Supporting Information

Orientational Perturbation in Patterned Self Assembled Monolayers Liquid Crystal Cells

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1. Simulation methods

In the numerical calculations, presented in the article, we take advantage of the tensor description of nematic liquid crystals, where nematic order is described by a traceless tensor $Q_{ij} = \frac{S}{2}(3n_i n_j - \delta_{ij}) + \frac{P}{2}\left(e_i^1 e_j^1 - e_i^2 e_j^2\right)$, where *S* is the degree of order (i.e. scalar order parameter), n the main ordering axis –the director. Possible biaxiality is described by the biaxial parameter *P* and a second director e^1. e^2 is an axis perpendicular to n and e^1. The $n \leftrightarrow -n$ symmetry is inherently incorporated in the tensor approach.

Numerical results are based on the minimization of the Landau-de Gennes free energy (1) combined with the free energy of a surface anchoring (2) (3):

$$F = \int_V \{\frac{A}{2}Q_{ij}Q_{ji} + \frac{B}{3}Q_{ij}Q_{jk}Q_{ki} + \frac{C}{4}(Q_{ij}Q_{ji})^2 + \frac{L_1 \partial Q_{ij}\partial Q_{ji}}{2\ \partial x_k\ \partial x_k} + \frac{L_2 \partial Q_{ij}\partial Q_{ik}}{2\ \partial x_j\ \partial x_k} + \frac{L}{2} + \int_{S^{uni}} \frac{1}{2}W^{uni}\left(Q_{ij} - Q_{ij}^0\right)^2 dS + \int_{S^{deg}} W^{deg}[\left(Q_{ij} - Q_{ij}^{\perp}\right)^2 + \left(Q_{ij}^2 - \frac{9}{4}S_S^2\right)^2]dS \quad (1)$$

,

where A, B, C are parameters tuning the nematic phase behavior. x_k is the k-th spatial coordinate. The corresponding derivatives of the tensor order parameter describe the effective elasticity, whose strength is given by the $L_1, L_2, and\ L_3$ tensorial elastic constants. They are connected to Frank elastic constants by the relations: $K_1 = \frac{9S^2}{4}(2L_1 + L_2 - L_3 S)$, $K_2 = \frac{9S^2}{4}(2L_1 - L_3 S)$, and $K_3 = \frac{9S^2}{4}(2L_1 + L_2 + 2L_3 S)$. Electric field contributions to the free energy consist of a term independent on the nematic ordering and a dielectric coupling between electric field and tensor order parameter, which tends to align the nematic molecules along the direction of the electric field. $\bar{\varepsilon}$ is the average permittivity and ε_a^{mol} the molecular dielectric anisotropy. W^{uni} is the strength of the uniform surface anchoring with Q_{ij}^0 being the surface-preferred order parameter tensor. W^{deg} is the strength of the planar-degenerate anchoring, which prefers the alignment along the surface with the degree of order of S_S.

(Meta)stable nematic configurations correspond to the minima of the free energy. To reach a minimum of a free energy, we use explicit relaxation algorithm for the Q-tensor to evolve from the initial conditions by the following rules:

$$\Gamma \partial_t Q_{ij} = h_{ij} - \frac{1}{3} h_{kk} \delta_{ij},$$

$$\Gamma^S \partial_t Q_{ij} = h_{ij}^S - \frac{1}{3} h_{kk}^S \delta_{ij},$$

according to bulk or surface (index *S*) position of the Q-tensor. Γ is the bulk (or surface) rotational relaxational constant (we take $\frac{\Delta t}{\Gamma} = \frac{\Delta t}{\Gamma^S} = 0.02 \frac{\Delta x^2}{L}$, where Δx is mesh resolution and Δt is a discrete time step) and h_{ij} are the molecular fields, defined as:

$$h_{ij} = -\frac{\partial F_{bulk}}{\partial Q_{ij}} + \partial x_k \frac{\partial F_{bulk}}{\partial \left(\frac{\partial Q_{ij}}{\partial x_k} \right)},$$

$$h_{ij}^S = -\frac{\partial F_{surface}}{\partial Q_{ij}} - \frac{\partial F_{bulk}}{\partial \left(\frac{\partial Q_{ij}}{\partial x_k} \right)} \nu_k,$$

where **ν** is the surface normal and F_{bulk} and $F_{surface}$ correspond to bulk or surface integrals in Eq. 1, respectively. Such relaxational procedure corresponds to the approximation of nematic dynamics without material flow (4) (5). More details on the numerical model can be found in (6).

Bibliography

1. P. G. de Gennes and J. Prost**,** *The Physics of Liquid Crystals,* Oxford University Press, New York, 1993.

2. J.-B. Fournier and P. Galatola*, Europhys. Lett*., 2005, **72**, 403.

3. M. Nobili and G. Durand, *Phys. Rev. A*, 1992**, 46,** R6174**.**

4. Anthony N. Beris and Brian J. Edwards, *Thermodynamics of Flowing Systems with Internal Microstructure*, Oxford University Press, New York, 1994.

5. T. Qian and P. Sheng, *Phys. Rev. E*, 1998, **58**, 7475.

6. M. Ravnik and S. Žumer, *Liq. Cryst*., 2009, **36**, 1201.