Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

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Version of record first published: 07 Oct 2011

To cite this article: C. Chiccoli, P. Pasini & C. Zannoni (2011): Is Internal Order in 2D Nematic Systems Destroyed by Boundary Disorder?, Molecular Crystals and Liquid Crystals, 549:1, 78-85

To link to this article: http://dx.doi.org/10.1080/15421406.2011.581143

Mol. Cryst. Liq. Cryst., Vol. 549: pp. 78–85, 2011

ISSN: 1542-1406 print/1563-5287 online
DOI: 10.1080/15421406.2011.581143

Is Internal Order in 2D Nematic Systems Destroyed by Boundary Disorder?

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Computer simulations of 2D nematic systems with quenched disorder placed on the oriented boundary have been performed to test the Feldman-Vinokur hypothesis which suggests that the long-range order is destroyed in that case. Our results for various system sizes and different percentages of disorder at the boundary do not necessarily confirm this hypothesis.

Keywords Monte Carlo; liquid crystals; nematic order; quenched disorder; Imry-Ma argument

1. Introduction

In a series of papers we have studied the effect of random frozen perturbations, e.g. dispersed silica nanoparticles, on the orientational order and the annealing capabilities of 3D nematic systems using a combination of Monte Carlo simulations and experiments [1–4]. We have proved that, for a model Sprinkled Spin System (SSS) where random frozen orientation spins are dispersed in the medium that the nature of the nematic ordering at finite disorder concentration is short-range while the long range order is suppressed [2]. Moreover we have observed that increasing the concentration of disorder can induce a nematic glassy state and memory effects [3,4]. In these studies, to detect the existence of long range order, we have typically focussed our attention on the second rank nematic order parameter $<P_2>$ and on the orientational correlation function $G_2(r)$. This function defines the probability of finding two particles *i,j* separated by a distance r aligned with respect to each other [5] and can be written as:

$$G_2(r) = <P_2[\mathbf{u}_{i\in C}\cdot\mathbf{u}_j(r)]> \quad (1)$$

where P_2 is a second rank Legendre polynomial and we have made the further assumption that one of the two particles belongs to a central cluster C of reference particles. For $r \to \infty$ the correlation $G_2(r)$ goes to $<P_2>^2$, that is to the square of the order parameter value measured for the overall system. Consequently, for nematic systems with long range order $G_2(r)$ decays to a finite plateau. If the $G_2(r)$ function decays exponentially as $\exp(-r/\zeta_N)$, then the system has only short range order and the decay length ζ_N is a quantitative measure

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of the nematic correlation length ζ [6,7]. The system can be considered to have a quasi-long range order when the $G_2(r)$ function decays more slowly, with a power law as $r^{-\zeta}$ [2]. In Fig. 1 we report the case that we studied in the past of a 3D SSS model of cubic shape with random internal disorder simulated for various system sizes L × L × L. It is clear that upon increasing the sample dimensions the long range order is destroyed in this case, with the orientational correlation functions calculated only for the nematic particles, $G_2{}^{NN}(r)$ that tends to decay to a zero value. The color coded snapshots allow us to observe the existence of correlated domains with similar orientation (color) and their size, giving a qualitative confirmation that, for the smaller systems, the majority of the particles are aligned along the common preferred direction (yellow).

In this work we wish to consider a related problem stimulated by the theoretical work of Feldman and Vinokur [8] who considered the case of random disorder only distributed at the border of the systems rather than embedded and dispersed. In particular they suggested that an arbitrary quenched disorder placed on the boundary of a 2D anisotropic system is sufficient to destroy its long-range order. The speculations of Feldman and Vinokur are based on the Imry-Ma argument [9] and they wrote [8]: "Let us consider a region of size L near the surface and compare the energies of ordered and disordered states of the region. If long-range order is broken on the scales of the order of L the loss in the bulk (elastic) energy is $E_{bulk} \sim L^D/L^2$, where D is the space dimension. The energy gain from the interaction with surface impurities scales as $E_{surface} \sim L^{(D-1)/2}$. If $D<3$ then $E_{surface} > E_{bulk}$. Hence, the

