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C_{2v} 对称性下液晶多张量模型的取向弹性推导

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摘 要

本文针对具有 C_{2v} 对称性的液晶分子形成的向列相，基于体积能稳定点和自由能的表达，推导了 C_{2v} 向列相的取向弹性。这种表达能够在一定程度上反映液晶相局部各向异性的对称性，并且其中的系数与分子参数有关，具有明确的物理意义。

关键词

向列相液晶，对称性，取向弹性

Derivation of Orientational Elasticity of Liquid Crystal Multitensor Model with C_{2v} Symmetry

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Abstract

In this paper, the orientational elasticity of C_{2v} nematic phase is derived based on the

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expression of the stability points of volume energy and free energy for the nematic phase formed by liquid crystal molecules with C_{2v} symmetry. This expression can reflect the symmetry of local anisotropy of liquid crystal phase to a certain extent, and the coefficients are related to molecular parameters, which has clear physical significance.

Keywords

Nematic Liquid Crystal, Symmetry, Orientational Elasticity

1. 引言

液晶是一种介于液态与固态的中间态, 向列相液晶具有局部各向异性的特点. 在数学上, 一般用点群描述液晶分子和局部液晶相各向异性的对称性 [1]. 弹性作为液晶均匀向列相的重要属性, 在液晶的数学建模过程中起着重要的作用. 局部各向异性是液晶向列相在平衡状态下的主要特征, 在此状态下, 弹性源于液晶相受边界与外力作用而发生的形变. 不同分子形成的不同向列相, 其弹性能的形式不尽相同. 具有 C_{2v} 对称性的液晶分子结构相对复杂, 并非简单的轴对称性, 能够形成多种向列相, 本文主要研究其形成的具有 C_{2v} 对称性的向列相的取向弹性.

常见的单轴向列相液晶的局部各向异性表现为简单的轴对称性质, 通常用单位指向矢 $\mathbf{n}$ 描述其局部最优取向. 当变形很小时, 指向的改变可以忽略不计, 因此可将局部最优取向取为位置是 $\mathbf{x}$ 的函数, 即 $\mathbf{n} = \mathbf{n}(\mathbf{x})$. 单轴向列相液晶的能量泛函可以通过 Oseen-Frank 能表达, 它是关于 $\mathbf{n}(\mathbf{x})$ 的泛函, 其中三项分别表示展曲, 扭曲, 弯曲所产生的能量 [2].

Oseen-Frank 能量对弹性常数 K_i 的测量具有重要意义. 在早期, Frederiks 等人研究了棒状分子的弹性常数 [3–5], 此后 Kaur 等人又针对由香蕉形分子形成的单轴相做出相应研究 [6–8], 并且 Sathyanarayana 等人研究了香蕉形分子类似物形成的单轴相的弹性常数 [9, 10] . 对于其它复杂结构的分子, 可能会表现出其他向列相, 如香蕉形分子形成的双轴向列相 [11, 12]. 对于双轴向列相, 已有工作研究了二阶取向弹性的形式, 并建立在动态模型中 [13–15].

在最近的研究中, Li. 和 Xu. 针对香蕉形分子形成的双轴向列相液晶建立了标架动力学模型 [16], 取向弹性对于模型在介观标架下的表达起着重要的作用. 模型中用两个线性无关的二阶序参量表达液晶相的局部各向异性, 即双轴向列相下的体积能稳定点, 得到了取向弹性的表达式, 其中

的系数均与分子物理参数相关联, 因此有明确的物理意义. 这在数值模拟方面具有重要的用途.

在建模过程中反应分子结构对弹性常数的影响具有重要意义. 基于 Onsager 分子理论建立的各种模型中, 模型系数与分子参数有关, 如基于分子理论的张量模型和由此推导出的标架模型等. 借助取向弹性, 又能将弹性常数通过这些系数表达出来, 因此, 研究不同液晶相下取向弹性的表达具有重要的应用价值. 取向弹性的推导基于标架的一阶导数, 能够从基于分子理论的张量模型中的自由能表达式推导得出 [17]. 本文针对具有 C_{2v} 对称性的分子形成的具有 C_{2v} 对称性的向列相液晶, 推导了其取向弹性的具体表达. 这种液晶相较双轴相具有更一般的对称性, 其指向弹性也更加复杂. 此推导过程仍源于基于 Onsager 分子理论的自由能表达, 最终得出的系数与分子参数有关, 具有物理意义.

本文在第二节介绍了推导取向弹性过程所需的基本理论, 如张量的运算和一些重要符号的说明. 第三节给出多张量模型中自由能的表达. 在第四节详细推导了具有 C_{2v} 对称性的液晶相下的取向弹性, 并简单阐述了它与其它向列相的取向弹性的关联. 最后在第五节总结了本文的主要结果和研究意义.

2. 张量与微分算子

本节给出推导取向弹性表达式过程中必需的基本理论, 其中对相同指标均使用 Einstein 求和约定.

首先介绍张量的相关概念和运算. 一般地, $\mathbb{R}^3$ 中的 n 阶张量 U 可以在参考正交标架 $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ 下表达为基与坐标的形式, 选取 $\mathbf{e}_{i_1}, \cdots, \mathbf{e}_{i_n}$ 的张量积作为基底, 其中 $i_1, \cdots, i_n \in \{1, 2, 3\}$, 此时 n 阶张量 U 表达为

$$U = U_{i_1 \cdots i_n} \mathbf{e}_{i_1} \otimes \cdots \otimes \mathbf{e}_{i_n},$$

这里 $U_{i_1 \cdots i_n}$ 为张量 U 在这组基底下的坐标. 两个张量间的点积符号表示张量的缩并运算, 将同阶张量 U 和 V 的缩并 $U \cdot V$ 定义为它们的坐标向量的数量积, 即相应分量乘积的和, 记为

$$U \cdot V = U_{i_1 \ldots i_n} V_{i_1 \ldots i_n},$$

并且$|U|^2 = U \cdot U$. 在此定义下, 两个同阶张量的缩并结果为一个标量.

如果对于 $\{1, \cdots, n\}$ 的任意排列 σ, n阶张量U的坐标总满足 $U_{i_{\sigma(1)} \cdots i_{\sigma(n)}} = U_{i_1 \cdots i_n}$, 则称其是 n 阶对称张量. 将张量的迹定义为针对其某两个指标的一阶缩并, 即一个 $n-2$ 阶张量

$$(\mathrm{tr} U)_{i_1 \ldots i_{n-2}} = U_{i_1 \ldots i_{n-2} kk}.$$

若对称张量 U 满足 $\mathrm{tr} U = 0$, 则称 U 为对称迹零张量.

对于 n 阶张量 $U = \mathbf{m}_1 \otimes \cdots \otimes \mathbf{m}_n \in \mathbb{R}^3$, 其分量形式为

$$U_{i_1 \cdots i_n} = (m_1)_{i_1} \cdots (m_n)_{i_n}, i_1, \cdots, i_n = 1, 2, 3.$$

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为便于在正交标架下表示对称张量, 可以使用单项式符号, 将 n 阶对称张量表示为 [1]

$$\mathbf{m}_1^{k_1}\mathbf{m}_2^{k_2}\mathbf{m}_3^{k_3} = \Big(\underbrace{\mathbf{m}_1\otimes\cdots\otimes\mathbf{m}_1}_{k_1}\otimes\underbrace{\mathbf{m}_2\otimes\cdots\otimes\mathbf{m}_2}_{k_2}\otimes\underbrace{\mathbf{m}_3\otimes\cdots\otimes\mathbf{m}_3}_{k_3}\Big)_{\text{sym}}. \tag{2.1}$$

其中 $k_1+k_2+k_3=n$. 对于任意的 n 阶张量, 可以将其表示为一个对称张量和一个反对称张量之和, 其中对称部分表示为

$$(U_{\text{sym}})_{i_1\cdots i_n} = \frac{1}{n!}\sum_{\sigma} U_{i_{\sigma(1)}\cdots i_{\sigma(n)}}.$$

(2.1) 的表达方式也同样适用于其它正交标架, 如局部正交标架 $\mathfrak{p}=(\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3)$.

