = 2.9 \times 10^{12}\,\mathrm{cm}^{-3}$ and the corresponding screening distance ξ is equal to $1.24\,\mu\mathrm{m}$ ($< D$) and $5.55\,\mu\mathrm{m}$ ($> D$), respectively.

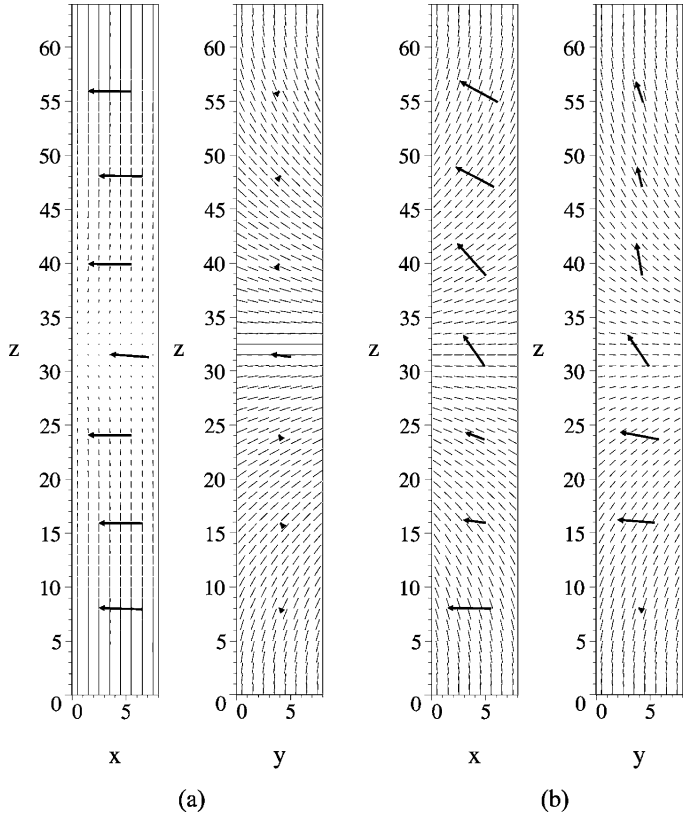

FIGURE 1 Projections of the director and particle configuration in the middle cross sections of the cell after equilibration of the system. The FN cell is subject to a magnetic field $\mathbf{H}_s = (-H_b, 0, H)$. Snapshots are taken at $h_b = 10$, $h = 20$ (a) and $h = 100$ (b); $U_p = 0.74$ ($W_p = 0.01$ erg cm^{-2}).

Typical snapshots of the ferronematic system after equilibration at $T^* = T_R^* = 0.0132$ are hown in Figures 1, 2 and 3(a) at different magnetic field strengths. When h is increased, the angles of rotation of ferroparticles and the orientational deformations of the LC matrix increase. It is seen from snapshots that the director and particle configurations differ structurally for different magnetic field as well as nematic-particle anchoring strengths. At small values of h and $U_p = 0.74$ (intermediate anchoring) the director's tilt angle increases from 0° (homeotropic orientation) at the lower cell plane to 90° in the middle of the cell and decreases to 0° at the upper plane, with the director rotating mainly in the y-z plane (Fig. 1(a)). At higher values