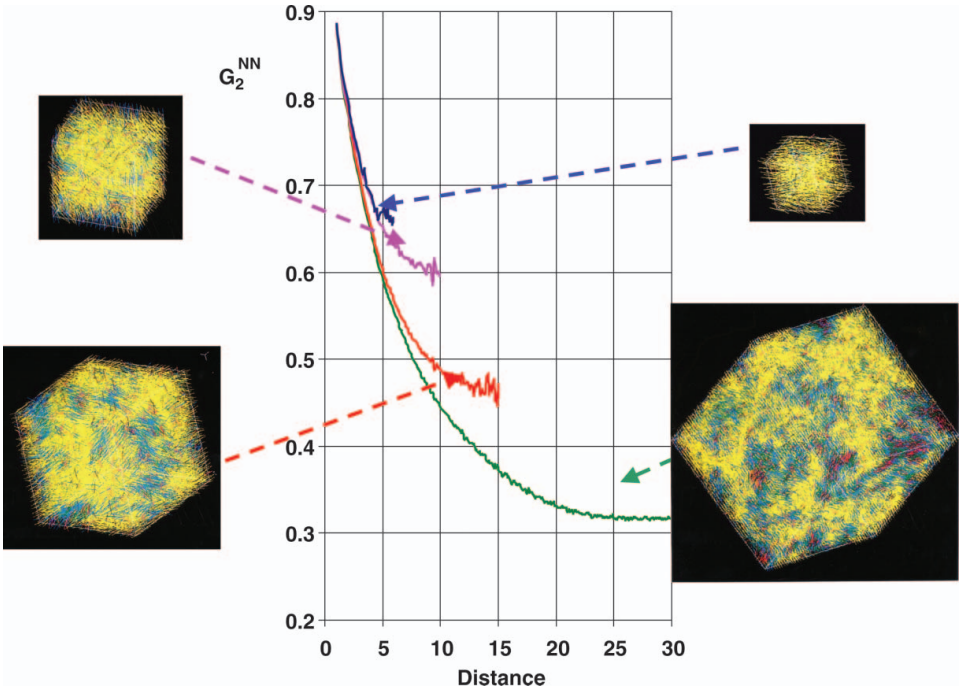

Figure 1. Dependence of the pair orientational correlation function on the distance from the central spins for a SSS system with a percentage of internal disorder p = 0.14 and a reduced temperature $T^* = 0.2$ (from Ref. [2]). The curves are for the following system sizes: 10 × 10 × 10 (blue), 16 × 16 × 16 (purple), 20 × 20 × 20 (red) and 50 × 50 × 50 (green). The spins in the snapshots are plotted with a color coding to appreciate their ordering with respect to the global director (yellow).

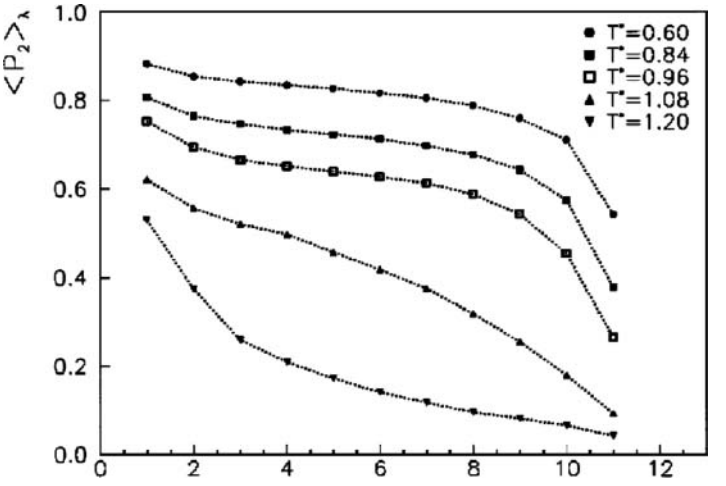

Figure 2. The second rank order parameter $<P_2>_\lambda$ vs distance from the droplet center in lattice units, r, at various scaled temperatures $T^* = kT/\varepsilon$ (from Ref. [10]. The droplet contains 5832 molecules (spins) and has fully random boundary surface.

disordered state should be favoured when $D<3$." And they conclude that long-range order should be absent for the arbitrarily weak disorder when $D < 3$.