当 $k_1+k_2+k_3=n$ 时, 可由一组线性无关的 n 阶对称张量构成基底, 使得任意对称张量都能用这组基底线性表出, 表达为 $\mathbf{m}_1,\mathbf{m}_2,\mathbf{m}_3$ 的齐次多项式. 二阶恒等张量 $\mathfrak{i}$ 表示为

$$\mathfrak{i} = \mathbf{m}_1^2+\mathbf{m}_2^2+\mathbf{m}_3^2,$$

其分量形式的表达可以借助 Kroneker 符号, 即 $\mathfrak{i}_{ij}=\delta_{ij}, i,j=1,2,3$, 其中

$$\delta_{ij} = \begin{cases} 1,\ i=j \\ 0,\ i\neq j \end{cases}.$$

另一个重要的符号为 Levi-Civita 符号, 表示为

$$\epsilon^{ijk} = \begin{cases} 1,\ (ijk)=(123),(231),(312) \\ -1,(ijk)=(132),(213),(321) \\ 0,\ 其它 \end{cases}.$$

行列式张量由此表达为 [18]

$$\begin{aligned}\epsilon &= \epsilon^{ijk}\mathbf{m}_i\otimes\mathbf{m}_j\otimes\mathbf{m}_k \\ &= \mathbf{m}_1\otimes\mathbf{m}_2\otimes\mathbf{m}_3+\mathbf{m}_2\otimes\mathbf{m}_3\otimes\mathbf{m}_1+\mathbf{m}_3\otimes\mathbf{m}_1\otimes\mathbf{m}_2 \\ &\quad -\mathbf{m}_1\otimes\mathbf{m}_3\otimes\mathbf{m}_2-\mathbf{m}_2\otimes\mathbf{m}_1\otimes\mathbf{m}_3-\mathbf{m}_3\otimes\mathbf{m}_2\otimes\mathbf{m}_1.\end{aligned} \tag{2.2}$$

这两个符号之间有一些重要的运算, 如

$$\epsilon^{ijk}\epsilon^{ipq} = \delta_{jp}\delta_{kq}-\delta_{jq}\delta_{kp},$$
$$\epsilon^{ijk}\epsilon^{pqr} = \det\begin{pmatrix}\delta_{ip} & \delta_{iq} & \delta_{ir} \\ \delta_{jp} & \delta_{jq} & \delta_{jr} \\ \delta_{kp} & \delta_{kq} & \delta_{kr}\end{pmatrix}.$$

此外, 用 $\langle\cdot\rangle$ 表示 $SO(3)$ 上的张量矩, 即函数 $\mathbf{m}_{i_1}\otimes\cdots\otimes\mathbf{m}_{i_n}$ 在 $SO(3)$ 上关于密度函数 $\rho(\mathfrak{p})$ 的平均可以表示为

$$\langle\mathbf{m}_{i_1}\otimes\cdots\otimes\mathbf{m}_{i_n}\rangle=\int_{SO(3)}\mathbf{m}_{i_1}(\mathfrak{p})\otimes\cdots\otimes\mathbf{m}_{i_n}(\mathfrak{p})\rho(\mathfrak{p})\mathrm{d}\mathfrak{p},\ i_1,\cdots i_n=1,2,3.$$

关于微分算子 ∇, 以一阶张量 $\mathbf{m}$ 为例, 给出张量的梯度, 散度以及旋度的求法:

$$(\nabla\mathbf{m})_{ij}=\partial_j m_i,\ \nabla\cdot\mathbf{m}=\partial_i m_i,\ (\nabla\times\mathbf{m})_i=\epsilon^{ijk}\partial_j m_k.$$

借助 $SO(3)$ 上的旋转微分算子, 能够求得正交标架的导数, 由此可以计算取向弹性的表达式. 在局部标架 $\mathfrak{p}(\mathbf{x})$ 下, $\mathbf{n}_\mu$ 沿着方向 $\mathbf{n}_\lambda$ 的导数为 $\mathbf{n}_\lambda\cdot\nabla\mathbf{n}_\mu$. 它在标架 $\mathfrak{p}$ 中的 ν 分量记为 $n_{\lambda i}n_{\nu j}\partial_i n_{\mu j}$. 由等式 $n_{\mu j}n_{\nu j}=\delta_{\mu\nu}$, 得到一个重要的关系:

$$n_{\lambda i}n_{\nu j}\partial_i n_{\mu j}=-n_{\lambda i}n_{\mu j}\partial_i n_{\nu j}.$$

由此算得, 标架 $\mathfrak{p}$ 的一阶导数有九个自由度 [15–17]:

$$\begin{cases}D_{11}=n_{1i}n_{2j}\partial_i n_{3j},\ D_{12}=n_{1i}n_{3j}\partial_i n_{1j},\ D_{13}=n_{1i}n_{1j}\partial_i n_{2j},\\ D_{21}=n_{2i}n_{2j}\partial_i n_{3j},\ D_{22}=n_{2i}n_{3j}\partial_i n_{1j},\ D_{23}=n_{2i}n_{1j}\partial_i n_{2j},\\ D_{31}=n_{3i}n_{2j}\partial_i n_{3j},\ D_{32}=n_{3i}n_{3j}\partial_i n_{1j},\ D_{33}=n_{3i}n_{1j}\partial_i n_{2j}.\end{cases}\tag{2.3}$$

3. 自由能与特征标架

在液晶的分子模型中, 能量的表达由二阶维里展开得到. 在空间均匀的情形中, 自由能形式为

$$F[f]=F_0+k_BT\Big(\int_{S^2}\mathrm{d}\mathbf{m}f(\mathbf{m})\log f(\mathbf{m})+\frac{1}{2}\int\int_{S^2\times S^2}\mathrm{d}\mathbf{m}\mathrm{d}\mathbf{m}'f(\mathbf{m})G(\mathbf{m},\mathbf{m}')f(\mathbf{m}')\Big).\tag{3.1}$$

其中 k_B 为 Boltzmann 常数, T 为绝对温度. 概率密度函数 $f(\mathbf{x},\mathbf{m})$ 代表在 $\mathbf{x}\in\Omega$ 处平行于指向 $\mathbf{m}$ 的分子的构型分布函数, $G(\mathbf{m},\mathbf{m}')$ 是分子间的相互作用核函数, 最后一项代表系统中分子间的相互作用势, 可以选取硬核势或 Maier-Saupe 势. 在张量模型中, 自由能可以通过对 (3.1) 中的密度函数 $f(\mathbf{x},\mathbf{m})$ 作 Taylor 展开得到, 其中的系数可由分子模型建立过程中所涉及的分子物理参数 k_B, T 表示, 且为正相关 [19].

具有 C_{2v} 对称性的分子所形成向列相的局部各向异性需要四个序参量描述 [1],

$$Q_1=\langle\mathbf{m}_1\rangle,\quad Q_2=\langle\mathbf{m}_1^2-\mathfrak{i}/3\rangle,\quad Q_3=\langle\mathbf{m}_2^2-\mathbf{m}_3^2\rangle,\quad Q_4=\langle\mathbf{m}_2\mathbf{m}_3\rangle,\tag{3.2}$$

其中 Q_1 是一阶张量, $Q_\alpha(\alpha=2,3,4)$ 是二阶对称迹零张量. 将这四个序参量记为向量形式, 即 $\mathbf{Q}=(Q_1,\cdots,Q_4)^T$.

