Nonequilibrium dynamics of liquid crystal films with chiral order

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カイラリティーをもった液晶分子によって構成された単分子膜は、分子の長軸が膜の法線に対して一様に傾いた２次元的な液晶相を形成し得る。この液晶膜を一方向に通過する水蒸気流束が存在するとき、膜面内の分子配向が集団的な回転運動をすることが実験的に観察されている [1]。我々は、この現象に対する簡単なモデルを構成し、それに基づいた数値シミュレーションを行うことにより、熱平衡状態ではカイラル秩序が現れないようなパラメータ領域において、水蒸気流束が存在する非平衡系においては、それが動的な秩序として現れ得ることを示す。

1 Introduction

Chiral liquid crystal monolayers/films are known to exhibit two-dimensional liquid crystal order such as Smectic-C phase in which long axes of constituent molecules are uniformly tilted to the layer normal. It has been observed in experiment that orientations of liquid crystal molecules in Smectic-C phase collectively rotate when the transmembrane vapor flux exists [1]. In this paper we construct a simple model of this phenomenon and carry out numerical simulations based on the model. The numerical results show that 'flux-induced chiral order' appears dynamically when the transmembrane flux exits, whereas no chiral order emerges in thermal equilibrium.

2 Model

Assuming that the tilt angles of molecules are constant and the monolayer/film is flat with layer normal $\hat{\boldsymbol{z}}$, we describe the director field as a two-dimensional unit vector $\boldsymbol{c} = \boldsymbol{c}(\boldsymbol{r}, t)$, the so-called c-director, at position $\boldsymbol{r} = (x, y)$ and time t. Introducing a chiral order parameter $\psi = \psi(\boldsymbol{r}, t)$, the free energy F of the system can be written as [2]

$$F = \int d\boldsymbol{r} \left[\frac{K_1}{2} (\nabla \cdot \boldsymbol{c})^2 + \frac{K_3}{2} (\nabla \times \boldsymbol{c})^2 - \chi \psi \nabla \times \boldsymbol{c} + \frac{D}{2} (\nabla \psi)^2 + f(\psi) \right], \tag{1}$$

where the K_1 and K_3 are the elastic constants and the third term with a coupling constant χ arises due to the absence of reflection symmetry. The last two terms in (1) are related to the chiral order parameter ψ only (D is constant). Here $f(\psi)$ is the free energy density associated with the chiral order ψ which is typically the Ginzburg-Landau type: $f(\psi) = (a/2)\psi^2 + (b/4)\psi^4 - h\psi$ with constants a, b, and an external field h.

When the transmembrane vapor flux exists, the flux can be dynamically coupled with torques exerting on the molecules due to the chirality, which causes the collective rotation of molecular orientation. This is a kind of Lehmann effect observed in cholestric liquid crystals [3]. The hydrodynamic theory of the Lehmann effect was developed by Leslie [3]. Taking into account this theory in a special case that there is no mass flow, we write kinetic equations of $\boldsymbol{c}$ and ψ as

$$\gamma \frac{\partial \boldsymbol{c}}{\partial t} = -\frac{\delta F}{\delta \boldsymbol{c}} - \nu(\psi)\boldsymbol{c} \times \boldsymbol{E}, \tag{2}$$

$$\frac{\partial \psi}{\partial t} = -L\frac{\delta F}{\delta \psi}, \tag{3}$$

where γ, $\nu(\psi)$, and L are transport coefficients and $\boldsymbol{E} \propto \hat{\boldsymbol{z}}$ is a constant field conjugate to the vapor flux. Here we have assumed that the transport coefficient ν depends on ψ as $\nu(\psi) = \nu_1\psi$ with constant ν_1. Note that the torque balance equation (2) should be evaluated on the transversal component because $|\boldsymbol{c}| = 1$.

3 Simulations and Result

We carry out numerical simulations based on (2) and (3), starting from a uniform initial state with a finite perturbation to ψ at the center of simulation box. The periodic boundary conditions are used.

We observe that a uniform nonchiral stationary state is stable for some parameter values in equilibrium systems ($\nu_1 = 0$). However, in nonequilibrium systems ($\nu_1 \neq 0$) the uniformly rotational state becomes unstable for the same parameter values except for ν_1. In this case spatio-temporal pattern of ψ which we call 'flux-induced chiral order' emerges.

The details will be presented at POSTER.

References

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