# Ordering kinetics of a conserved binary mixture with a nematic liquid crystal component

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# Abstract

A numerical study on the phase separation and ordering kinetics of a binary mixture of a nematic liquid crystal and a flexible polymer modeled with a Ginzburg-Landau free energy is presented. The system couples a generalized Cahn-Hilliard equation, which incorporates the nematic elastic energy as well as mixing, with a de Gennes-Prost evolution equation for the liquid crystal's director field. The effects of the liquid crystal micro-structure on the phase separation and morphology dynamics during spinodal decomposition is investigated numerically in two dimensions. It is found that the orientational distortion of the director field induced by interfacial anchoring dramatically affects both the morphology, the ordering kinetics of the binary mixture, and the coarsening rate.

Keywords: Canh-Hilliard equation, ordering dynamics, anchoring, Model B

# 1. Introduction

Phase separation of binary mixtures quenched rapidly from a homogeneous phase is characterized by a fast transition into an ordered phase, where domains rich in either component form followed by a slow coarsening of these domains. It is a fascinating problem that has been investigated for several decades due to its fundamental and practical relevance in materials processing. Binary alloys and polymer blends have been extensively studied (see e.g. [7, 6]) and systems in which one of the components is a liquid crystal are receiving increased attention [27, 30, 21, 26, 9, 8].

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In this work we investigate numerically the phase separation kinetics of a two-dimensional binary system in which one of the components is a nematic liquid crystal and the other component is a flexible polymer with a Ginzburg-Landau free energy. Our focus is to examine the effects of the orientational distortion in the nematic-rich phase and interfacial anchoring on the morphology and coarsening rate of phase domains. We find that these effects are dramatic. The late stage morphology of the phase separated system can be largely controlled by the type of interfacial anchoring and the coarsening rate is significantly affected by both long-range orientational distortion and by the orientational interfacial anisotropy induced by anchoring.

The system is modeled through an order parameter or phase field  $\phi$ , which is a measure of the volume fraction of one of the components, and a director field **n**, which quantifies the mean orientational order in the nematic liquid crystal phase. The dynamics are driven by energy minimization with conserved  $\phi$  (Model B in the nomenclature of of Hohenberg and Halperin [19]). Phase field models like this one have been used extensively for the investigation of phase separation with and without an underlying flow [15, 25, 20, 4, 1, 2, 22, 23, 5, 32, 34, 33, 3, 35, 13, 36, 12, 28, 18, 29]. In particular, the model that we employ stems from that considered in [32] with the essential difference that we keep both elastic and anchoring terms in the order parameter (Cahn-Hilliard) equation.

The rest of the paper is organized as follows. Section 2 is devoted to the description of the mathematical model and the numerical method is summarized in Section 3. This is followed by the presentation and discussion of results in Section 5. Details on the calculation of the structure function are given in Appendix A.

#### 2. The Model

We consider a binary mixture of a nematic liquid crystal and a flexible polymer with a Ginzburg-Landau free energy. The system can be described with a phase field  $\phi$  related to the species concentration and with the director field **n** which is a measure of the mean molecular orientation in the nematic liquid crystal phase. The pure, bulk phases are identified with  $\phi = 1$  and  $\phi = -1$  for the nematic liquid crystal and the flexible polymer component, respectively. A narrow neighborhood of the level set  $\phi = 0$  provides a diffuse interface between the two species. The free energy density of the system consists of three parts: a mixing energy density  $f_{\text{mix}}$ , a bulk, orientational distortion energy density of the nematic,  $f_{\text{bulk}}$ , and the anchoring energy density of the liquid crystal molecules on the interface,  $f_{\text{anch}}$  [32]:

$$f(\phi, \mathbf{n}, \nabla \phi, \nabla \mathbf{n}) = f_{\text{mix}} + \frac{1+\phi}{2} f_{\text{bulk}} + f_{\text{anch}}, \qquad (1)$$

where

$$f_{\rm mix} = \frac{\lambda_c}{2} \left[ |\nabla \phi|^2 + \frac{(\phi^2 - 1)^2}{2\varepsilon_c^2} \right],$$
(2)