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假设向列相液晶分子浓度为常数 c, 其自由能由体积能和弹性能构成, 即 [19]

$$\frac{\mathcal{F}(\mathbf{Q},\nabla\mathbf{Q})}{k_BT} = \int \mathrm{d}\mathbf{x}\left(\frac{1}{\varepsilon}F_{\mathrm{b}}(\mathbf{Q}) + F_{\mathrm{e}}(\mathbf{Q},\nabla\mathbf{Q})\right), \tag{3.3}$$

其中 k_B 是 Boltzmann 常数, T 是绝对温度. 其中 F_{b} 和 F_{e} 分别表示体积能密度和弹性能密度. 小参数 ε 描述刚性液晶分子和液晶局部之间的平方相对尺度 $\tilde{L}$. 体积能密度 F_{b} 包括熵项和 $\mathbf{Q}$ 的二次项, 即

$$F_{\mathrm{b}} = cF_{\mathrm{entropy}} + \frac{c^2}{2}\big(c_{01}|Q_1|^2 + c_{02}|Q_2|^2 + 2c_{03}Q_2\cdot Q_3 + c_{04}|Q_3|^2 + c_{05}|Q_4|^2\big), \tag{3.4}$$

熵项 F_{entropy} 对于保持自由能稳态起到关键作用. 弹性能密度 F_{e} 包括 $\nabla\mathbf{Q}$ 的线性项和二次项, 即

$$F_{\mathrm{e}} = \frac{c^2}{2}\left(F_{1,\mathrm{elastic}} + F_{2,\mathrm{elastic}}\right), \tag{3.5}$$

$$\begin{aligned} F_{1,\mathrm{elastic}} = {}& c_{10}\nabla\cdot Q_1 + c_{11}Q_1\cdot(\nabla\cdot Q_2) + c_{12}Q_1\cdot(\nabla\cdot Q_3)\\ &+ c_{13}Q_2\cdot\nabla\times Q_4 + c_{14}Q_3\cdot\nabla\times Q_4, \end{aligned} \tag{3.6}$$

$$\begin{aligned} F_{2,\mathrm{elastic}} = {}& c_{21}|\nabla Q_1|^2 + c_{22}|\nabla Q_2|^2 + 2c_{23}\nabla Q_2\cdot\nabla Q_3 + c_{24}|\nabla Q_3|^2\\ &+ c_{25}|\nabla Q_4|^2 + c_{26}|\nabla\cdot Q_1|^2 + c_{27}|\nabla\cdot Q_2|^2 + 2c_{28}(\nabla\cdot Q_2)\cdot(\nabla\cdot Q_3)\\ &+ c_{29}|\nabla\cdot Q_3|^2 + c_{2,10}|\nabla\cdot Q_4|^2 + c_{2,13}(\nabla\times Q_1)\cdot(\nabla\cdot Q_4). \end{aligned} \tag{3.7}$$

其中的系数 c_{ij} 由分子参数决定.

下面在局部正交标架 $(\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3)$下描述向列相. 在参考文献 [20]中, Xu. 通过通过提取张量的非零分量, 对体积能稳定点进行分析, 得到不同向列相的特征标架. 当液晶分子的对称性为 C_{2v} 时, 根据其体积能的系数, 适当选取自由参数 ν, 使得矩阵

$$\begin{pmatrix} c_{01} & & & \\ & c_{02} & c_{03} & \\ & c_{03} & c_{04} & \\ & & & c_{05} \end{pmatrix}$$

是非负定的, 在稳定点就可得到其 C_{2v} 向列相的特征标架为 [20,21]

$$\begin{aligned} &Q_1 = d_1\mathbf{n}_1, \quad Q_2 = s_2\Big(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}\Big) + b_2(\mathbf{n}_2^2 - \mathbf{n}_3^2),\\ &Q_3 = s_3\Big(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3}\Big) + b_3(\mathbf{n}_2^2 - \mathbf{n}_3^2), \quad Q_4 = d_4\mathbf{n}_2\mathbf{n}_3. \end{aligned} \tag{3.8}$$

当 (3.8) 中的系数 d_1, d_4, b_2, b_3 为 0 时, 即为具有 $C_{\infty v}$ 对称性的向列相. 对于一些高阶对称迹零张量，也可以在由标架 $(\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3)$ 生成的不同基底下线性表出.

4. 取向弹性

利用二阶恒等张量 $\mathfrak{i} = \mathbf{n}_1^2 + \mathbf{n}_2^2 + \mathbf{n}_3^2$, 可将 (3.8) 中的 $Q_\alpha(\alpha = 2, 3)$ 变形为

$$\begin{aligned} Q_\alpha =& s_\alpha \left(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3} \right) + b_\alpha \left(\mathbf{n}_2^2 - \mathbf{n}_3^2 \right) \\ =& s_\alpha \left(\mathbf{n}_1^2 - \frac{\mathfrak{i}}{3} \right) + b_\alpha \left(\mathbf{n}_2^2 - \mathfrak{i} + \mathbf{n}_1^2 + \mathbf{n}_2^2 \right) \\ =& \left(s_\alpha + b_\alpha \right) \mathbf{n}_1^2 + 2b_\alpha \mathbf{n}_2^2 - \left(\frac{1}{3} s_\alpha + b_\alpha \right) \mathfrak{i}, \quad \alpha = 2, 3. \end{aligned} \tag{4.1}$$

为了计算取向弹性的系数, 分别考虑自由能中的线性一阶导数项, 二次一阶导数项, 即一阶弹性能密度 (3.6) 和二阶弹性能密度 (3.7).

由 (3.8) 和 (4.1), 算得一阶弹性能密度 (3.6) 中各项分别为

$$\begin{aligned} \nabla \cdot Q_1 =& d_1 \partial_i n_{1i}, \\ Q_1 \cdot (\nabla \cdot Q_\alpha) =& d_1 n_{1i} \partial_j \left[\left(s_\alpha + b_\alpha \right) \mathbf{n}_1^2 + 2b_\alpha \mathbf{n}_2^2 - \left(\frac{1}{3} s_\alpha + b_\alpha \right) \mathfrak{i} \right]_{ij} \\ =& d_1 n_{1i} \left[\left(s_\alpha + b_\alpha \right) \left(\partial_j n_{1i} n_{1j} + n_{1i} \partial_j n_{1j} \right) + 2b_\alpha \left(\partial_j n_{2i} n_{2j} + n_{2i} \partial_j n_{2j} \right) \right] \\ =& d_1 (s_\alpha + b_\alpha) \partial_j n_{1j} + 2 d_1 b_\alpha n_{1i} n_{2j} \partial_j n_{2i}, \quad \alpha = 2, 3. \\ Q_\alpha \cdot \nabla \times Q_4 =& \frac{1}{2} \left[\left(s_\alpha + b_\alpha \right) n_{1i} n_{1j} + 2b_\alpha n_{2i} n_{2j} - \left(\frac{1}{3} s_\alpha + b_\alpha \right) \delta_{ij} \right] d_4 \varepsilon^{jkl} \partial_k \left(n_{2l} n_{3i} + n_{3l} n_{2i} \right) \\ =& \frac{1}{2} d_4 (s_\alpha + b_\alpha) \epsilon^{jkl} n_{1i} n_{1j} \left(\partial_k n_{2l} n_{3i} + n_{2l} \partial_k n_{3i} + \partial_k n_{3l} n_{2i} + n_{3l} \partial_k n_{2i} \right) \\ &+ d_4 b_\alpha \epsilon^{jkl} n_{2i} n_{2j} \left(\partial_k n_{2l} n_{3i} + n_{2l} \partial_k n_{3i} + \partial_k n_{2i} n_{3l} + n_{2i} \partial_k n_{3l} \right) \\ &- \frac{1}{6} d_4 (s_\alpha + 3b_\alpha) \epsilon^{jkl} \delta_{ij} \left(\partial_k n_{2l} n_{3i} + n_{2l} \partial_k n_{3i} + \partial_k n_{3l} n_{2i} + n_{3l} \partial_k n_{2i} \right) \\ =& \frac{1}{2} d_4 (s_\alpha + b_\alpha) \left(\epsilon^{jkl} n_{1i} n_{1j} n_{2l} \partial_k n_{3i} + \epsilon^{jkl} n_{1i} n_{1j} n_{3l} \partial_k n_{2i} \right) \\ &+ d_4 b_\alpha \left(\epsilon^{jkl} n_{2i} n_{2j} n_{2l} \partial_k n_{3i} + \epsilon^{jkl} n_{2j} \partial_k n_{3l} \right) \\ &- \frac{1}{6} d_4 (s_\alpha + 3b_\alpha) \epsilon^{ikl} \left(\partial_k n_{2l} n_{3i} + n_{2l} \partial_k n_{3i} + \partial_k n_{3l} n_{2i} + n_{3l} \partial_k n_{2i} \right) \\ =& \frac{1}{2} d_4 (s_\alpha + b_\alpha) \left(\epsilon^{jkl} n_{1i} n_{1j} n_{2l} \partial_k n_{3i} + \epsilon^{jkl} n_{1i} n_{1j} n_{3l} \partial_k n_{2i} \right) \\ &+ d_4 b_\alpha \epsilon^{jkl} n_{2j} \partial_k n_{3l}, \quad \alpha = 2, 3. \end{aligned}$$

