Irreducible function bases for fluids & liquid crystal films

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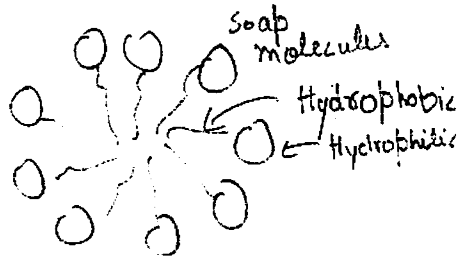
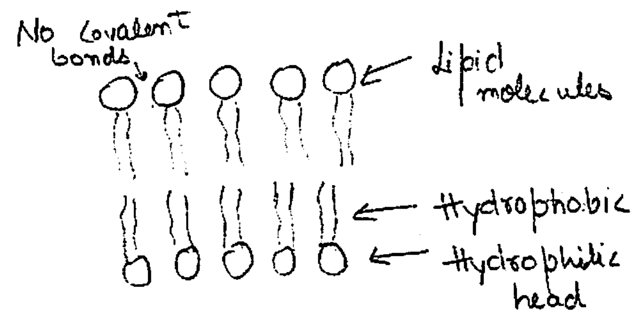
Liquid crystals → Materials with properties between a solid and a liquid. These can flow like a liquid but the molecules are oriented in a crystal-like way (solid) & they maintain that orientation while flowing.

Ex →



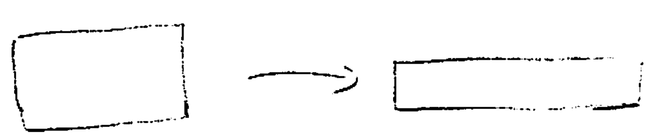
Micelle

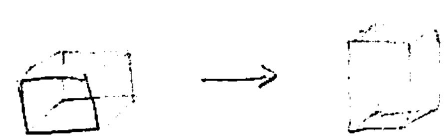


Lipid bilayer

In plane Lipid bilayer behave like a fluid but since molecules cannot change their orientation hence some bending energy is associated with curved surfaces unlike liquids!

Liquid crystal films	Simple fluids
Unimodular transformations are allowed in 2-d	Unimodular transformations are allowed in 3-d





Material symmetry group →

(page-49 Notes)

$\mathcal{U} = \{ \underline{A} \in \mathrm{Lin} : |\det \underline{A}| = 1 \}$ — group of unimodular tensors

$\mathcal{U}^{+} = \{ \underline{A} \in \mathrm{Lin} : \det \underline{A} = 1 \}$ — proper unimodular tensors.

Function basis $\rightarrow$

It is a list of scalar valued functions of tensor variables whose elements are invariant under a group of local transformations which characterizes the symmetries inherent in a material.

For ex – for isotropic materials

function basis for $\underline{\underline{C}} = I_c, II_c, III_c, I_c^2, I_c II_c$.

Irreducible function basis $\longrightarrow$

There is no single valued function yielding any member of the list in terms of the others. Therefore only I_c, II_c, III_c are part of irreducible function basis.

Under Unimodular transformations $\rightarrow$

Given $\rightarrow$ $\psi(\underline{\underline{C}}, \underline{\underline{K}}) = \psi(\underline{R}\,\underline{\underline{C}}\,\underline{R}^t, \pm \underline{R}\,\underline{\underline{K}}\,\underline{R}^t)$ $\forall$ $\underline{R} \in \underline{U}$.

where $\underline{\underline{C}} = \underline{F}^T \underline{F}$ $\rightarrow$ Right cauchy green strain tensor.

$\underline{\underline{K}} = \underline{F}^T \underline{\underline{b}}\,\underline{F}$, $\underline{\underline{b}}$ = curvature tensor.

To show $\rightarrow$ Irreducible functions of $\underline{\underline{C}}, \underline{\underline{K}}$ from isotropy

(lecture 28)

$I_1(\underline{\underline{C}}) = tr(\underline{\underline{C}})$

$I_2(\underline{\underline{C}}) = det(C)$

$I_3(\underline{\underline{K}}) = tr(\underline{\underline{K}})$

$I_4(\underline{\underline{K}}) = det\,\underline{\underline{K}}$

$I_5(\underline{\underline{C}}, \underline{\underline{K}}) = tr(\underline{\underline{C}}\,\underline{\underline{K}})$

$I_6(\underline{\underline{C}}, \underline{\underline{K}}) = tr(\underline{\underline{C}}\,\underline{\underline{K}}\,\underline{\underline{C}})$

$\xrightarrow{\text{reduces to}}$

$I_2(\underline{\underline{C}}) = det(\underline{\underline{C}})$

$I_4(\underline{\underline{K}}) = det(\underline{\underline{K}})$

$I_7(\underline{\underline{C}}, \underline{\underline{K}}) = tr\,\underline{\underline{C}}\; tr\underline{\underline{K}} - tr\,\underline{\underline{C}}\,\underline{\underline{K}}$

under unimodular transformations.