$$f_{\text{bulk}} = \frac{K_c}{2} \left[ \nabla \mathbf{n} : (\nabla \mathbf{n})^T + \frac{(|\mathbf{n}|^2 - 1)^2}{2\delta_c^2} \right],\tag{3}$$

$$f_{\rm anch} = \begin{cases} \frac{A_c}{2} (\mathbf{n} \cdot \nabla \phi)^2 & \text{(planar anchoring)} \\ \frac{A_c}{2} [|\mathbf{n}|^2 |\nabla \phi|^2 - (\mathbf{n} \cdot \nabla \phi)^2] & \text{(homeotropic anchoring).} \end{cases}$$
(4)

In (2),  $\lambda_c$  is the mixing energy density constant, given in units of J/m, and  $\varepsilon_c$  is the capillary width, with units of length. Equation (3) is the regularized Frank energy density in which the elastic constants for splay, twist, and bend are all equal to  $K_c$  and  $(|\mathbf{n}| - 1)^2/(2\delta_c)$  is a penalty term to approximately enforce the constraint  $|\mathbf{n}| = 1$ . In (3)  $K_c$  has units of J/m and  $\delta_c$  has units of length. Finally, in (4),  $A_c$  is the strength of the anchoring, and is given in J/m. The planar anchoring energy density favors alignment of the director tangential to the interface whereas for the homeotropic anchoring the alignment of  $\mathbf{n}$  is perpendicular to it.

The free energy terms can be nondimensionalized as follows: Consider a characteristic length scale  $\mathcal{L}_c$  and a characteristic energy scale  $\mathcal{E}_c$  and define the dimensionless parameters  $\lambda = \lambda_c \mathcal{L}_c / \mathcal{E}_c$ ,  $\varepsilon = \varepsilon_c / \mathcal{L}_c$ ,  $\delta = \delta_c / \mathcal{L}_c$ ,  $K = K_c \mathcal{L}_c / \mathcal{E}_c$ ,  $A = A_c \mathcal{L}_c / \mathcal{E}_c$ , then we can write the energy densities in

dimensionless form as

$$\widetilde{f}_{\text{mix}} = \frac{\lambda}{2} \left[ |\nabla \phi|^2 + \frac{(\phi^2 - 1)^2}{2\varepsilon^2} \right],$$
(5)

$$\widetilde{f}_{\text{bulk}} = \frac{K}{2} \left[ \nabla \mathbf{n} : (\nabla \mathbf{n})^T + \frac{(|\mathbf{n}|^2 - 1)^2}{2\delta^2} \right],\tag{6}$$

$$\widetilde{f}_{\text{anch}} = \begin{cases} \frac{A}{2} (\mathbf{n} \cdot \nabla \phi)^2 & \text{(planar anchoring)} \\ \\ \frac{A}{2} [|\mathbf{n}|^2 |\nabla \phi|^2 - (\mathbf{n} \cdot \nabla \phi)^2] & \text{(homeotropic anchoring).} \end{cases}$$
(7)

In what follows we will drop the tilde for ease of notation.

We consider a cylindrical domain of the form  $V = \Omega \times [0, d]$  (in dimensionless variables), and assume that neither  $\phi$  nor **n** depend on the z variable. Then the total free energy is

$$F = d \int_{\Omega} f(\phi, \mathbf{n}, \nabla \phi, \nabla \mathbf{n}) d\mathbf{x}.$$
 (8)

Defining a chemical potential

$$\mu = \left(\frac{\delta F}{\delta \phi}\right),\tag{9}$$

the corresponding Cahn-Hilliard equation [10, 11] governing the dynamics of the order parameter is

$$\frac{\partial \phi}{\partial t} = \nabla \cdot \left[ \gamma \nabla \mu \right], \tag{10}$$

where  $\gamma$  is the mobility, which in this work is assumed to be a constant. Taking all the contributions to the energy, (5)-(7), we have