其中上式的最后一个等式用了下列关系:

$$\begin{aligned} &\epsilon^{jkl} n_{2i} n_{2j} n_{2l} \partial_k n_{3i} \\ &\quad = n_{2i} n_{2j} (n_{3j} n_{1k} - n_{1j} n_{3k}) \partial_k n_{3i} = 0, \\ &\epsilon^{ikl} \partial_k n_{2l} n_{3i} + \epsilon^{ikl} n_{2l} \partial_k n_{3i} + \epsilon^{ikl} \partial_k n_{3l} n_{2i} + \epsilon^{ikl} n_{3l} \partial_k n_{2i} \end{aligned}$$

$$
\begin{aligned}
&= (n_{1k}n_{2l} - n_{1l}n_{2k})\partial_k n_{2l} + (n_{3i}n_{1k} - n_{1i}n_{3k})\partial_k n_{3i} \\
&\quad + (n_{3k}n_{1l} - n_{1k}n_{3l})\partial_k n_{3l} + (n_{2k}n_{1i} - n_{1k}n_{2i})\partial_k n_{2i} \\
&= 0.
\end{aligned}
$$

将上述结果代入一阶弹性项 $F_{1,elastic}$, 可以得到

$$
\begin{aligned}
F_{1,elastic} =& c_{10}d_1\partial_i n_{1i} + c_{11}\left[d_1(s_2+b_2)\partial_j n_{1j} + 2d_1b_2n_{1i}n_{2j}\partial_j n_{2i}\right] \\
&+ c_{12}\left[d_1(s_3+b_3)\partial_j n_{1j} + 2d_1b_3n_{1i}n_{2j}\partial_j n_{2i}\right] \\
&+ c_{13}\left[\frac{1}{2}d_4(s_2+b_2)\big(\epsilon^{jkl}n_{1i}n_{1j}n_{2l}\partial_k n_{3i} + \epsilon^{jkl}n_{1i}n_{1j}n_{3l}\partial_k n_{2i}\big) + d_4b_\alpha\epsilon^{jkl}n_{2j}\partial_k n_{3l}\right] \\
&+ c_{14}\left[\frac{1}{2}d_4(s_3+b_3)\big(\epsilon^{jkl}n_{1i}n_{1j}n_{2l}\partial_k n_{3i} + \epsilon^{jkl}n_{1i}n_{1j}n_{3l}\partial_k n_{2i}\big) + d_4b_\alpha\epsilon^{jkl}n_{2j}\partial_k n_{3l}\right] \\
=& d_1\big[c_{10} + c_{11}(s_2+b_2) + c_{12}(s_3+b_3)\big]\partial_i n_{1i} + 2d_1(c_{11}b_2 + c_{12}b_3)n_{1i}n_{2j}\partial_j n_{2i} \\
&+ \frac{1}{2}d_4\big[c_{13}(s_2+b_2) + c_{14}(s_3+b_3)\big](\epsilon^{jkl}n_{1i}n_{1j}n_{2l}\partial_k n_{3i} + \epsilon^{jkl}n_{1i}n_{1j}n_{3l}\partial_k n_{2i}) \\
&+ d_4(c_{13}b_2 + c_{14}b_3)\epsilon^{jkl}n_{2j}\partial_k n_{3l} \\
=& J_{11}\partial_i n_{1i} + J_{12}n_{1i}n_{2j}\partial_j n_{2i} \\
&+ J_{13}(\epsilon^{jkl}n_{1i}n_{1j}n_{2l}\partial_k n_{3i} + \epsilon^{jkl}n_{1i}n_{1j}n_{3l}\partial_k n_{2i}) + J_{14}\epsilon^{jkl}n_{2j}\partial_k n_{3l},
\end{aligned}
\tag{4.2}
$$

其中系数 J_{1i} 为 $d_1, d_4, s_i, b_i\ (i = 2, 3)$ 的函数, 且

$$
\begin{aligned}
&J_{11} = d_1\big[c_{10} + c_{11}(s_2+b_2) + c_{12}(s_3+b_3)\big], \quad J_{12} = 2d_1(c_{11}b_2 + c_{12}b_3), \\
&J_{13} = \frac{1}{2}d_4\big[c_{13}(s_2+b_2) + c_{14}(s_3+b_3)\big], \quad J_{14} = d_4(c_{13}b_2 + c_{14}b_3).
\end{aligned}
$$

下面通过 (2.3) 中的九个量 $D_{ij}(i, j = 1, 2, 3)$ 表示 (4.2) 中的导数项, 计算出如下结果,

$$
\begin{aligned}
&\partial_i n_{1i} = \delta_{ij}\partial_i n_{1j} = (n_{2i}n_{2j} + n_{3i}n_{3j})\partial_i n_{1j} = D_{32} - D_{23}, \\
&n_{1i}n_{2j}\partial_i n_{2i} = D_{23}, \\
&\epsilon^{jkl}n_{1i}n_{1j}n_{2l}\partial_k n_{3i} = n_{1i}n_{1j}(n_{3j}n_{1k} - n_{1j}n_{3k})\partial_k n_{3i} = D_{32}, \\
&\epsilon^{jkl}n_{1i}n_{1j}n_{3l}\partial_k n_{2i} = n_{1i}n_{1j}(n_{1j}n_{2k} - n_{2j}n_{1k})\partial_k n_{2i} = D_{23}, \\
&\epsilon^{jkl}n_{2j}\partial_k n_{3l} = (n_{3k}n_{1l} - n_{1k}n_{3l})\partial_k n_{3l} = -D_{32},
\end{aligned}
$$

将这些结果带入到 (4.2) 式中, 得到其用 $D_{ij}(i, j = 1, 2, 3)$ 的表达为

$$
\begin{aligned}
F_{1,elastic} =& J_{11}(D_{32} - D_{23}) + J_{12}D_{23} + J_{13}(D_{32} + D_{23}) - J_{14}D_{32} \\
=& (-J_{11} + J_{12} + J_{13})D_{32} + (J_{11} + J_{13} - J_{14})D_{23} \\
=& K_{23}D_{23} + K_{32}D_{32},
\end{aligned}
\tag{4.3}
$$

其中相应的弹性系数为

$$K_{23}=-J_{11}+J_{12}+J_{13},\quad K_{32}=J_{11}+J_{13}-J_{14}. \tag{4.4}$$

接下来考虑自由能中的二次一阶导数项, 需要分别计算二阶弹性项 $F_{2,elastic}$ 中的梯度项, 散度项和混合项, 过程类似于讨论线性一阶导数项. 首先计算 $F_{2,elastic}$ 中的梯度项为

