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The generalized equations of bulk and interfacial nematostatics in terms of the tensor order parameter are derived using calculus of variations, taking into account long and short range nematic bulk free energies as well as anchoring and saddle–splay surface free energies. A general expression for the surface stress tensor order parameter for a nematic liquid crystal/isotropic fluid (NLC/I) interface has been derived, and found to represent normal, shear, and bending stresses. It is shown that the surface stress tensor is asymmetric. It is also found that anchoring energy contributes to bending and normal stresses, while saddle–splay energy contributes to normal and shear stresses. The rotational identifies governing the bulk and surface stress tensors are derived and used to show that the equations of nematostatics are fully consistent with the general balance equations of polar fluids. The equations presented provide a theoretical framework for solving interfacial problems involving NLCs that is applicable to cases where variations in liquid crystalline order and saddle–splay energy play significant roles.

1. Introduction

The equations of bulk and interfacial nematostatics are necessary for describing problems involving interfaces and free surfaces. Cases of current interest include nematic droplets, freely standing thin films, filled nematics, and nematic in porous media, to name a few [1–3].

The bulk and interfacial *torque* balance equations of nematostatics using director theories are well known [4–7]. Several formulations that take into account surface gradient energy, known as saddle–splay energy, have been presented (see, for example, the reviews [8, 9], and references therein), and its importance has been established. On the other hand, the interfacial *force* balance equation including saddle–splay energy has not been considered in any detail. We should note here that although the bulk force and torque balance equations are not independent of each other [4], the same is not the case for the interfacial counterparts. Thus a better understanding of the interfacial force balance equation that includes saddle–splay energy is necessary.

Interfacial problems in nematostatics usually involve changes in the order parameters and development of biaxiality [8, 10–12]. Thus formulations of interfacial problems must use the tensor order parameter **Q**, which accounts for nematic ordering as well as orientation. The equation of bulk nematostatics at the tensor order parameter level are well known and have been given by several authors; see, for example, [13, 14]. On the other hand, the interfacial equations using a tensor order parameter and including saddle–splay energies have not been given in the literature. The present paper aims at generalizing the existing nematostatic formulations by deriving balance equations for the tensor order parameter, and by including saddle–splay energy.

An important recent observation regarding the interfacial nematostatics in the absence of saddle–splay energy is that surface stress tensor is a 2×3 tensor with normal and bending components, but no shear components [15, 16]. The unique contribution of saddle–splay energy to the surface stress tensor will be shown to be the source of interfacial shear stresses, thus completing the nature of possible surface stresses. In addition, given that the surface stress tensor has not been widely used in the LC literature, its nature, symmetry, and its restrictions arising from material objectivity must be established.

Continuum theories of materials with microstructure are known as polar fluid theories [17]. These theories take into account the internal structure of the material and use force and angular momentum balance equations. The general balance equations for polar fluids are exactly the same as those for nematics, since torques as well as forces are taken into account. A key signature in the bulk torque balance equation is the presence of the asymmetric stress [17]. In bulk nematostatics this term originates from the Ericksen stress [17]. It will be shown here that the analogous term in the interfacial torque balance equation is saddle–splay distortion stresses.

The objectives of this paper are: (1) to develop the bulk and interfacial nematostatic equations in terms of the tensor order parameter, including saddle–splay energy

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for NLC/I interfaces; (2) to identify the origin of the components of the surface stress tensor for a NLC/I interface, and to establish the restrictions on the surface stress tensor arising from material objectivity; (3) to show that the derived nematostatic equations are consistent with the continuum mechanical theory of polar fluids.

2. Nematic free energies

The system considered in this paper is a static interface between a nematic liquid crystal and an isotropic fluid. The interface is assumed to be isothermal, and both phases are incompressible. The NLC occupies region R^N, and the isotropic fluid region R^I. The orientation of the interface between the R^N/R^I regions, denoted by NLC/I, is characterized by a unit normal $\mathbf{k}$, directed from R^N into R^I. The NLC structure is given by the symmetric, traceless, 3×3 tensor order parameter $\mathbf{Q}$, usually parametrized as follows [7]:

$$\mathbf{Q} = S(\mathbf{nn} - \mathbf{I}/3) + P(\mathbf{mm} - \mathbf{II})/3 \qquad (1)$$

The total free energy of the NLC in the absence of external fields is given by [8, 11, 18–21]:

$$F = F_H + F_{el} + F_{an} + F_{is} \qquad (2)$$

where F_H is the homogeneous, F_{el} the elastic, F_{an} the anchoring, and F_{is} the isotropic free energies. The homogeneous free energy is responsible for the nematic–isotropic phase transition and is given by:

$$F_H = \int f_H(\mathbf{Q})\,dV; \qquad (3\,a)$$

$$f_H(\mathbf{Q}) = f_H(0) + a\,\mathrm{tr}\,\mathbf{Q}^2 - b\,\mathrm{tr}\,\mathbf{Q}^3 + c(\mathrm{tr}\,\mathbf{Q}^2)^2 \qquad (3\,b)$$

where a, b, c are the Landau coefficients. The elastic free energy F_{el}, also known as Frank energy, contains long range gradient contributions and is given by:

$$F_{el} = \int f_g\,dV \qquad (4)$$

where the gradient free energy density f_g is taken to be [19, 20]:

$$f_g(\nabla\mathbf{Q}) = \frac{L_1}{2}\,\mathrm{tr}\,\nabla\mathbf{Q}^2 + \frac{L_2}{2}(\nabla\cdot\mathbf{Q})\cdot(\nabla\cdot\mathbf{Q}) + \frac{L_3}{2}(\nabla\mathbf{Q})\vdots(\nabla\mathbf{Q}) \qquad (5)$$

where $\{L_i\}$; $i = 1, 2, 3$ are the Frank elastic constants [19, 20]. More complete expressions for f_g are found in the literature [21–25], but for the objective of this paper, expression (5) will suffice. Using the identity:

$$(\nabla\mathbf{Q})\vdots(\nabla\mathbf{Q}) = (\nabla\cdot\mathbf{Q})\cdot(\nabla\cdot\mathbf{Q}) - \nabla\cdot[\mathbf{Q}\cdot(\nabla\cdot\mathbf{Q}) - \mathbf{Q}:\nabla\mathbf{Q}] \qquad (6)$$