In the past we have studied a small 3D nanodroplet (5832 spins) with random orientations (complete disorder) at the surface but we have found that a nematic order is present inside the system and this order is maintained up to the proximity of the boundary [10] (see Fig. 2). This is also true for a larger droplet (approximately 100 times larger) for which the behavior of the order starting form the center of the system is similar, as can be seen from the second rank order parameter $<P_2>_\lambda$ (obtained by as the largest eigenvalues of the ordering matrix Q [5]) plotted versus distance from the center reported in Fig. 3.

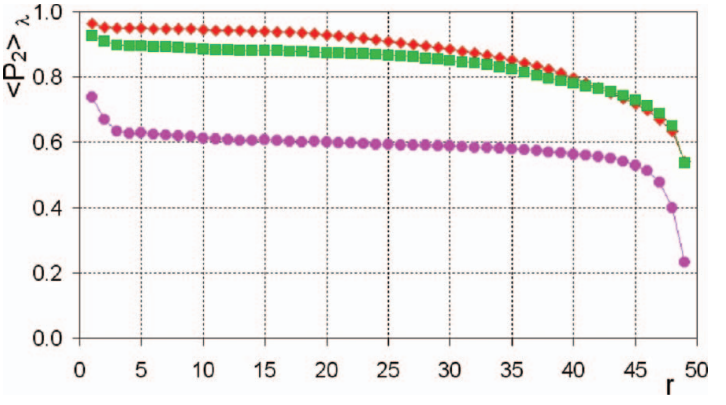

Figure 3. The dependence of $<P_2>_\lambda$ on the distance from the center for a droplet with 527,560 molecules and a disordered enclosing surface. The temperatures are $T^* = kT/\varepsilon$ 0.2 (upper curve), 0.4 (middle curve) and 1.0 (lower curve).

Here we aim to study by means of MC simulations a 2D system of various sizes and with different percentage of disorder at the boundaries to test the Feldman hypothesis.

This is of interest also in view of recent applications of quasi two dimensional nematic thin films employed as biosensors, where the boundary disorder could be provided by nanoparticles absorbed at the confining walls [11].

2. The Simulation Model

The Monte Carlo simulations were based on the simple and well studied Lebwohl - Lasher (LL) lattice spin model [12]. The particles interact through the attractive nearest neighbors LL pair potential

$$U_{i,j} = -\varepsilon_{i,j} \mathrm{P}_2(\mathbf{u}_\mathrm{i} \cdot \mathbf{u}_\mathrm{j}), \tag{2}$$

where

$$\varepsilon_{ij} = \begin{cases} \varepsilon, & \varepsilon > 0 \quad \textit{for i,j nearest neighbours} \\ 0 & \textit{otherwise}, \end{cases} \tag{3}$$

$\mathbf{u}_i$, $\mathbf{u}_j$ are unit vectors along the axis of the two particles ("spins") and. The spins represent a cluster of neighboring molecules whose short range order is assumed to be maintained through the temperature range examined [13]. The three dimensional bulk Nematic-Isotropic (*NI*) transition for this model occurs at a reduced temperature $T^* \equiv kT/\varepsilon = 1.1232$ [5,14]. Here we assume the model to be planar, with the spins reorienting in three dimensions but with their positions on a 2D square lattice and in this case the model with periodic boundary conditions has a quasi long range order [6].