$$\begin{aligned}
|\nabla Q_1|^2 =& d_1^2(\partial_i n_{1j})^2,\\
|\nabla Q_4|^2 =& \frac{1}{4}d_4^2\left(\partial_k n_{2i}n_{3j}+\partial_k n_{3j}n_{2i}+\partial_k n_{3i}n_{2j}+\partial_k n_{2j}n_{3i}\right)^2\\
=&\frac{1}{4}d_4^2\big[\left(\partial_k n_{2i}\right)^2+\left(\partial_k n_{3j}\right)^2+\left(\partial_k n_{3i}\right)^2+\left(\partial_k n_{2j}\right)^2\\
&+\partial_k n_{2i}n_{3j}\partial_k n_{2j}n_{3i}+\partial_k n_{3j}n_{2i}\partial_k n_{3i}n_{2j}\\
&+\partial_k n_{3j}n_{2i}\partial_k n_{3i}n_{2j}+\partial_k n_{2i}n_{3j}\partial_k n_{2j}n_{3i}\big]\\
=&\frac{1}{2}d_4^2\big((\partial_i n_{2j})^2+(\partial_i n_{3j})^2+2n_{2j}\partial_i n_{3j}n_{2k}\partial_i n_{3k}\big),\\
\nabla Q_\alpha\cdot\nabla Q_\beta =& \partial_i\left[\left(s_\alpha+b_\alpha\right)\mathbf{n}_1^2+2b_\alpha\mathbf{n}_2^2-\left(\frac{1}{3}s_\alpha+b_\alpha\right)\mathfrak{i}\right]_{jk}\\
&\partial_i\left[\left(s_\beta+b_\beta\right)\mathbf{n}_1^2+2b_\beta\mathbf{n}_2^2-\left(\frac{1}{3}s_\beta+b_\beta\right)\mathfrak{i}\right]_{jk}\\
=&\left[\left(s_\alpha+b_\alpha\right)\left(\partial_i n_{1j}n_{1k}+n_{1j}\partial_i n_{1k}\right)+2b_\alpha\left(\partial_i n_{2j}n_{2k}+n_{2j}\partial_i n_{2k}\right)\right]\\
&\left[\left(s_\beta+b_\beta\right)\left(\partial_i n_{1j}n_{1k}+n_{1j}\partial_i n_{1k}\right)+2b_\beta\left(\partial_i n_{2j}n_{2k}+n_{2j}\partial_i n_{2k}\right)\right]\\
=&\left(s_\alpha+b_\alpha\right)\left(s_\beta+b_\beta\right)\left(\partial_i n_{1j}\right)^2+\left(s_\alpha+b_\alpha\right)\left(s_\beta+b_\beta\right)\left(\partial_i n_{1k}\right)^2\\
&+4b_\alpha b_\beta\left(\partial_i n_{2j}^2\right)+4b_\alpha b_\beta\left(\partial_i n_{2k}^2\right)\\
&+2\left(s_\alpha+b_\alpha\right)b_\beta\left(\partial_i n_{1j}n_{1k}n_{2j}\partial_i n_{2k}+n_{1j}\partial_i n_{1k}\partial_i n_{2j}n_{2k}\right)\\
&+2\left(s_\beta+b_\beta\right)b_\alpha\left(n_{1j}\partial_i n_{1k}\partial_i n_{2j}n_{2k}+\partial_i n_{1j}n_{1k}n_{2j}\partial_i n_{2k}\right)\\
=&2(s_\alpha+b_\alpha)(s_\beta+b_\beta)(\partial_i n_{1j})^2+8b_\alpha b_\beta(\partial_i n_{2j})^2\\
&+4[b_\alpha(s_\beta+b_\beta)+b_\beta(s_\alpha+b_\alpha)]n_{1j}\partial_i n_{2j}n_{2k}\partial_i n_{1k},\quad \alpha,\beta=2,3.
\end{aligned}$$

其次, 计算散度项的结果为

$$\begin{aligned}
|\nabla\cdot Q_1|^2 =& d_1^2(\partial_i n_{1i})^2,\\
|\nabla\cdot Q_4|^2 =& \partial_i Q_{4ik}\partial_j Q_{4jk}\\
=&\frac{1}{4}d_4^2\left(\partial_i n_{2i}n_{3k}+\partial_i n_{3k}n_{2i}+\partial_i n_{3i}n_{2k}+\partial_i n_{2k}n_{3i}\right)\\
&\left(\partial_j n_{2j}n_{3k}+\partial_j n_{3k}n_{2j}+\partial_j n_{3j}n_{2k}+\partial_j n_{2k}n_{3j}\right)\\
=&\frac{1}{4}d_4^2\big(\partial_i n_{2i}\partial_j n_{2j}+\partial_i n_{2i}n_{3k}\partial_j n_{2k}n_{3j}+\partial_i n_{2i}n_{3k}\partial_j n_{3j}n_{2k}\\
&+\partial_i n_{3k}n_{2i}\partial_j n_{3k}n_{2j}+\partial_i n_{3k}n_{2i}\partial_j n_{2k}n_{3j}+\partial_i n_{3k}n_{2i}\partial_j n_{3j}n_{2k}
\end{aligned}$$

$$
\begin{aligned}
&+\partial_i n_{3i} n_{2k} \partial_j n_{2j} n_{3k}+\partial_i n_{3i} n_{2k} \partial_j n_{3k} n_{2j}+\partial_i n_{3i} \partial_j n_{3j} \\
&+\partial_i n_{2k} n_{3i} \partial_j n_{2j} n_{3k}+\partial_i n_{2k} n_{3i} \partial_j n_{3k} n_{2j}+\partial_i n_{2k} n_{3i} \partial_j n_{2k} n_{3j}) \\
=&\frac{1}{4} d_4^2\Big(|\nabla \cdot \mathbf{n}_2|^2+|\nabla \cdot \mathbf{n}_3|^2+n_{3j} n_{3i} \partial_j n_{2k} \partial_i n_{2k} \\
&+n_{2j} n_{2i} \partial_j n_{3k} \partial_i n_{3k}+2 n_{3j} n_{2i} \partial_j n_{2k} \partial_i n_{3k} \\
&+2 n_{3k} n_{3j} \partial_j n_{2k}(\nabla \cdot \mathbf{n}_2)+2 n_{2j} n_{2k} \partial_j n_{3k}(\nabla \cdot \mathbf{n}_3)\Big)
\end{aligned}
$$

$$
\begin{aligned}
(\nabla \cdot Q_\alpha) \cdot (\nabla \cdot Q_\beta)=&\left[(s_\alpha+b_\alpha)\left(\partial_i n_{1i} n_{1k}+n_{1i} \partial_i n_{1k}\right)+2 b_\alpha\left(\partial_i n_{2i} n_{2k}+n_{2i} \partial_i n_{2k}\right)\right] \\
&\left[(s_\beta+b_\beta)\left(\partial_j n_{1j} n_{1k}+n_{1j} \partial_j n_{1k}\right)+2 b_\beta\left(\partial_j n_{2j} n_{2k}+n_{2j} \partial_j n_{2k}\right)\right] \\
=&(s_\alpha+b_\alpha)(s_\beta+b_\beta)\big(\partial_i n_{1i} \partial_j n_{1j}+n_{1i} n_{1j} \partial_i n_{1k} \partial_j n_{1k}\big) \\
&+4 b_\alpha b_\beta\big(\partial_i n_{2i} \partial_j n_{2j}+n_{2i} n_{2j} \partial_i n_{2k} \partial_j n_{2k}\big) \\
&+2 b_\alpha(s_\beta+b_\beta)\Big(n_{1k} n_{2k} \partial_j n_{2j} \partial_i n_{1i}+n_{2j} n_{1k} \partial_j n_{2k} \partial_i n_{1i} \\
&+n_{1i} n_{2k} \partial_j n_{2j} \partial_i n_{1k}+n_{1i} n_{2j} \partial_i n_{1k} \partial_j n_{2k}\Big) \\
&+2 b_\beta(s_\alpha+b_\alpha)\Big(n_{1k} n_{2k} \partial_j n_{1j} \partial_i n_{2i}+n_{1j} n_{2k} \partial_j n_{1k} \partial_i n_{2i} \\
&+n_{2i} n_{1k} \partial_j n_{1j} \partial_i n_{2k}+n_{2i} n_{1j} \partial_i n_{2k} \partial_j n_{1k}\Big) \\
=&(s_\alpha+b_\alpha)(s_\beta+b_\beta)\big(|\nabla \cdot \mathbf{n}_1|^2+n_{1i} n_{1j} \partial_i n_{1k} \partial_j n_{1k}\big) \\
&+4 b_\alpha b_\beta\big(|\nabla \cdot \mathbf{n}_2|^2+n_{2i} n_{2j} \partial_i n_{2k} \partial_j n_{2k}\big) \\
&+2\big[b_\alpha(s_\beta+b_\beta)+b_\beta(s_\alpha+b_\alpha)\big]\Big(n_{1i} n_{2j} \partial_i n_{1k} \partial_j n_{2k} \\
&+n_{1k} n_{2j} \partial_j n_{2k}(\nabla \cdot \mathbf{n}_1)+n_{1i} n_{2k} \partial_i n_{1k}(\nabla \cdot \mathbf{n}_2)\Big), \quad \alpha, \beta=2,3 .
\end{aligned}
$$

除此之外, 算得混合项 $(\nabla \times Q_1) \cdot (\nabla \cdot Q_4)$ 为

$$
\begin{aligned}
(\nabla \times Q_1) \cdot (\nabla \cdot Q_4)=&\varepsilon^{ijk} \partial_j Q_{1k} \partial_l Q_{4il} \\
=&\frac{1}{2} d_1 d_4 \epsilon^{ijk} \partial_j n_{1k}\big(\partial_l n_{2l} n_{3i}+n_{2l} \partial_l n_{3i}+\partial_l n_{3l} n_{2i}+n_{3l} \partial_l n_{2i}\big) .
\end{aligned}
$$