$$\mu = \lambda \left[ -\nabla^2 \phi + \frac{\phi(\phi^2 - 1)}{\varepsilon^2} \right] + \frac{K}{4} \left[ \nabla \mathbf{n} : (\nabla \mathbf{n})^T + \frac{(|\mathbf{n}|^2 - 1)^2}{2\delta^2} \right] + \mu_{\text{anch}}, \quad (11)$$

where

$$\mu_{\rm anch} = \begin{cases} -A\nabla \cdot \left[ (\mathbf{n} \cdot \nabla \phi) \mathbf{n} \right] & \text{(planar anchoring)} \\ -A\nabla \cdot \left[ |\mathbf{n}|^2 \nabla \phi - (\mathbf{n} \cdot \nabla \phi) \mathbf{n} \right] & \text{(homeotropic anchoring)} \end{cases}$$
(12)

The director evolves following the simplified Leslie-Ericksen theory due to de Gennes and Prost [16] and used by Yue, Feng, Liu, and Shen [32]

$$\frac{1}{\tau}\frac{\partial \mathbf{n}}{\partial t} = -\frac{\delta F}{\delta \mathbf{n}},\tag{13}$$

where  $\tau$  is a measure of the relaxation time of the director. Hence the coupled system of equations governing the phase separation of the mixture is

$$\frac{\partial \phi}{\partial t} = \gamma \nabla^2 \left[ \lambda \left( -\nabla^2 \phi + \frac{\phi^3 - \phi}{\varepsilon^2} \right) + \frac{K}{4} \left( \nabla \mathbf{n} : (\nabla \mathbf{n})^T + \frac{(|\mathbf{n}|^2 - 1)^2}{2\delta^2} \right) + \mu_{\text{anch}} \right],$$
(14)

$$\frac{1}{\tau}\frac{\partial \mathbf{n}}{\partial t} = K \left[ \nabla \cdot \left( \frac{1+\phi}{2} \nabla \mathbf{n} \right) - \frac{1+\phi}{2} \frac{(|\mathbf{n}|^2 - 1)\mathbf{n}}{\delta^2} \right] - \mathbf{g}, \quad (15)$$

where  $\mu_{\text{anch}}$  is given by (12) and

$$\mathbf{g} = \begin{cases} A(\mathbf{n} \cdot \nabla \phi) \nabla \phi & \text{(planar anchoring)}, \\ A[|\nabla \phi|^2 \mathbf{n} - (\mathbf{n} \cdot \nabla \phi) \nabla \phi] & \text{(homeotropic anchoring)}. \end{cases}$$
(16)

A more general combination of planar and homeotropic anchoring interfacial conditions can also be considered by writing the anchoring energy as

$$f_{\rm anch} = \frac{A}{2} \left[ C_{\rm p}(\mathbf{x}) (\mathbf{n} \cdot \nabla \phi)^2 + C_{\rm h}(\mathbf{x}) \left( |\mathbf{n}|^2 |\nabla \phi|^2 - (\mathbf{n} \cdot \nabla \phi)^2 \right) \right], \qquad (17)$$

where  $C_{\rm p}(\mathbf{x})$  and  $C_{\rm h}(\mathbf{x})$  are spatially varying weights determining the strength of each anchoring term:  $0 \leq C_{\rm p}(\mathbf{x}), C_{\rm h}(\mathbf{x}) \leq 1$  and  $C_{\rm p}(\mathbf{x}) + C_{\rm h}(\mathbf{x}) = 1$ . With this anchoring energy we have

$$\mu_{\rm anch} = A\nabla \cdot \left[ (C_{\rm p} - C_{\rm h})(\mathbf{n} \cdot \nabla \phi) \mathbf{n} + C_{\rm h}(|\mathbf{n}|^2 \nabla \phi) \right], \qquad (18)$$

$$\mathbf{g} = A \left[ (C_{\rm p} - C_{\rm h}) (\mathbf{n} \cdot \nabla \phi) \nabla \phi + C_{\rm h} |\phi|^2 \mathbf{n} \right].$$
(19)

We select continuous weights to create smooth transitions between the anchoring types. Specifically, on a  $L \times L$  periodic domain, we take  $C_{\rm p}(x, y) = 0.5 + 0.5 \sin(2\pi x/L)$  and  $C_{\rm h}(x, y) = 0.5 - 0.5 \sin(2\pi x/L)$ . Since  $C_{\rm p}$ ,  $C_{\rm h}$  only vary in x in this case, this anchoring favors planar on the left half of the domain and homeotropic on the right.