and the divergence theorem, the elastic free energy F_{el} becomes:

$$F_{el} = \int f_{bg}\,dV + \int f_{sg}\,dS \qquad (7\,a)$$

$$f_{bg}(\nabla\mathbf{Q}) = \frac{L_1}{2}\,\mathrm{tr}\,\nabla\mathbf{Q}^2 + \frac{L_2 + L_3}{2}(\nabla\cdot\mathbf{Q})\cdot(\nabla\mathbf{Q}) \qquad (7\,b)$$

where f_{bg} is the bulk gradient elastic free energy density, and f_{sg} is the surface gradient free energy density given by:

$$f_{sg} = \mathbf{k}\cdot\mathbf{g}; \quad \mathbf{g} = \frac{L_3}{2}[\mathbf{Q}:\nabla\mathbf{Q} - \mathbf{Q}\cdot(\nabla\cdot\mathbf{Q})]. \qquad (8\,a,b)$$

The total bulk energy and its density are:

$$F_{bulk} = \int f\,dV; \quad f = f_{bg} + f_H.$$

The anchoring energy F_{an} is given by [8]:

$$F_{an} = \int \gamma_{an}\,dS \qquad (9\,a)$$

$$\gamma_{an} = \beta_{11}\mathbf{k}\cdot\mathbf{N} + \beta_{20}\mathbf{Q}:\mathbf{Q} + \beta_{21}\mathbf{N}\cdot\mathbf{N} + \beta_{22}(\mathbf{k}\cdot\mathbf{N})^2; \quad \mathbf{N} = \mathbf{Q}\cdot\mathbf{k} \qquad (9\,b)$$

where γ_{an} is the anchoring energy density, and $\{\beta_{ij}\}$, $ij =$ 11, 20, 22, 22, are the anchoring coefficients (energy/area). Discussions and different uses of equation (9 *b*) can be found in the literature [1, 8, 10–12, 26, 27]. The isotropic free energy F_{is} is the surface integral of the usual isotropic interfacial tension γ_{is}. The total surface free energy F_s and its density γ are given in terms of the following sum of isotropic, anchoring, and gradient contributions:

$$F_s = \int \gamma\,dS \qquad (10\,a)$$

$$\gamma(\mathbf{Q}, \mathbf{k}, \nabla_s\mathbf{Q}) = \gamma_{is} + \gamma_{an} + f_{sg} = \gamma_{is} + \gamma_{an} + \mathbf{k}\cdot\mathbf{g} \qquad (10\,b)$$

which now depends on $\nabla_s\mathbf{Q}$ as well as $\mathbf{k}$, and $\mathbf{Q}$; the symbol ∇_s represents the surface gradient. By decomposing the gradient vector as $\nabla(*) = \mathbf{kk}\cdot\nabla(*) + \nabla_s(*)$, it is possible to show that only surface gradients enter in equation (14), and $\gamma = \gamma(\mathbf{Q}, \mathbf{k}, \nabla_s\mathbf{Q})$.

3. Bulk and interfacial static torque balance equations

The bulk and interfacial static torque balance equations are the static limit of the internal angular momentum balance equations. The bulk static torque balance equation is well known [14], and details can be found in the literature. These equations follow from a variation of the tensor order parameter $\mathbf{Q}(\mathbf{r}) \to \mathbf{Q}'(\mathbf{r})$. For a NLC in contact with an isotropic fluid, the variation of the energy due to a variation of $\mathbf{Q}$ leads to:

$$\delta F = \int \left[\frac{\partial f}{\partial \mathbf{Q}} : \delta\mathbf{Q} + \frac{\partial f}{\partial \nabla \mathbf{Q}} \vdots \delta(\nabla \mathbf{Q})^{\mathrm{T}} \right]^{[\mathrm{s}]} \mathrm{d}V + \int \left[\frac{\partial \gamma}{\partial \mathbf{Q}} : \delta\mathbf{Q} + \frac{\partial \gamma}{\partial \nabla_{\mathrm{s}} \mathbf{Q}} \vdots \delta(\nabla_{\mathrm{s}} \mathbf{Q})^{\mathrm{T}} \right]^{[\mathrm{s}]} \mathrm{d}S \quad (11)$$

where [s] denotes symmetric and traceless, and arises because $\mathbf{Q} = \mathbf{Q}^{\mathrm{T}}$, and $\mathbf{Q} : \mathbf{I} = 0$. Using the divergence theorem the volume integral is written as:

$$\int_{V^{\mathrm{N}}} \left[\frac{\partial f}{\partial \mathbf{Q}} : \delta\mathbf{Q} + \frac{\partial f}{\partial \nabla \mathbf{Q}} \vdots \delta(\nabla \mathbf{Q})^{\mathrm{T}} \right]^{[\mathrm{s}]} \mathrm{d}V = \int_{V^{\mathrm{N}}} \left[\frac{\partial f}{\partial \mathbf{Q}} - \nabla \ \left(\frac{\partial f}{\partial \nabla \mathbf{Q}} \right) \right]^{[\mathrm{s}]} : \delta\mathbf{Q}\, \mathrm{d}V + \int_S \left[\mathbf{k} \ \frac{\partial f}{\partial \nabla \mathbf{Q}} \right]^{[\mathrm{s}]} : \delta\mathbf{Q}\, \mathrm{d}S. \quad (12)$$

Likewise using the surface divergence theorem the surface integral becomes:

$$\int_S \left[\frac{\partial \gamma}{\partial \mathbf{Q}} : \delta\mathbf{Q} + \frac{\partial \gamma}{\partial \nabla_{\mathrm{s}} \mathbf{Q}} \vdots \delta(\nabla_{\mathrm{s}} \mathbf{Q})^{\mathrm{T}} \right]^{[\mathrm{s}]} \mathrm{d}S = \int_S \left[\frac{\partial \gamma}{\partial \mathbf{Q}} - \nabla_{\mathrm{s}} \ \left(\frac{\partial \gamma}{\partial \nabla_{\mathrm{s}} \mathbf{Q}} \right) \right]^{[\mathrm{s}]} : \delta\mathbf{Q}\, \mathrm{d}S \quad (13)$$

where edge terms have been omitted. Collecting bulk and surface terms, the variation δF vanishes if:

$$\left[\frac{\partial f}{\partial \mathbf{Q}} - \nabla \ \left(\frac{\partial f}{\partial \nabla \mathbf{Q}} \right) \right]^{[\mathrm{s}]} = 0; \quad (14\,a)$$

$$\left[\mathbf{k} \ \left(\frac{\partial f}{\partial \nabla \mathbf{Q}} \right) + \frac{\partial \gamma}{\partial \mathbf{Q}} - \nabla_{\mathrm{s}} \ \left(\frac{\partial \gamma}{\partial \nabla_{\mathrm{s}} \mathbf{Q}} \right) \right]^{[\mathrm{s}]} = 0 \quad (14\,b)$$

which are known as the bulk and interfacial torque balance equations. These two equations are not independent of the force balance equations and can be expressed in terms of the asymmetric components of the bulk and surface stress tensors, as shown below.