因此, 将得到的梯度项, 散度项和混合项结果代入二阶弹性能密度的表达式 (3.7) 中有

$$
\begin{aligned}
F_{2,elastic}=&c_{21} d_1^2(\partial_i n_{1j})^2 \\
&+c_{22}\left[2(s_2+b_2)^2(\partial_i n_{1j})^2+8 b_2^2(\partial_i n_{2j})^2+8 b_2(s_2+b_2) n_{1j} \partial_i n_{2j} n_{2k} \partial_i n_{1k}\right] \\
&+c_{23}\big[2(s_2+b_2)(s_3+b_3)(\partial_i n_{1j})^2+8 b_2 b_3(\partial_i n_{2j})^2 \\
&+4[b_3(s_2+b_2)+b_2(s_3+b_3)] n_{1j} \partial_i n_{2j} n_{2k} \partial_i n_{1k}\big] \\
&+c_{24}\left[2(s_3+b_3)^2(\partial_i n_{1j})^2+8 b_3^2(\partial_i n_{2j})^2+8 b_3(s_3+b_3) n_{1j} \partial_i n_{2j} n_{2k} \partial_i n_{1k}\right] \\
&+c_{25}\left[\frac{1}{2} d_4^2\big((\partial_i n_{2j})^2+(\partial_i n_{3j})^2+2 n_{2j} \partial_i n_{3j} n_{2k} \partial_i n_{3k}\big)\right] \\
&+c_{26} d_1^2(\partial_i n_{1i})^2
\end{aligned}
$$

$$
\begin{aligned}
&+c_{27}\Big[(s_2+b_2)^2\big(|\nabla\cdot\mathbf{n}_1|^2+n_{1i}n_{1j}\partial_i n_{1k}\partial_j n_{1k}\big)+4b_2^2\big(|\nabla\cdot\mathbf{n}_2|^2+n_{2i}n_{2j}\partial_i n_{2k}\partial_j n_{2k}\big)\\
&+4\big[b_2(s_2+b_2)\big]\Big(n_{1i}n_{2j}\partial_i n_{1k}\partial_j n_{2k}+n_{1k}n_{2j}\partial_j n_{2k}(\nabla\cdot\mathbf{n}_1)+n_{1i}n_{2k}\partial_i n_{1k}(\nabla\cdot\mathbf{n}_2)\Big)\Big]\\
&+c_{28}\Big[(s_2+b_2)(s_3+b_3)\big(|\nabla\cdot\mathbf{n}_1|^2+n_{1i}n_{1j}\partial_i n_{1k}\partial_j n_{1k}\big)\\
&+4b_2b_3\big(|\nabla\cdot\mathbf{n}_2|^2+n_{2i}n_{2j}\partial_i n_{2k}\partial_j n_{2k}\big)\\
&+2\big[b_2(s_3+b_3)+b_3(s_2+b_2)\big]\Big(n_{1i}n_{2j}\partial_i n_{1k}\partial_j n_{2k}\\
&+n_{1k}n_{2j}\partial_j n_{2k}(\nabla\cdot\mathbf{n}_1)+n_{1i}n_{2k}\partial_i n_{1k}(\nabla\cdot\mathbf{n}_2)\Big)\Big]\\
&+c_{29}\Big[(s_3+b_3)^2\big(|\nabla\cdot\mathbf{n}_1|^2+n_{1i}n_{1j}\partial_i n_{1k}\partial_j n_{1k}\big)+4b_3^2\big(|\nabla\cdot\mathbf{n}_2|^2+n_{2i}n_{2j}\partial_i n_{2k}\partial_j n_{2k}\big)\\
&+4\big[b_3(s_3+b_3)\big]\Big(n_{1i}n_{2j}\partial_i n_{1k}\partial_j n_{2k}+n_{1k}n_{2j}\partial_j n_{2k}(\nabla\cdot\mathbf{n}_1)+n_{1i}n_{2k}\partial_i n_{1k}(\nabla\cdot\mathbf{n}_2)\Big)\Big]\\
&+c_{210}\Big[\frac{1}{4}d_4^2\Big(|\nabla\cdot\mathbf{n}_2|^2+|\nabla\cdot\mathbf{n}_3|^2+n_{3j}n_{3k}\partial_j n_{2i}\partial_k n_{2i}\\
&+n_{2j}n_{2k}\partial_j n_{3i}\partial_k n_{3i}+2n_{3j}n_{2k}\partial_j n_{2i}\partial_k n_{3i}\\
&+2n_{3i}n_{3j}\partial_j n_{2i}(\nabla\cdot\mathbf{n}_2)+2n_{2i}n_{2k}\partial_k n_{3i}(\nabla\cdot\mathbf{n}_3)\Big)\Big]\\
&+c_{213}\Big[\frac{1}{2}d_1d_4\epsilon^{ijk}\partial_j n_{1k}\big(\partial_l n_{2l}n_{3i}+n_{2l}\partial_l n_{3i}+\partial_l n_{3l}n_{2i}+n_{3l}\partial_l n_{2i}\big)\Big]\\
=&J_{21}(\partial_i n_{1j})^2+J_{22}(\partial_i n_{2j})^2+J_{23}(\partial_i n_{3j})^2\\
&+J_{24}n_{1j}\partial_i n_{2j}n_{2k}\partial_i n_{1k}+J_{25}n_{2j}\partial_i n_{3j}n_{2k}\partial_i n_{3k}\\
&+J_{26}|\nabla\cdot\mathbf{n}_1|^2+J_{27}|\nabla\cdot\mathbf{n}_2|^2+J_{28}|\nabla\cdot\mathbf{n}_3|^2\\
&+J_{29}n_{1i}\partial_i n_{1k}n_{1j}\partial_j n_{1k}+J_{2,10}n_{2i}\partial_i n_{2k}n_{2j}\partial_j n_{2k}\\
&+J_{2,11}\Big(n_{1i}\partial_i n_{1k}n_{2j}\partial_j n_{2k}+n_{1k}n_{2j}\partial_j n_{2k}(\nabla\cdot\mathbf{n}_1)+n_{1i}n_{2k}\partial_i n_{1k}(\nabla\cdot\mathbf{n}_2)\Big)\\
&+J_{2,12}\Big(n_{3j}n_{3i}\partial_j n_{2k}\partial_i n_{2k}+n_{2j}n_{2i}\partial_j n_{3k}\partial_i n_{3k}+2n_{3j}n_{2i}\partial_j n_{2k}\partial_i n_{3k}\\
&+2n_{3k}n_{3j}\partial_j n_{2k}(\nabla\cdot\mathbf{n}_2)+2n_{2j}n_{2k}\partial_j n_{3k}(\nabla\cdot\mathbf{n}_3)\Big)\\
&+J_{2,13}\epsilon^{ijk}\partial_j n_{1k}(\partial_l n_{2l}n_{3i}+n_{2l}\partial_l n_{3i}+\partial_l n_{3l}n_{2i}+n_{3l}\partial_l n_{2i}),
\end{aligned}
\tag{4.5}
$$

其中系数 J_{1i} 也为 $d_1, d_4, s_i, b_i\ (i=2,3)$ 的函数, 表示为

$$
\begin{aligned}
&J_{21}=c_{21}d_1^2+2\big[c_{22}(s_2+b_2)^2+2c_{23}(s_2+b_2)(s_3+b_3)+c_{24}(s_3+b_3)^2\big],\\
&J_{22}=8(c_{22}b_2^2+2c_{23}b_2b_3+c_{24}b_3^2)+\frac{1}{2}c_{25}d_4^2,\quad J_{23}=\frac{1}{2}c_{25}d_4^2,\\
&J_{24}=8\big[c_{22}b_2(s_2+b_2)+c_{23}(b_2s_3+2b_2b_3+b_3s_2)+c_{24}b_3(s_3+b_3)\big],\\
&J_{25}=c_{25}d_4^2,\quad J_{26}=c_{26}d_1^2+c_{27}(s_2+b_2)^2+2c_{28}(s_2+b_2)(s_3+b_3)+c_{29}(s_3+b_3)^2,\\
&J_{27}=4(c_{27}b_2^2+2c_{28}b_2b_3+c_{29}b_3^2)+\frac{1}{4}c_{2,10}d_4^2,\quad J_{28}=\frac{1}{4}c_{2,10}d_4^2,
\end{aligned}
$$

$$
\begin{aligned}
&J_{29}=c_{27}(s_2+b_2)^2+2c_{28}(s_2+b_2)(s_3+b_3)+c_{29}(s_3+b_3)^2,\\
&J_{2,10}=4(c_{27}b_2^2+2c_{28}b_2b_3+c_{29}b_3^2),\\
&J_{2,11}=4\big[c_{27}b_2(s_2+b_2)+c_{28}(b_2s_3+2b_2b_3+b_3s_2)+c_{29}b_3(s_3+b_3)\big],\\
&J_{2,12}=\frac{1}{4}c_{2,10}d_4^2,\quad J_{2,13}=\frac{1}{2}c_{2,13}d_1d_4.
\end{aligned}\tag{4.6}
$$