The different boundary conditions are mimicked assuming a layer of outside particles with a fixed orientation consistent with the desired type of alignment at the border. As we have mentioned before, in this work we need to consider a certain amount of disorder at the system boundaries. To this purpose we extract from random distributions the orientations and the positions of the disordered particles, which we shall then keep fixed during the simulation, since they belong to the additional "ghost" layer. The anchoring strength at the boundary can be tuned by considering a different value of ε_{ij} when the spin j belongs to the additional layers. In the present work we have considered for simplicity only the case that the coupling with the boundary as the interaction is the same as that between the nematic spins inside the sample. To generate the lattice configurations we have used the standard Metropolis Monte Carlo procedure [15] where one spin at a time is updated as described in [5,12,14].

3. Simulation Results

We have considered a 2D LL model on a disc with a different percentage (p = 0%, 30%, 60%, 90% and 100%) of disordered sites at the boundaries where the other spins are by default aligned along z. We have investigated two system sizes with $N = 2{,}852$ and $N = 31{,}508$ nematic particles. The boundary particles are 172 and 568 respectively and are kept fixed during the simulations performed at the reduced very low temperature $\mathrm{T}^* = 0.2$. To equilibrate the systems we have performed, for each independent simulation, at least 400,000 Monte Carlo cycles, where a cycle is a complete attempt of updating the system.

We have also tried to start from two completely different initial configurations: all the nematic particles aligned along z or all random. As mentioned before we concentrate our attention on the second rank nematic order parameter $<P_2>_\lambda$ and on the orientational correlation function $G_2(r)$.

To calculate $G_2(r)$ we have considered a central cluster of 12 reference particles. The results are presented in Fig. 4 and in Fig. 5, respectively. We observe that the fully aligned spins on the rim (p = 0% case) induce long range order inside, with respect to the period boundary case [6], as indicated by the plateau in the correlation. We also notice from

