Flow and Texture Modeling of Liquid Crystalline Materials

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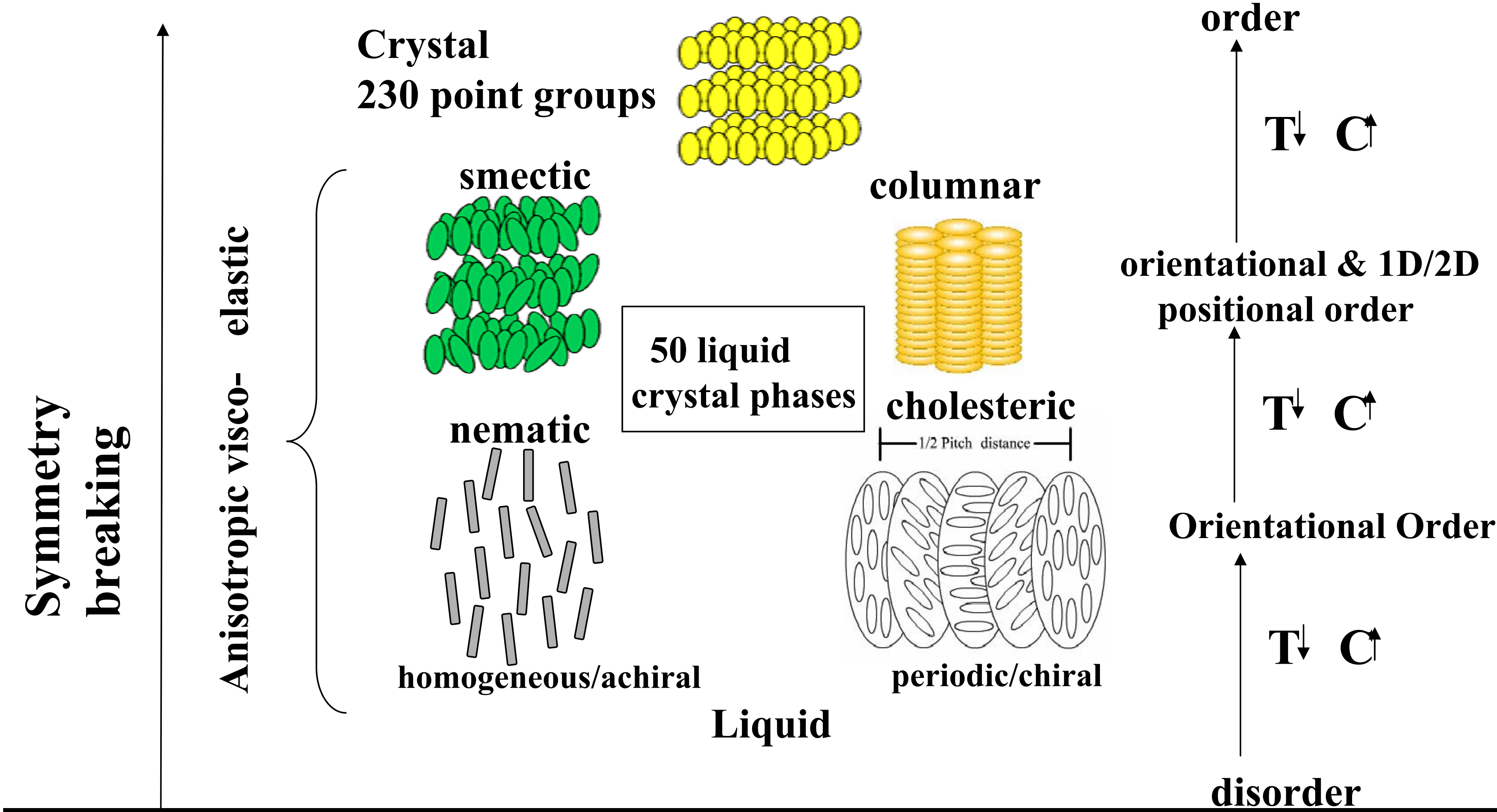
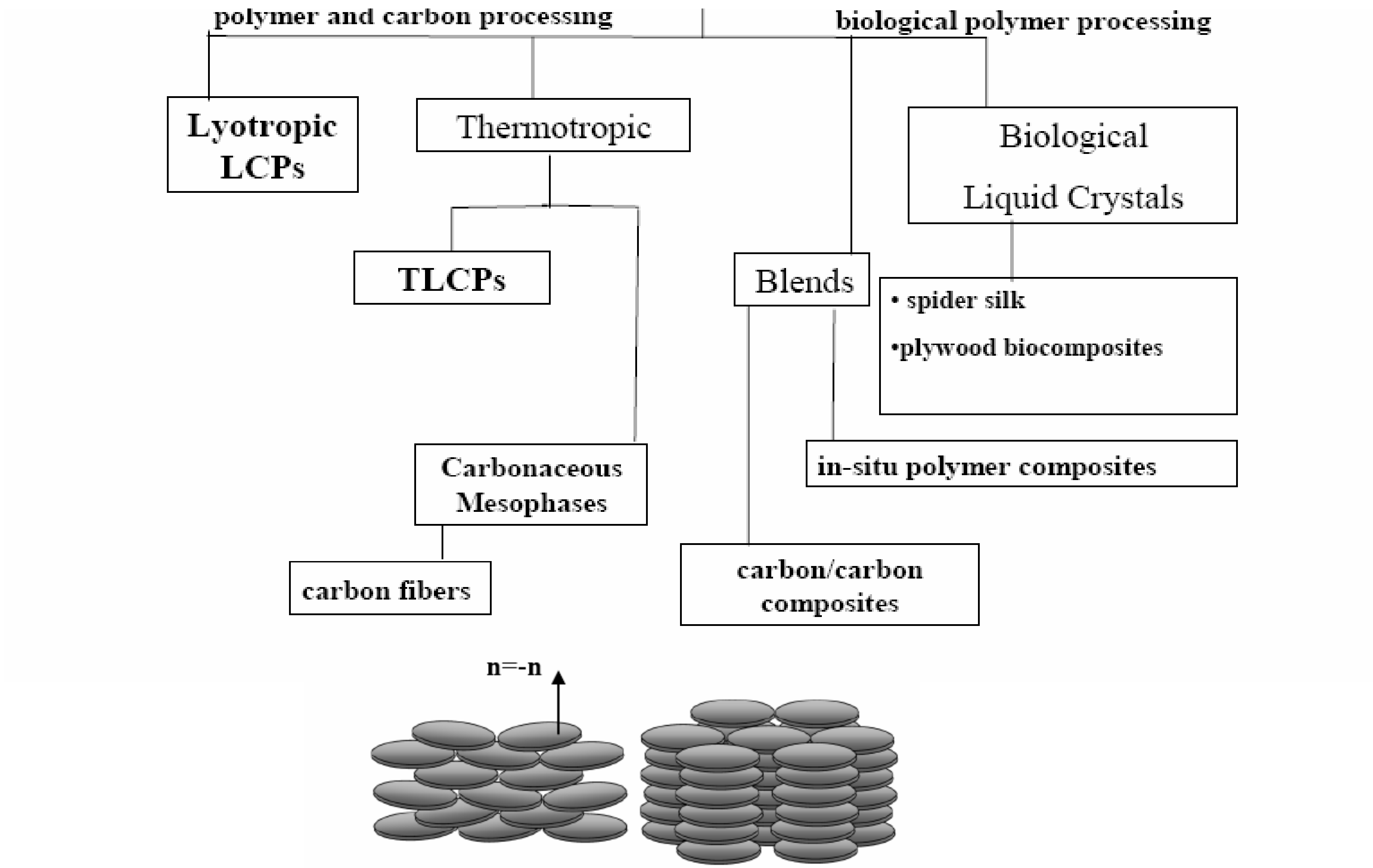
Christopher Cox
Amod Ogale
Dan Edie

Rheology of complex fluids: modeling and numerics
Ecole de Ponts-Peking University Workshop
January 5-9th 2009
Paris

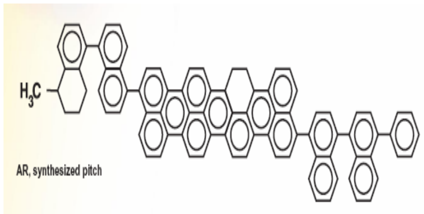
Classification



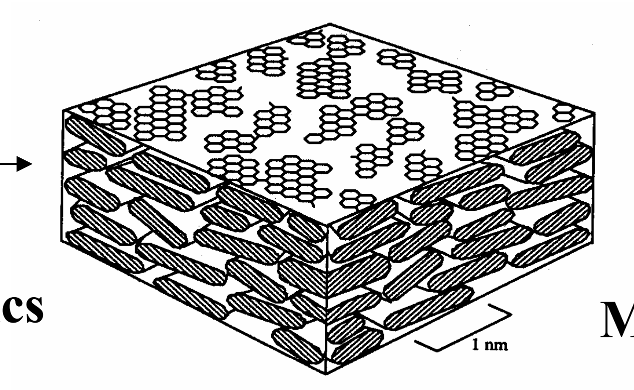
Liquid Crystalline Precursors for Structural Materials

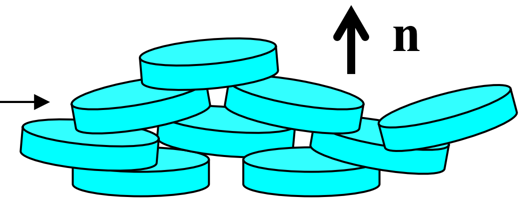


Carbonaceous Mesophases



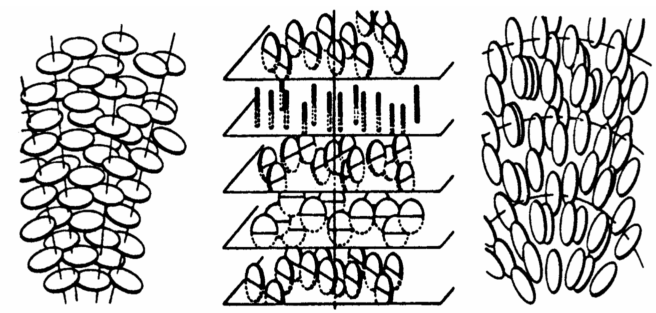
polycyclic aromatics





MW=o(500g/mol)

Elasticity



splay twist bend

Topological Defects

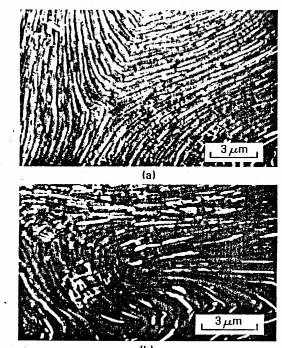
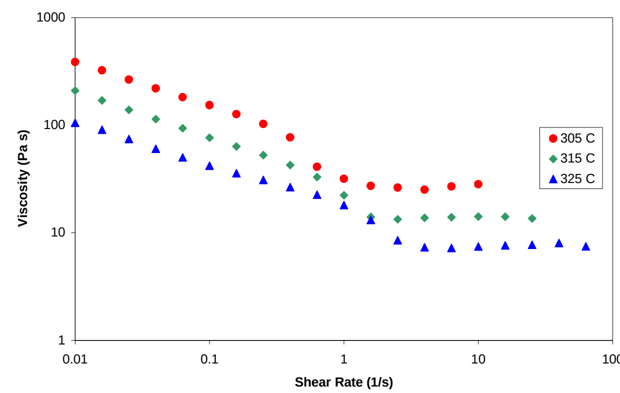


Fig. 28. Scanning electron micrographs of wedge disclinations in the fine fibrous structure of a heat-treated needle coke. (a) Wedge disclination of strength $S = -1/2$; (b) wedge disclination of strength $S = +1/2$. Reprinted from White and Zimmer [60] by courtesy of the Royal Society of Chemistry.