$\underline{\underline{\varepsilon}} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

Simple fluids →

By (M.S) we have

$$\Psi(\underline{\underline{C}}) = \Psi(\underline{\underline{R}}\,\underline{\underline{C}}\,\underline{\underline{R}}^T) \quad \forall\ \underline{\underline{C}} \in \text{sym}^+ \ \&\ \underline{\underline{R}} \in \mathcal{U},$$

$\underline{\underline{F}}^T\underline{\underline{F}}$

Principal invariants of $\underline{\underline{C}}$ constitute an irreduci-ble function basis of $\underline{\underline{C}}$ under $\underline{\underline{O}}$.

$$\Rightarrow \Psi(\underline{\underline{C}}) = \Psi(\text{principal invariants of } \underline{\underline{C}})$$

Let $\underline{\underline{C}}^* \in \text{sym}^+$, if there exists $\underline{\underline{R}} \in \mathcal{U}$ s.t $\underline{\underline{R}}\,\underline{\underline{C}}^*\,\underline{\underline{R}}^T$ & $\underline{\underline{C}}$ have same invariants.

$$\Rightarrow \Psi(\underline{\underline{C}}) = \Psi(\underline{\underline{C}}^*) = \Psi(\text{principal invariants of } \underline{\underline{C}}).$$

In 2-d, let

$$\underline{\underline{C}} = \text{diag}(c_1, c_2).$$

then $\underline{\underline{C}}^* = \sqrt{\det \underline{\underline{C}}}\,(1,1)$.

Let $\underline{\underline{R}} = \text{diag}\left(a, \frac{1}{a}\right) \in U^+$.

To show → Invariants of $\underline{\underline{C}}$ & $\underline{\underline{R}}\,\underline{\underline{C}}^*\,\underline{\underline{R}}^T$ are same.

$$\text{tr}(\underline{\underline{R}}\,\underline{\underline{C}}^*\,\underline{\underline{R}}^T) = \left(a^2 + \frac{1}{a^2}\right)\sqrt{c_1 c_2}$$

$$\det(\underline{\underline{R}}\,\underline{\underline{C}}^*\,\underline{\underline{R}}^T) = \det \underline{\underline{C}}^* = \det \underline{\underline{C}}.$$

Now for $\text{tr}(\underline{\underline{R}}\,\underline{\underline{C}}^*\,\underline{\underline{R}}^T) = \text{tr}(\underline{\underline{C}})$

$$\left(a^2 + \frac{1}{a^2}\right)\sqrt{c_1 c_2} = c_1 + c_2$$

for $a = \left(\frac{c_1}{c_2}\right)^{1/4}$

$\Rightarrow$ For any $\underline{\underline{C}}$ there exists a $\underline{\underline{C}}^*$ & $\underline{\underline{R}}$ s.t $\underline{\underline{R}}\,\underline{\underline{C}}^*\,\underline{\underline{R}}^T$ & $\underline{\underline{C}}$ have same invariants.

Invariants of $\underline{\underline{C}}^*$ are $\rightarrow$

$I_1 = \det \underline{\underline{C}}$ & $II_2 = 2\sqrt{\det \underline{\underline{C}}}$.

$\therefore$ The only unique independent principal invariant is $\det \underline{\underline{C}}$.

$$\Rightarrow \quad \Psi(\underline{\underline{C}}) = \Psi(\det \underline{\underline{C}})$$ is the complete representation.