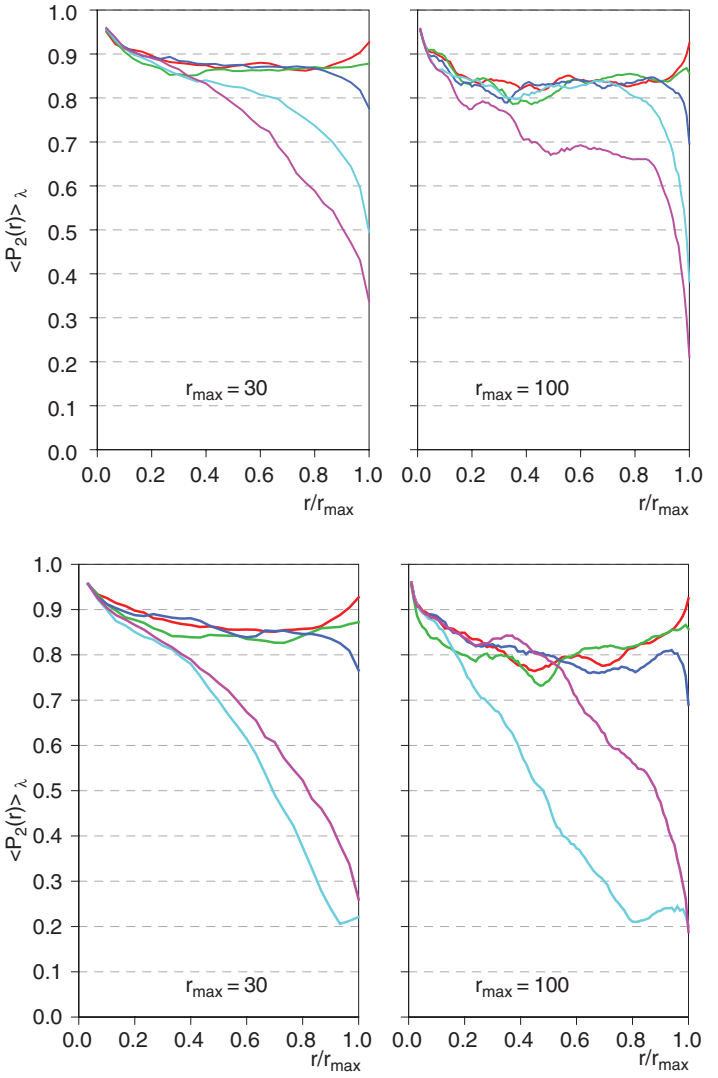

Figure 4. Order Parameter $<P_2\ (r)>_\lambda$ vs reduced distance r/r_{max} from the center of the systems. The percentages of disorder at the boundary are p = 0% (red), 30% (green), 60%)(blue), 90% (cyan) and 100% (purple). The starting configuration was all aligned along z (top plates) and random (bottom plates).

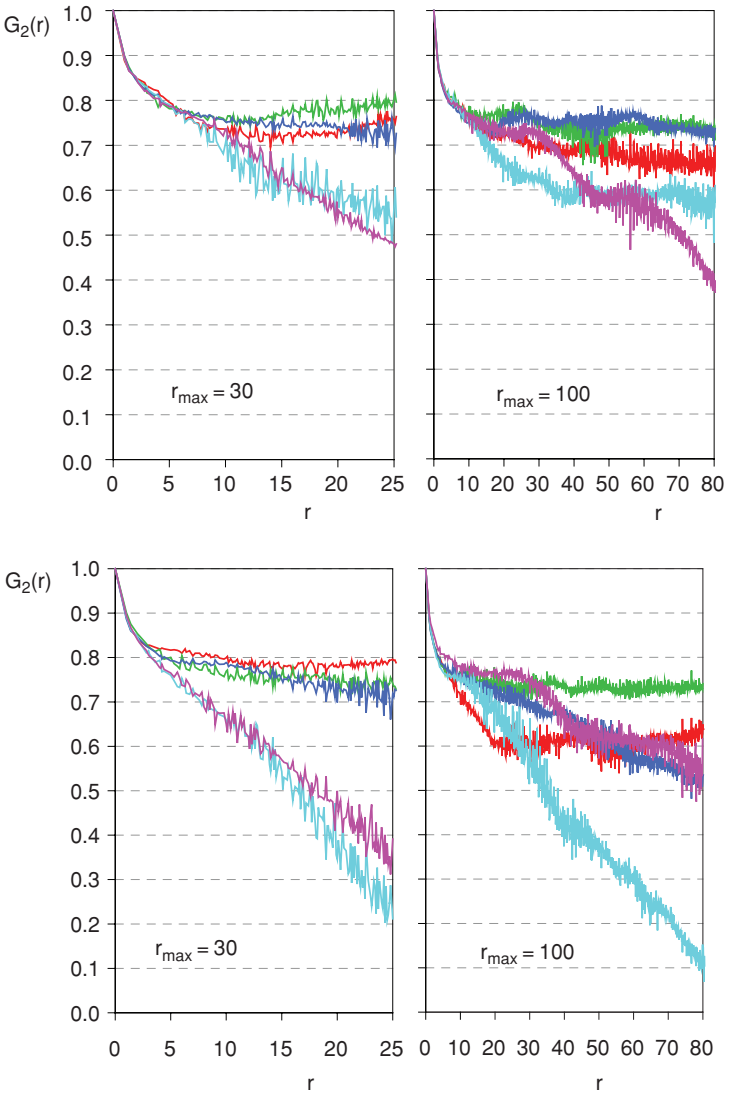

Figure 5. Orientational correlation function G_2 (r) vs distance r for two system sizes. The starting configuration was all aligned along z (top plates) and random (bottom plates). The percentages of disorder are p = 0% (red), 30% (green), 60% (blue), 90% (cyan), 100% (purple).

the values of $<P_2>_\lambda$, plotted against the distance from the center of the disc, that the system tends to be ordered up to the vicinity of the boundary also for a large percentage concentration of random disordered spins placed on the frontier line.

