Control of the phase separation pattern in a mixture of an isotropic liquid and liquid crystal

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等方液体・液晶混合系では，相分離と等方・ネマティック転移という２種類の秩序化が競合しながら進行する．この系のスピノーダル分解は，相分離初期においてどちらの秩序化が支配的かによって，等方スピノーダル (ISD) とネマティックスピノーダル (NSD) に分類することができる．我々は，この混合系の外場下における相分離ダイナミクスに関する数値シミュレーションを行った．その結果，NSD の方が ISD に比べ相分離パターンに対する外場の影響が大きいことが分かった．このようにして制御された異方的相分離パターンは初期の外場の影響を効率よく記憶することができ，この特徴は PDLC などの光学デバイスの開発に有用であると考えている．

We demonstrate field-induced stripe domain formation in phase separation of a mixture of an isotropic liquid and a nematic liquid crystal. The dynamics of such a mixture is described by two types of order parameters, namely, a conserved compositional (ϕ) and a non-conserved orientational (Q_{ij}) order parameter. The free energy functional of the mixture is given by

$$\begin{aligned}\mathcal{F}\{\phi, Q_{ij}\} &= k_{\mathrm{B}}T\int dV\Big\{-\frac{\tau}{2}\phi^2+\frac{u}{4}\phi^4+\frac{1}{2}a(\phi)Q_{ij}Q_{ji}-\frac{b}{3}Q_{ij}Q_{jk}Q_{ki}+\frac{c}{4}(Q_{ij}Q_{ji})^2\\ &+ \frac{K_\phi}{2}|\nabla\phi|^2+\frac{K_Q}{2}(\partial_k Q_{ij})^2+w\partial_i\phi\partial_j\phi Q_{ij}-\chi e_i e_j Q_{ij}\Big\}. \qquad (1)\end{aligned}$$

The first five terms describe the bulk free energy of the mixture. They give the typical phase diagram, which is composed of the coexistence curve and the isotropic-nematic (I-N) transition line, as shown in Figure 1. The sixth and seventh terms are the gradient energies, which lead to the interface tension and Frank elasticity of nematic solvent, respectively. The eighth term describes the anchoring of the director field on the interface. And the ninth one is the coupling between Q_{ij} and the external field e_i. We numerically solve the following dynamic equations,

$$\frac{\partial}{\partial t}\phi=\frac{D}{k_{\mathrm{B}}T}\nabla^2\frac{\delta\mathcal{F}}{\delta\phi}+\theta, \qquad \frac{\partial}{\partial t}Q_{ij}=-\frac{L}{k_{\mathrm{B}}T}\left(\frac{\delta\mathcal{F}}{\delta Q_{ij}}-\frac{1}{d}\delta_{ij}\mathrm{Tr}\frac{\delta\mathcal{F}}{\delta Q_{ij}}\right)+\lambda_{ij}, \qquad (2)$$

where θ and λ_{ij} are the thermal fluctuations for ϕ and Q_{ij}, respectively.

In the mixture of an isotropic liquid and a liquid crystal, spinodal decomposition can be classified into two types: isotropic (ISD) and nematic (NSD) spinodal decomposition. Figures 2(a), (b) and (c) show the simulated pattern evolution of mixtures under a horizontal external

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field. Since all the mixtures are almost symmetric, they are unstable for compositional ordering. In other words, phase separation proceeds via spinodal decomposition. While, the stability for the orientational ordering depends upon the quench depth [see the points (a)-(c) in Fig.1]. In the early stage of mixture (a), phase separation proceeds before nematic ordering and, thus, the isotropic domain pattern is formed even under the external field. In mixture (c), on the other hand, the nematic order develops before phase separation. The director field is aligned along the external field without interference from concentration fluctuation. Thus, the anisotropic stripe domain pattern emerges from the ordered nematic phase along the external field. Since the director field in the LC-rich phase tends to be parallel to the external field, the domain interface also tends to align along the field owing to the coupling between $\nabla\phi$ and Q_{ij} at the interface. Once isotropic domains are formed in the early stage as in Fig. 2(a), however, it is not easy to control the morphology by the external field since it takes a quite long time for domains to be deformed.

As shown in Fig. 2(c), the application of an external field to the nematic ordering before phase separation is a very promising way to control the domain pattern. We revealed that the kinetic pathway in the two-dimensional order parameter space is a key to the field-induced stripe formation. We confirmed that the anisotropic pattern has a memory of orientation of the applied external field, which may be used for device applications.

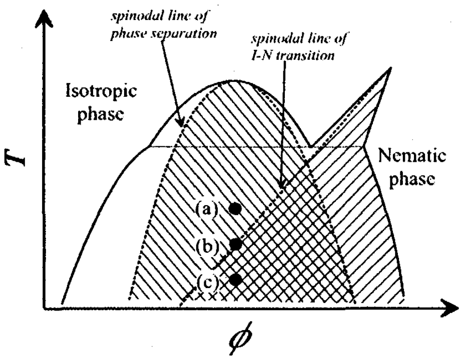

Figure 1: Schematic phase diagram of an IL-LC mixture. Points (a), (b) and (c) correspond to simulations (a), (b) and (c) in Figures 2, respectively.

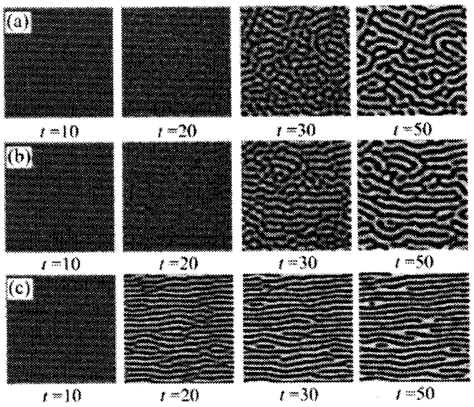

Figure 2: Simulated domain pattern evolution of symmetric mixtures under the external field. Phase separation in (a), (b) and (c) proceed via ISD, neutral SD and NSD, respectively.

References

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