Rheology



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Outline

1. Introduction: Liquid crystals

2. Modeling Overview

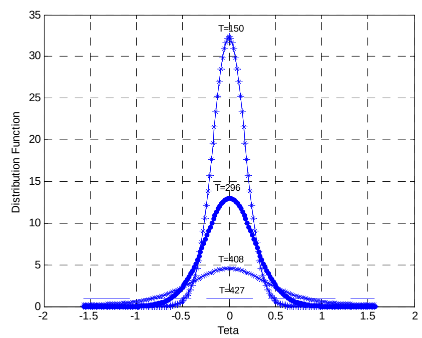
3. Leslie-Ericksen Nematodynamics

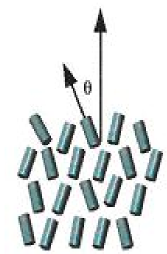
4. Landau de Gennes Nematodynamics

5. Applications

Order Parameters: n and Q

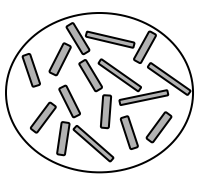
$$\Psi(\mathbf{u}) = \frac{1}{4\pi} + \frac{3x5}{4\pi x2}\mathbf{Q} : (\mathbf{uu} - \mathbf{I}/3) + \ldots$$



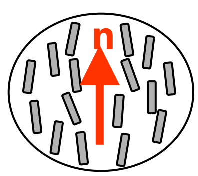


$$S = \frac{3}{2}\langle \cos^2\theta \rangle - \frac{1}{2}$$

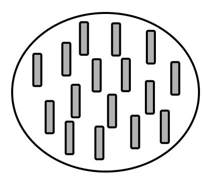
Orientation n and Alignment S



S=0



S=1/2



S=1

Orientation & alignment Q

$$Q = S\left(nn - \frac{\delta}{3}\right)$$

Quadrupolar order parameter Q

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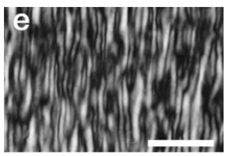
Computational Flow-Modeling Paradigm

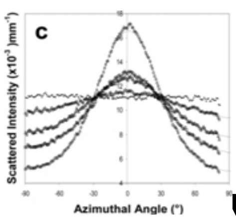
$$\Delta = \mathbf{T}^s : \mathbf{A} - \frac{\delta F}{\delta \mathbf{Q}} : \left(\frac{d\mathbf{Q}}{dt}\right)$$

$$\begin{pmatrix} \mathbf{T}^s \\ \frac{d\mathbf{Q}}{dt} \end{pmatrix} = \begin{pmatrix} \mathbf{a} & -\lambda \\ \lambda & \boldsymbol{\beta} \end{pmatrix} \otimes \begin{pmatrix} \mathbf{A} \\ -\frac{\delta F}{\delta \mathbf{Q}} \end{pmatrix}$$

λ: coupling parameter

Flow-Induced Orientation/Back-Flow Cycle





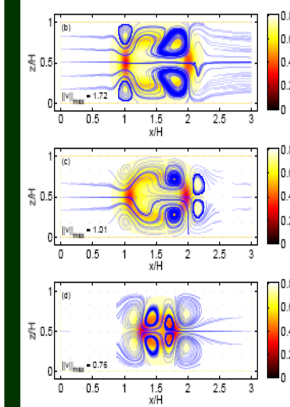
Flow velocity $v \Rightarrow \mathbf{A} = (\nabla \mathbf{v})^s$

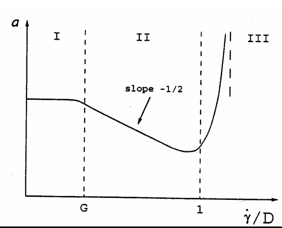
$$\begin{pmatrix} \mathbf{T}^s \end{pmatrix} = \begin{pmatrix} & -\lambda \end{pmatrix} \otimes \begin{pmatrix} -\frac{\delta F}{\delta \mathbf{Q}} \end{pmatrix}$$

Flow-induced orientation — **defects** — **Back-flow**

$$\begin{pmatrix} \frac{d\mathbf{Q}}{dt} \end{pmatrix} = \begin{pmatrix} \lambda & \end{pmatrix} \otimes \begin{pmatrix} \mathbf{A} \end{pmatrix}$$

Q- velocity $d\mathbf{Q}/dt \Rightarrow \delta F/\delta \mathbf{Q}$

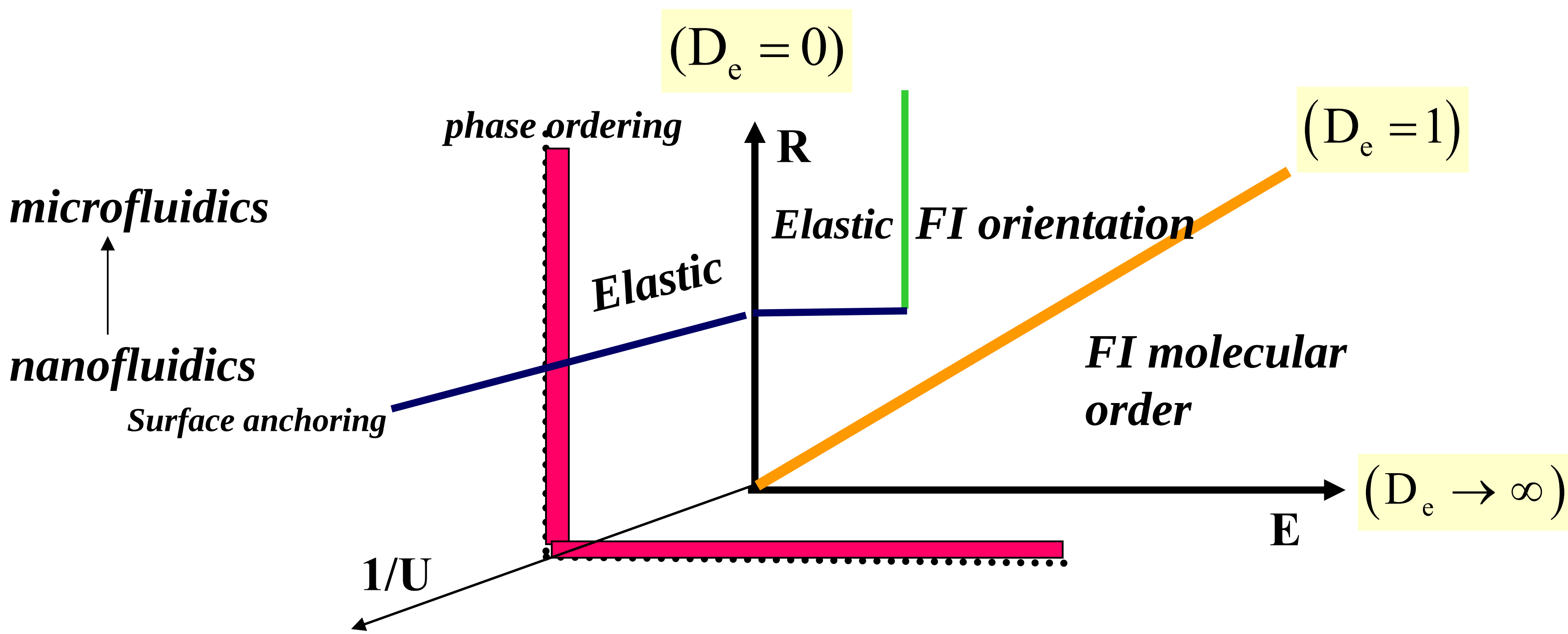




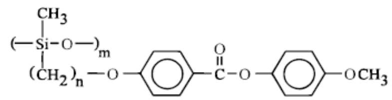
$$E = \frac{\tau_o}{\tau_f}; R = \left(\frac{H}{\ell}\right)^2 \rightarrow D_e = \frac{E}{R}$$

Parametric Space

$$R=\left(\frac{H}{\xi}\right)^2,\ \mathbf{E}=\dot{\gamma}\boldsymbol{\tau}_n,\ \ U=\left(\frac{T^*}{T}\right),\qquad \mathbf{D}_e=\frac{\mathbf{E}}{\mathbf{R}}=\dot{\gamma}\boldsymbol{\tau}_s$$

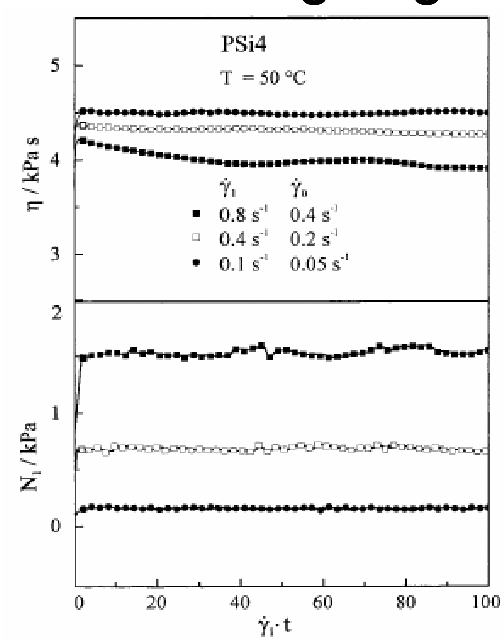


Flow-Alignment $\lambda = \frac{\alpha_3 + \alpha_2}{\alpha_2 - \alpha_3} = \frac{\text{strain}}{\text{vorticity}}$



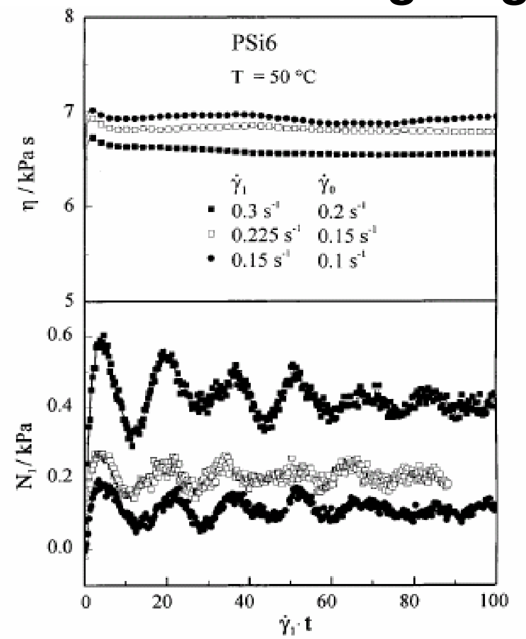
mers studied, presented in Scheme 1, consist of a polysiloxane backbone and a 4-methoxyphenyl-4'-alkyloxybenzoate side chain. The mesogen is connected to the backbone via a flexible spacer of four or six methylene units for PSi4 and PSi6, respectively. The synthesis was carried out as described by

Flow-aligning



$\lambda > 1$

Non-flow-aligning



$0 < \lambda < 1$

Quijada-Garrido et al., *Macromolecules*, (2000)