4. Bulk and interfacial static stress balance equations

The bulk and interfacial static stress balance equations are the static limit of the linear momentum balance equations. The bulk static force balance equation is well known [14], and details can be found in the literature. These equations follow from a displacement: $\mathbf{r} \to \mathbf{r}' = \mathbf{r} + \mathbf{u}$ at constant tensor order parameter: $\mathbf{Q}(\mathbf{r}) = \mathbf{Q}'(\mathbf{r}')$. For a NLC in contact with an isotropic fluid, the variation of the energy due to a displacement $\mathbf{u}$ leads to:

$$\delta F = \int_{V^{\mathrm{N}}} \left[f \nabla \ \mathbf{u} + \frac{\partial f}{\partial \nabla \mathbf{Q}} \vdots \delta(\nabla \mathbf{Q})^{\mathrm{T}} \right] \mathrm{d}V + \int_S \left[\Pi_{\mathrm{o}} \mathbf{u} \ \mathbf{k} + \gamma \nabla_{\mathrm{s}} \ \mathbf{u} + \frac{\partial \gamma}{\partial \mathbf{k}} \ \delta\mathbf{k} + \frac{\partial \gamma}{\partial \nabla_{\mathrm{s}} \mathbf{Q}} \vdots \delta(\nabla_{\mathrm{s}} \mathbf{Q})^{\mathrm{T}} \right] \mathrm{d}S + \int_{V^{\mathrm{I}}} -p^{\mathrm{I}} \nabla \ \mathbf{u}\, \mathrm{d}V \quad (15)$$

where Π_{o} is a constant (hydrostatic pressure), and p^{I} is the pressure in the isotropic phase. The variations $\delta\mathbf{k}$ and $\delta(\nabla_{\mathrm{s}} \mathbf{Q})^{\mathrm{T}}$ in terms of the surface displacement gradient $(\nabla_{\mathrm{s}} \mathbf{u})^{\mathrm{T}}$ are simply:

$$\delta\mathbf{k} = -\mathbf{k} \ (\nabla_{\mathrm{s}} \mathbf{u})^{\mathrm{T}}; \quad \delta(\nabla_{\mathrm{s}} \mathbf{Q})^{\mathrm{T}} = -(\nabla_{\mathrm{s}} \mathbf{Q})^{\mathrm{T}} \ (\nabla_{\mathrm{s}} \mathbf{u})^{\mathrm{T}} \quad (16)$$

which yield:

$$\delta F = \int_{V^{\mathrm{N}}} \left[f\mathbf{I} - \frac{\delta f}{\partial \nabla \mathbf{Q}} : (\nabla \mathbf{Q})^{\mathrm{T}} \right] : (\nabla \mathbf{u})^{\mathrm{T}} \mathrm{d}V + \int_S \left\{ \left[\mathbf{I}_{\mathrm{s}} \gamma - \mathbf{I}_{\mathrm{s}} \ \frac{\partial \gamma}{\partial \mathbf{k}} \mathbf{k} - \mathbf{I}_{\mathrm{s}} \ \frac{\partial \gamma}{\partial \nabla_{\mathrm{s}} \mathbf{Q}} : (\nabla_{\mathrm{s}} \mathbf{Q})^{\mathrm{T}} \right] : (\nabla_{\mathrm{s}} \mathbf{u})^{\mathrm{T}} + \Pi_{\mathrm{o}} \mathbf{u} \ \mathbf{k} \right\} \mathrm{d}S + \int_{V^{\mathrm{I}}} (-p^{\mathrm{I}} \mathbf{I}) : (\nabla \mathbf{u})^{\mathrm{T}} \mathrm{d}V. \quad (17)$$

Using the divergence theorem the volume integral in the nematic phase becomes:

$$\int_{V^{\mathrm{N}}} \left[f\mathbf{I} - \frac{\partial f}{\partial \nabla \mathbf{Q}} : (\nabla \mathbf{Q})^{\mathrm{T}} \right] : (\nabla \mathbf{u})^{\mathrm{T}} \mathrm{d}V = -\int_{V^{\mathrm{N}}} \left\{ \nabla \ \left[f\mathbf{I} - \frac{\partial f}{\partial \nabla \mathbf{Q}} : (\nabla \mathbf{Q})^{\mathrm{T}} \right] \right\} \ \mathbf{u}\, \mathrm{d}V + \int_S \mathbf{k} \ \left\{ \left[f\mathbf{I} - \frac{\partial f}{\partial \nabla \mathbf{Q}} : (\nabla \mathbf{Q})^{\mathrm{T}} \right] \ \mathbf{u} \right\} \mathrm{d}S. \quad (18)$$