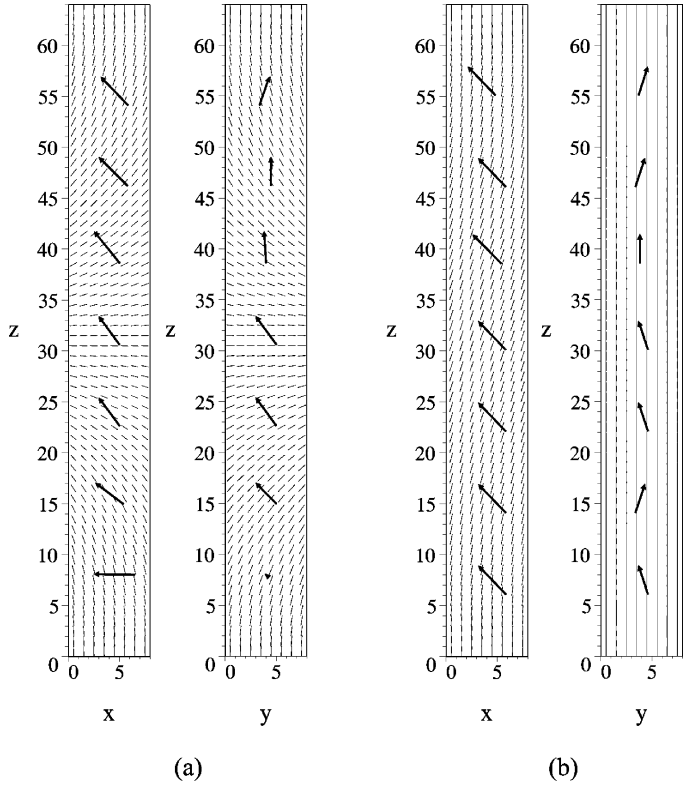

FIGURE 2 The same as Figure 1 for $h_b = 10$, $h = 200$ (a) and $h = 300$ (b).

of h the director rotate between the planes x-z and y-z when moving from one cell plate to the other. In addition the long axes of the ferroparticles leave the x-z plane inside the FN cell (Figs. 1(b) and 2(a)). Possible explanation for the observed behavior is the small extent of the distortion induced by an individual particle (a quarter of the cell thickness).

On further increasing the magnetic field strength the nematic director is decoupled from the ferroparticles and the orientational deformations of the LC matrix decrease (Figs. 2(b) and 3(b)). The angles ϕ_m and ψ_m in Figure 3(b) are measured from the z-axis and the x-axis, respectively, in the x-z plane. Similar phenomenon was found numerically in Ref. [13] and predicted theoretically in Ref. [17].

At sufficiently weak anchoring $\xi > D$ and the orientational distribution of ferroparticles is uniform throughout the height of the FN cell (Fig. 3(a)). In this case the extent of distortion of the nematic

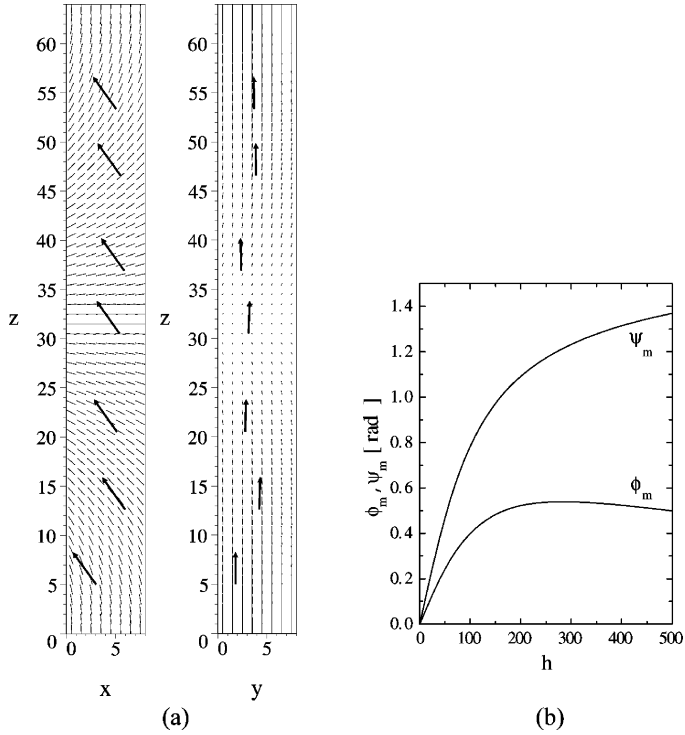

FIGURE 3 (a) Projections of the director and particle equilibrium configuration in the middle cross sections of the cell. Snapshots are taken at $h_b = 10$ and $h = 100$; $U_p = 0.037$ ($W_p = 5 \times 10^{-4}\,\mathrm{erg\,cm^{-2}}$). (b) The angle of maximum deviation of the nematic director inside the cell ϕ_m and the corresponding angle of the ferroparticle ψ_m vs the normalized magnetic field calculated with the continuum theory of FN [8] for $W_p = 0.01\mathrm{erg\,cm^{-2}}$.

orientational order, induced by an individual particle, is greater than the cell thickness.

CONCLUSIONS

In this paper we presented results of MC simulations of the ferronematic cell subject to an external magnetic field. We employed the Gruhn-Hess lattice model and a modification of the Lebwohl-Lasher potential for interaction between clusters of the LC molecules and the ferroparticle surface. Our simulations demonstrated that, depending on nematic-particle anchoring and magnetic field strengths, the FN system can display unexpected physical properties. For intermediate

anchoring strengths we observed a 3D reorientation of the ferroparticles and the nematic director. In moderate magnetic fields the nematic director can decouple from the ferroparticles.

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