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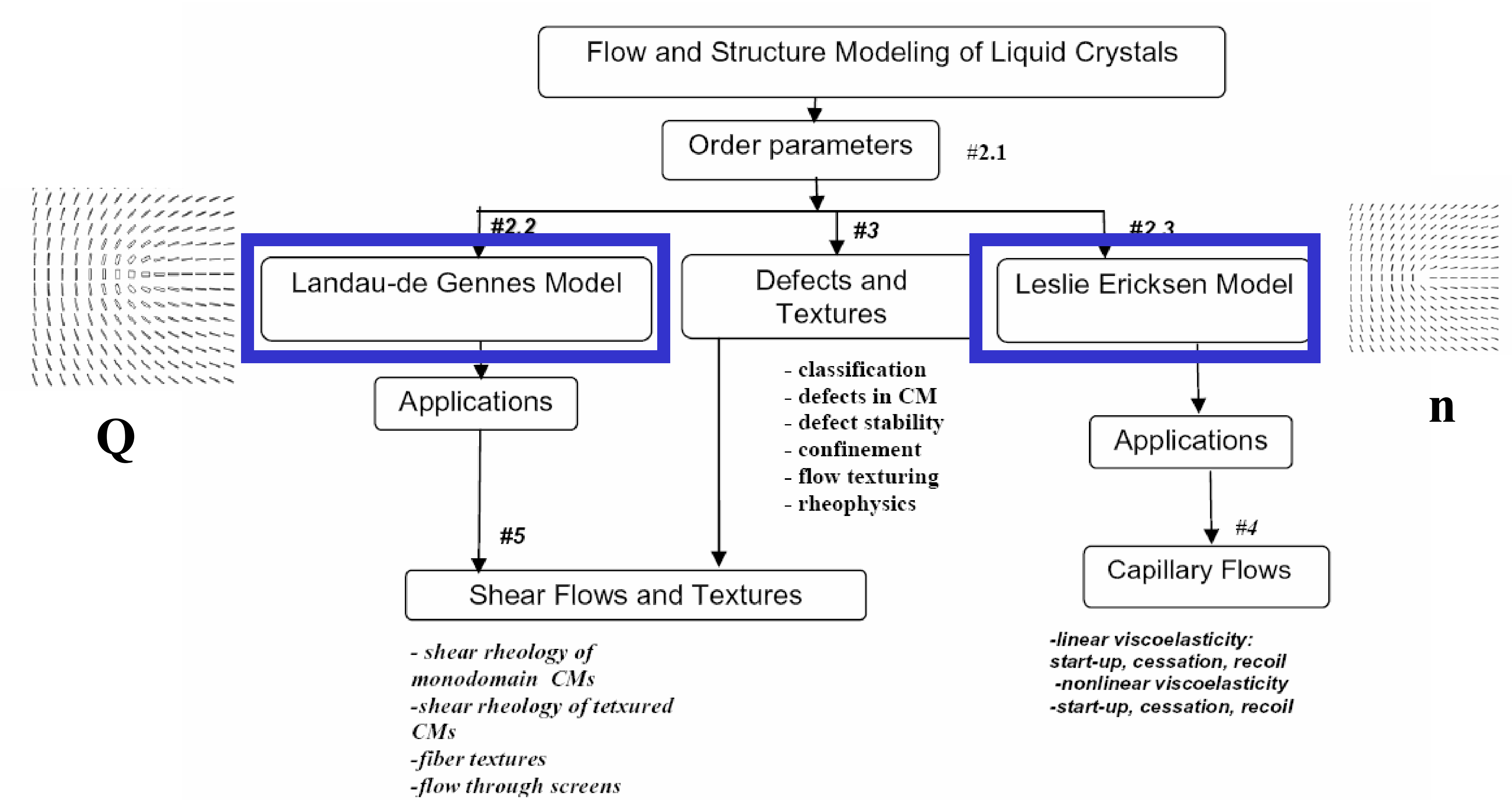
Flow-Modeling



Leslie-Ericksen Nematodynamics

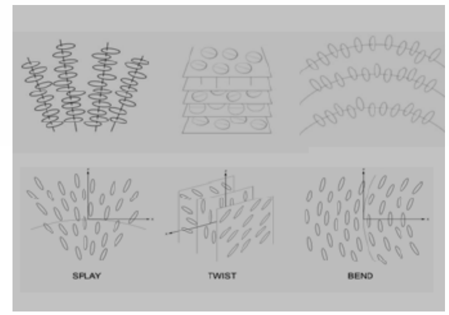
$$\nabla \cdot \mathbf{v} = 0\,, \qquad \rho\dot{\mathbf{v}} = \mathbf{f} + \nabla \cdot \mathbf{T}$$

$$\Delta = \mathbf{T}^s : \mathbf{A} - \frac{\delta F}{\delta \mathbf{n}} : \left(\frac{d\mathbf{n}}{dt}\right)$$

$$\begin{pmatrix} \mathbf{T}^s \\ \frac{d\mathbf{n}}{dt} \end{pmatrix} = \begin{pmatrix} \mathbf{a} & -\lambda \\ \lambda & \boldsymbol{\beta} \end{pmatrix} \otimes \begin{pmatrix} \mathbf{A} \\ -\frac{\delta F}{\delta \mathbf{n}} \end{pmatrix}$$

$$\mathbf{T} = -p\mathbf{I} - \frac{\partial F_g}{(\partial \nabla \mathbf{n})^T} \cdot \nabla \mathbf{n} + \alpha_1(\mathbf{nn}:\mathbf{A})\mathbf{nn} + \alpha_2 \mathbf{nN} + \alpha_3 \mathbf{Nn} + \alpha_4 \mathbf{A} + \alpha_5 \mathbf{nn} \cdot \mathbf{A} + \alpha_6 \mathbf{A} \cdot \mathbf{nn}$$

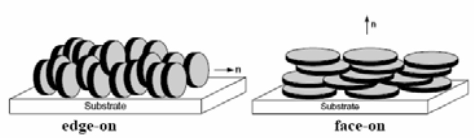
$$2\mathbf{A} = (\nabla \mathbf{v} + (\nabla \mathbf{v})^T), \quad \mathbf{N} = \dot{\mathbf{n}} - \mathbf{W} \cdot \mathbf{n}, \quad 2\mathbf{W} = (\nabla \mathbf{v} - (\nabla \mathbf{v})^T)$$



$$2f_g = K_{11}(\nabla \cdot \mathbf{n})^2 + K_{22}(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_{33}(\mathbf{n} \times \nabla \times \mathbf{n})^2$$

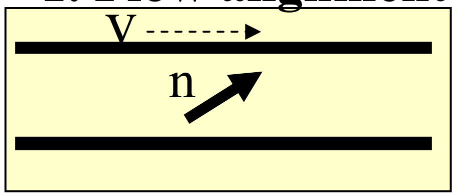
$$\boldsymbol{\Gamma}^v + \boldsymbol{\Gamma}^e = 0\,, \boldsymbol{\Gamma}^v = \mathbf{n} \times \mathbf{h}^v \equiv -\mathbf{n} \times (\gamma_1 \mathbf{N} + \gamma_2 \mathbf{A} \cdot \mathbf{n})\,, \boldsymbol{\Gamma}^e = \mathbf{n} \times \mathbf{h}^e \equiv -\mathbf{n} \times \left(\frac{\partial f_g}{\partial \mathbf{n}} - \nabla \cdot \frac{\partial f_g}{\partial (\nabla \mathbf{n})^T} \right)$$

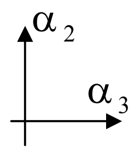
$$\boldsymbol{\Gamma}^{se} + \boldsymbol{\Gamma}^{sv} = \mathbf{0} \qquad \boldsymbol{\Gamma}^{se} = \mathbf{n} \times \mathbf{h}^s_e\;; \qquad \boldsymbol{\Gamma}^{sv} = -\mathbf{n} \times \mathbf{h}^s_v$$



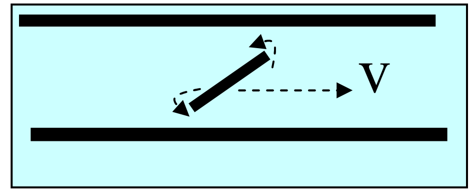
Four Dynamical Laws

1. Flow alignment

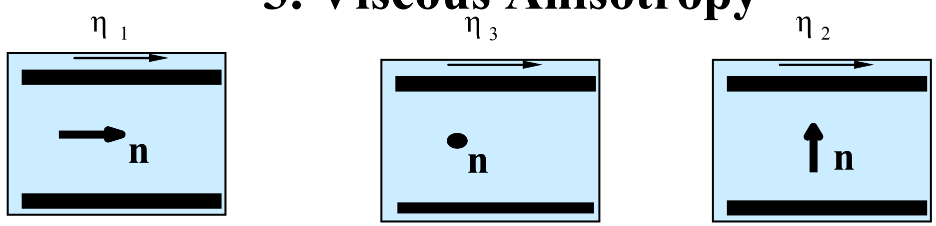




2. Back-flow



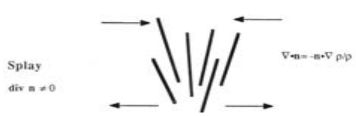
3. Viscous Anisotropy



$$\eta_1 > \eta_3 > \eta_2$$

4. Three Visco-elastic Modes

$$\left(K_{11}, \gamma_1 - \frac{\alpha_3^2}{\eta_1}\right) \qquad \left(K_{22}, \gamma_1 - 0\right) \qquad \left(K_{33}, \gamma_1 - \frac{\alpha_2^2}{\eta_2}\right)$$

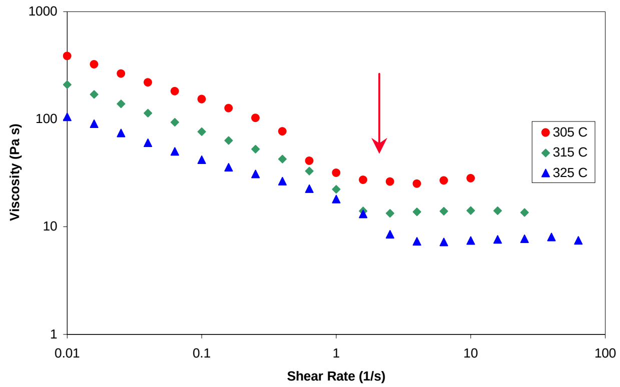


Leslie-Ericksen Nematorheology

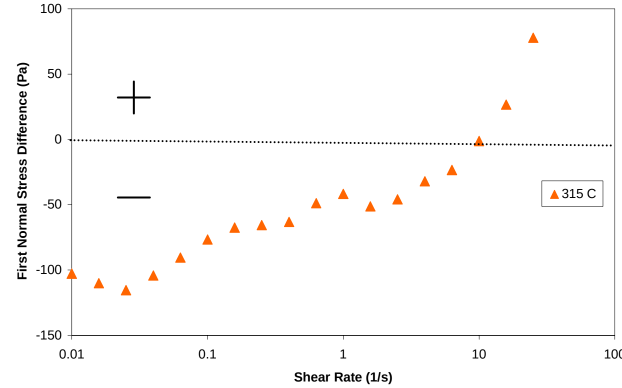
- **Flow alignment** $\eta_{al} = \frac{1}{2}(\eta_1 + \eta_2 - \gamma_1) + \frac{1}{4}\alpha_1\left(1 - \left(\frac{1}{\lambda}\right)^2\right)$
- **Shear viscosities** $\eta_1 = (\alpha_3 + \alpha_4 + \alpha_6)/2 \ , \ \eta_2 = (-\alpha_2 + \alpha_4 + \alpha_5)/2 \ , \ \eta_3 = \alpha_4/2$
- **Back-flow** $\eta_{twist} = \gamma_1, \quad \eta_{splay} = \gamma_1 - \alpha_3{}^2/\eta_1, \quad \eta_{bend} = \gamma_1 - \alpha_2{}^2/\eta_2$
- **Secondary flow** $T_{ij}^{extra} = C_{ijkl}A_{lk} + D_{ijk}N_k$
- **First normal stress difference** $N_1 = t_{xx} - t_{yy} = \dot{\gamma} n_x n_y \left(\gamma_2 + \alpha_1\left(n_y^2 - n_x^2\right)\right)$
- **Shear thinning** $\eta_s = \frac{\eta - \eta_{al}}{\eta_0 - \eta_{al}} = \left[1 + (\tau E_r)^a\right]^{\frac{n-1}{a}}$