Using the surface divergence theorem, the surface integral omitting edge terms becomes:

$$\int \left\{ \left[\mathbf{I}_{\mathrm{s}} \gamma - \mathbf{I}_{\mathrm{s}} \ \frac{\partial \gamma}{\partial \mathbf{k}} \mathbf{k} - \mathbf{I}_{\mathrm{s}} \ \frac{\partial \gamma}{\partial \nabla_{\mathrm{s}} \mathbf{Q}} : (\nabla_{\mathrm{s}} \mathbf{Q})^{\mathrm{T}} \right] : (\nabla_{\mathrm{s}} \mathbf{u})^{\mathrm{T}} + \Pi_{\mathrm{o}} \mathbf{u} \ \mathbf{k} \right\} \mathrm{d}S = \int - \left\{ \left(\nabla_{\mathrm{s}} \ \left[\mathbf{I}_{\mathrm{s}} \gamma - \mathbf{I}_{\mathrm{s}} \ \frac{\partial \gamma}{\partial \mathbf{k}} \mathbf{k} - \mathbf{I}_{\mathrm{s}} \ \frac{\partial \gamma}{\partial \nabla_{\mathrm{s}} \mathbf{Q}} : (\nabla_{\mathrm{s}} \mathbf{Q})^{\mathrm{T}} \right] \right) \ \mathbf{u} + \Pi_{\mathrm{o}} \mathbf{u} \ \mathbf{k} \right\} \mathrm{d}S. \quad (19)$$

Using the divergence theorem, the volume integral in the isotropic phase becomes

$$\int_{V^{\mathrm{I}}}(-p^{\mathrm{I}}\mathbf{I}):(\nabla\mathbf{u})^{\mathrm{T}}\,\mathrm{d}V=-\int_{V^{\mathrm{I}}}[\nabla\cdot(-p^{\mathrm{I}}\mathbf{I})]\cdot\mathbf{u}\,\mathrm{d}V-\int_{S}\mathbf{k}\cdot[(-p^{\mathrm{I}}\mathbf{I})\cdot\mathbf{u}]\,\mathrm{d}S. \quad (20)$$

Thus the force balance equation in the bulk nematic phase is:

$$\nabla\cdot\left[f\mathbf{I}-\frac{\partial f}{\partial\nabla\mathbf{Q}}:(\nabla\mathbf{Q})^{\mathrm{T}}\right]=0. \quad (21)$$

Since Π_{o} is a constant and appears in the corresponding surface term, we will include it in equation (21) and find:

$$\nabla\cdot\left[(f+\Pi_{\mathrm{o}})\mathbf{I}-\frac{\partial f}{\partial\nabla\mathbf{Q}}:(\nabla\mathbf{Q})^{\mathrm{T}}\right]=0. \quad (22)$$

It is customary to express the term in brackets in terms of the following mechanical quantities:

$$p^{\mathrm{N}}=-(f+\Pi_{\mathrm{o}});\quad \mathbf{T}^{\mathrm{E}}=-\frac{\partial f}{\partial\nabla\mathbf{Q}}:(\nabla\mathbf{Q})^{\mathrm{T}};\quad (23\,a,b)$$

$$\mathbf{T}^{\mathrm{N}}=-p^{\mathrm{N}}\mathbf{I}+\mathbf{T}^{\mathrm{E}} \quad (23\,c)$$

where p^{N} is the pressure, $\mathbf{T}^{\mathrm{E}}$ is the Ericksen stress tensor, and $\mathbf{T}^{\mathrm{N}}$ is the total bulk stress tensor. The force balance in the isotropic bulk phase is obtained from equation (20):

$$\nabla\cdot\mathbf{T}^{\mathrm{I}}=0 \quad (24)$$

with $\mathbf{T}^{\mathrm{I}}=-p^{\mathrm{I}}\mathbf{I}$.

The surface integral in equation (17) leads, with the use of equations (18–20) to the following interfacial stress balance equation:

$$\int[\mathbf{k}\cdot(\mathbf{T}^{\mathrm{N}}-\mathbf{T}^{\mathrm{I}})-\nabla_{\mathrm{s}}\cdot\mathbf{t}]\cdot\mathbf{u}\,\mathrm{d}S=0 \quad (25)$$

where $\mathbf{t}$ is the total surface stress tensor:

$$\mathbf{t}=\mathbf{I}_{\mathrm{s}}\gamma-\mathbf{I}_{\mathrm{s}}\cdot\left(\frac{\partial\gamma}{\partial\mathbf{k}}\mathbf{k}\right)-\mathbf{I}_{\mathrm{s}}\cdot\frac{\partial\gamma}{\partial\nabla_{\mathrm{s}}\mathbf{Q}}:(\nabla_{\mathrm{s}}\mathbf{Q})^{\mathrm{T}}. \quad (26)$$

Thus the interfacial stress balance equation is:

$$-\mathbf{k}\cdot(\mathbf{T}^{\mathrm{I}}-\mathbf{T}^{\mathrm{N}})=\nabla_{\mathrm{s}}\cdot\mathbf{t} \quad (27)$$

which is indeed the classical expression for interfacial stress jumps across an interface.

5. Surface stress tensor

In this section we discuss in more detail the surface stress tensor $\mathbf{t}$, given that very little discussion has been presented in the experimental or theoretical literature. For an interface between an isotropic substrate and a NLC, the most general surface elastic stress tensor $\mathbf{t}$ is a 2×3 tensor given by the sum of the normal (tension) $\mathbf{t}^{\mathrm{n}}$, bending $\mathbf{t}^{\mathrm{b}}$, and distortion $\mathbf{t}^{\mathrm{d}}$ stresses:

$$\mathbf{t}=\mathbf{t}^{\mathrm{n}}+\mathbf{t}^{\mathrm{b}}+\mathbf{t}^{\mathrm{d}}. \quad (28)$$

The surface stress tensor can naturally be decomposed into the following physically significant contributions:

(a) Normal surface stresses $\mathbf{t}^{\mathrm{n}}$:

$$\mathbf{t}^{\mathrm{n}}(\mathbf{Q},\mathbf{k},\nabla_{\mathrm{s}}\mathbf{Q})=\gamma\mathbf{I}_{\mathrm{s}}. \quad (29)$$

These are the classical 2×2 tension stresses arising in all interfaces. For the NLC/I interface, the tension stresses are a function of $\mathbf{Q}$, $\mathbf{k}$, and $\nabla_{\mathrm{s}}\mathbf{Q}$, in addition to the usual temperature dependence. In particular, surface gradients of the tensor order parameter $\nabla_{\mathrm{s}}\mathbf{Q}$ affect $\mathbf{t}^{\mathrm{n}}$.