# 3. Numerical Scheme

The numerical scheme is a linearly implicitly discretization, as the one considered in [1] and [37], in which the implicit part is discretized using a second-order backward difference formula (BDF) and the explicit part corresponds to a second order Adams-Bashforth method. The scheme can be written as follows

$$\frac{\frac{3}{2}\phi^{n+1} - 2\phi^n + \frac{1}{2}\phi^{n-1}}{\Delta t} = \gamma\lambda \left[\frac{\alpha}{\varepsilon^2}\nabla^2\phi^{n+1} - \nabla^4\phi^{n+1}\right] + 2\mathcal{F}(\phi^n, \mathbf{n}^n) - \mathcal{F}(\phi^{n-1}, \mathbf{n}^{n-1}),$$
(20)

$$\frac{1}{\tau} \frac{\frac{3}{2} \mathbf{n}^{n+1} - 2\mathbf{n}^n + \frac{1}{2} \mathbf{n}^{n-1}}{\Delta t} = K \beta \nabla^2 \mathbf{n}^{n+1} + 2\mathcal{G}(\phi^n, \mathbf{n}^n) - \mathcal{G}(\phi^{n-1}, \mathbf{n}^{n-1}), \quad (21)$$

where

$$\mathcal{F}(\phi, \mathbf{n}) = \gamma \nabla^2 \left[ \lambda \left( \frac{\phi^3 - \phi}{\varepsilon^2} \right) + \frac{K}{4} \left( \nabla \mathbf{n} : (\nabla \mathbf{n})^T + \frac{(|\mathbf{n}|^2 - 1)^2}{2\delta^2} \right) + \mu_{\mathrm{anch}} \right] - \gamma \lambda \frac{\alpha}{\varepsilon^2} \nabla^2 \phi,$$
(22)

$$\mathcal{G}(\phi, \mathbf{n}) = K \left[ \nabla \cdot \left( \frac{1+\phi}{2} \nabla \mathbf{n} \right) - \frac{1+\phi}{2} \frac{(|\mathbf{n}|^2 - 1)\mathbf{n}}{\delta^2} \right] - \mathbf{g}$$
(23)  
$$- K\beta \nabla^2 \mathbf{n}.$$

Here,  $\alpha$  and  $\beta$  are numerical parameters introduced to relax the time step stability constraint [1]. In the simulations reported in this work we take  $\alpha = 2$  and  $\beta = 1$ . In addition, to limit the terms  $(1 + \phi)/2$  from exceeding 1 due to numerical overshoot, we approximate this term by  $(1 + s\phi)/2$ , where s = 0.95. These equations are solved on a square  $[0, L] \times [0, L]$  with periodic boundary conditions. The spatial derivatives are handled spectrally, using the FFTW package in Fortran, on a uniform grid.

# 4. Parameters

Guided by [32], we consider a square domain of dimensionless side length L = 3.974 and we choose the dimensionless parameters  $\lambda = 1.342 \times 10^{-2}$ ,  $\gamma = 4 \times 10^{-5}$ ,  $\delta = 6.325 \times 10^{-2}$ ,  $\varepsilon = 1.265 \times 10^{-2}$ ,  $\tau = 1$ , and  $A = 6.708 \times 10^{-3}$ . With K/A = 1, the choice of K is set to A. The numerical scheme is run on a  $512 \times 512$  grid, leading to  $\Delta x = \Delta y \approx 7.76 \times 10^{-3}$ , and we impose periodic

boundary conditions on each side. The timestep is initially set to  $\Delta t = 10^{-3}$ , but can be increased at later times.

