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Perturbative Approach to the Structure of a Planar Interface in the Landau-de Gennes Model

— Elastic Anisotropy Effects —

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The main focus of this contribution are the effects of elastic anisotropy on the propagation and structure of the flat interface between the nematic (N) and isotropic liquid (I) phases. We consider two configurations singled out by the underlying symmetries, i.e. the in-plane and homeotropic alignment of the optical axis at the interface. The problem is studied within the framework provided by the Landau-de Gennes theory with the dynamics governed by the time-dependent Ginzburg-Landau equation (TDGL) together with the assumption of isothermic condition. To account for the full elastic anisotropy of the nematic liquid crystal we extend the elastic free energy to include a third order term, i.e.

$$\mathcal{F}_e = \frac{1}{2}L_1\partial_i Q_{jk}\partial_i Q_{jk} + \frac{1}{2}L_2\partial_i Q_{ik}\partial_j Q_{jk} + \frac{1}{2}L_3Q_{ij}\partial_i Q_{kl}\partial_j Q_{kl}, \quad (1)$$

where $\hat{Q} = [Q_{ij}]$ ($i, j = 1, 2, 3$) is the symmetric, traceless, second-rank tensor order parameter of the nematic liquid crystal, L_1, L_2, L_3 are the elastic coefficients, and for repeated indices the Einstein summation convention is assumed. Although the addition of the third order term is not a unique procedure [1], the particular term we include was reported to be sufficient to reproduce correctly the temperature dependence of the Oseen-Frank elastic constants for a typical nematogen PAA (*p*-azoxyanisole) [2]. The solutions of the TDGL equation corresponding to the moving flat interface are obtained within a consistent perturbative scheme. The fact that the first order corrections to \hat{Q} are found to be two orders of magnitude smaller than the zeroth order solution provides a good justification of that approach. Corrections to the order parameter are obtained order by order as solutions of ordinary, linear differential equations, while corrections to the velocity of the interface follow from certain integrability conditions, which are due to the existence of the translational zero mode.

With the corresponding solutions a number of physical effects are revealed, see Figs. 1, 2.

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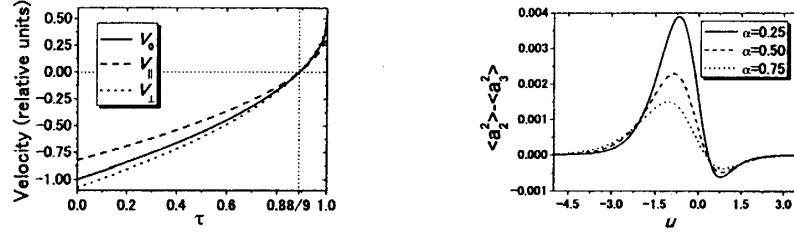


Figure 1: Left: Elastic anisotropy corrections to the temperature dependence of the interface velocity for the in-plane (V_{\parallel}) and homeotropic (V_{\perp}) director alignment. The solid line shows the velocity for the unperturbed interface (V_0) which is equivalent to the de Gennes' variational solution. The elastic parameter values adopted in the calculations are those of PAA and $\tau = (T - T^*)/(T^{\dagger} - T^*)$, where the temperature interval (T^* , T^{\dagger}) marks the phase coexistence region ($\tau = 8/9$ corresponds to the N/I equilibrium point). Right: Degree of biaxiality (in-plane alignment). The parameter α maps monotonically the temperature interval (T^* , T^{\dagger}) onto (0, 1). The value $\alpha = 0.5$ corresponds to the N/I equilibrium point. $\langle a_i^2 \rangle$ denotes the mesoscopic average for the i -th component of the unit vector aligning with the molecular long axis. The x^3 -axis is normal to the interface plane and the unit of the dimensionless coordinate u corresponds to the coherence length at equilibrium.

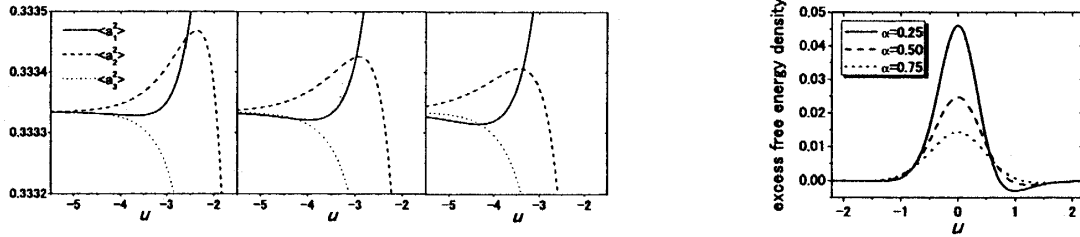


Figure 2: Left: Symmetry restoring feature for the in-plane configuration observed on the I-phase side. The region of the oblate uniaxial order (negative scalar order parameter) interpolates between the regions of the prolate order with the mutually perpendicular in-plane directors, unlike it was suggested in [3]. Right: Excess free energy density for in-plane alignment (arbitrary units). The region of lowered tension on the N-phase side is exclusively due to the nonequivalence of the splay and bend deformations.

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