(b) Bending stresses $\mathbf{t}^{\mathrm{b}}$:

$$\mathbf{t}^{\mathrm{b}}(\mathbf{Q},\mathbf{k},\nabla\mathbf{Q})=-\mathbf{I}_{\mathrm{s}}\cdot\left(\frac{\partial\gamma}{\partial\mathbf{k}}\mathbf{k}\right)=-\mathbf{I}_{\mathrm{s}}\cdot\left(\frac{\partial\gamma_{\mathrm{an}}}{\partial\mathbf{k}}\mathbf{k}\right)-\mathbf{I}_{\mathrm{s}}\cdot\mathbf{gk}. \quad (30)$$

These are non-classical 2×3 bending stresses. For the NLC/I interface, the bending stresses are a function of $\mathbf{Q}$, $\mathbf{k}$, and $\nabla\mathbf{Q}$, in addition to the usual temperature dependence. In particular, gradients of the tensor order parameter $\nabla\mathbf{Q}$ at the interface, including surface gradients $\nabla_{\mathrm{s}}\mathbf{Q}$ and normal gradients $\mathbf{kk}\cdot\nabla\mathbf{Q}$ at the interface affect $\mathbf{t}^{\mathrm{b}}$. The bending stress tensor $\mathbf{t}^{\mathrm{b}}$ is obviously not symmetric, and hence neither is $\mathbf{t}$.

(c) Tension and shear distortion stresses $\mathbf{t}^{\mathrm{d}}$:

$$\mathbf{t}^{\mathrm{d}}(\mathbf{Q},\mathbf{k},\nabla_{\mathrm{s}}\mathbf{Q})=-\mathbf{I}_{\mathrm{s}}\cdot\frac{\partial\gamma}{\partial\nabla_{\mathrm{s}}\mathbf{Q}}:(\nabla_{\mathrm{s}}\mathbf{Q})^{\mathrm{T}}=-\mathbf{I}_{\mathrm{s}}\cdot\frac{\partial(\mathbf{g}\cdot\mathbf{k})}{\partial\nabla_{\mathrm{s}}\mathbf{Q}}:(\nabla_{\mathrm{s}}\mathbf{Q})^{\mathrm{T}}. \quad (31)$$

These are non-classical 2×2 shear and tension stresses. These stresses are the 2D analogue of the 3×3 bulk Ericksen stresses. Since $\mathbf{t}^{\mathrm{d}}$ is not traceless, it contains both shear components (i.e. components 12 and 21) and tension components (i.e. components 11 and 22). For the NLC/I interface, the distortion stresses are a function of $\mathbf{Q}$, $\mathbf{k}$, and $\nabla_{\mathrm{s}}\mathbf{Q}$, in addition to the usual temperature dependence. In particular, surface gradients of the tensor order parameter $\nabla_{\mathrm{s}}\mathbf{Q}$ affect $\mathbf{t}^{\mathrm{d}}$. The distortion stress tensor is not symmetric. Using the expression for f_{sg}, we find that the distortion surface stress tensor is given by:

$$\mathbf{t}^{\mathrm{d}}(\mathbf{Q},\mathbf{k},\nabla_{\mathrm{s}}\mathbf{Q})=-\mathbf{I}_{\mathrm{s}}\cdot\frac{\partial\gamma}{\partial\nabla_{\mathrm{s}}\mathbf{Q}}:(\nabla_{\mathrm{s}}\mathbf{Q})^{\mathrm{T}}=-\frac{\partial\gamma}{\partial\nabla_{\mathrm{s}}\mathbf{Q}}:(\nabla_{\mathrm{s}}\mathbf{Q})^{\mathrm{T}}=-\frac{L_3}{2}\{\mathbf{I}_{\mathrm{s}}\cdot\mathbf{Qk}-\mathbf{I}_{\mathrm{s}}\mathbf{k}\cdot\mathbf{Q}\}:(\nabla_{\mathrm{s}}\mathbf{Q})^{\mathrm{T}}$$

which clearly is not symmetric.

The surface stress tensor given here is consistent with previous work [28]. To check the validity of the expression for the surface stress tensor $\mathbf{t}$ given in equations (28–31), we assume uniaxiality (set $P=0$ in equation (1)), neglect saddle–splay energy (set $\mathbf{g}=0$, $f_{sg}=0$ in equations (8*a*,*b*)), and obtain:

$$\mathbf{t}=\mathbf{I}_s(\gamma_{is}+\gamma_{an})-\mathbf{I}_s\ C(\mathbf{n}\ \ \mathbf{k})\ \ \mathbf{nk} \qquad (32)$$

in perfect agreement with the surface stress tensor expression previously derived by Ericksen [5], Jenkins and Barrat [6], and Virga [4]. Here C is a given constant.

6. Rotational identities for the bulk and surface stress tensors

In this section we find expressions for the asymmetric components of the bulk and interfacial stress tensors in terms of derivatives of the free energy densities; the expressions are known as rotational identities [7]. These equations will then be used to establish the connection between the bulk and interfacial torque and the stress equations. In what follows we have to present operations with third order tensors and shall use the following transposition nomenclature:

$$(\mathbf{A}^{\mathrm{T}_{123}})_{ijk}=\mathbf{A}_{ijk};\quad (\mathbf{A}^{\mathrm{T}_{231}})_{ijk}=\mathbf{A}_{jki}; \qquad (33\,a,b)$$

$$(\mathbf{A}^{\mathrm{T}_{321}})_{ijk}=\mathbf{A}_{jki};\quad (\mathbf{A}^{\mathrm{T}_{132}})_{ijk}=\mathbf{A}_{ikj}. \qquad (33\,c,d)$$

2.1. *Rotational invariance of the surface stress tensor*

The surface stress tensor $\mathbf{t}$ obeys a rotational identity, since the energy of the system is invariant when subjected to a rotation. Let the rotation be defined as the following rotation tensor [4]:

$$\mathbf{R}=\mathbf{I}+\sin\alpha\mathbf{W}+(1-\cos\alpha)\mathbf{W}\ \ \mathbf{W} \qquad (34)$$

where

$$\mathbf{W}=-\boldsymbol{\varepsilon}\ \ \mathbf{N};\quad \mathbf{W}\ \ \mathbf{W}=-(\mathbf{I}-\mathbf{NN}) \qquad (35\,a,b)$$

and $\boldsymbol{\varepsilon}$ is the alternator unit tensor. Then since $\mathbf{N}$ is the axis of rotation, the rotation of a vector $\mathbf{k}$ by an angle α is $\mathbf{R}\ \ \mathbf{k}$. Since a rotation leaves the energy invariant, we find:

$$\gamma(\mathbf{Q},\mathbf{k},\nabla_s\mathbf{Q})=\gamma(\mathbf{Q}^*,\mathbf{k}^*,\nabla_s^*\mathbf{Q}^*) \qquad (36)$$

where the starred quantities are:

$$\mathbf{Q}^*=\mathbf{R}\ \ \mathbf{Q}\ \ \mathbf{R}^{\mathrm{T}},\quad \mathbf{k}^*=\mathbf{R}\ \ \mathbf{k},\quad \nabla_s^*=\mathbf{R}\ \ \nabla_s. \qquad (37\,a,b,c)$$