To understand the scaling of the parameters, we start with an estimate on the order of  $10^{-11} N$  for the elastic energy constant  $K_c$  [24] and  $10^{-3} - 10^{-6} J/m^2$  for the surface anchoring strength  $W_c$  [24], which is related to  $A_c$  by  $W_c = 2\sqrt{2}A_c/3\varepsilon_c$  [32]. To balance anchoring and elastic energy, we select  $K_c = A_c$ . Then with the definition of  $W_c$ , a range for  $\varepsilon_c$  can be recovered, which places  $\varepsilon \approx 10^{-5} - 10^{-8} m$ . Using this range for  $\varepsilon_c$  and the nondimensional value  $\varepsilon$ , a range for a length scale can be produced:  $\mathcal{L}_c \approx 10^{-3} - 10^{-6} m$ . From [24], realistic values for the ratio  $K_c/W_c$  are  $10^{-5} - 10^{-8} m$ . Utilizing the relationship between  $W_c$  and  $A_c$ , and that  $K_c/A_c = 1$ , the choice of parameters from [32] in the simulations places  $K_c/W_c$  in  $10^{-5} - 10^{-8} m$ , which is within the bounds of the values in [24].

#### 5. Results

We consider spinodal decomposition starting from the slightly, randomly perturbed homogeneous phase  $\phi \equiv 0$ . To this end, we take the initial order parameter  $\phi_0$  at each grid point  $(x_i, y_j)$  to be  $\phi_0(x_i, y_j) = \xi_{ij}$ , where  $\xi_{ij} \in$  $U(-\varepsilon, \varepsilon)$ , that is  $\xi_{ij}$  is a uniformly distributed random number in  $(-\varepsilon, \varepsilon)$ . The small parameter  $\varepsilon$  here is the same as that in the mixing energy (5), i.e. a measure of the interfacial thickness. The initial director field  $\mathbf{n}_0$  is given by  $\mathbf{n}_0(x_i, y_j) = (1, \omega_{ij})/\sqrt{1 + \omega_{ij}^2}$  where  $\omega_{ij} \in U(-0.05, 0.05)$ .

We examine the effect of the liquid crystal anchoring at the interface between flexible polymer-rich and liquid crystal-rich phases on the coarsening and morphology of the separating mixture. We consider first phase separation with planar anchoring. Figure 1 shows a time series of the phase separation and the formation of a coarsening pattern with a bicontinuous structure. The polymer-rich phase is shown in solid color and the liquid crystal-rich phase is white with the (subsampled) director field depicted with arrows. The long range orientational distortion of the director field significantly affects the spinodal pattern and the strong planar anchoring favors the formation of horizontal lamellae.

The simulation in Fig. 1 is run with timestep  $\Delta t = 10^{-3}$  up to t = 1000and then the timestep is increased tenfold to  $\Delta t = 10^{-2}$  until reaching t =10000. At early times in the simulation (around t = 500) the polymer- and liquid crystal-rich phases separate relative to the orientation of the director field and the anchoring type. These effects lead to long, finger-like connected



Figure 1: Time sequence of spinodal decomposition with planar anchoring.

regions of each phase, running horizontally. Since the interface is primarily parallel to the orientation of the director, the distortion of this field near the interface is not evident, but it can be observed near the finger tips of the polymer-rich phase. As the mixture coarsens, the smaller structures begin to merge and some form regions islands, which can been seen in the data at t = 1000. At later times, the islands and fingers merge with larger formations and several horizontal lamellae develop. At t = 5000, five lamellae are present for each phase and only four by t = 10000, each roughly equally spaced and with straight edges. The initial condition on the liquid crystal phase has a large influence on the morphology, creating structures not typically seen in standard Canh-Hilliard phase separation. While this analysis is based on a single time series, these characteristics have been observed in additional simulations with the same parameters and defferent initial data for  $\phi$  and **n**.

