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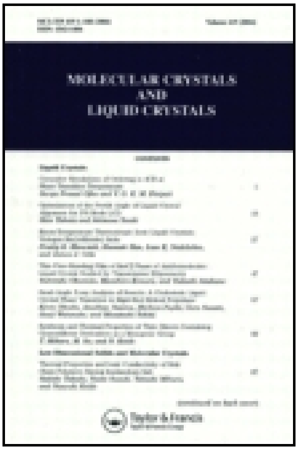

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How to Simulate Anchoring: Confining the Director

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How to Simulate Anchoring: Confining the Director

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We present a method to manipulate the average direction of linear model molecules. In contrast to a hard constraint, we use a soft confinement potential linked to the director orientation. The method is applied to a mixture of Gay-Berne molecules at high density, where smectic demixing occurs. Other possible applications, such as the simulation of " easy directions" in anchoring and the evaluation of elastic coefficients, are discussed.

1 CONFLICTING DIRECTIONS IN MODEL SYSTEMS

A simulation box defines a number of preferred directions. In the case of a cubic box these are the box sides, the space diagonal, and the diagonals of compound boxes made up of a row or column of periodic replicas of the basic cell. Quite generally, the introduction of periodic cells entails a spurious crystalline structure, and the Bragg angles of that crystal are "preferred" in some ill-defined way. The extent to which this artificial anisotropy may affect the calculated averages has been discussed before [1], but was never assessed in a definitive manner.

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An additional complication arises when the molecules are themselves carrying a directional vector. If at some density and temperature the particles tend to align more or less parallel to each other, then the predominant orientation – the *director* **d** – must compete with the predefined directions due to the geometry of the simulation box.

We have encountered this problem when simulating a mixture of ellipsoidal Gay-Berne molecules [2] of different length-to-width ratios l/d. An equimolar mixture of such particles, with $l/d = 3.0$ and 1.5 (the latter being nearly spherical) displays spontaneous demixing at high density. This separation leads to an alternating sequence of layers of pure components, with a layer normal that is approximately equal to the director of the longer particle species.

However, these smectic layers are stable only as long as their normal vector **s** points into one of the Bragg directions. Moreover, the period Δs of the layers must coincide with the Fourier wavelength λ of that Bragg mode. If one of these conditions is not met, the periodic boundary conditions act to disrupt the layered structure. Since the reorientational motion of the director is very slow, it then takes a long time until a new allowed orientation can be found and the layers reappear.

Even if a successful lock-in has occured, the resulting structure is stable only at the given density. In the course of a simulation experiment the system is frequently compressed or expanded. This gives rise to changes in the Fourier-Bragg wavelengths, and in consequence to a mismatch between Δs and λ.

It may seem that the source of these difficulties is the use of constant volume ensembles (NVT and NVE) in the simulations, and that in constant pressure experiments a match between Δs and λ could be attained more easily. To investigate this point we are currently preparing (NpT) Monte Carlo simulations on the same systems as studied here. However, we do not expect a marked technical advantage from such an approach, for the following reason. On compression the *average* volume at any given pressure will change in much the same manner as the exact volume in an (NV) experiment, and the fluctuation of the volume around that average tends to be small at fluid densities. The situation with regard to eligible Bragg angles and Fourier modes thus remains the same as in (NV) ensembles.

It seemed desirable, then, to investigate more closely the inter-

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action between the director, the nematic normal, and the various preferred orientations in the simulated system. To this end we devised a method that permits the manipulation of the director.

In his investigations of model nematics, Allen [3] suggested to constrain the director such that it is at all times oriented along some given vector, which he took to be one axis of the box. Sarman et al., in their nonequilibrium calculations on sheared nematics, used an equivalent method [4].