Equation (36) implies that the derivative of the surface free energy density with respect to the rotation angle α vanishes:

$$\frac{\partial\gamma(\mathbf{Q}^*,\mathbf{k}^*,\nabla_s^*\mathbf{Q})}{\partial\alpha}=\frac{\partial\gamma}{\partial\mathbf{Q}^*}:\frac{\partial(\mathbf{Q}^*)^{\mathrm{T}}}{\partial\alpha}+\frac{\partial\gamma}{\partial\mathbf{k}^*}\ \ \frac{\partial(\mathbf{k}^*)^{\mathrm{T}}}{\partial\alpha}+\frac{\partial\gamma}{\partial\nabla_s^*\mathbf{Q}^*}\vdots\frac{\partial(\nabla_s^*\mathbf{Q}^*)^{\mathrm{T}}}{\partial\alpha}=0. \qquad (38)$$

Since the derivative vanishes for any α, if we pick $\alpha=0$ we obtain:

$$\mathbf{W}^{\mathrm{T}}:\left[\frac{\partial\gamma}{\partial\mathbf{Q}}\ \ \mathbf{Q}+\left(\frac{\partial\gamma}{\partial\mathbf{Q}}\right)^{\mathrm{T}}\ \ \mathbf{Q}+\frac{\partial\gamma}{\partial\mathbf{k}}\mathbf{k}+\frac{\partial\gamma}{\partial\nabla_s\mathbf{Q}}:(\nabla_s\mathbf{Q})^{\mathrm{T}}+\left(\frac{\partial\gamma}{\partial\nabla_s\mathbf{Q}}\right)^{\mathrm{T}_{321}}:(\nabla_s\mathbf{Q})+\left(\frac{\partial\gamma}{\partial\nabla_s\mathbf{Q}}\right)^{\mathrm{T}_{231}}:(\nabla_s\mathbf{Q})\right]=0. \qquad (39)$$

Thus the tensor $\boldsymbol{\Sigma}$:

$$\boldsymbol{\Sigma}=\frac{\partial\gamma}{\partial\mathbf{Q}}\ \ \mathbf{Q}+\left(\frac{\partial\gamma}{\partial\mathbf{Q}}\right)^{\mathrm{T}}\ \ \mathbf{Q}+\frac{\partial\gamma}{\partial\mathbf{k}}\mathbf{k}+\frac{\partial\gamma}{\partial\nabla_s\mathbf{Q}}:(\nabla_s\mathbf{Q})^{\mathrm{T}}+\left(\frac{\partial\gamma}{\partial\nabla_s\mathbf{Q}}\right)^{\mathrm{T}_{321}}:(\nabla_s\mathbf{Q})+\left(\frac{\partial\gamma}{\partial\nabla_s\mathbf{Q}}\right)^{\mathrm{T}_{231}}:(\nabla_s\mathbf{Q}) \qquad (40)$$

is symmetric, $\boldsymbol{\Sigma}-\boldsymbol{\Sigma}^{\mathrm{T}}=0$. Expressing the second and third terms of $\boldsymbol{\Sigma}$ in terms of the surface stress tensor $\mathbf{t}$, we find:

$$\frac{\partial\gamma}{\partial\mathbf{k}}\mathbf{k}+\frac{\partial\gamma}{\partial\nabla_s\mathbf{Q}}:(\nabla_s\mathbf{Q})^{\mathrm{T}}=-\mathbf{t}+\left(\mathbf{k}\ \ \frac{\partial\gamma}{\partial\mathbf{k}}\right)\mathbf{kk}+\gamma\mathbf{I}_s \qquad (41)$$

and

$$\boldsymbol{\Sigma}=-\mathbf{t}+\left(\mathbf{k}\ \ \frac{\partial\gamma}{\partial\mathbf{k}}\right)\mathbf{kk}+\gamma\mathbf{I}_s+\left[\frac{\partial\gamma}{\partial\mathbf{Q}}+\left(\frac{\partial\gamma}{\partial\mathbf{Q}}\right)^{\mathrm{T}}\right]\ \ \mathbf{Q}+\left[\left(\frac{\partial\gamma}{\partial\nabla_s\mathbf{Q}}\right)^{\mathrm{T}_{321}}+\left(\frac{\partial\gamma}{\partial\nabla_s\mathbf{Q}}\right)^{\mathrm{T}_{231}}\right]:(\nabla_s\mathbf{Q}). \qquad (42)$$

Using the symmetry of $\boldsymbol{\Sigma}$, we finally arrive at the rotational identity obeyed by the surface stress tensor:

$$\begin{aligned}\mathbf{t}-\mathbf{t}^{\mathrm{T}}=&\left\{\left[\frac{\partial\gamma}{\partial\mathbf{Q}}+\left(\frac{\partial\gamma}{\partial\mathbf{Q}}\right)^{\mathrm{T}}\right]\ \mathbf{Q}\right.\\&\left.+\left[\left(\frac{\partial\gamma}{\partial\nabla_{\mathrm{s}}\mathbf{Q}}\right)^{\mathrm{T}_{321}}+\left(\frac{\partial\gamma}{\partial\nabla_{\mathrm{s}}\mathbf{Q}}\right)^{\mathrm{T}_{231}}\right]:(\nabla_{\mathrm{s}}\mathbf{Q})\right\}\\&-\left\{\left[\frac{\partial\gamma}{\partial\mathbf{Q}}+\left(\frac{\partial\gamma}{\partial\mathbf{Q}}\right)^{\mathrm{T}}\right]\ \mathbf{Q}\right.\\&\left.+\left[\left(\frac{\partial\gamma}{\partial\nabla_{\mathrm{s}}\mathbf{Q}}\right)^{\mathrm{T}_{321}}+\left(\frac{\partial\gamma}{\partial\nabla_{\mathrm{s}}\mathbf{Q}}\right)^{\mathrm{T}_{231}}\right]:(\nabla_{\mathrm{s}}\mathbf{Q})\right\}^{\mathrm{T}}.\end{aligned}\tag{43}$$

This expression has not been presented before in the literature but is the exact analogue of the bulk expression, shown in what follows.