为了用 (2.3) 中的九个量表示 (4.5), 需要建立其中的导数项和这些量之间的关系. 对于二次一阶导数项, 计算 (4.5) 的梯度项分别为

$$
\begin{aligned}
(\partial_i n_{1j})^2=&\delta_{jl}\delta_{ik}\partial_k n_{1l}\partial_i n_{1j}\\
=&(n_{2j}n_{2l}+n_{3j}n_{3l})(n_{1i}n_{1k}+n_{2i}n_{2k}+n_{3i}n_{3k})\partial_k n_{1l}\partial_i n_{1j}\\
=&\big(n_{1i}n_{2j}n_{1k}n_{2l}+n_{2i}n_{2j}n_{2k}n_{2l}+n_{3i}n_{2j}n_{3k}n_{2l}+n_{1i}n_{3j}n_{1k}n_{3l}\\
&+n_{2i}n_{3j}n_{2k}n_{3l}+n_{3i}n_{3j}n_{3k}n_{3l}\big)\partial_k n_{1l}\partial_i n_{1j}\\
=&D_{12}^2+D_{22}^2+D_{32}^2+D_{13}^2+D_{23}^2+D_{33}^2,\\
(\partial_i n_{2j})^2=&\delta_{jl}\delta_{ik}\partial_k n_{2l}\partial_i n_{2j}\\
=&(n_{1j}n_{1l}+n_{3j}n_{3l})(n_{1i}n_{1k}+n_{2i}n_{2k}+n_{3i}n_{3k})\partial_k n_{2l}\partial_i n_{2j}\\
=&D_{11}^2+D_{21}^2+D_{31}^2+D_{13}^2+D_{23}^2+D_{33}^2,\\
(\partial_i n_{3j})^2=&\delta_{jl}\delta_{ik}\partial_k n_{3l}\partial_i n_{3j}\\
=&(n_{1j}n_{1l}+n_{2j}n_{2l})(n_{1i}n_{1k}+n_{2i}n_{2k}+n_{3i}n_{3k})\partial_k n_{3l}\partial_i n_{3j}\\
=&D_{11}^2+D_{21}^2+D_{31}^2+D_{12}^2+D_{22}^2+D_{32}^2,\\
n_{2j}\partial_i n_{3j}n_{2k}\partial_i n_{3k}=&\delta_{is}\delta_{jl}n_{2j}n_{2k}\partial_i n_{3l}\partial_s n_{3k}\\
=&(n_{1i}n_{1s}+n_{2i}n_{2s}+n_{3i}n_{3s})n_{2l}n_{2k}\partial_i n_{3l}\partial_s n_{3k}\\
=&D_{11}^2+D_{21}^2+D_{31}^2,\\
n_{1j}\partial_i n_{2j}n_{2k}\partial_i n_{1k}=&\delta_{jq}\delta_{ip}n_{1j}\partial_i n_{2q}n_{2k}\partial_p n_{1k},\\
=&n_{1q}n_{2k}(n_{1i}n_{1p}+n_{2i}n_{2p}+n_{3i}n_{3p})\partial_i n_{2q}\partial_p n_{1k}\\
=&-(D_{13}^2+D_{23}^2+D_{33}^2).
\end{aligned}
$$

计算二次散度项的结果为

$$
\begin{aligned}
\partial_i n_{2i}=&(n_{1i}n_{1j}+n_{3i}n_{3j})\partial_i n_{2j}=D_{13}-D_{31},\\
\partial_i n_{3i}=&(n_{1i}n_{1j}+n_{2i}n_{2j})\partial_i n_{3j}=D_{21}-D_{12},\\
n_{1i}\partial_i n_{1k}n_{1j}\partial_j n_{1k}=&\delta_{kl}n_{1i}n_{1j}\partial_i n_{1k}\partial_j n_{1l}\\
=&(n_{2k}n_{2l}+n_{3k}n_{3l})n_{1i}n_{1j}\partial_i n_{1k}\partial_j n_{1l}\\
=&D_{13}^2+D_{12}^2,\\
n_{2i}\partial_i n_{2k}n_{2j}\partial_j n_{2k}=&\delta_{kl}n_{2i}n_{2j}\partial_i n_{2k}\partial_j n_{2l}
\end{aligned}
$$

$$
\begin{aligned}
&=(n_{1k}n_{1l}+n_{3k}n_{3l})n_{2i}n_{2j}\partial_i n_{2k}\partial_j n_{2l}\\
&=D_{23}^2+D_{21}^2,\\
n_{3j}\partial_i n_{2k}n_{3i}\partial_j n_{2k} &=\delta_{kl}n_{3i}n_{3j}\partial_i n_{2l}\partial_j n_{2k}\\
&=(n_{1k}n_{1l}+n_{3k}n_{3l})n_{3i}n_{3j}\partial_i n_{2l}\partial_j n_{2k}\\
&=D_{31}^2+D_{33}^2,\\
n_{2j}\partial_i n_{3k}n_{2i}\partial_j n_{3k} &=\delta_{kl}n_{2i}n_{2j}\partial_i n_{3l}\partial_j n_{3k}\\
&=(n_{1k}n_{1l}+n_{2k}n_{2l})n_{2i}n_{2j}\partial_i n_{3l}\partial_j n_{3k}\\
&=D_{21}^2+D_{22}^2,\\
n_{3j}\partial_i n_{3k}n_{2i}\partial_j n_{2k} &=\delta_{kl}n_{2i}n_{3j}\partial_i n_{3l}\partial_j n_{2k}\\
&=n_{1k}n_{1l}n_{2i}n_{3j}\partial_i n_{3l}\partial_j n_{2k}\\
&=-D_{22}D_{33},\\
n_{1i}\partial_i n_{1k}n_{2j}\partial_j n_{2k} &=\delta_{kl}n_{1i}n_{2j}\partial_i n_{1l}\partial_j n_{2k}\\
&=n_{3k}n_{3l}n_{1i}n_{2j}\partial_i n_{1l}\partial_j n_{2k}\\
&=-D_{21}D_{12}.
\end{aligned}
$$

它满足

$$
2n_{3j}n_{2k}\partial_j n_{2i}\partial_k n_{3i}=-2D_{22}D_{33}=-2D_{23}D_{32}+\underbrace{2(D_{23}D_{32}-D_{22}D_{33})}_{\text{表面项}}. \tag{4.7}
$$