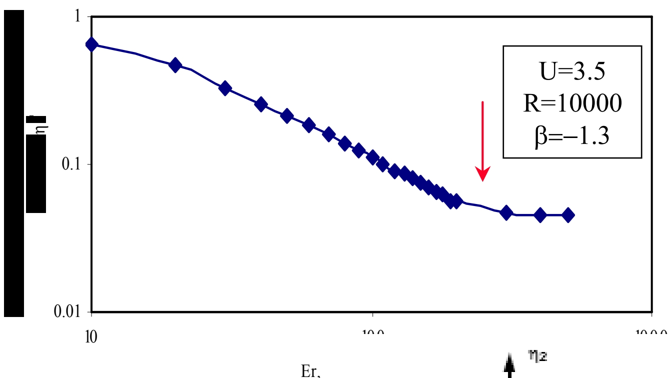
Rheological Characterization

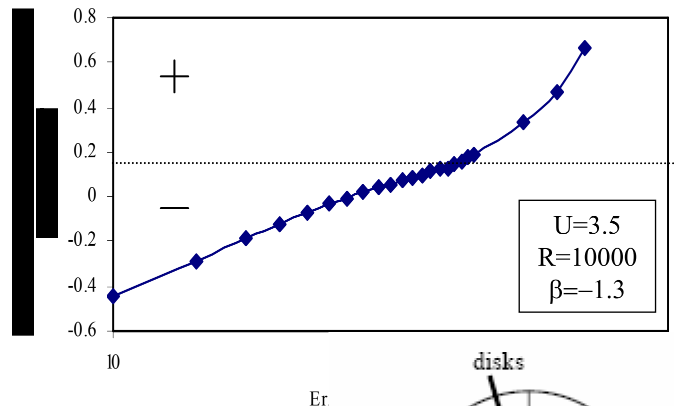
shear viscosity



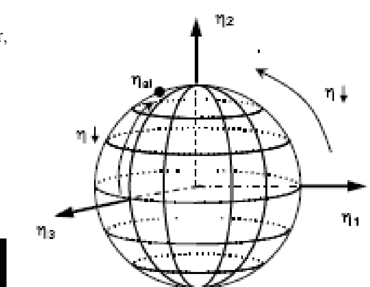
1st normal stress difference



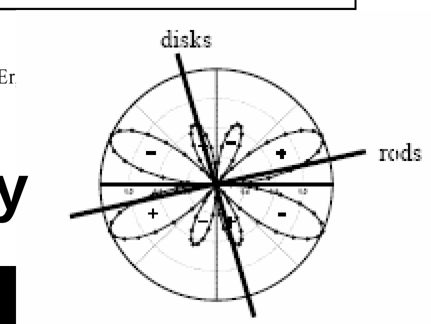




anisotropy



nonlinearity



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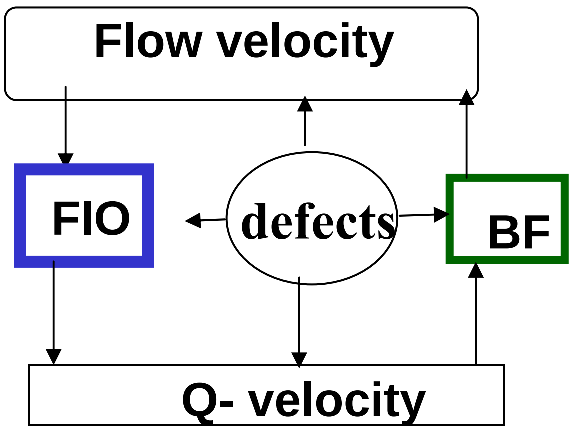
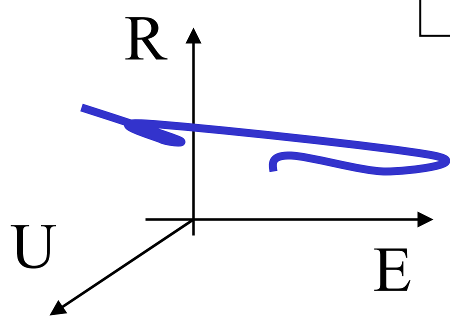
Landau-de Gennes Nematodynamics

$$\Delta = \mathbf{T}^s : \mathbf{A} - \frac{\delta F}{\delta \mathbf{Q}} : \left(\hat{\mathbf{Q}}\right)$$

$$\begin{pmatrix}\mathbf{T}^s \\ \hat{\mathbf{Q}}\end{pmatrix} = \begin{pmatrix}\mathbf{a} & -\beta \\ \beta & c\end{pmatrix} \otimes \begin{pmatrix}\mathbf{A} \\ -\dfrac{\delta F}{\delta \mathbf{Q}}\end{pmatrix}$$

$$\begin{aligned}
Er\hat{Q}^* &= Er\left[\frac{2}{3}\beta A^* + \beta\left[A^*\cdot Q + Q\cdot A^* - \frac{2}{3}(A^*:Q)\mathbb{I}\right]\right. \\
&\quad -\frac{1}{2}\beta\left[(A^*:Q)Q + A^*\cdot Q\cdot Q + Q\cdot A^*\cdot Q + Q\cdot Q\cdot A^* - \{(Q\cdot Q):A^*\}\mathbb{I}\right] \\
&\quad -\frac{3}{U}\cdot\frac{R}{\left(1-\frac{3}{2}Q:Q\right)^2}\left[\left(1-\frac{1}{3}U\right)Q - UQ\cdot Q + U\left\{(Q:Q)Q + \frac{1}{3}(Q:Q)\mathbb{I}\right\}\right] \\
&\quad +\frac{3}{\left(1-\frac{3}{2}Q:Q\right)^2}\left[\nabla^{*2}Q + \frac{1}{2}L_2^*\left[\nabla^*(\nabla^*\cdot Q) + \{\nabla^*(\nabla^*\cdot Q)\}^{\mathrm{T}}\right.\right. \\
&\quad \left.\left.\left. -\frac{2}{3}\mathrm{tr}\{\nabla^*(\nabla^*\cdot Q)\}\mathbb{I}\right]\right]\right] \\
\hat{Q} &= \frac{\partial Q}{\partial t} + (v\cdot\nabla)Q - W^*\cdot Q + Q\cdot W^* \\
A^* &= \frac{1}{2}\left(\nabla v + (\nabla v)^{\mathrm{T}}\right) \\
W^* &= \frac{1}{2}\left(\nabla v - (\nabla v)^{\mathrm{T}}\right)
\end{aligned}$$



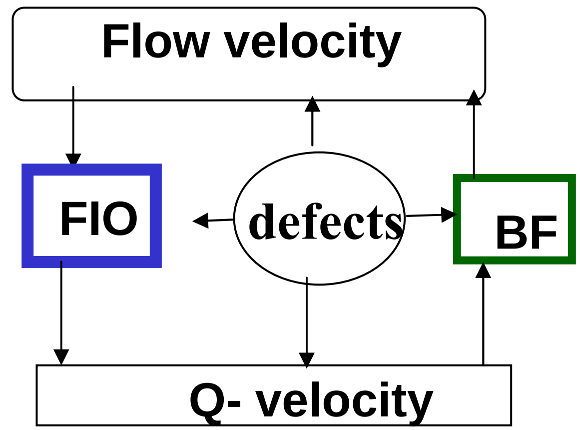


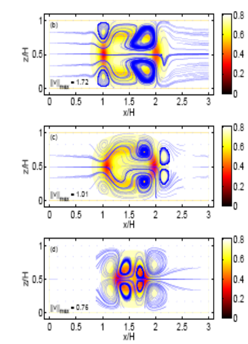
Landau-de Gennes Nematodynamics

$$\mathbf{t}^{t} = \mathbf{t}^{s} + \mathbf{t}^{a} + \mathbf{t}^{Er}$$

$$\begin{pmatrix} \mathbf{T}^{s} \\ \hat{\mathbf{Q}} \end{pmatrix} = \begin{pmatrix} \mathbf{a} & -\beta \\ \beta & \mathbf{c} \end{pmatrix} \otimes \begin{pmatrix} \mathbf{A} \\ \mathbf{H} \end{pmatrix}$$

$$\begin{aligned}
\tilde{\mathbf{t}}^{t} = {} & \frac{Er}{\mathbb{R}}\left(\nu_1^{*}\mathbf{A}^{*} + \nu_2^{*}\left\{\mathbf{Q}\cdot\mathbf{A}^{*} + \mathbf{A}^{*}\cdot\mathbf{Q} - \frac{2}{3}(\mathbf{Q}{:}\mathbf{A}^{*})\,\mathbf{I}\right\}\right) + \\
& \frac{Er}{\mathbb{R}}\left(\nu_4^{*}\left[(\mathbf{A}^{*}:\mathbf{Q})\mathbf{Q} + \mathbf{A}^{*}\cdot\mathbf{Q}\cdot\mathbf{Q} + \mathbf{Q}\cdot\mathbf{A}^{*}\cdot\mathbf{Q} + \mathbf{Q}\cdot\mathbf{Q}\cdot\mathbf{A}^{*} - \{(\mathbf{Q}\cdot\mathbf{Q}){:}\mathbf{A}^{*}\}\,\mathbf{I}\right]\right) + \\
& \frac{3}{U}\left[-\frac{2}{3}\beta\,\mathbf{H} - \beta\left\{\mathbf{H}\cdot\mathbf{Q} + \mathbf{Q}\cdot\mathbf{H} - \frac{2}{3}(\mathbf{H}:\mathbf{Q})\,\mathbf{I}\right\}\right] + \\
& \frac{3}{2U}\beta\left[(\mathbf{H}{:}\mathbf{Q})\,\mathbf{Q} + \mathbf{H}\cdot\mathbf{Q}\cdot\mathbf{Q} + \mathbf{Q}\cdot\mathbf{H}\cdot\mathbf{Q} + \mathbf{Q}\cdot\mathbf{Q}\cdot\mathbf{H} - \{(\mathbf{Q}\cdot\mathbf{Q}){:}\mathbf{H}\}\,\mathbf{I}\right] \\
& + \frac{3}{U}(\mathbf{H.Q} - \mathbf{Q.H}) + \frac{3}{R}\left[-\nabla^{*}\mathbf{Q}{:}(\nabla^{*}\mathbf{Q})^{T} - \frac{L_2}{L_1}(\nabla^{*}\cdot\mathbf{Q})\cdot(\nabla^{*}\mathbf{Q})^{T}\right]
\end{aligned}$$





LdG Nematorheology

LdG → LE

$$\alpha_1 = \bar{\eta}\left(2\nu_4^* S^2 - \beta^2 S^2 (\frac{8}{9} - \frac{8}{9} S + \frac{S^2}{12})\right)$$

$$\alpha_2 = \bar{\eta}\left(-S^2 - \frac{1}{3}\beta S(2 + S - \frac{S^2}{2})\right)$$

$$\alpha_3 = \bar{\eta}\left(S^2 - \frac{1}{3}\beta S(2 + S - \frac{S^2}{2})\right)$$

$$\alpha_5 = \bar{\eta}\left(\nu_2^* S + \frac{1}{3}\beta S(2 + S - \frac{1}{2}S^2) + \frac{1}{3}\beta^2 S(4 - S - S^2)\right)$$

$$\alpha_6 = \bar{\eta}\left(\nu_2^* S - \frac{1}{3}\beta S(2 + S - \frac{1}{2}S^2) + \frac{1}{3}\beta^2 S(4 - S - S^2)\right)$$

$$\alpha_4 = \bar{\eta}\left(\nu_1^* - \frac{2}{3}\nu_2^* S + \frac{1}{3}\nu_4^* S^2 + \frac{4}{9}\beta^2 (1 - S - \frac{S^2}{4})\right)$$