6.2. *Rotational identity of the bulk stress tensor*

The bulk stress tensor $\mathbf{T}^{\mathrm{N}}$ also obeys a rotational identity, since the bulk energy of the system is invariant when subjected to a rotation. Since a rotation leaves the bulk energy invariant, we find:

$$f(\mathbf{Q},\nabla\mathbf{Q})=f(\mathbf{Q}^*,\nabla^*\mathbf{Q}^*)\tag{44}$$

where the starred quantities are:

$$\mathbf{Q}^*=\mathbf{R}\ \ \mathbf{Q}\ \ \mathbf{R}^{\mathrm{T}},\quad \nabla^*=\mathbf{R}\ \ \nabla.\tag{45 a,b}$$

Equation (44) implies that the derivative of the bulk free energy density with respect to the rotation angle α vanishes:

$$\frac{\partial f(\mathbf{Q}^*,\nabla^*\mathbf{Q}^*)}{\partial\alpha}=\frac{\partial f}{\partial\mathbf{Q}^*}:\frac{\partial(\mathbf{Q}^*)^{\mathrm{T}}}{\partial\alpha}+\frac{\partial f}{\partial\nabla^*\mathbf{Q}^*}\vdots\frac{\partial(\nabla^*\mathbf{Q}^*)^{\mathrm{T}}}{\partial\alpha}=0.\tag{46}$$

Since the derivative vanishes for any α, if we pick $\alpha=0$ we obtain:

$$\begin{aligned}\mathbf{W}^{\mathrm{T}}:&\left[\frac{\partial f}{\partial\mathbf{Q}}\ \mathbf{Q}+\left(\frac{\partial f}{\partial\mathbf{Q}}\right)^{\mathrm{T}}\ \mathbf{Q}+\frac{\partial f}{\partial\nabla\mathbf{Q}}:(\nabla\mathbf{Q})^{\mathrm{T}}\right.\\&\left.+\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)^{\mathrm{T}_{321}}:(\nabla\mathbf{Q})+\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)^{\mathrm{T}_{231}}:(\nabla\mathbf{Q})\right]=0.\end{aligned}\tag{47}$$

Thus the tensor $\boldsymbol{\Psi}$:

$$\begin{aligned}\boldsymbol{\Psi}=&\frac{\partial f}{\partial\nabla\mathbf{Q}}:(\nabla\mathbf{Q})^{\mathrm{T}}+\left[\frac{\partial f}{\partial\mathbf{Q}}+\left(\frac{\partial f}{\partial\mathbf{Q}}\right)^{\mathrm{T}}\right]\ \mathbf{Q}\\&+\left[\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)^{\mathrm{T}_{321}}+\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)^{\mathrm{T}_{231}}\right]:(\nabla\mathbf{Q})\end{aligned}\tag{48}$$

is symmetric, $\boldsymbol{\Psi}-\boldsymbol{\Psi}^{\mathrm{T}}=0$. Expressing the first terms of $\boldsymbol{\Psi}$ in term of the bulk stress tensor $\mathbf{T}^{\mathrm{N}}$, we find:

$$\frac{\partial f}{\partial\nabla\mathbf{Q}}:(\nabla\mathbf{Q})^{\mathrm{T}}=-\mathbf{T}^{\mathrm{N}}-p\mathbf{I}\tag{49}$$

and

$$\begin{aligned}\boldsymbol{\Psi}=&-\mathbf{T}^{\mathrm{N}}-p\mathbf{I}+\left[\frac{\partial f}{\partial\mathbf{Q}}+\left(\frac{\partial f}{\partial\mathbf{Q}}\right)^{\mathrm{T}}\right]\ \mathbf{Q}\\&+\left[\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)^{\mathrm{T}_{321}}+\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)^{\mathrm{T}_{231}}\right]:(\nabla\mathbf{Q}).\end{aligned}\tag{50}$$

Using the symmetry of $\boldsymbol{\Psi}$, we finally arrive at the rotational identity obeyed by the bulk stress tensor:

$$\begin{aligned}\mathbf{T}^{\mathrm{N}}-(\mathbf{T}^{\mathrm{N}})^{\mathrm{T}}=&\left\{\left[\frac{\partial f}{\partial\mathbf{Q}}+\left(\frac{\partial f}{\partial\mathbf{Q}}\right)^{\mathrm{T}}\right]\ \mathbf{Q}\right.\\&\left.+\left[\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)^{\mathrm{T}_{321}}+\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)^{\mathrm{T}_{231}}\right]:(\nabla\mathbf{Q})\right\}\\&-\left\{\left[\frac{\partial f}{\partial\mathbf{Q}}+\left(\frac{\partial f}{\partial\mathbf{Q}}\right)^{\mathrm{T}}\right]\ \mathbf{Q}\right.\\&\left.+\left[\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)^{\mathrm{T}_{321}}+\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)^{\mathrm{T}_{231}}\right]:(\nabla\mathbf{Q})\right\}^{\mathrm{T}}.\end{aligned}\tag{51}$$

This expression has already been presented in the literature [14]. Comparing the rotational identities for the bulk (equation (51)) and surface (equation (43)) stress tensors we find that they are completely analogous.