We now consider homeotropic anchoring, taking the same parameters as in the previously discussed planar achoring case but with a different seed for the random initial data. Figure 2 shows snapshots of the corresponding separating mixture. Around t = 500, the polymer-rich phase has separated into long vertical domains, including a few fingers branching off of these areas and an island on the left-side of the domain. This is due to the directors of the liquid crystal-rich phase being oriented left to right, initially, and the polymer-rich phase adapting to have a perpendicular director at the interface. Locally, near the finger tips or in the vicinity of the island, the liquid crystal has adjusted to match the anchoring. By t = 1000, the island has disappeared and several of the polymer-rich domains have consolidated into larger regions. At t = 5000, the polymer-rich phase has formed two small ellipsoidal nuclei of the liquid crystal-rich phase. By this time, three lamellae have formed, albeit with one including both an island and a finger extending from it. The director field is largely influenced by the anchoring in areas where parts of the interface are close together, such as inside the nuclei and near the finger tip upper-right corner. At the end of the simulation (t = 10000) the two liquid crystal-rich nuclei and the finger have merged with the larger structures to form three lamellae, two of which are fairly straight on the sides and a large third lamellae that extends to the other side of the domain via the periodic boundary conditions. At this point, the liquid crystal has largely oriented itself back to its original left-to-right direction.

The importance of the elastic and anchoring contributions to the coarsening dynamics and the phase morphology can also be gauged by considering an often used simplified model in which these effects are neglected in the



Figure 2: Time sequence of spinodal decomposition with homeotropic anchoring.



Figure 3: Comparison of order parameter and the director field during spinodal decomposition with planar anchoring for the full model (a) and the simplified model (b) at t = 1000for the same initial conditions.

Cahn-Hilliard equation [32], that is

$$\frac{\partial \phi}{\partial t} = \gamma \lambda \nabla^2 \left[ -\nabla^2 \phi + \frac{\phi^3 - \phi}{\varepsilon^2} \right],\tag{24}$$

$$\frac{1}{\tau}\frac{\partial \mathbf{n}}{\partial t} = K\left[\nabla \cdot \left(\frac{1+\phi}{2}\nabla \mathbf{n}\right) - \frac{1+\phi}{2}\frac{(|\mathbf{n}|^2 - 1)\mathbf{n}}{\delta^2}\right] - \mathbf{g}.$$
 (25)

Figure 3 shows the striking contrast between the solution of the full system (14)-(15) and the simplified model (24)-(25) for the same parameters and initial conditions. While more tractable computationally, the simpler model (24)-(25) has no coupling of  $\phi$  with **n** in (24) and thus it fails to capture the important nematic elastic effects, the interfacial anisotropy of the director field due to anchoring, and the proper energy dissipation. A model using the Allen-Cahn equation instead of the Cahn-Hilliard equation with the correct energy dissipation has been recently proposed [31].

The effect of the director's interfacial configuration can be also examined by comparing the spinodal late morphology for the cases of homeotropic anchoring and a combination of planar and homeotropic (mixed) anchoring as shown in Fig. 4. While homeotropic anchoring favors the formation of vertical lamellae despite the initial perturbed horizontal alignment, mixed anchoring



Figure 4: The spinodal pattern at t = 1000 for (a) homeotropic anchoring and (b) mixed anchoring.

leads to a more complex coarsening pattern where both liquid crystal-rich and flexible polymer-rich nuclei develop on the left (planar) region of the domain. A long range distortion of the director is clearly visible on the left side of the flexible polymer-rich nucleus.

To quantify the influence of the nematic component on the coarsening rate of the separated phases, we estimate a time-dependent length scale L(t)characterizing the domain growth. This characteristic length scale is obtained from the first moment  $k_1(t)$  of the structure function s(k,t) (see Appendix A for details) and  $L(t) \sim 1/k_1(t)$  [37]. Simple scaling arguments [6] show that  $L(t) \sim t^{1/3}$  for the Cahn-Hilliard equation with a Ginzburg-Landau energy. The assumption of a single characteristic length scale L(t) implies that the structure function obeys the scaling

$$s(k,t) = L(t)^d g(kL(t))$$
(26)

for sufficiently long times, where d is the space dimension. Equivalently,  $s(\mathbf{k},t) = k_1(t)^{-d}g(k/k_1(t)).$ 

For the case of planar anchoring, after an initial transient phase, the structure function and subsequently the coarsening rate are computed from  $\phi$ . For this case, we employ an ensemble average of twelve simulations with the same parameters, but different random initial data.



