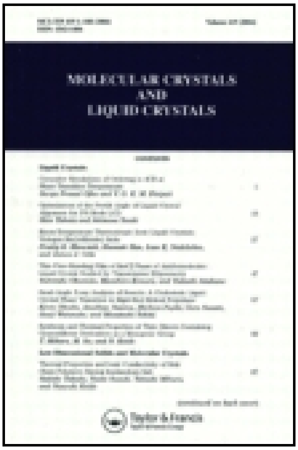

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Cluster Formation of Colloids in Nematics

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Cluster Formation of Colloids in Nematics

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Colloidal suspension show interesting phenomena which are mediated by the solvent. Recently, colloids in nematic liquid crystal phase used as anisotropic solvent have been investigated experimentally and have inspired theoretical work[1–3]. In relation to these work, effective pair potential between spherical colloidal particles suspended in nematic liquid crystals has been suggested[4,5]. The interparticle interaction can cause nontrivial collective behavior that results in formation of new spatial structures in colloidal particle systems. We determine these structures by particle dynamics simulations using these effective pair-interaction.

Keywords: Colloidal particles; Nematic Liquid Crystal Phase

INTRODUCTION

Systems of colloidal particles dispersed in nematic liquid crystal(NLC) give rise to interesting structure. A chain like structure where the colloidal particles line up in a row is one example[1-3]. The type of defects and structure which appear in these systems also give novel information concerning the interaction at the interface *i.e.* the type of anchoring of NLC at the surface of the colloidal particles. Poulin et al[1] concluded that when the surrounding NLC align normal at the surface of the colloidal particles (normal anchoring), the chain structure align along the nematic (N_D) director. On the other hand, planar alignment (planer anchoring) at the colloidal surface give rise to chains inclined roughly $\pm$ 30° from the nematic (N_C) director.

To describe the interaction working between the colloidal particles, several pairwise potentials have been suggested[2,4,5]. Among these potentials, colloidal interactions arising purely from the anisotropic elastic energy of the host fluid, *i.e.* the surrounding NLC, are reported in [4,5]. They separate the effect of physical properties of the colloidal particle itself (such as charge, dipole moment, etc.) and try to determine the nature of the interparticle interaction due to the anchoring strength and the direction of anisotropy of the host fluid alone.

In a situation where 3 body effect is absent or negligible, the proposed potentials can be used as pairwise additive potentials to investigate many body systems. This paper treats such case, and obtain some possible stable configurations of colloidal clusters in NLC's.

MODEL AND METHODS

In this work, we use two models which consider the elastic deformation energy of nematics and the anchoring energy at the surface of the colloidal particle. The essence of the models [4,5] are given by the pair-wise colloidal interaction potentials

$$\begin{aligned} U_{ij} &= \frac{d}{r_{ij}^5}(9 - 20\cos 2\theta_{ij} + 35\cos 4\theta_{ij}) \\ &= \frac{d}{r_{ij}^5}(64 - 320\cos^2\theta_{ij} + 280\cos^4\theta_{ij}) \end{aligned} \tag{1}$$

[4] and

$$U_{ij} = \frac{d}{r_{ij}^5}(3 - 30\cos^2\theta_{ij} + 35\cos^4\theta_{ij}) \tag{2}$$

[5] respectively, where r_{ij} is the distance between particles i and j, and θ_{ij} is the angle of the r_{ij} against the background nematic director. We take the nematic director to be parallel to the z-direction; $\cos\theta_{ij} = (\mathbf{r}_{ij}\cdot\mathbf{z})/|\mathbf{r}_{ij}|$ where $\mathbf{z}$ is the unit vector in z-direction.

The above potential do not contain the excluded volume of the colloid, thus not suited for dense concentration of colloids. We add a term $(d/r_{ij})^{-12}$ which represent the colloidal core to overcome this situation. This term avoids the colloids to collapse into each other when attractive force are working between particle i and j. The two potentials Eqs.(1) and (2) with the term $(d/r_{ij})^{-12}$ representing the core of the particles (U'_{ij}), are called model I and II, respectively, throughout this article. We conduct particle dynamics simulation to obtain possible stable configurations of the colloidal particles in NLC. No boundary condition have been applied so the particles freely expand in space. During particle dynamics simulations, particles are moved with kinetic energy $T^* = 1$ using the 6-value 2nd order Gear predictor-corrector algorithm, until all the particles halt and attain total potential energy $U_i = \sum_{j \neq i} U'_{ij} = 0$. Interaction between particles whthin the distance of $10d$ are all considered. In other words, the cut-off length in the simulation is $10d$. We start from the same initial conditions in each case for both model I and II, and compare the final stable configurations.