"Hard" constraints of some kind or other have been used by simulators for a long time. Ryckaert et al. [5] showed how to include holonomic constraints in an efficient manner in the multiparticle dynamics. However, it should be kept in mind that hard constraints define an ensemble which may be inappropriate to the given physical problem. In extreme cases, of which the original application of Ryckaert's method, i.e. flexible chains with rigid bond lengths, is an example, averages over this modified ensemble may deviate considerably from the canonical averages.

It is sometimes unavoidable to resort to hard constraints. In chain molecules, for instance, the bonds between successive atomic groups could alternatively be confined to a narrow interval by the use of strong springs. However, the fast oscillations of these springs would require an extremely small time step, rendering the method inefficient. In contrast, the fluctuations of a collective property such as the director are usually rather slow as compared to the single particle dynamics. We have no reason, therefore, to apply hard, unphysical constraints. It seems more natural to keep the director aligned near some desired orientation by an appropriately defined smooth potential.

2 DIRECTOR POTENTIAL AND TORQUE

The director in a system of linear molecules with individual orientation vectors $\mathbf{u}_i$, $i = 1, \ldots N$ is usually defined in terms of the order tensor $\mathbf{Q}$ with elements

$$Q_{\alpha\beta} = \frac{3}{2N} u_{i\alpha} u_{i\beta} - \frac{1}{2}\delta_{\alpha\beta} \qquad (1)$$

where the summation over double indices is implied. If λ_1 is the

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largest eigenvalue of **Q** (i.e.the *order parameter*), then the corresponding eigenvector is the director **d**.

Consider a potential of the form

$$U_d = c\,|\mathbf{d} - \mathbf{d}_0|^2 \qquad (2)$$

where $\mathbf{d}_0$ is a unit vector defining the desired orientation of the director **d**. By adding such a potential to the system Hamiltonian we can keep the director in the vicinity of $\mathbf{d}_0$.

We note in passing that the added potential (2) is linked only to the orientation of the director **d**, and not to the order parameter $P_2 \equiv \lambda_1$. The molecules are thus not forced to align their individual direction vectors parallel to each other; only the average orientation of their main axes is manipulated. A differently defined potential might include a factor proportional to some even power of P_2, mimicking the action of an aligning field.

Since **d** is the eigenvector corresponding to the *largest* eigenvalue of **Q**, and the distinction of being the largest may sometimes go from one eigenvalue to another, the director is apt to make discontinuous jumps over angles of $\pi/2$. In such cases the director confinement energy will also change discontinuously. However, such erratic behaviour can occur only for low values of the order parameter, i.e. just in those cases when the physical significance of the director is nil. Whenever the molecules are to some extent aligned, a cross-over of the largest and second largest eigenvalues of **Q** is very improbable.

In the framework of a Monte Carlo simulation it is sufficient to include the additional potential energy given by equ. 2 in the evaluation of the transition probabilities. In the molecular dynamics setting we also need, for each particle k, the torque deriving from the potential 2. Writing $\mathbf{e} \equiv \mathbf{d} - \mathbf{d}_0$, this torque is given by

$$\mathbf{T}_k = -\mathbf{u}_k \times \nabla_k U_d == -2c\mathbf{u}_k \times (\nabla_k \mathbf{d}) \cdot \mathbf{e} \qquad (3)$$

where ∇_k is the derivative with respect to the orientation vector of particle k. In component notation, the torque is

$$T_{k\eta} = -2cA_{\eta\beta\gamma}u_{k\beta}\frac{\partial d_\alpha}{\partial u_{k\gamma}}e_\alpha \qquad (4)$$

where $A_{\eta\beta\gamma}$ are the elements (0 or ±1) of the Levi-Civita pseudotensor **A** defining the vector product.

When it comes to differentiate **d** with respect to the components $u_{k\eta}$ of the individual vectors $\mathbf{u}_k$, we encounter the difficulty that neither **d** nor λ are given as explicit, differentiable expressions, but are rather implicitly defined as solutions to the eigenvector and eigenvalue equations of **Q**.