It is interesting to notice that the two sample sizes investigated, although very different, show essentially the same behavior. Of course for the lower values of boundary disorder the smaller disc has a greater degree of order (about 0.87) in comparison with the larger size for which $<P_2>_\lambda$ fluctuates around 0.83 for at least the 80% of the central part of the sample. For the values of boundary disorder greater than 90% we can observe that also in that case

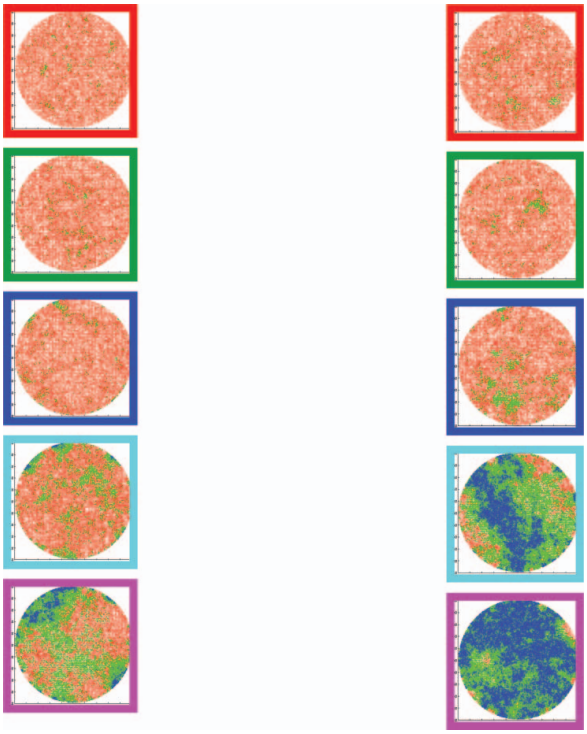

Figure 6. Snapshots of 2D systems (disc with r = 100) containing 31508 particles for a different percentage, p, of randomly oriented spins at the boundaries,with the other boundary spins parallel to z. The simulations were performed at the reduced nematic temperature $T^* = 0.2$. The snapshots are taken after 500,000 Monte Carlo cycles. The results are for an all aligned starting configuration (left column) and for a random one (right column). The red color of the spins indicate the alignment along z.

a large portion in the center of the disc is ordered. The results are not significantly affected by the starting configurations, aligned or random (Fig. 4 top or bottom plates, respectively).

These results are confirmed by the calculation of the orientational correlation function reported on Fig. 5.

4. Conclusions

We have performed Monte Carlo simulations of 2D nematic systems with different percentage of random disorder at the boundary. Our simulations are based on the simplest successful Lebwohl-Lasher lattice potential put forward to describe nematic liquid crystals. We have employed a standard Metropolis Monte Carlo method. We have tried to verify Feldman- Vinokur hypothesis that an arbitrary quenched disorder placed on the boundary of a 2D oriented system is sufficient to destroy the long-range order. Monte Carlo simulations of a 2D system with different percentage of disorder at the boundary do not necessarily confirm the hypothesis.

In fact orientational correlation functions calculated from the center of two systems of different size indicate the presence of long range order in the nematic phase at least up to a percentage of boundary disorder of 60%. The achievement is also supported by a qualitative investigation by looking at the snapshots of the system studied. These results,

shown in Fig 6, corresponding to the various cases of disorder are presented with a color coding to better appreciate the ordering of the systems.

The alignment of the spins along z is indicated in red and it is then confirmed that the system is ordered at least up to a percentage of boundary disorder of 60% both starting from a complete ordered or random initial configuration. When the boundary tend to be completely disordered we can observe the appearance of ordered domains inside the systems. The core of the disc, far from the boundary, is however ordered because the aligning properties of the potential overcome the disordering effect of the surface. The correlation length, extracted from the initial slope of the orientational correlation functions seems to be about 10 lattice spacings for all the cases.

Acknowledgments

C.C. and P.P. thank INFN (grant I.S. BO62) for support.

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