RESULTS

In multi-body clusters, even strong repulsive forces can cancel out by neighboring particles in the opposite direction. So there is a possibility that even clusters including i-j pairs with repulsive interaction can stabilize due to other neighboring particle interaction. We show such several stabilized clusters in the following which are not reported in [6].

Fig. 1 show clusters of N=20 colloidal particles arising from models I and II. Particles are initially aligned in a zig-zag configuration. The particles expanded to give a structure consistent of three chains approximately parallel to the director as shown in Fig. 1. Note that models I and II can not give rise to a isolated single chain parallel to the director of colloidal particles since the pair-wise interactions only yield repulsive force when two particles i and j align along the director($\theta_{ij} = 0$). However the clusters can give rise to chain structures due to the neighboring particles. The particles in oblique direction in the neighboring chains are the source of attractive forces which stabilize the chain structure in this case. As evident in Fig.1(a) and (c), the chains are approximately parallel to the director. Since models I and II assume normal anchoring as an easy axis, this result is in accord with the experimental results reported in [1]. Although these results seem to be different from experimental results in a sense that the chain structure of colloids seems to be fairly isolated from other colloidal particles in experiments (Fig.3(a) of [1]). In experiment [1] the nematic orientation is induced by a wedge. We suggest that there might be a possibility that the walls of the wedge have significant effect (similar to that of the neighboring particles in our simulation) to the colloidal chain structure.

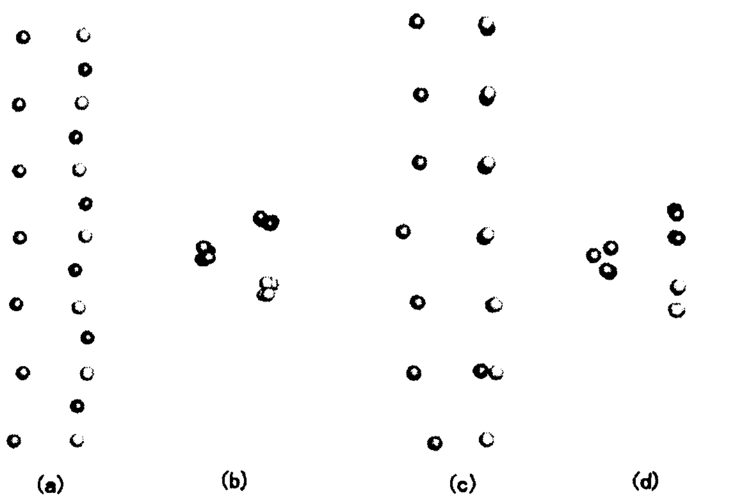

FIGURE 1 Configuration for N=20 obtained for models I((a), (b)) and II((c), (d)); In (a) and (c) director is parallel to vertical axis (side view). In (b) and (d) director is perpendicular to the plane of figure (bird view). Different tone of gray-scale are used to distinguish different chain structure.

Figure 2 show stable configurations obtained for $N = 16$. The initial configuration was 4 layers of a rhombus stacked alternately as one edge particle become in the middle of the next rhombus. Both models give rise to layer structures perpendicular to the director. Model I give rise to a stable configuration with 3 layers;a middle layer of hexatic like structure sandwiched by two layers of deformed rhombi. In contrast, model II give rise to a two layer structure with both layers having a triangular lattice like structure shifted from each other. For both models, alignment in direction perpendicular to the director ($\cos\theta_{ij} = 0$), give rise to repulsive interaction. So the particles in the same layer, should be stabilized by particles in other layers or by not aligning truly perpendicular to the director.