Let us consider the eigenvalues first. They are readily computed as the 3 solutions to

$$F(\{\mathbf{u}_i, \lambda\}) \equiv |\mathbf{Q}(\{\mathbf{u}_i\}) - \lambda \mathbf{I}| = 0 \tag{5}$$

To compute the derivative $\partial\lambda/\partial u_{k\eta}$ of any of the eigenvalues we use the theorem on implicit functions, $\partial\lambda/\partial u_{k\eta} = -(\partial F/\partial u_{k\eta})/(\partial F/\partial\lambda)$. Writing out the determinant F and using the notation $S_{\alpha\beta} \equiv Q_{\alpha\beta} - \lambda\delta_{\alpha\beta}$, we have

$$F(\{\mathbf{u}_i, \lambda\}) = S_{xx}S_{yy}S_{zz} + 2S_{xy}S_{xz}S_{yz} - S_{xy}^2S_{zz} - S_{xz}^2S_{yy} - S_{yz}^2S_{xx} \tag{6}$$

Using $\partial Q_{\alpha\beta}/\partial u_{k\eta} = (3/2N)(u_{k\alpha}\delta_{\beta\eta} + u_{k\beta}\delta_{\alpha\eta})$, we find for the required partial derivatives

$$\begin{aligned}\frac{\partial F}{\partial u_{kx}} &= \frac{3}{N}\Big[u_{kx}(S_{yy}S_{zz} - S_{yz}^2) + u_{ky}(S_{xz}S_{yz} - S_{xy}S_{zz}) \\ &\quad + u_{kz}(S_{xy}S_{yz} - S_{xz}S_{yy})\Big]\end{aligned} \tag{7}$$

et mut. mut., and

$$\frac{\partial F}{\partial\lambda} = -S_{yy}S_{zz} - S_{xx}S_{zz} - S_{xx}S_{yy} + S_{xz}^2 + S_{xy}^2 + S_{yz}^2 \tag{8}$$

Next we treat the director **d**. Application of the implicit functions theorem would be possible, but is unnecessarily complicated. Instead, we construct an explicit expression for the components d_β of the director in terms of $u_{k\eta}$ [4]. Such an expression can be found from the eigenvector equation

$$[\mathbf{Q} - \lambda_1\mathbf{I}] \cdot \mathbf{d} = 0 \tag{9}$$

which states that every row of the matrix $\mathbf{S} = \mathbf{Q} - \lambda_1\mathbf{I}$ is orthogonal to **d**. (λ_1 is now the *largest* of the three eigenvalues.) Accordingly, we can write **d** as the normalized vector product of two such rows, say $\mathbf{S}_x$ and $\mathbf{S}_y$ [4]:

$$\mathbf{d} = (\mathbf{S}_x \times \mathbf{S}_y)\,|\mathbf{S}_x \times \mathbf{S}_y|^{-1} \tag{10}$$

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In component notation, the row vectors $\mathbf{S}_x$ and $\mathbf{S}_y$ are given by

$$S_{\alpha\beta} = \frac{3}{2N} u_{i\alpha} u_{i\beta} - \left(\lambda_1 + \frac{1}{2}\right) \delta_{\alpha\beta} \ , \quad \alpha = x, y; \ \beta = x, y, z \qquad (11)$$

The pertinent derivatives of $S_{\alpha\beta}$ may now be evaluated according to

$$\frac{\partial S_{\alpha\beta}}{\partial u_{k\eta}} = \frac{3}{2N} \left[u_{k\alpha} \delta_{\beta\eta} + u_{k\beta} \delta_{\alpha\eta} \right] - \frac{\partial \lambda_1}{\partial u_{k\eta}} \delta_{\alpha\beta} \ , \quad \alpha = x, y; \ \ \eta, \beta = x, y, z \qquad (12)$$

for $k = 1, \ldots N$.