$$\lambda = \frac{\beta\left(4 + 2S - S^2\right)}{6\,S}$$

Trial by Fire

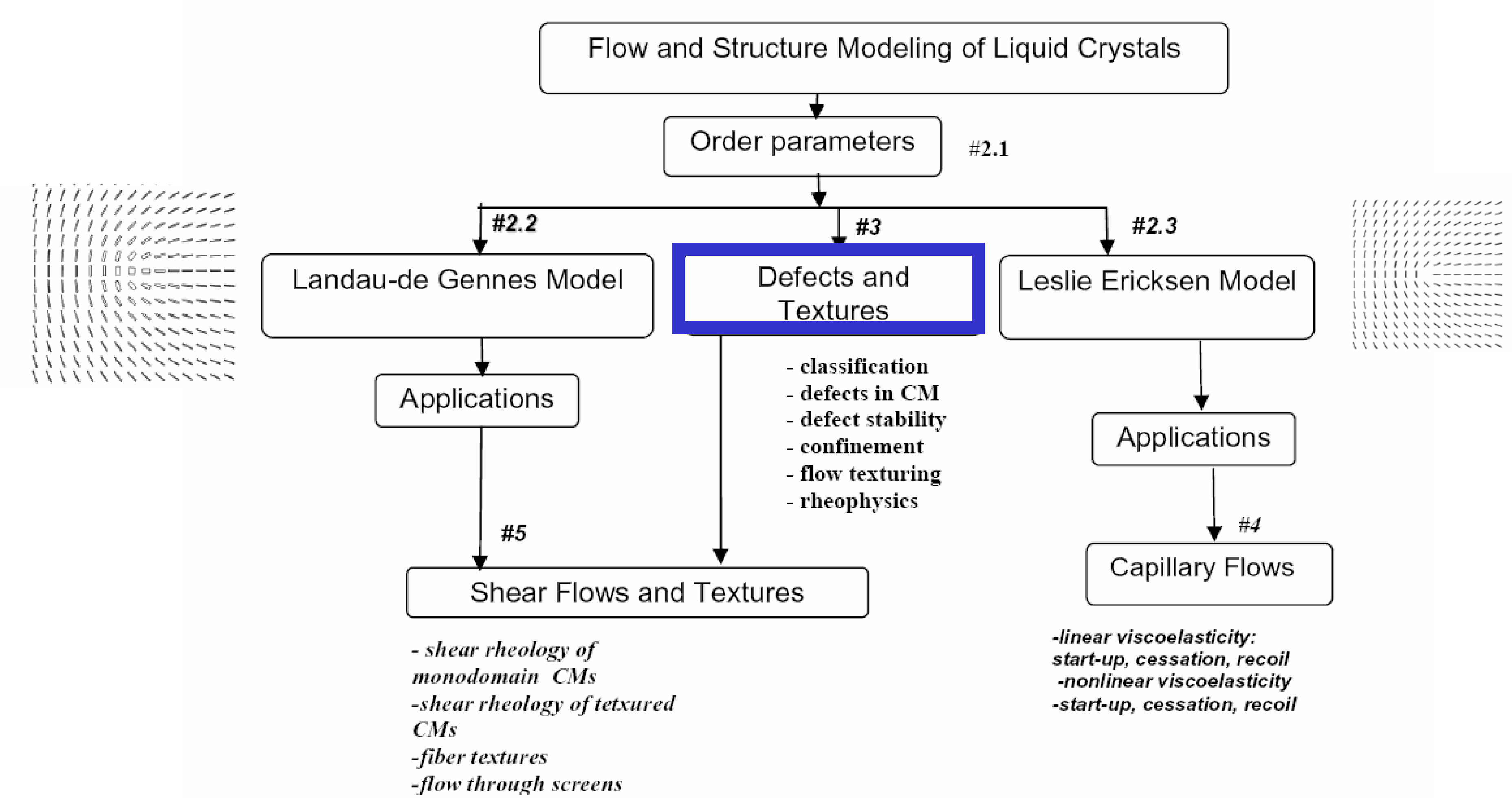
$$\eta_1 + \eta_2 + 8\eta_3 = C_1 + C_2\left(\eta_1 - \eta_2\right) \qquad 2.77 < C_2 < 3.84$$

Hess-Doi models respect reality only if λ<0 for rods!

$$C_2 = \frac{8\beta^2 + 16\nu_2^*}{\nu_2^* + 4\beta} \longrightarrow \lambda = \frac{\beta\left(4 + 2S - S^2\right)}{6\,S} > 0$$

69. M. Simoes, S.M. Domiciano, and F.S, Alves, Liquid Crystals, **33** (7) 849 (2006).
70. M. Simoes, S.M. Domiciano, Physical Review E, **68** , 011705 (2003).

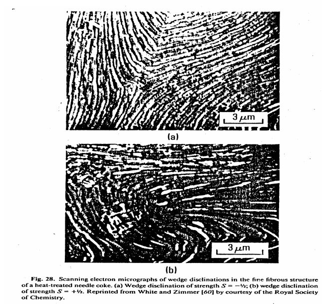
Flow-Modeling

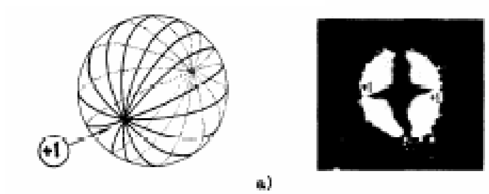


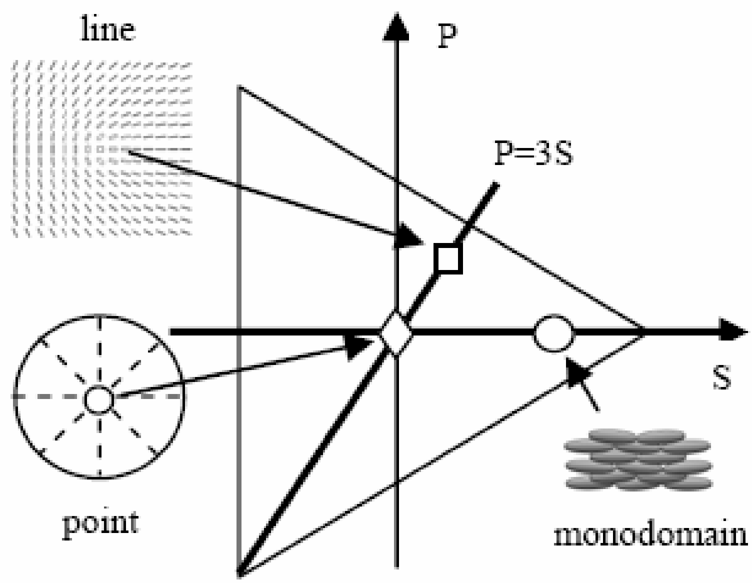
Topological Defects

$$\left(1-\frac{1}{3}U\right)\mathbf{Q}-U\mathbf{Q}\cdot\mathbf{Q}+U\left\{(\mathbf{Q}:\mathbf{Q})\mathbf{Q}+\frac{1}{3}(\mathbf{Q}:\mathbf{Q})\ \mathbf{I}\right\}=0$$

$$\mathbf{Q}=\mathrm{S}\left(\mathbf{nn}-\frac{\delta}{3}\right)+\frac{\mathrm{P}}{3}(\mathbf{mm}-\mathbf{ll})$$



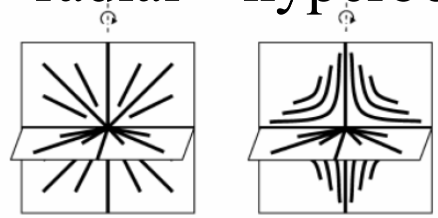


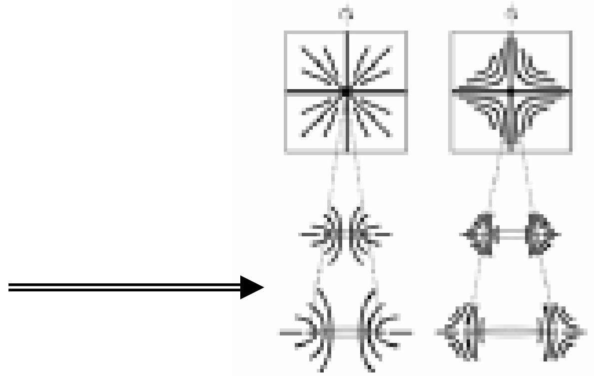


Point Defects

$$M_p = \left| \frac{1}{8\pi} \oiint d\mathbf{S} \cdot \boldsymbol{\varepsilon} : (\nabla \mathbf{n} \times \nabla \mathbf{n}) \cdot \mathbf{n} \right|$$

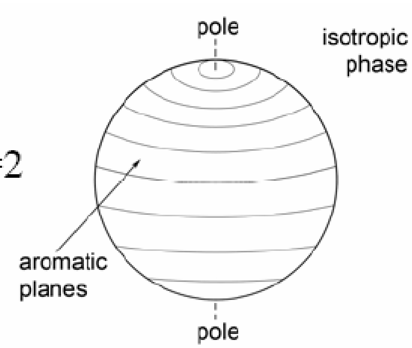
radial hyperbolic



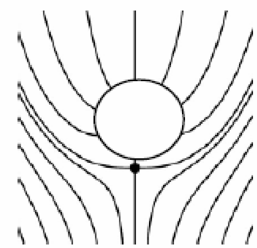


Brooks-Taylor Spherulites

$$\chi = \frac{1}{2\pi} \oiint \frac{1}{R^2} dS = 2$$



Micron-range Gas Bubbles



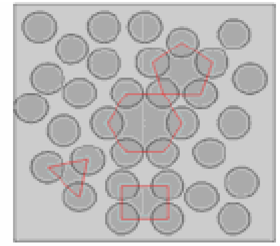
bubble-defect dipole:

d=1.2-1.5 R

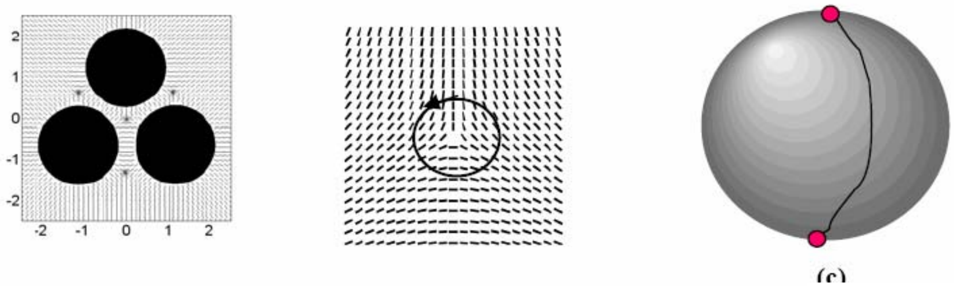
Disclination Lines in c/c Composites

Zimmer's Rule: $S = -(N-2)/2$ ⟵ Poincare theorem

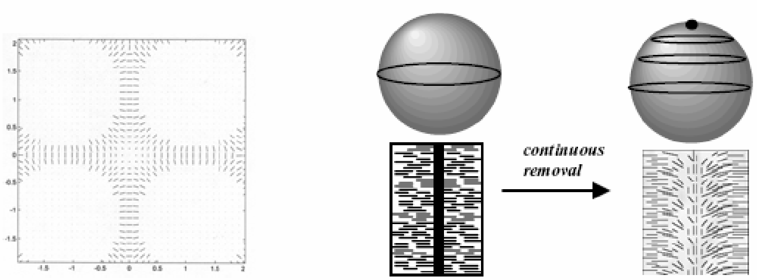
Fiber Array	Disclination strength	Core structure
Triangular	-1/2	Singular
Square	-1	Escape
Pentagonal	-3/2	Singular
Hexagonal	-2	Escape



singular core
(3,5,7..)

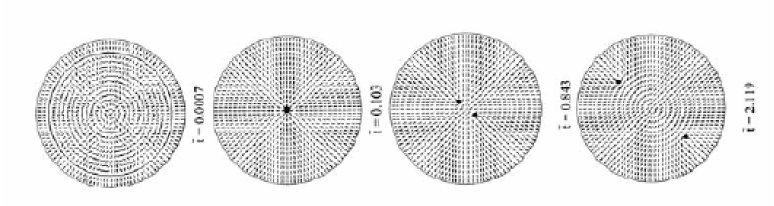


escape core
(4,6,..)

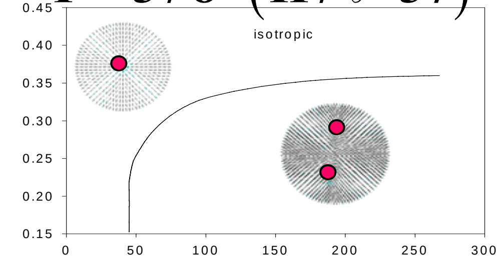


Defect-Defect Reactions

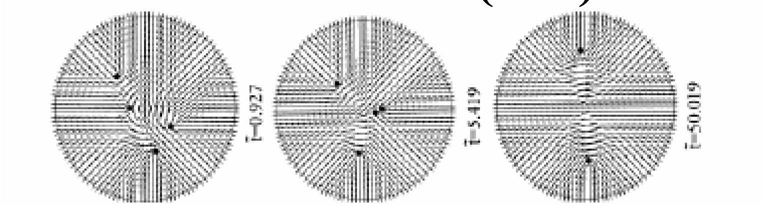
splitting: M=+1→ 2 M=+1/2



$$\tilde{T} = 3/8 - \left(H/\ell - 37\right)^{0.65}$$

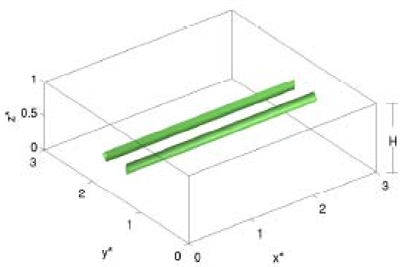


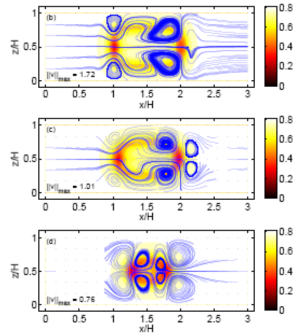
annihilation:1/2+(-1/2)=0



$$F \propto \frac{M_1 M_2}{d}$$

asymmetric annihilation with HI



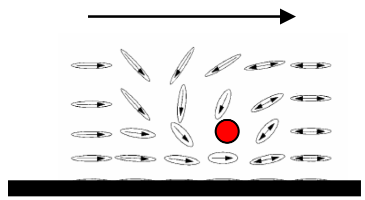


$$T_{ij}^{extra} = C_{ijkl} A_{lk} + D_{ijk} N_k$$

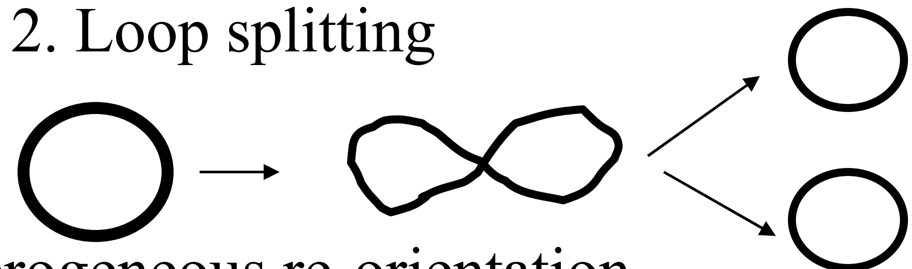
Defect Rheo-physics:Nucleation $|\lambda| > 1$