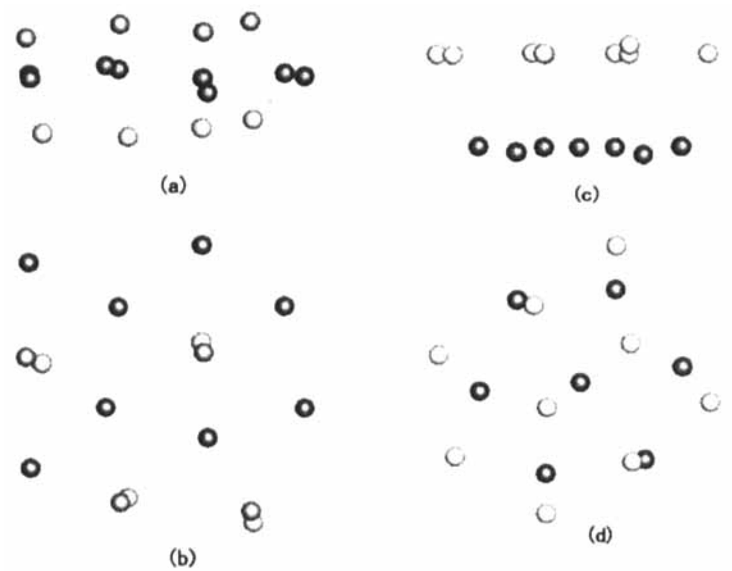

FIGURE 2 Configuration for N=16 obtained for models I((a), (b)) and II((c), (d)); In (a) and (c) director is parallel to vertical axis (side view). In (b) and (d) director is perpendicular to the plane of figure (bird view). Different tone of gray scale are used to distinguish different layers.

Depending on the initial configuration, sometimes beautiful configurations with nearly complete symmetry appear in these colloidal clusters. In the case where an double-shell icosahedron is used as initial configuration, the final stable configurations are shown in Fig. 3. It is interesting that even clusters with quite complicated symmetry can appear with special initial configuration.

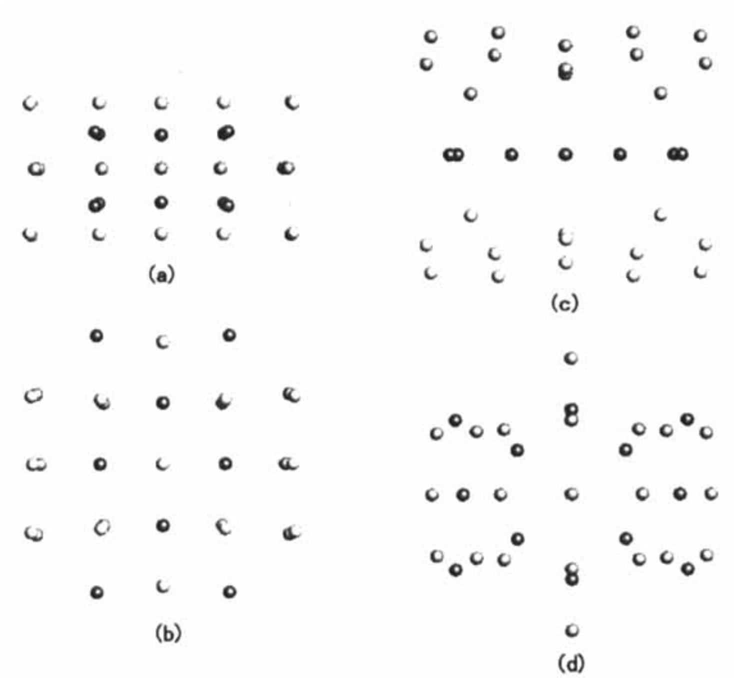

FIGURE 3 Configuration for N=55 obtained for models I((a), (b)) and II((c), (d)); In (a) and (c) director is parallel to vertical axis (side view). In (b) and (d) director is perpendicular to the plane of figure (bird view).

CONCLUDING REMARKS

We have conducted particle dynamics simulation to obtain possible colloidal cluster structures in nematics, using model effective potentials which consider the elastic deformation energies with anchoring energies at the colloidal surface. The simulations in this paper only treat the effective interaction between the colloidal particles and obtain stabilized configurations when all particles attain total energy $U_i = 0$. So to discuss which final configurations are more energetically favorable can not be done within the exent of this work:it can only be done through comparison of the energy of the background nematic director field. However, when a dynamical evolution from the same initial configuration is conducted, the arising difference for models I and II not only deepen our understanding of both models but also suggests that even pair-additive multi-body effects can lead to quit complicated results which is difficult to perceive by just examining the pair potential itself.

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