Rewriting the unnormalized director $\mathbf{d}' \equiv \mathbf{S}_x \times \mathbf{S}_y$ in component notation, we have

$$d'_\beta \equiv \{\mathbf{S}_x \times \mathbf{S}_y\}_\beta = A_{\beta\gamma\epsilon} S_{x\gamma} S_{y\epsilon} \qquad (13)$$

The 9 elements of $\nabla_k \mathbf{d}'$ are then

$$D_{\eta\beta} \equiv \frac{\partial d'_\beta}{\partial u_{k\eta}} = A_{\beta\gamma\epsilon} \left[\frac{\partial S_{x\gamma}}{\partial u_{k\eta}} S_{y\epsilon} + \frac{\partial S_{y\epsilon}}{\partial u_{k\eta}} S_{x\gamma} \right] \qquad (14)$$

where the expressions for $\partial S_{x\gamma} / \partial u_{k\eta}$ etc. may be inserted from 12. Finally, the derivative of the normalized vector $\mathbf{d}$ is obtained from

$$\frac{\partial d_\beta}{\partial u_{k\eta}} = D_{\eta\beta} \left| \mathbf{d}' \right|^{-1} - d'_\beta \left| \mathbf{d}' \right|^{-3} D_{\eta\epsilon} d'_\epsilon \qquad (15)$$

A procedure for confined director dynamics then consists of the following steps:

- Given all momentary molecular orientations, compute the 9 elements $Q_{\alpha\beta}$ of the order matrix (equ. 1), the order parameter λ_1 (eq. 5), and the 2×3 elements $S_{x\beta}$, $S_{y\beta}$ of the first two rows in $\mathbf{S}$ (equ. 11).

- For each particle k, compute the 3 elements of $\partial \lambda_1 / \partial u_{k\eta}$ (using $\partial \lambda / \partial u_{k\eta} = -\left(\partial F / \partial u_{k\eta} \right) / \left(\partial F / \partial \lambda \right)$ and equs. 7-8), the 18 elements $\partial S_{\alpha\beta} / \partial u_{k\eta}$ (equ. 12), and from these the 9 components $\partial d_\beta / \partial u_{k\eta}$ of $\nabla_k \mathbf{d}$ (equ. 15).

- The torque acting on particle k can now be evaluated using equ. 3. It is added to the mechanical torques due to the anisotropic interparticle potential.

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3 APPLICATION TO A GAY-BERNE MIXTURE

An equimolar mixture of Gay-Berne molecules with lengths $\sigma_p = 3.0$ (species 1) and 1.5 (species 2) was investigated. MC calculations using $N = 512$ particles as well as MD simulations with $N = 500$ and 864 were performed. The MC simulations are part of a thorough investigation of the structure and thermodynamics of Gay-Berne systems in the range $l/d = 1.5 \ldots 5.0$, both pure and mixed [6].

The usual parametrisation of the GB potential was applied, with $\mu = 2$, $\nu = 1$, and $epsilon_{ss}/\epsilon_{ee} = 5$ (see [7]); the Lorentz-Berthelot rule was applied in defining the interaction between unlike particles.

Preparatory simulations: For a test of the confined director method we chose the isotherm $T = 1.25$, which in the case of a pure species-1 system would correspond to a supercritical fluid (see [7]). The density of the system was slowly increased, with frequent re-expansion and -compression over moderate density intervals, so as to avoid metastable, glassy states. In the density interval $\rho = 0.48 - 0.56$ the system clearly goes from a isotropic to a nematic, then to a smectically demixed state. This is evident from a steep increase of the order parameter P_2, from a distinctly oscillatory structure of the species-1 pair correlation function projected onto the director, and finally from the visual inspection of the particle configurations (Figures 1-4). Alternating layers of pure 1- and 2- phases appeared in which the longer particles were well aligned (with an order parameter in the range $0.7 - 0.9$), while the shorter molecules had no significant orientational order; in fact, they tended to "lie down" in the plane of their layers.