7. Asymmetric stresses in the surface and bulk torque balance equations

Alternative expressions for the static limit of the interfacial and bulk internal angular momentum balance equations are obtained by introducing the following duals of the asymmetric components of the interfacial and bulk stress tensors:

$$\mathbf{T}_x^{\mathrm{N}}=-\boldsymbol{\varepsilon}:\frac{1}{2}[\mathbf{T}^{\mathrm{N}}-(\mathbf{T}^{\mathrm{N}})^{\mathrm{T}}]=-\boldsymbol{\varepsilon}:\mathbf{T}^{\mathrm{N}}\tag{52}$$

$$\mathbf{t}_x^{\mathrm{N}}=-\boldsymbol{\varepsilon}:\frac{1}{2}[\mathbf{t}-(\mathbf{t})^{\mathrm{T}}]=-\boldsymbol{\varepsilon}:\mathbf{t}\tag{53}$$

where $\boldsymbol{\varepsilon}$ is the alternating third order tensor [17]. The static limit of the bulk and interfacial internal angular momentum equations read, respectively [17]:

$$\mathbf{T}_x^{\mathrm{N}}+\nabla\ \ \mathbf{C}_{\mathrm{b}}=0\tag{54}$$

$$\mathbf{t}_x^{\mathrm{N}}+\nabla_{\mathrm{s}}\ \ \mathbf{C}_{\mathrm{s}}=\mathbf{k}\ \ \mathbf{C}_{\mathrm{b}}\tag{55}$$

where $\mathbf{C}_{\mathrm{b}}$ is the bulk couple stress tensor, and $\mathbf{C}_{\mathrm{s}}$ is the surface couple stress tensor. The purpose of this section is to show that the present equations follow the well known classical format of polar fluids [17]. Similar polar fluid equations with applications to liquid crystals have been given previously by Papenfuss and Muschik [29].

7.1. *Alternative expression of the surface torque balance equation*

Operating on the interfacial torque balance equation (14 *b*) as follows:

$$\left[\mathbf{k}\;\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)+\frac{\partial\gamma}{\partial\mathbf{Q}}-\nabla_{\mathrm{s}}\;\left(\frac{\partial\gamma}{\partial\nabla_{\mathrm{s}}\mathbf{Q}}\right)\right]^{[\mathrm{s}]}\;\mathbf{Q}$$
$$-\mathbf{Q}\;\left[\mathbf{k}\;\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)+\frac{\partial\gamma}{\partial\mathbf{Q}}-\nabla_{\mathrm{s}}\;\left(\frac{\partial\gamma}{\partial\nabla_{\mathrm{s}}\mathbf{Q}}\right)\right]^{[\mathrm{s}]}=0 \tag{56}$$

we find after some algebra and with the use of the rotational identity (43) that equation (56) becomes:

$$-\mathbf{k}\;\;(\mathbf{X}-\mathbf{X}^{\mathrm{T}})=[\mathbf{t}^{\mathrm{N}}-(\mathbf{t}^{\mathrm{N}})^{\mathrm{T}}]-[(\nabla_{\mathrm{s}}\;\;\mathbf{x})-(\nabla_{\mathrm{s}}\;\;\mathbf{x})^{\mathrm{T}}] \tag{57}$$

where the bulk $\mathbf{X}$ and surface $\mathbf{x}$ third order tensor are:

$$\mathbf{X}=\left[\frac{\partial f}{\partial\nabla\mathbf{Q}}+\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)^{\mathrm{T}_{231}}\right]\;\mathbf{Q};$$
$$\mathbf{x}=\left[\frac{\partial\gamma}{\partial\nabla_{\mathrm{s}}\mathbf{Q}}+\left(\frac{\partial\gamma}{\partial\nabla_{\mathrm{s}}\mathbf{Q}}\right)^{\mathrm{T}_{231}}\right]\;\mathbf{Q}. \tag{58}$$

Introducing the following bulk $\mathbf{C}_{\mathrm{b}}$ and surface $\mathbf{C}_{\mathrm{s}}$ couple stress tensors:

$$\mathbf{C}_{\mathrm{b}}=\mathbf{X}:\boldsymbol{\varepsilon};\quad \mathbf{C}_{\mathrm{s}}=\mathbf{x}:\boldsymbol{\varepsilon} \tag{59 a,b}$$

we find that the contraction of equation (57) with the alternating tensor $\boldsymbol{\varepsilon}$ becomes:

$$\mathbf{k}\;\;\mathbf{C}_{\mathrm{b}}=\mathbf{t}_x^{\mathrm{N}}+\nabla_{\mathrm{s}}\;\;\mathbf{C}_{\mathrm{s}} \tag{60}$$

which agrees with the classical interfacial equation for polar fluids; see equation (4.2-10) of reference [17].

7.2. *Alternative expression of the bulk torque balance equation*

Operating on the bulk torque balance equation, equation (14 *a*), as follows:

$$\left[\frac{\partial f}{\partial\mathbf{Q}}-\nabla\;\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)\right]^{[\mathrm{s}]}\;\mathbf{Q}$$
$$-\mathbf{Q}\;\left[\frac{\partial f}{\partial\mathbf{Q}}-\nabla\;\left(\frac{\partial f}{\partial\nabla\mathbf{Q}}\right)\right]^{[\mathrm{s}]}=0 \tag{61}$$

we find, after some algebra and with the use of the rotational identity (51), that equation (61) becomes:

$$0=[\mathbf{T}^{\mathrm{N}}-(\mathbf{T}^{\mathrm{N}})^{\mathrm{T}}]-[(\nabla\;\;\mathbf{X})-(\nabla\;\;\mathbf{X})^{\mathrm{T}}]. \tag{62}$$

Taking the double contraction of this equation with the alternator tensor $\boldsymbol{\varepsilon}$, we find:

$$0=\mathbf{T}_x^{\mathrm{N}}+\nabla\;\;\mathbf{C}_{\mathrm{b}} \tag{63}$$

which agrees with the classical interfacial equation for polar fluids; see equation (4.1-8) of reference [17].

8. Conclusions

The generalized equations of nematostatics in terms of the tensor order parameter have been derived using the calculus of variations, and taking into account interfacial and bulk nematic free energies. The complete expression for the surface tensor order parameter has been derived, and is found to contain normal, shear, and bending stresses. In addition, anchoring energy contributes to bending and normal stresses, while saddle–splay energy contributes to normal and shear stresses. The rotational identities governing the bulk and surface stress tensors are derived and used to show that the equations of nematostatics are fully consistent with the general balance equations of polar fluids.

The equations presented provide a theoretical framework for solving interfacial problems involving nematic liquid crystals that is applicable to cases where variations in liquid crystalline order and saddle–splay energy play significant roles.

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