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Three-dimensional coarsening dynamics of a conserved, nematic liquid crystal-isotropic fluid mixture

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ABSTRACT

We present a numerical investigation of the three-dimensional coarsening dynamics of a nematic liquid crystal-isotropic fluid mixture using a conserved phase field model. The model is a coupled system for a generalized Cahn–Hilliard equation for the order parameter ϕ, related to the volume fraction of the nematic component, and a simplified de Gennes–Prost evolution equation for the director field $\mathbf{n}$, which describes the mean orientation of the rigid rod-like, liquid crystal molecules. We find that, as in the two-dimensional system, the orientational distortion induced by interfacial anchoring has profound effects both on the morphology and the coarsening rate. However, we identify significant differences in the three-dimensional and two-dimensional coarsening processes. In particular, we find a remarkable, new 3-stage late coarsening process with markedly different coarsening rates in the three-dimensional bicontinuous phase separation with homeotropic anchoring, unseen in the two-dimensional system.

1. Introduction

Phase separation of binary mixtures is a fundamental process in materials processing. The important phenomenon is characterized by a fast transition into an ordered phase consisting of domains rich in either component and followed by a very slow coarsening process until a steady state is reached [6,7].

Mixtures in which one of the components is a liquid crystal or a liquid crystalline polymer offer a significant potential for applications and have received increased attention [8,9,21,27–29,36].

We focus here on the three-dimensional phase separation and coarsening dynamics of a binary mixture of a nematic liquid crystal and an isotropic fluid, like a polymer. We use a conserved phase field model (Model B in the nomenclature of Hohenberg and Halperin [19]) which couples a generalized Cahn–Hilliard equation for the order parameter ϕ, related to the volume fraction of the species, with a simplified de Gennes–Prost evolution equation [17] for the director field $\mathbf{n}$, which describes the mean orientation of the rigid rod-like, liquid crystal molecules. The same model, which stems from that considered in [37], has been used in the two-dimensional study of Mata et al. [27] and the current work is a follow-up report on our findings for the corresponding three-dimensional system. Similar phase field models have been used extensively in phase separation [1–5,12–14,18,20,22,23,26,31,35,37–41]. A more general model of de Gennes type, using a tensor order parameter, is described in [33].

We find that the global distortion of the orientational field in the nematic-rich phase, induced by strong interfacial anchoring, has a profound effect on the morphology and coarsening rate, just as it happens in 2D. Specifically, the steady-state morphology of the system can be largely controlled by the type of interfacial anchoring and the coarsening rate is significantly affected by anchoring-induced long-range orientational distortion. However, we observe substantial differences between the three-dimensional and two-dimensional coarsening dynamics. In particular, we identify a remarkable, new 3-stage late coarsening process with markedly different coarsening rates in the three-dimensional bicontinuous phase separation with homeotropic anchoring ($\mathbf{n}$ perpendicular to the surface), unseen in the two-dimensional system. We also obtain a notable minimal surface (a Schwarz

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P Surface) for one instance of 3D phase separation with planar anchoring conditions.

The rest of the paper is organized as follows. In Section 2 we provide a description of the phase field model and the numerical methodology employed is described in Section 3. A summary of our numerical results is given in Section 4 and some concluding remarks are given in Section 5. Finally, data of an accuracy and convergence test of the numerical method are provided in the Appendix.

2. Mathematical model

We focus on a system consisting of a conserved mixture of a nematic liquid crystal and an isotropic fluid, which undergoes phase separation in three dimensional space. The model is the same as that used in [27] except that here our domain is three-dimensional. The system can be described with an order parameter ϕ related to the species concentration ($(1+\phi)/2$ represents the nematic liquid crystal concentration and $(1-\phi)/2$ the isotropic fluid concentration) and with the director field $\mathbf{n}$, 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 isotropic fluid, 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 has three parts: a mixing energy f_{mix}, a bulk, orientational distortion energy of the nematic, f_{bulk}, and the anchoring energy related to the preferential orientation of the liquid crystal molecules at interfaces, f_{anch} [37]:

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

where

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

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

$$f_{\text{anch}} = \begin{cases} \dfrac{A}{2}(\mathbf{n}\cdot\nabla\phi)^2 & \text{(planar anchoring)}, \\ \dfrac{A}{2}\left[|\mathbf{n}|^2|\nabla\phi|^2 - (\mathbf{n}\cdot\nabla\phi)^2 \right] & \text{(homeotropic anchoring)}. \end{cases} \tag{4}$$

The parameter λ in (2) is the strength of the mixing energy density and ε is the capillary width. Eq. (3) is the regularized Frank energy in which the elastic constants for splay, twist, and bend are all equal to K and $(|\mathbf{n}|-1)^2/(2\delta^2)$ is a penalty term to approximately enforce the constraint $|\mathbf{n}| = 1$. Finally, in (4), A is the *volumetric* anchoring strength, which is related to the *surface* anchoring strength W by $\varepsilon W = (2\sqrt{2}/3)A$ [37]. Some bounds on the parameter A are necessary for thermodynamic stability [16]. The specific choice of f_{anch} for planar (homeotropic) anchoring in (4) favors alignment of the director field $\mathbf{n}$ tangential (normal) to nematic-isotropic fluid interfaces.