In their investigations of bidisperse Gay-Berne fluids, Bemrose et al. [8] did not encounter smectic demixing. However, in that study the two particle species were of similar lengths (3.0 and 3.5); the tendency to demix is probably linked to the more or less spherical shape of one of the components.

Upon close scrutiny we found that in the $N = 512$ system the director for the species-1 particles, $\mathbf{d}(1)$, did not coincide with the

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smectic vector **s**. It was suspected [9] that this smectic C phase was just an artefact of the simulation, created by the interplay of molecular and cell geometry. It must be remembered that regular layers of single species can only develop if their normal vectors are pointing into Bragg orientations of the supercrystal made up by the periodic cells.

Indeed, the smectic vector $\mathbf{s} \approx (-0.29, 0.91, 0.31)$ which had developed spontaneously at compression to $\rho = 0.55$ is reasonably near to the Bragg-allowed Fourier vector $\mathbf{k}_0 = (-1/3/1)/\sqrt{11} = (-0.30, 0.90, 0.30)$. At that density this arrangement allowed for four smectic layers within the periodic cell, with a distance of only $\Delta s = 2.94$ between successive layers. Such a distance is obviously insufficient to accomodate a layer of *upright* $\sigma = 3.0$ particles plus a layer of shorter molecules. (Incidentally, the shorter molecules tend to squeeze into the free volumes between the tapering ends of the longer ones, such that a layer period nearer to 3.0 than to 4.0 results). The longer molecules, then, compromise by tilting their director with respect to **s**.

In the $N = 864$ molecular dynamics system at the same density (0.55) the tilted phase did not appear. A smectic vector $\mathbf{s} \approx (-0.24/0.55/0.80)$ formed spontaneously, in agreement with the Bragg Fourier vector $\mathbf{k}_0 = (-1/2/3)/\sqrt{14} = (-0.27/0.53/0.80)$. This allowed for 5 periodic layers with a wave length of $\lambda_k = 3.11$. Thus there was no need for tilting **d** relative to **s**.

Confined director simulations: To study in more detail the influence of cell geometry upon the structure we performed a series of confined director MD simulations with various choices regarding the required director orientation: z-direction, face diagonal, space diagonal, and no required orientation.

It would be preferable to be able to control the smectic vector **s** instead of the director **d**. Such a technique is simple to devise and will be described elsewhere [10]. It consists in introducing a potential which is a function of the Fourier modes of concentration (say, of species 1). By forcing certain Fourier modes to remain small and permitting others to grow, we can favour demixing along the corresponding direction.

For the time being we proceeded on the assumption that **s** would never be very different from **d**. Thus, if **d** is forced to remain in the

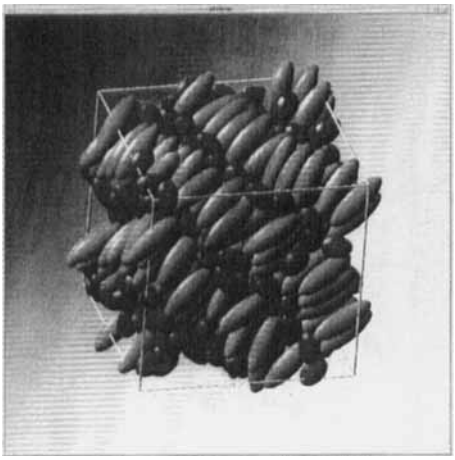

Figure 1: The 000 system at $\rho = 0.56$

proximity of a fixed $\mathbf{d}_0$, then $\mathbf{s}$ will settle for the same or some nearby Bragg-allowed direction. Depending on the Fourier wavelength of that Bragg mode, the $\sigma = 3.0$ particles can be accomodated either parallel to $\mathbf{s}$ or tilted.