In 3-d $\longrightarrow$

Let
$$\underline{\underline{C}}^* = (\det \underline{\underline{C}})^{1/3} \operatorname{diag}(1, 1, 1).$$
$$\underline{\underline{C}} = \operatorname{diag}(c_1, c_2, c_3)$$
$$\underline{\underline{R}} = \operatorname{diag}\left(a, b, \frac{1}{ab}\right) \in U^+.$$

Now
$$\det \underline{\underline{R}}\,\underline{\underline{C}}^*\underline{\underline{R}}^T = \det \underline{\underline{C}} \quad \text{—— } *$$
$$\operatorname{tr}(\underline{\underline{R}}\,\underline{\underline{C}}^*\underline{\underline{R}}^T) = \left(a^2 + b^2 + \frac{1}{a^2b^2}\right)(c_1c_2c_3)^{1/3} \quad \text{—— } **$$
$$\frac{1}{2}\left[\left(\operatorname{tr}(\underline{\underline{R}}\,\underline{\underline{C}}^*\underline{\underline{R}}^T)\right)^2 - \operatorname{tr}(\underline{\underline{R}}\,\underline{\underline{C}}^*\underline{\underline{R}}^T)^2\right] = \frac{1}{2}\left[\left(a^2 + b^2 + \frac{1}{a^2b^2}\right)^2 - a^4 \cancel{b} - b^4 - \frac{1}{a^4b^4}\right] \times (c_1c_2c_3)^{\frac{2}{3}}$$
$$= \frac{1}{2}\left[2\left(\frac{1}{b^2}\right) + 2\frac{1}{a^2} + 2a^2b^2\right](c_1c_2c_3)^{2/3}$$
$$= \left[\frac{1}{a^2} + \frac{1}{b^2} + a^2b^2\right](c_1c_2c_3)^{2/3} \quad \text{—— } ***$$

For $a^2 = \left(\frac{c_1^2}{c_2c_3}\right)^{1/3}$, $b^2 = \left(\frac{c_2}{c_1c_3}\right)^{1/3}$, $** = c_1 + c_2 + c_3 = \operatorname{tr}(\underline{\underline{C}})$

& $*** = c_1c_2 + c_2c_3 + c_3c_1 = \frac{1}{2}\left[(\operatorname{tr}(\underline{\underline{C}}))^2 - \operatorname{tr}(\underline{\underline{C}})^2\right]$

I_{C^*}, II_{C^*}, III_{C^*} are all functions of $\det \underline{\underline{C}}$

$\therefore$ Only independent principal invariant is $\det \underline{\underline{C}}$.

$$\Rightarrow \quad \Psi(\underline{\underline{C}}) = \Psi(\det \underline{\underline{C}}).$$

Liquid Crystal Films $\rightarrow$

From isotropy, using orthogonal transformations etc. can be shown that $\rightarrow$

$$\Psi(\underline{\underline{C}}, \underline{\underline{K}}) = \Psi(I_1, I_2, I_3, I_4, I_5, I_6).$$

Ref $\Rightarrow$ Zheng, 1994.

Now define a $\mathcal{U}$ equivalent set $(\underline{\underline{C}}^*, K^*)$ s.t there exists a $\underline{\underline{R}} \in \mathcal{U}^+$ so that both $(\underline{\underline{R}}\,\underline{\underline{C}}^*\underline{\underline{R}}^T, \underline{\underline{R}}\,\underline{\underline{K}}^*\underline{\underline{R}}^T)$ & $(\underline{\underline{C}}, \underline{\underline{K}})$ have the same basis function...

Follow the same strategy as used in 2-d fluids i.e for given $\underline{\underline{C}} = \mathrm{diag}(c_1, c_2)$ & $\underline{\underline{K}} = \begin{pmatrix} K_{11} & K_{12} \\ K_{12} & K_{22} \end{pmatrix}$.

Define $\rightarrow$ $\underline{\underline{C}}^* = \sqrt{c_1 c_2}\, \mathrm{diag}(1, 1)$, $\quad \underline{\underline{K}}^* = \begin{pmatrix} \sqrt{\frac{c_2}{c_1}} K_{11} & -K_{12} \\ -K_{12} & \sqrt{\frac{c_1}{c_2}} K_{22} \end{pmatrix}$

$\underline{\underline{R}} = \mathrm{diag}\left(a, \frac{1}{a}\right)$

For this system for $a = \left(\frac{c_1}{c_2}\right)^{1/4}$

$\det \underline{\underline{R}}\,\underline{\underline{C}}^*\underline{\underline{R}}^T = \det \underline{\underline{C}}$