We consider a domain $\Omega = [0, L] \times [0, L] \times [0, L]$. The total free energy is

$$F = \int_\Omega f(\phi, \mathbf{n}, \nabla\phi, \nabla\mathbf{n}) dx. \tag{5}$$

The evolution of the order parameter is governed by the Cahn–Hilliard equation [10,11]

$$\frac{\partial\phi}{\partial t} = \nabla\cdot[\gamma\nabla\mu], \tag{6}$$

where γ is the mobility, which in this work is taken to be constant, and

$$\mu = \frac{\delta F}{\delta\phi}. \tag{7}$$

Using (2)–(4) we obtain

$$\mu = \lambda\left[-\nabla^2\phi + \frac{\phi(\phi^2-1)}{\varepsilon^2} \right] + \frac{K}{4}\left[\nabla\mathbf{n} : (\nabla\mathbf{n})^T + \frac{(|\mathbf{n}|^2-1)^2}{2\delta^2} \right] + \mu_{\text{anch}}, \tag{8}$$

where

$$\mu_{\text{anch}} = \begin{cases} -A\nabla\cdot[(\mathbf{n}\cdot\nabla\phi)\mathbf{n}] & \text{(planar anchoring)}, \\ -A\nabla\cdot\left[|\mathbf{n}|^2\nabla\phi - (\mathbf{n}\cdot\nabla\phi)\mathbf{n} \right] & \text{(homeotropic anchoring)}. \end{cases} \tag{9}$$

We evolve the director field using the simplified Leslie-Ericksen theory of de Gennes and Prost [17], first used by Yue et al. [37], and in the two-dimensional work of Mata et al. [27],

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

where τ is Leslie twist viscosity, which can be physically measured [17]. Then the coupled system of equations governing the phase separation of the mixture is

$$\frac{1}{\gamma}\frac{\partial\phi}{\partial t} = \nabla^2\left[\lambda\left(-\nabla^2\phi + \frac{\phi^3-\phi}{\varepsilon^2} \right) + \frac{K}{4}\left(\nabla\mathbf{n} : (\nabla\mathbf{n})^T + \frac{(|\mathbf{n}|^2-1)^2}{2\delta^2} \right) + \mu_{\text{anch}} \right], \tag{10}$$

$$\frac{1}{\tau}\frac{\partial\mathbf{n}}{\partial t} = K\left[\nabla\cdot\left(\frac{1+\phi}{2}\nabla\mathbf{n} \right) - \frac{1+\phi}{2}\frac{(|\mathbf{n}|^2-1)\mathbf{n}}{\delta^2} \right] - \mathbf{g}_{\text{anch}}, \tag{11}$$

where μ_{anch} is given by (9) and

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

We non-dimensionalize the system (9)–(12) by selecting characteristic time, length, and energy scales t_c, L_c, and E_c, respectively. Then, the free energy parameters K, A, and λ are made dimensionless with E_c/L_c, γ with $L_c^5/(E_c t_c)$, and τ with $L_c^3/(E_c t_c)$. We choose the characteristic length scale $L_c = L/2$, i.e. one half the domain size. Denoting by K_c and τ_c characteristic values of the Frank elastic constant and the Leslie twist viscosity, respectively, we define characteristic energy and time scales by $E_c = aK_cL_c$, $t_c = bL_c^3/(E_c\tau_c)$, respectively, where a and b are dimensionless constants. Following [27,37], we take $a = 1/(6.708\times10^{-3})$ and $b = 1$. We use the same letters to denote the dimensionless variables and parameters, so (9)–(12) can be considered to be in dimensionless form. We consider here only *periodic boundary conditions*.

3. Numerical methodology

We employ the same discretization as in [27], except that here we write the Cahn–Hilliard equation as a second order system to avoid a direct discretization of the fourth order, biharmonic operator and to use an efficient linear multigrid method [12,13]. The spatial discretization is second order with standard finite differences and periodic boundary conditions. The time integration is a linearly implicit scheme, as the one considered in [1,12], 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

$$\frac{\frac{3}{2}\phi_1^{n+1} - 2\phi_1^n + \frac{1}{2}\phi_1^{n-1}}{\Delta t} = \gamma\lambda\nabla^2\phi_2^{n+1} + 2\mathcal{F}^n - \mathcal{F}^{n-1}, \tag{13}$$

$$\phi_2^{n+1} = \frac{\alpha}{\varepsilon^2}\phi_1^{n+1} - \nabla^2\phi_1^{n+1}, \tag{14}$$