The onset of smectic ordering was detected in the following manner. Let L be the side length of the cubic cell, and let

$$\rho(\mathbf{k}) \equiv \frac{1}{L^3} \sum_{j=1}^{N_1} e^{-i\mathbf{k} \cdot \mathbf{r}_j} \tag{16}$$

denote the Fourier component of the species-1 concentration corresponding to a Fourier vector $\mathbf{k}$. A high value of some $S(\mathbf{k}) \equiv |\rho(\mathbf{k})|^2$ will then indicate the presence of a planar concentration mode with wave vector $\mathbf{k}$.

The periodic boundary conditions impose restrictions on the Fourier vectors $\mathbf{k}$. Only "Bragg-allowed" vectors need be taken into account. These Bragg vectors have components $2\pi k_{x,y,z}/L$, with the integers $k_x, k_y, k_z \epsilon [-k_{max}, k_{max}]$. The zero vector is excluded, and for symmetry reasons ($\mathbf{k} \rightarrow -\mathbf{k}$) one of the components, say k_z, may be

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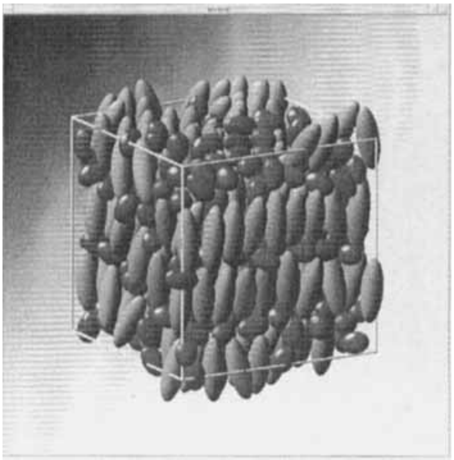

Figure 2: The 001_0 system at $\rho = 0.56$

restricted to non-negative values. For the same reason, if $k_z = 0$, then $k_y > 0$, and if $k_z = k_y = 0$, then $k_x > 0$. Considering these selection rules, the total number of relevant Bragg vectors is

$$K = k_{max}\left[1 + (2k_{max} + 1) + (2k_{max} + 1)^2\right] \qquad (17)$$

For $k_{max} = 2/3/4/5$, $K = 62/171/364/665$. The wave number corresponding to $\mathbf{k}$ is $k = 2\pi\sqrt{k_x^2 + k_y^2 + k_z^2}/L$.

We ordered the $S(\mathbf{k})$ by value and watched out for the appearance of a single high maximum $S_0 \equiv max_{\mathbf{k}}(S(\mathbf{k}))$; the respective vector $\mathbf{k}_0$ must be the smectic normal.

Scattering experiments performed on smectics have shown that the concentration (or density) oscillations present in such systems are nearly sinusoidal, leading to a single peak in the experimental $S(\mathbf{k})$.[11] A paraphrase to this experimental fact is our finding that

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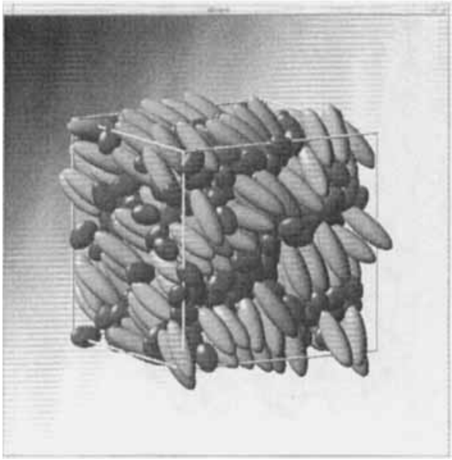

Figure 3: The 011_0 system at $\rho = 0.56$

S_0 was generally much higher than the next smaller $S(\mathbf{k})$.