$\mathrm{tr}\,\underline{\underline{R}}\,\underline{\underline{C}}^*\underline{\underline{R}}^T = c_1 + c_2 = \mathrm{tr}\,\underline{\underline{C}}$

$\det \underline{\underline{R}}\,\underline{\underline{K}}^*\underline{\underline{R}}^T = \det \underline{\underline{K}}$

$\mathrm{tr}\,\underline{\underline{R}}\,\underline{\underline{K}}^*\underline{\underline{R}}^T = \mathrm{tr}\,\underline{\underline{K}}$

$\mathrm{tr}\,(\underline{\underline{R}}\,\underline{\underline{C}}^*\underline{\underline{R}}^T\underline{\underline{R}}\,\underline{\underline{K}}^*\underline{\underline{R}}^T) = \mathrm{tr}\,(\underline{\underline{C}}\,\underline{\underline{K}})$

$\mathrm{tr}\,(\underline{\underline{R}}\,\underline{\underline{C}}^*\underline{\underline{R}}^T\underline{\underline{R}}\,\underline{\underline{K}}^*\underline{\underline{R}}^T\underline{\underline{\epsilon}}) = \mathrm{tr}\,(\underline{\underline{\epsilon}}\,\underline{\underline{K}}\,\underline{\underline{\epsilon}})$

$\Rightarrow$ $(\underline{\underline{C}}^*, \underline{\underline{K}}^*)$ and $(\underline{\underline{C}}, \underline{\underline{K}})$ are $\mathcal{U}$ equivalent.

Hence, $\Psi(\underline{\underline{C}}, \underline{\underline{K}}) = \Psi(\underline{\underline{C}}^*, \underline{\underline{K}}^*)$

Now function basis of (C^*, K^*) consists of $\rightarrow$

$I_1 = 2\sqrt{\det \underline{\underline{C}}}$ $\qquad I_4 = \det \underline{\underline{K}}$

$I_2 = \sqrt{\det \underline{\underline{C}}}$ $\qquad I_5 = \operatorname{tr}\underline{\underline{C}}\operatorname{tr}\underline{\underline{K}} - \operatorname{tr}\underline{\underline{C}}\,\underline{\underline{K}}$

$I_3 = \dfrac{\operatorname{tr}\underline{\underline{C}}\operatorname{tr}\underline{\underline{K}} - \operatorname{tr}\underline{\underline{C}}\,\underline{\underline{K}}}{\sqrt{\det \underline{\underline{C}}}}$ $\qquad I_6 = 0$

This involves only three independent invariants

I_2, I_4, $I_7 = \operatorname{tr}\underline{\underline{C}}\operatorname{tr}\underline{\underline{K}} - \operatorname{tr}\underline{\underline{C}}\,\underline{\underline{K}}$

I_2, I_4 are already $\mathcal{U}^+$ invariant, we still need to show that I_7 is a $\mathcal{U}^+$ invariant too.

For this let's use Cayley Hamilton

$$\underline{\underline{A}}^2 - I_A \underline{\underline{A}} + II_A \underline{\underline{I}} = \underline{\underline{0}}.$$

$$\Rightarrow \quad II_A \underline{\underline{A}}^{-1} = I_A \underline{\underline{I}} - \underline{\underline{A}}.$$

Now $I_7 = \operatorname{tr}\underline{\underline{C}}\operatorname{tr}\underline{\underline{K}} - \operatorname{tr}\underline{\underline{C}}\,\underline{\underline{K}}$

$= \operatorname{tr}\left((\operatorname{tr}\underline{\underline{C}})\underline{\underline{K}} - \underline{\underline{C}}\,\underline{\underline{K}}\right)$

$= \operatorname{tr}\left(\left((\operatorname{tr}\underline{\underline{C}})\underline{\underline{I}} - \underline{\underline{C}}\right)\underline{\underline{K}}\right)$

$= \operatorname{tr}\left(\left(II_C \underline{\underline{C}}^{-1}\right)\underline{\underline{K}}\right).$

$= II_C \operatorname{tr}(\underline{\underline{C}}^{-1}\underline{\underline{K}})$

$= (\det \underline{\underline{C}}) \operatorname{tr}(\underline{\underline{C}}^{-1}\underline{\underline{K}})$