$$N \propto \sqrt{E - E_c} \Rightarrow \ell \propto \frac{1}{\sqrt{E - E_c}}$$

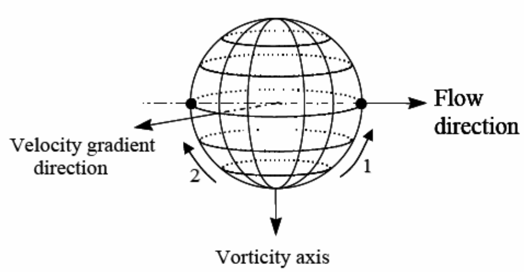
1. Frank-Reid loop emission

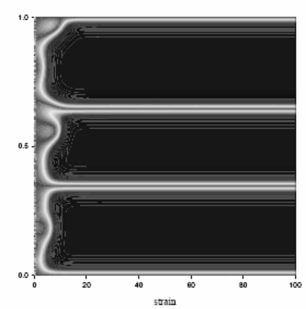


2. Loop splitting



3. Heterogeneous re-orientation

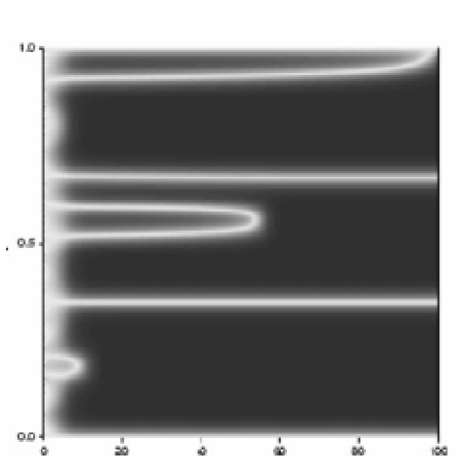


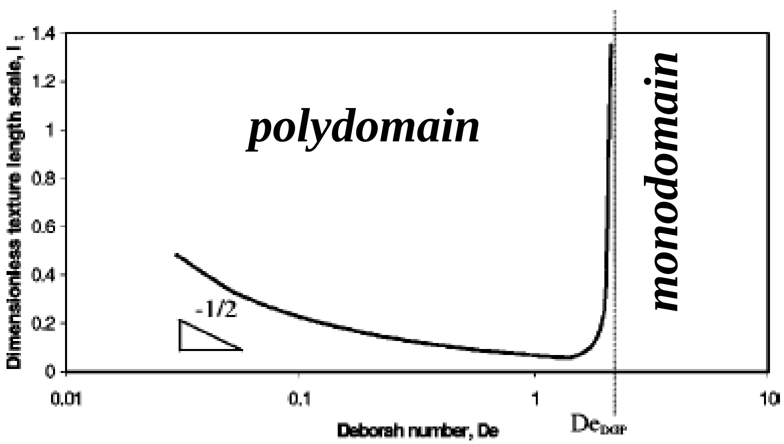


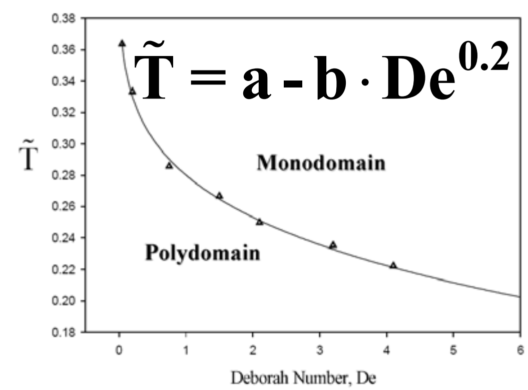
Defect Rheo-physics: Coarsening Rate f(De)

1. defect-interface annihilation

2. defect-defect annihilation





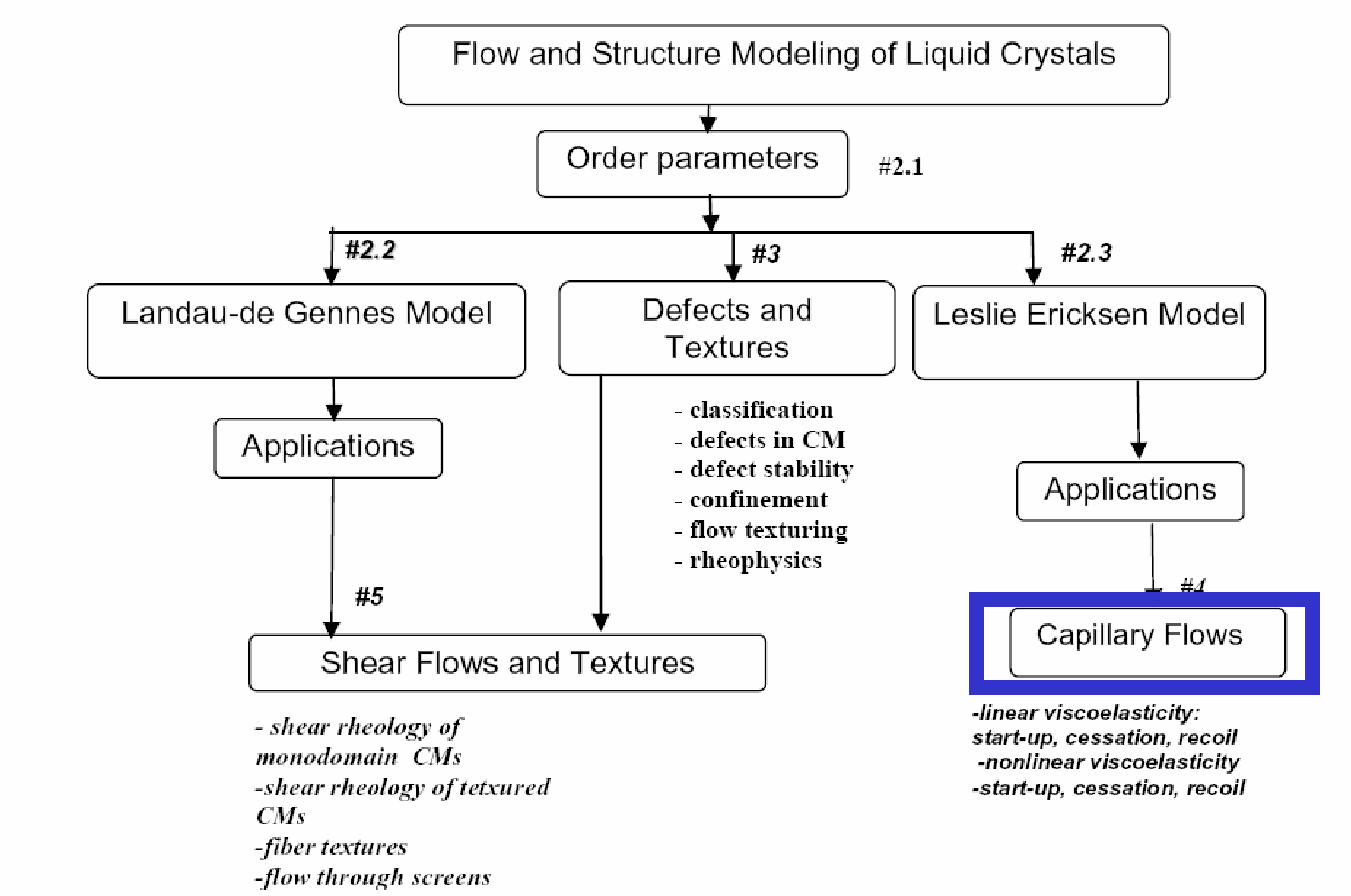


Materials Modeling Research Group

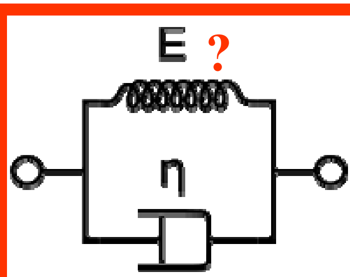
Outline

1. Introduction: Liquid crystals
2. Modeling Overview
3. Leslie-Ericksen Nematodynamics
4. Landau de Gennes Nematodynamics
5. Applications

Multiscale Flow-Modeling



MONOCRYSTAL LINEAR VISCOELASTICITY



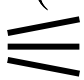
$$\boldsymbol{\tau} = \underbrace{\boldsymbol{\eta}(\mathbf{n}):\mathbf{A}}_{\text{viscous}} + \underbrace{\alpha_2 \mathbf{nN} + \alpha_3 \mathbf{Nn}}_{\text{visco-elastic}}$$

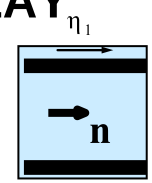
$\mathbf{A} = (\nabla \mathbf{v})^s$

$$\mathbf{N} = \boldsymbol{\omega}\text{-}\mathbf{w} = (\mathbf{I} - \mathbf{nn}) \cdot \left\{ \lambda (\mathbf{A}.\mathbf{n}) - \frac{\delta F}{\delta \mathbf{n}} \right\}$$

SPLAY

$$\alpha_3 = (1-\lambda)\frac{\gamma_1}{2}$$

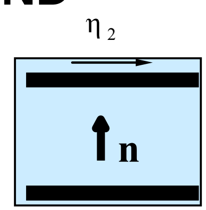




$$\begin{cases} \tau = \eta_1 \dot{\gamma} + \alpha_3 \dot{\theta}, \\ \gamma_1 \dot{\theta} = K_{11} \dfrac{\partial^2 \theta}{\partial y^2} - \alpha_3 \dot{\gamma} \end{cases}$$

BEND

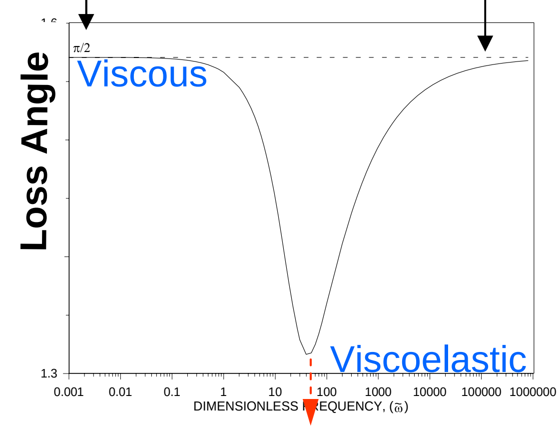
$$\alpha_2 = -(1+\lambda)\frac{\gamma_1}{2}$$



$$\begin{cases} \tau = \eta_2 \dot{\gamma} + \alpha_2 \dot{\theta}, \\ \gamma_1 \dot{\theta} = K_{33} \dfrac{\partial^2 \theta}{\partial y^2} - \alpha_2 \dot{\gamma} \end{cases}$$