对于二次混合项, 利用行列式张量 ϵ 的表达式 (2.2), 有如下结果

$$
\begin{aligned}
\epsilon^{ijk}n_{3i}\partial_j n_{1k} &=(n_{1j}n_{2k}-n_{2j}n_{1k})\partial_j n_{1k}=-D_{13},\\
\epsilon^{ijk}n_{2i}\partial_j n_{1k} &=(n_{3j}n_{1k}-n_{1j}n_{3k})\partial_j n_{1k}=-D_{12},\\
\epsilon^{ijk}\partial_j n_{1k}n_{2l}\partial_l n_{3i} &=\delta_{ip}\delta_{jq}\delta_{ks}\epsilon^{ijk}\partial_q n_{1s}n_{2l}\partial_l n_{3p}\\
&=(n_{1i}n_{1p}+n_{2i}n_{2p})(n_{1j}n_{1q}+n_{2j}n_{2q}+n_{3j}n_{3q})\\
&\quad\times(n_{2k}n_{2s}+n_{3k}n_{3s})\epsilon^{ijk}\partial_q n_{1s}n_{2l}\partial_l n_{3p}\\
&=n_{1p}n_{2q}n_{3s}\partial_q n_{1s}n_{2l}\partial_l n_{3p}-n_{1p}n_{3q}n_{2s}\partial_q n_{1s}n_{2l}\partial_l n_{3p}\\
&\quad+n_{2p}n_{1q}n_{3s}\partial_q n_{1s}n_{2l}\partial_l n_{3p}\\
&=-D_{22}^2-D_{21}D_{12}-D_{22}D_{33},\\
\epsilon^{ijk}\partial_j n_{1k}n_{3l}\partial_l n_{2i} &=\delta_{ip}\delta_{jq}\delta_{ks}\epsilon^{ijk}\partial_q n_{1s}n_{3l}\partial_l n_{2p}\\
&=(n_{1i}n_{1p}+n_{3i}n_{3p})(n_{1j}n_{1q}+n_{2j}n_{2q}+n_{3j}n_{3q})\\
&\quad\times(n_{2k}n_{2s}+n_{3k}n_{3s})\epsilon^{ijk}\partial_q n_{1s}n_{3l}\partial_l n_{2p}\\
&=n_{1p}n_{2q}n_{3s}\partial_q n_{1s}n_{3l}\partial_l n_{2p}-n_{1p}n_{3q}n_{2s}\partial_q n_{1s}n_{3l}\partial_l n_{2p}\\
&\quad+n_{3p}n_{1q}n_{2s}\partial_q n_{1s}n_{3l}\partial_l n_{2p}
\end{aligned}
$$

$$= D_{33}^2 + D_{31}D_{13} + D_{22}D_{33}.$$

这样, 利用上述梯度项, 散度项及二次混合项和九个不变量之间的关系, 得到

$$\begin{aligned} F_{2,elastic} =& (D_{13}^2 + D_{23}^2 + D_{33}^2 + D_{12}^2 + D_{22}^2 + D_{32}^2)J_{21} \\ &+ (D_{13}^2 + D_{23}^2 + D_{33}^2 + D_{11}^2 + D_{21}^2 + D_{31}^2)J_{22} \\ &+ (D_{12}^2 + D_{11}^2 + D_{22}^2 + D_{21}^2 + D_{32}^2 + D_{31}^2)J_{23} \\ &+ (-D_{13}^2 - D_{23}^2 - D_{33}^2)J_{24} + (D_{11}^2 + D_{21}^2 + D_{31}^2)J_{25} \\ &+ (D_{32}^2 + D_{23}^2 - 2D_{32}D_{23})J_{26} + (D_{13}^2 + D_{31}^2 - 2D_{13}D_{31})J_{27} \\ &+ (D_{12}^2 + D_{21}^2 - 2D_{12}D_{21})J_{28} + (D_{13}^2 + D_{12}^2)J_{29} + (D_{23}^2 + D_{21}^2)J_{210} \\ &+ (-D_{23}^2 - D_{13}^2 + D_{23}D_{32} + D_{31}D_{13} - D_{12}D_{21})J_{211} \\ &+ (3D_{31}^2 + 3D_{21}^2 + D_{22}^2 + D_{33}^2 - 2D_{22}D_{33} - 2D_{31}D_{13} - 2D_{12}D_{21})J_{212} \\ &+ (D_{33}^2 + D_{12}^2 - D_{13}^2 - D_{22}^2 + 2D_{31}D_{13} - 2D_{12}D_{21})J_{213} \\ =& K_{1111}D_{11}^2 + K_{2121}D_{21}^2 + K_{3131}D_{31}^2 + K_{1212}D_{12}^2 \\ &+ K_{2222}D_{22}^2 + K_{3232}D_{32}^2 + K_{1313}D_{13}^2 + K_{2323}D_{23}^2 + K_{3333}D_{33}^2 \\ &+ K_{1221}D_{12}D_{21} + K_{1331}D_{13}D_{31} + K_{2332}D_{23}D_{32}, \end{aligned} \tag{4.8}$$

其中忽略了表面项

$$\partial_i(n_{1j}\partial_j n_{1i} - n_{1i}\partial_j n_{1j}) = 2(D_{23}D_{32} - D_{22}D_{33}),$$

(4.8) 中的系数表达为

$$\begin{aligned} &K_{1111} = J_{22} + J_{23} + J_{25}, \quad K_{2121} = J_{22} + J_{23} + J_{25} + J_{28} + J_{2.10} + 3J_{2,12}, \\ &K_{3131} = J_{22} + J_{23} + J_{25} + J_{27} + 3J_{2,12}, \quad K_{1212} = J_{21} + J_{23} + J_{28} + J_{29} + J_{2,13}, \\ &K_{2222} = J_{21} + J_{23} + J_{2,12} - J_{2,13}, \quad K_{3232} = J_{21} + J_{23} + J_{26}, \\ &K_{1313} = J_{21} + J_{22} - J_{24} + J_{27} + J_{29} - J_{2,11} - J_{2,13}, \\ &K_{2323} = J_{21} + J_{22} - J_{24} + J_{26} + J_{2,10} - J_{2,11}, \\ &K_{3333} = J_{21} + J_{22} - J_{24} + J_{2,12} + J_{2,13}, \quad K_{1221} = -2J_{28} - J_{2,11} - 2J_{2,12} - 2J_{2,13}, \\ &K_{1331} = -2J_{27} + J_{2,11} - 2J_{2,12} + 2J_{2,13}, \quad K_{2332} = -2J_{26} + J_{2,11} - 2J_{2,12}. \end{aligned} \tag{4.9}$$

经过上述讨论, 我们得到了 C_{2v} 对称下的取向弹性, 其表达反映了向列相局部各向异性的对称性, 具体形式如下

$$\begin{aligned} F_{e,C_{2v}} = \frac{c^2}{2}\big(&K_{23}D_{23} + K_{32}D_{32} \\ &+ K_{1111}D_{11}^2 + K_{2121}D_{21}^2 + K_{3131}D_{31}^2 + K_{1212}D_{12}^2 \end{aligned}$$

$$+ K_{2222}D_{22}^2 + K_{3232}D_{32}^2 + K_{1313}D_{13}^2 + K_{2323}D_{23}^2 + K_{3333}D_{33}^2 + K_{1221}D_{12}D_{21} + K_{1331}D_{13}D_{31} + K_{2332}D_{23}D_{32}\big). \tag{4.10}$$

其中的系数均来源于体积能稳定点中的系数 $s_2, s_3, b_2, b_3, d_1, d_4$ 和弹性能密度表达式中的系数 c_{ij}, 因此均源于分子参数, 具有明确的物理意义. 由以上的计算过程可知, 当弹性能密度表达式相同时, 可以得到一些其它向列相下的取向弹性. 如当 $d_1 = d_4 = b_2 = b_3 = 0$ 时, 即为 $C_{\infty v}$ 向列相下的取向弹性. 除此之外, 通过对比不同向列相的特征标架及弹性能密度的表达, 可以借助本文推导过程的部分结果, 在一定程度上简化取向弹性的计算.

弹性取向的研究对于液晶数学模型的建立具有重要的作用. 对于具有 C_{2v} 对称的液晶分子形成的液晶相, 难以通过实验观测其局部各向异性, 因此可以考虑通过取向弹性对自由能中系数进行研究, 建立系数具有物理意义的数学模型.

5. 总结与展望

本文基于具有 C_{2v} 对称性的分子形成的向列相液晶, 由其体积能稳定点和弹性能密度的表达, 推导了 C_{2v} 向列相下取向弹性的表达式. 此种表达形式反映了向列相液晶局部各向异性的对称性, 并且系数源于分子参数, 因此具有明确的物理意义, 可用于数值模拟的相关研究. 此外, 由于取向弹性的上述优点, 可将其用于基于 Onsager 分子理论的标架模型的建立, 包括静力学模型和动力学模型. 最后, 本文的推导过程可帮助简化其它液晶相下取向弹性的相关计算. 因此, 本文的研究对于液晶数学模型的建立及模型的数值模拟具有重要的作用. 向列相在显示器的制造中有着广泛应用, 其弹性性质, 缺陷, 以及在外场作用下的行为都是重要的论题. 弹性能的引入使模型可以考察边界作用几何限制效应, 浸润和缺陷等含有空间变化的情形.

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