Now $\det \underline{\underline{C}}$ is already $\mathcal{U}$-invariant

$$\mathrm{tr}\left((\underline{\underline{R}}\,\underline{\underline{C}}\,\underline{\underline{R}}^t)^{-1}\,\underline{\underline{R}}\,\underline{\underline{K}}\,\underline{\underline{R}}^t\right) = \mathrm{tr}\left((\underline{\underline{C}}\,\underline{\underline{R}}^t)^{-1}\,\underline{\underline{R}}^{-1}\,\underline{\underline{R}}\,\underline{\underline{K}}\,\underline{\underline{R}}^t\right)$$

$$= \mathrm{tr}\left(\underline{\underline{R}}^{t^{-1}}\,\underline{\underline{C}}^{-1}\,\underline{\underline{K}}\,\underline{\underline{R}}^t\right)$$

$$= \mathrm{tr}\left(\underline{\underline{C}}^{-1}\,\underline{\underline{K}}\,\underline{\underline{R}}^t\,\underline{\underline{R}}^{t^{-1}}\right)$$

$$= \mathrm{tr}\left(\underline{\underline{C}}^{-1}\,\underline{\underline{K}}\right). \qquad \left(\mathrm{tr}(\underline{\underline{A}}\,\underline{\underline{B}}) = \mathrm{tr}(\underline{\underline{B}}\,\underline{\underline{A}})\right)$$

$\Rightarrow$ I_7 is invariant under Unimodular transformation.

So far we have considered only $\underline{\underline{R}} \in \mathcal{U}^+$ transformations, for $\underline{\underline{R}} \in \mathcal{U}\backslash\mathcal{U}^+$.

ex $\rightarrow$ $\underline{\underline{B}} = \mathrm{diag}(1,-1)$

$I_2(\underline{\underline{B}}\,\underline{\underline{C}}\,\underline{\underline{B}}^t) = I_2(\underline{\underline{C}})$, $I_4(-\underline{\underline{B}}\,\underline{\underline{K}}\,\underline{\underline{B}}^T) = I_4(\underline{\underline{K}})$, $I_7(\underline{\underline{B}}\,\underline{\underline{C}}\,\underline{\underline{B}}, -\underline{\underline{B}}\,\underline{\underline{K}}\,\underline{\underline{B}}^T) = -I_7(\underline{\underline{C}}, \underline{\underline{K}})$

$\Rightarrow$ ψ must be an even function of I_7^2.

$$\psi(\underline{\underline{C}}, \underline{\underline{K}}) = \psi(I_2, I_4, I_7^2).$$

Check irreducibility of $I_2, I_4, I_7 \rightarrow$

let $\underline{\underline{B}} = \mathrm{diag}(1,2)$, $\underline{\underline{B}}_1 = \mathrm{diag}(2,1)$ $\underline{\underline{B}}_2 = \mathrm{diag}(\frac{3}{2}, 1)$.

$$\left\{\begin{array}{l} \underline{\underline{C}} = \underline{\underline{B}},\ \underline{\underline{K}}_1 = \underline{\underline{B}},\ \underline{\underline{K}}_2 = \underline{\underline{B}}_1 \\ \underline{\underline{C}} = \underline{\underline{B}},\ \underline{\underline{K}}_2 = \underline{\underline{B}},\ \underline{\underline{K}}_2 = \underline{\underline{B}}_2 \\ \underline{\underline{C}} = \underline{\underline{B}},\ \underline{\underline{C}}_2 = \underline{\underline{B}}_2,\ \underline{\underline{K}} = \underline{\underline{B}} \end{array}\right\} \Rightarrow \left\{\begin{array}{l} I_4(\underline{\underline{K}}_1) = I_4(\underline{\underline{K}}_2) = 2,\ I_7(\underline{\underline{C}}, \underline{\underline{K}}_1) = 4,\ I_7(\underline{\underline{C}}, \underline{\underline{K}}_2) = 5 \\ I_4(K_1) = 2,\ I_4(K_2) = 3/2,\ I_7(\underline{\underline{C}}, K_1) = I_7(\underline{\underline{C}}, \underline{\underline{K}}_2) = 4 \\ I_2(\underline{\underline{C}}_1) = 2,\ I_2(\underline{\underline{C}}_2) = \frac{3}{2},\ I_7(\underline{\underline{C}}_1, \underline{\underline{K}}) = I_7(\underline{\underline{C}}_2, \underline{\underline{K}}) = 4. \end{array}\right.$$

$\Rightarrow$ I_7, I_4 & I_2 cannot be single valued functions of the remaining invariants.