4 RESULTS

The thermodynamic state $\rho = 0.56$, $T = 1.25$, just above the nematic-smectic transition, was studied in detail. The total number of particles in the equimolar mixture was $N = 500$. Four sets of simulations were performed, with the required directors chosen as follows: $\mathbf{d}_0 = (0,0,1)$, $(0,1,1)$, $(1,1,1)$, and none. Each set was started at density $\rho = 0.1$; as in the preparatory simulations, care was taken to avoid metastable states during the compression stage.

The results of these simulations may be summarized as follows:

- The method of "softly" confined (vs. strictly constrained) directors was found to be feasible and efficient. The configuration snapshots in Figs. 1-4 clearly show the formation of smectic, demixed layers whose normal vectors point in the approximate

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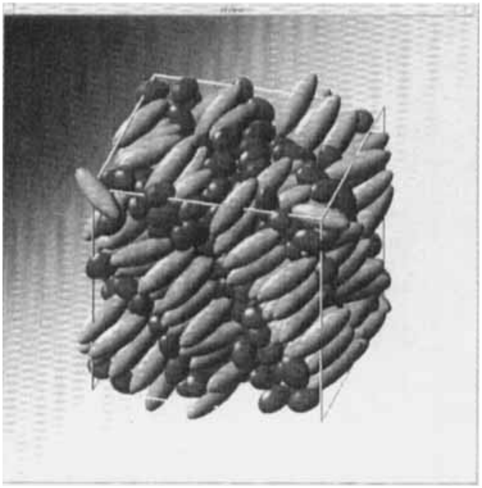

Figure 4: The 111_0 system at $\rho = 0.56$

direction of the required director. Quantitative insight may be gained from $g_{||}$, i. e. the strongly oscillating pair correlation function of the longer particles, resolved parallel to the actual director; and by the "smectic ratio" S_0/S_1 between the largest and the second largest Fourier component of the species-1 concentration (see Table of results).

- The coupling coefficient c in (2) was adjusted experimentally so as to keep $\mathbf{d}$ aligned near $\mathbf{d}_0$; values of c in the range $100 - 120$ were used at different stages of the compression-decompression steps. When the systems had reached their equilibrium layered configurations at $\rho = 0.56$, the value of c was set to zero, and an additional equilibration run was performed. As expected, the layers remained stable at that density, indicating that the respective configuration was at least metastable. The thermodynamic data given in the Table show that all final states have comparable pressures and energies.

- Run 000: no director potential; the system was free to find an optimal Bragg vector to lock in to. It settled for $\mathbf{k}_0 = (2,1,2)/3$, with a natural period of $\lambda_0 = 3.21$. The actual period of the layers, as determined from $g_{||}$, was 3.17, and the angle between the director of the species-1 particles and the smectic layer normal was small: 3.48^0.

- Runs 001 and 001_0: Desired director $\mathbf{d}_0 = (0,0,1)$. The optimal Bragg vector to lock in was $\mathbf{k}_0 = (0,-1,3)/\sqrt{10}$, with a natural wave length of 3.045. Layer period: $\Delta s = 3.11$; the director is distinctly tilted with respect to the smectic normal: 11.0^0 while the potential was on, 7.7^0 afterwards. Also, the actual director strayed quite far from the desired director: 7.8^0 and 11.1^0, respectively, with and without director potential.
- Runs 011 and 011_0: $(-1,2,2)/3$ was the stable Bragg vector, with a natural period of 3.21 and an actual layer spacing of 3.2 (3.11 after the potential was switched off). The director is tilted against the smectic normal by some $8-12^0$. The order parameter was smaller than in the 000 and 001 runs, and so was the smectic ratio S_0/S_1 (between the largest and second largest concentration modes); this indicates that the smectic demixing is imperfect. The reason for this is unclear, as the Bragg vector $(-1,2,2)/3$ could easily accomodate clean smectic layers. Conceivably, a small number $(1-2)$ of particles trapped in a metastable, tilted orientation are spoiling the layers.
- Runs 111 and 111_0: In this case the reason for the defective layering is obvious: the Bragg vector $(2,2,2)/\sqrt{12}$ was approached, but with its period of 2.78 it was not suited to accomodate clean demixed layers. Accordingly, the order parameter remained below 0.85 (vs. $0.90-0.91$ in the 000 and 001 runs), and the smectic ratio S_0/S_1 was small. In a system with $N = 690$ instead of 500 the natural wave length of the $(2,2,2)$ mode would be 3.09 (at a density of 0.56). In this case the layers would fit into the Bragg period. A closer study of such a system, as well as a further investigation of the 011-system, will be reported soon.