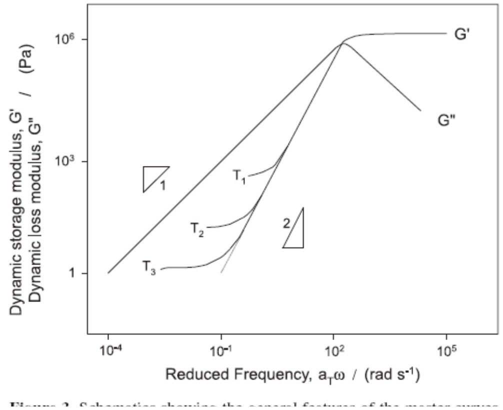
$\dot{\theta} = 0$

$\dfrac{\partial^2 \theta}{\partial y^2} = 0$

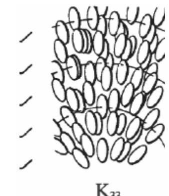


Polycrystal Linear Viscoleasticity: G’ and G”

$$\Delta = \mathbf{T}^s : \mathbf{A} - \frac{\delta F}{\delta \mathbf{n}} : \left(\frac{d\mathbf{n}}{dt} \right)$$



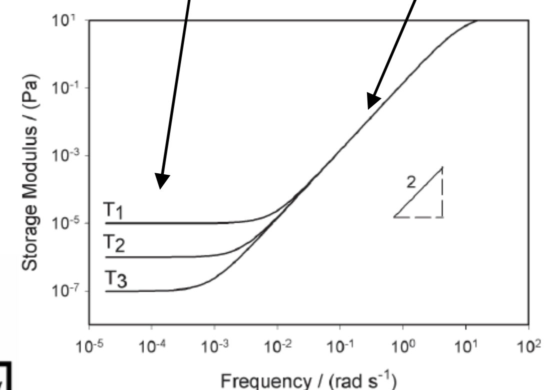
24. Sakai, M.; Sato, Y.; Inagaki, M.; *Carbon’90: Extended Abstracts and Program – International Carbon Conference*, Paris, 1990, p. 298.
25. Hara, R.; *Carbon’90: Extended Abstracts and Program – International Carbon Conference*, Paris, 1990, p. 290.

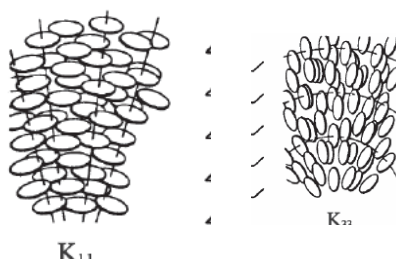


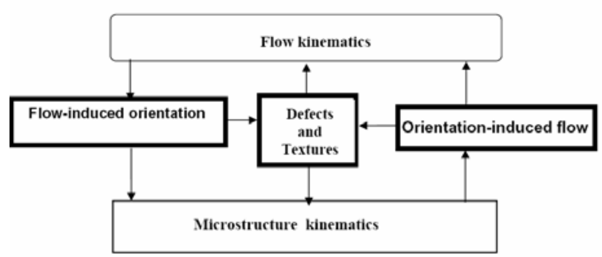
$$\tilde{G}'(\tilde{\omega},\mathbf{n},T) = \frac{P_1 U_2(\tilde{\omega})}{U_2(\tilde{\omega})^2 + \left(P_2 - U_1(\tilde{\omega})\right)^2}\,\tilde{\omega}$$

$$\tilde{G}''(\tilde{\omega},\mathbf{n},T) = \frac{P_1\left(P_2 - U_1(\tilde{\omega})\right)}{U_2(\tilde{\omega})^2 + \left(P_2 - U_1(\tilde{\omega})\right)^2}\,\tilde{\omega}$$

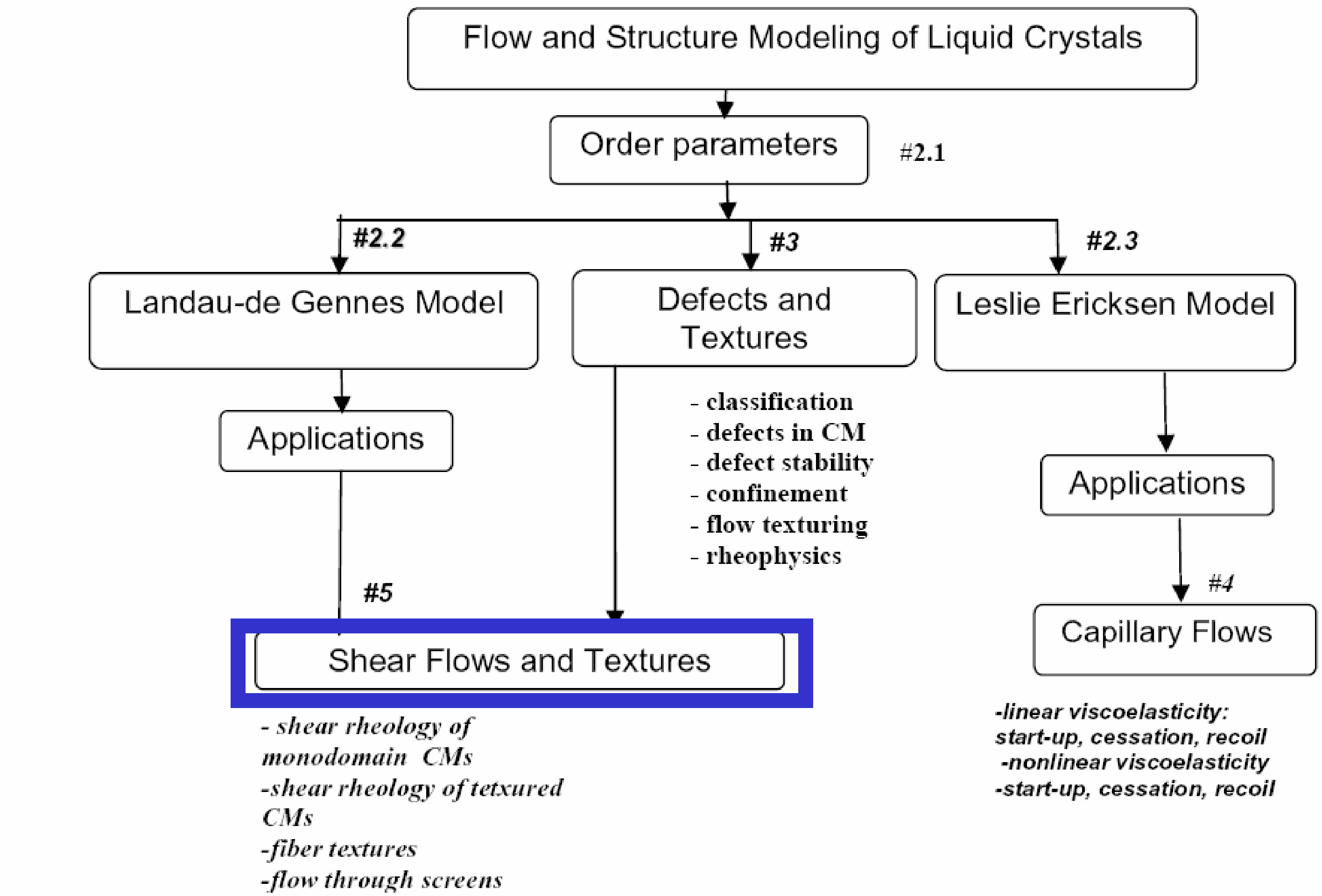
$$G'_{texture} = \varphi_{splay} G'_{splay} + G'_{bend}\,\varphi_{bend} + G'_{defect}$$



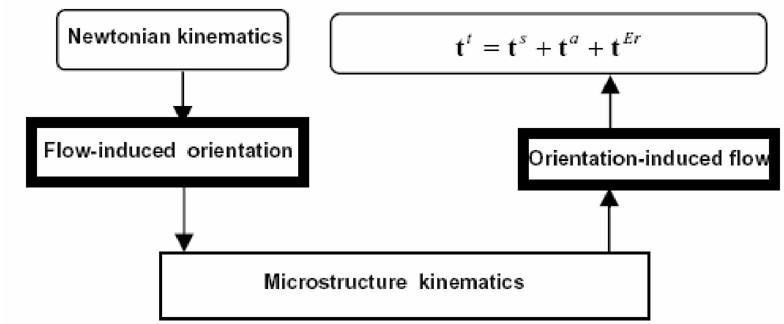




Multiscale Flow-Modeling

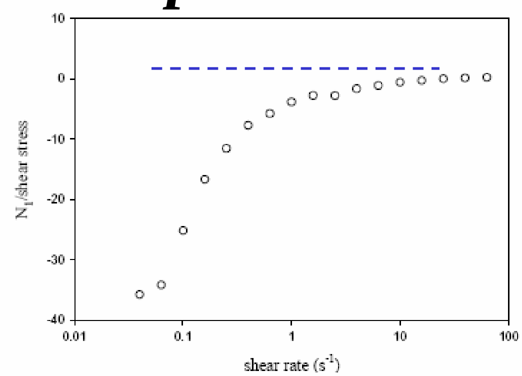


Monodomain Shear Rheology of CMs

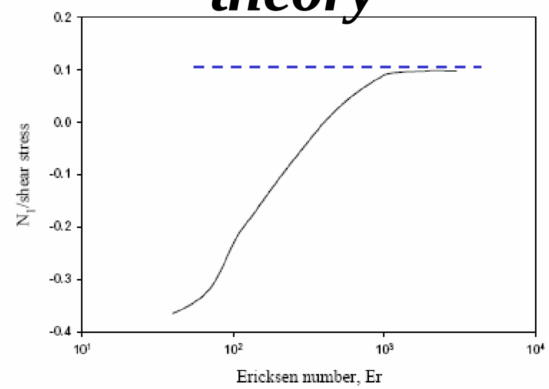


$$\begin{pmatrix}\mathbf{T}^{s}\\ \hat{\mathbf{Q}}\end{pmatrix} = \begin{pmatrix} \mathbf{a} & -\beta \\ \beta & \mathbf{c}\end{pmatrix} \otimes \begin{pmatrix}\mathbf{A}\\ \mathbf{H}\end{pmatrix}$$

experiments



theory



(b)

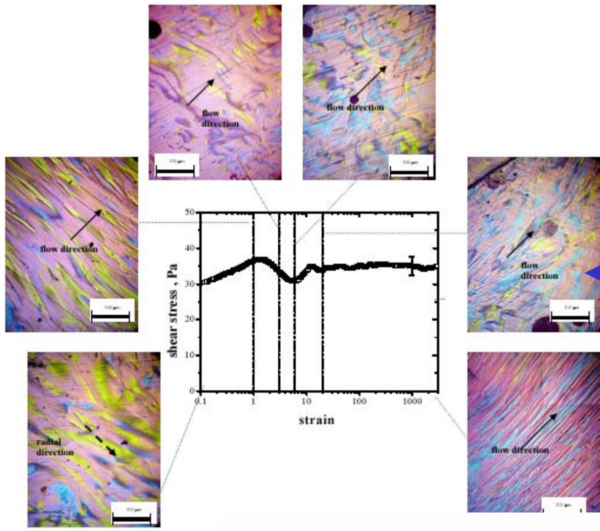
$$\left.\frac{N}{t_{xy}}\right|_{\text{flow-alignment}} = \frac{\dfrac{\sqrt{\lambda^2-1}}{2\lambda}\left(\gamma_2 - \dfrac{\alpha_1}{\lambda}\right)}{\dfrac{1}{2}(\eta_1+\eta_2-\gamma_1)+\dfrac{\alpha_1}{2}\left(\dfrac{\lambda^2-1}{\lambda^2}\right)} \longrightarrow \lambda = \frac{\beta\left(4+2S-S^2\right)}{6\,S} < -1$$