Figure 5: Bicontinuous system with planar anchoring: (a) the structure function s(k,t) and (b) the scaled structure function  $k_1^2 s(k,t)$  as a function of  $k/k_1$ .

In Fig. 5, the first plot is the structure function from t = 2000 to t = 10000. As time increases, the maximum of the structure function, moves closer to zero, indicating that the growth of the characteristic domain size. The second plot has the structure function at late times (near t = 10000), scaled as  $k/k_1$  and  $k_1^2s(k,t)$ . With this scaling, the data at the five times shown collapse onto a single curve, demonstrating the aforementioned scaling  $s(k,t) = L(t)^d g(kL(t))$ . With homeotropic anchoring conditions a similar self-similarity is obtained as Fig. 6 demonstrates.

Utilizing the data at incremental times and computing the first moment,  $k_1$ , of the structure function at these times, the coarsening exponent can be estimated. Assuming a relation of the form  $L(t) \sim t^{\alpha}$  and using  $k_1(t) = 1/L(t)$ , we can cast the rate of coarsening in terms of the first moment as  $k_1(t) \sim t^{-\alpha}$ . As a point of comparison, the exponent related to Cahn-Hilliard is  $\alpha = 1/3$ . In order to remove the effect of the initial transient in the simulations, we estimate the coarsening rate from t = 3200 (when the transient visually appears to end) to t = 10000.

The coarsening rate for planar anchoring is estimated to be  $\alpha = 0.2317$ . This indicates that for the planar anchoring the domains grow with a characteristic length scale which is shorter than that in standard Cahn-Hilliard dynamics.

Similar to the planar anchoring case, we run twelve simulations for the homeotropic anchoring case to compute the structure function and subsequently the coarsening rate. The transient stage ends around t = 4800 and



Figure 6: Bicontinuous system with homeotropic anchoring: (a) the structure function s(k,t) and (b) the scaled structure function  $k_1^2 s(k,t)$  as a function of  $k/k_1$ .



Figure 7: Time behavior of the first moment  $k_1(t)$ :  $L(t) \sim k_1^{-1}(t) \sim t^{\alpha}$ . The best fit line for (a) planar anchoring from time 3,200 to 10,000 leads to  $\alpha = 0.2317$  and (b) for homeotropic anchoring from time 4,800 to 10,000 leads to  $\alpha = 0.4006$ .

using the data from this point to t = 10000, the coarsening rate is estimated to be  $\alpha = 0.4006$ . This is larger than both the corresponding Cahn-Hilliard value and the planar anchoring exponent of 0.2317. Thus, the homeotropic anchoring leads to a higher coarsening rate than in the previously mentioned cases.

In Fig. 7 we present the time behavior of  $k_1 \sim L^{-1}$  for planar and homeotropic anchoring, respectively, corresponding to the cases shown in Figs. 5 and 6.

We now consider the phase separation which takes place from an initially perturbed homogeneous state with one majority phase, close to the end of the spinodal interval. The other phase will nucleate in the majority phase-rich matrix and the system will coarsen. We first take the initial condition  $\phi_0(x_i, y_j) = 0.5 + \xi_{ij}$ , where  $\xi_{ij} \in U(-\varepsilon, \varepsilon)$ . This corresponds to a small random perturbation of the homogeneous state  $\phi \equiv 0.5$  where the liquid crystal is the dominant component. The initial director field is selected as before,  $\mathbf{n}_0(x_i, y_j) = (1, \omega_{ij})/\sqrt{1 + \omega_{ij}^2}$  where  $\omega_{ij} \in U(-0.05, 0.05)$ .

Figure 8 displays both the order parameter and the director field of the nematic matrix at a late time of the phase separation (t = 1000). With planar anchoring [Fig. 8(a)] the orientational distortion in the liquid crystal-rich matrix is more pronounced around the largest flexible polymer-rich nuclei but remains somewhat localized. In contrast, with homeotropic anchoring [Fig. 8(b)], the nearly horizontal initial director field undergoes a global reordering into a predominantly vertical alignment to accommodate for the perpendicular interfacial distribution of the director field. Similar results are displayed in Fig. 9 where the majority and minority roles are reversed.