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Run	000	$001/001_0$	$011/011_0$	$111/111_0$
$P_2(1)$	0.903	0.908/0.912	0.813/0.850	0.797/0.842
$\mathbf{k}_0$	2/1/2	0/ − 1/3	−1/2/2	2/2/2
λ_0	3.210	3.045/3.045	3.212/3.210	2.780/2.780
Δs	3.17	3.11/3.11	3.2/3.11	2.94/3.00
S_0/S_1	20.91	72.50/51.99	3.21/6.35	1.86/1.81
α_1	3.49	10.97/7.714	11.88/0.80	2.13/5.21
α_2	–	18.43/18.43	19.47/19.47	0.00/0.00
α_3	–	7.81/11.14	7.97/19.49	2.13/5.21
T	1.253	1.267/1.281	1.284/1.268	1.243/ 1.239
U_i	−2.575	−2.713/−2.704	−2.245/−2.504	−2.498/−2.593
E_t	0.5574	0.4550/0.4990	0.9655/0.6655	0.6093/0.5052
p	14.35	13.95/14.12	15.50/14.76	14.74/ 14.41

Table 1: Results. The simulation runs are characterized by the desired director, thus: 000 for no director potential, 001 for $\mathbf{d}_0 = (0,0,1)$, etc. The suffix $\ldots_0$ denotes a continuation run after the director potential has been switched off (and a thermalisation period of $\approx$ 10000 steps has elapsed). We list the order parameter P_2 of species 1, the Fourier-Bragg vector $\mathbf{k}_0$ of the strongest concentration mode of species 1, the corresponding wave length λ_0, the actual layer period Δs, and the "smectic ratio" S_0/S_1 between the strongest and second strongest concentration modes (see text). Also listed are the angles α between the actual director $\mathbf{d}(1)$ of species 1, the stable Fourier vector $\mathbf{k}_0$, and the desired director $\mathbf{d}_0$:
$\alpha_1 \equiv \alpha(\mathbf{d}(1),\mathbf{k}_0)$; $\alpha_2 \equiv \alpha(\mathbf{k}_0,\mathbf{d}_0)$; $\alpha_3 \equiv \alpha(\mathbf{d}(1),\mathbf{d}_0)$ Furthermore, the values of the thermodynamic observables T, U_i (configurational internal energy), E_t (total energy), and p (pressure) are given.

5 OUTLOOK: OTHER APPLICATIONS

In its present form the method applies to a desired director $\mathbf{d}_0$ and a coupling coefficient c (see equ. 2) that are independent of position. Also, the degree of orientational order does not enter into the synthetic potential. Now that the basic feasibility of the method has been demonstrated, generalisations may be explored that would open up interesting possibilities. One such modification is the introduction of a position-dependent coefficient $c(\mathbf{r})$. In this way a preferred or "easy" direction within a certain domain – say, near a wall – may be introduced.

Also, the desired director itself may vary in space: $\mathbf{d}_0 = \mathbf{d}_0(\mathbf{r})$. The system must then find a way to interpolate between those differently aligned domains, thus revealing its elastic coefficients.

Finally, the potential energy may include an even power of the order parameter P_2, mimicking the action of an applied field that not only defines a preferred direction but also exerts a torque that aligns the particles parallel to each other.

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