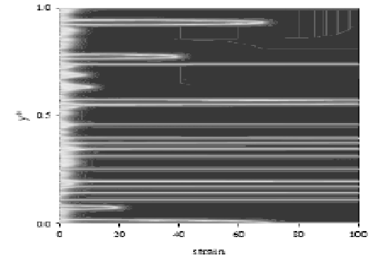
Materials Modeling Research Group

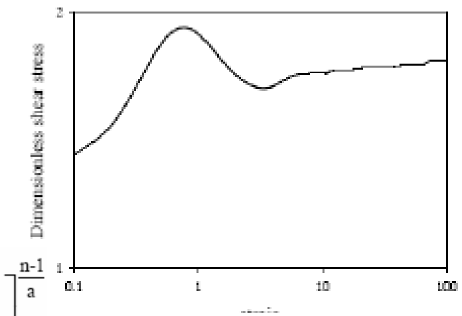
Shear Flow-Alignment and Texturing

Experiments | **Simulations**

transient

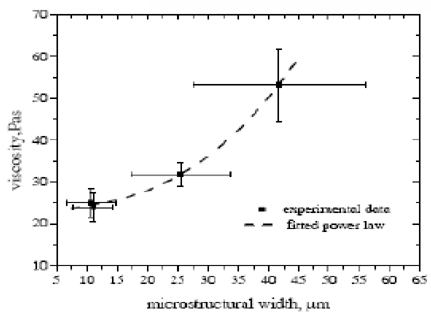


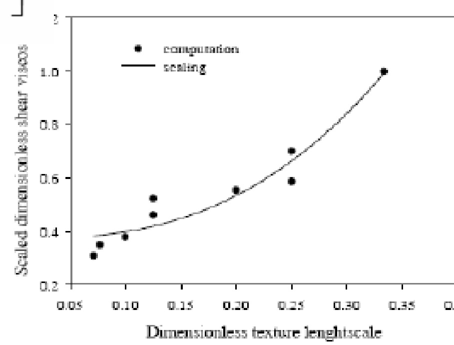




$$\eta_s = \frac{\eta-\eta_{al}}{\eta_0-\eta_{al}} = cl_t^{\,2(1-n)}\left[(cl_t)^{2a} + \left(\tau H^2 + (cl_t)^2\,\tau Er_{ADL}\right)^a\right]^{\frac{n-1}{a}}$$

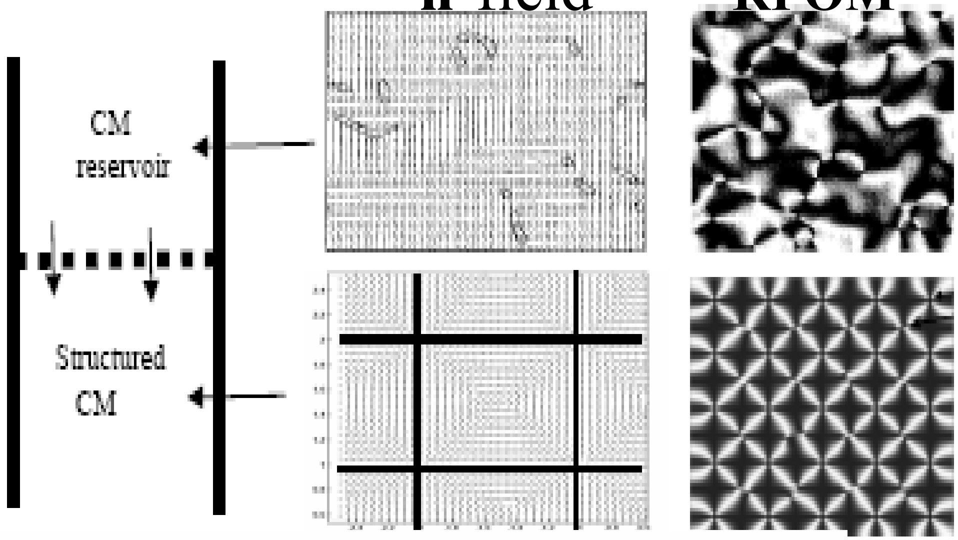
steady



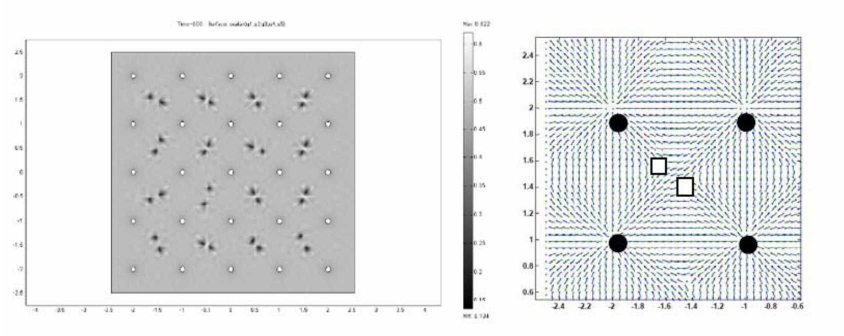


Structuring by Flow Through Screens

Nucleation of Disclination Lattices



Experiments



$$Charge = (+1/4)\times 4 + (-1/2)\times 2$$

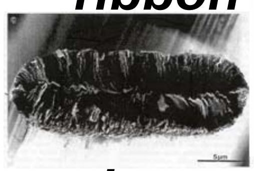
Fiber Texture Engineering

Heat transfer appl.

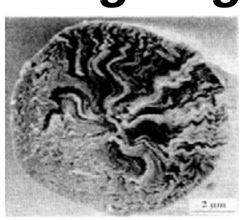
circular

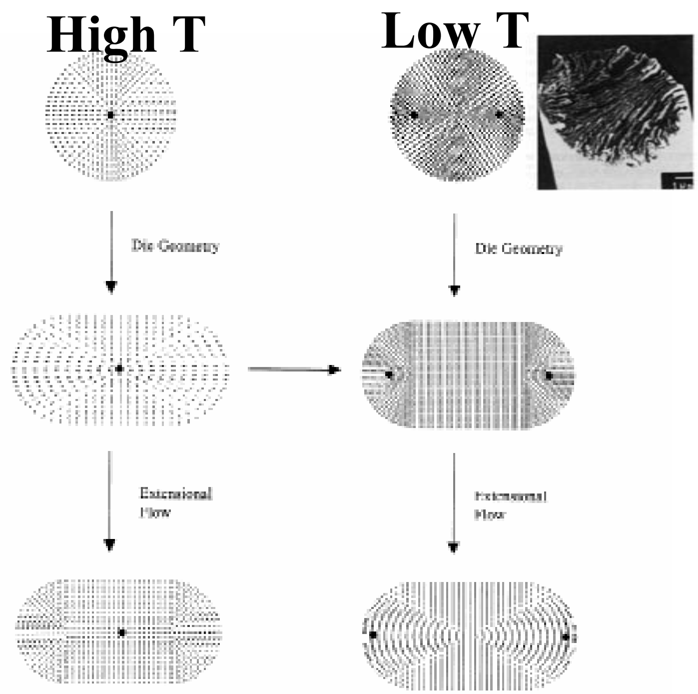
ribbon

ribbon

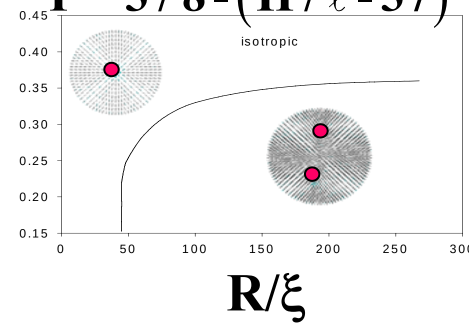


Zig-Zag

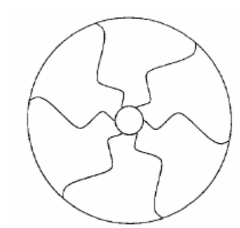


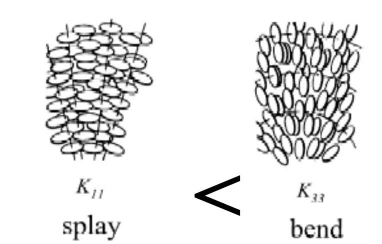


$$\tilde{T} = 3/8 - \left(H/\ell - 37\right)^{0.65}$$



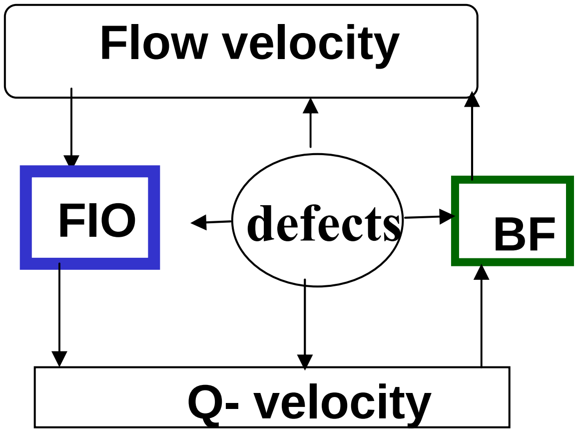
$$\mathbf{A} = \begin{bmatrix} -\frac{1}{2}\dot{\varepsilon}(1+b) & 0 & 0 \\ 0 & -\frac{1}{2}\dot{\varepsilon}(1-b) & 0 \\ 0 & 0 & \dot{\varepsilon} \end{bmatrix}$$



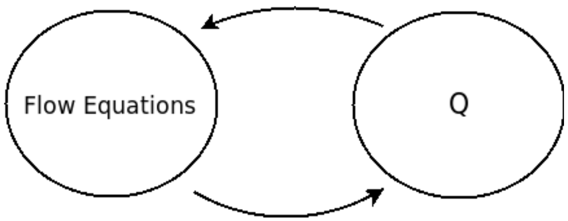


elastic instability

Computational Textured Nematodynamics



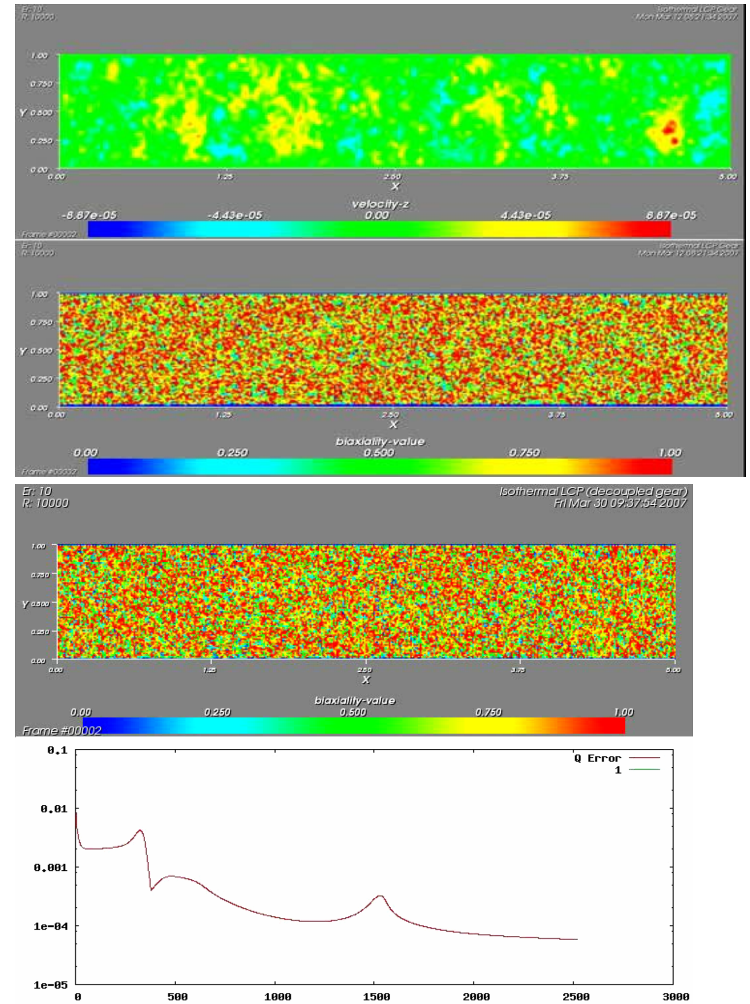
Numerical Scheme



$$-\nabla \cdot (\nabla v + \nabla v^T) + \nabla p + (1-\alpha)\nabla \cdot (G + G^T) = \nabla \cdot \tau_{LCP}$$

where $\tau_{\mathrm{LCP}} = \tau_{total} - \alpha(G + G^T)$ and $0 \le \alpha \le 1$

$$\nabla \cdot v = 0 \qquad G - \nabla v = 0$$



Materials Modeling Research Group

Outlook

Models

- Need further development in molecular models to remove current inconsistencies in fitting shear viscosities
- Further develop interfacial and contact line nematodynamics
- Stress boundary conditions for outflows
- Incorporate couple stresses

Computation

- Multiscale multidimensional DNS
- Resolve banded texture enigma