#### 6. Discussion

In summary, we have presented a numerical study of the phase separation and ordering kinetics of a binary mixture comprised of a nematic liquid crystal and a flexible polymer. We have considered both planar and homeotropic anchoring, and demonstrated that the presence of the nematic liquid crystal in the blend can impact significantly both the resulting morphology, the ordering kinetics, and the coarsening rates of the binary mixture. Specifically, the morphology and coarsening are found to be dramatically affected by the orientational anisotropy introduced by anchoring and by long-range orientational distortion of the nematic phase.



Figure 8: The order parameter and the director field for nucleation of a flexible polymer phase in a liquid crystal matrix with (a) planar anchoring and (b) homeotropic anchoring at t = 1000 with the same initial conditions.



Figure 9: The order parameter and the director field for nucleation of a liquid crystal phase in a flexible polymer matrix with (a) planar anchoring and (b) homeotropic anchoring at t = 1000 with the same initial conditions.

While the model considered here has several limitations, the results unequivocally point to strong effects that a liquid crystal component can have on phase separating mixture and underline a potential mechanism for controlling morphology. It would be interesting to examine the how these effects are modified in the presence of a flow (Model H) and in a three-dimensional system.

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#### Appendix A. Structure Function

The structure function, also referred to as the time-dependent structure factor [14], is defined as:

$$S(\mathbf{k},t) = \left\langle \frac{1}{N} \left| \sum_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}} \left[ \psi(\mathbf{r},t) - \langle \psi \rangle \right] \right|^2 \right\rangle.$$
(A.1)

In this definition, the sum runs over the lattice of linear size L and  $N = L^2$ is the total number of points in the lattice and the  $\langle \cdot \rangle$  notation is spatial averaging over the lattice for  $\phi$  and an ensemble average for the outer braces. Using this, and assuming isotropy, the circularly-averaged structure function, S(k, t), is computed.

Note that the discrete Fourier transform is similar to the summation in **r**:

$$\Psi(\mathbf{n}) = \sum_{\mathbf{r}} \psi(\mathbf{r}) e^{-2\pi i \mathbf{n} \cdot (\mathbf{r}/\mathbf{L})}.$$
 (A.2)

Then define  $\mathbf{k} = 2\pi \mathbf{n}/\mathbf{L}$ , so that:

$$\Psi(\mathbf{k}) = \sum_{\mathbf{r}} \psi(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}.$$
(A.3)

If we examine the summation terms in the structure function, we can compute the summations by interpreting it as a discrete Fourier transform of a discrete convolution [17]. The circular average is the average over all wave vectors of magnitude between  $k - \frac{1}{2}\Delta k$  and  $k + \frac{1}{2}\Delta k$  [17]. The value of  $\Delta k$  is chosen to be of the form  $(2\pi/L) \times c$ , where c is a value near one for which the plot of the structure function is smooth. Then S(k, t) can be written in discrete form as

$$S(k,t) = \frac{\sum_{\substack{k-\frac{1}{2}\Delta k < |\mathbf{k}| \le k+\frac{1}{2}\Delta k}} S(\mathbf{k},t)}{\sum_{\substack{k-\frac{1}{2}\Delta k < |\mathbf{k}| \le k+\frac{1}{2}\Delta k}} 1}.$$
 (A.4)

For  $n_1, n_2 > L/2$ , we reassign  $n_1 = L - n_1 + 1$ ,  $n_2 = L - n_2 + 1$ .

The structure function can then be normalized to

$$s(k,t) = \frac{S(k,t)}{\langle \psi^2(t) \rangle - \langle \psi \rangle^2}.$$
 (A.5)

The the first moment of s(k, t) is calculated as

$$k_1(t) = \frac{\sum_k ks(k,t)}{\sum_k s(k,t)}.$$
(A.6)

This is in lieu of  $k_m(t) = \operatorname{argmax}_k s(k, t)$  since  $k_m(t)$  is difficult to calculate due to the discrete nature of k [37]. The typical length scale of the domain is then  $L(t) = 1/k_1(t)$ .

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