MESOSCALE DESCRIPTION OF DEFECTED MATERIALS

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Linear bubble model of abnormal grain growth

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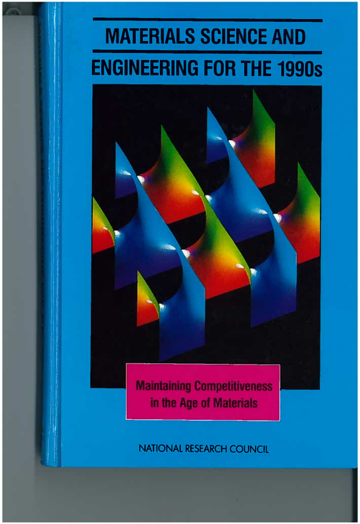
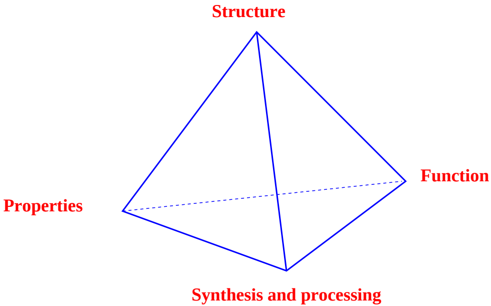
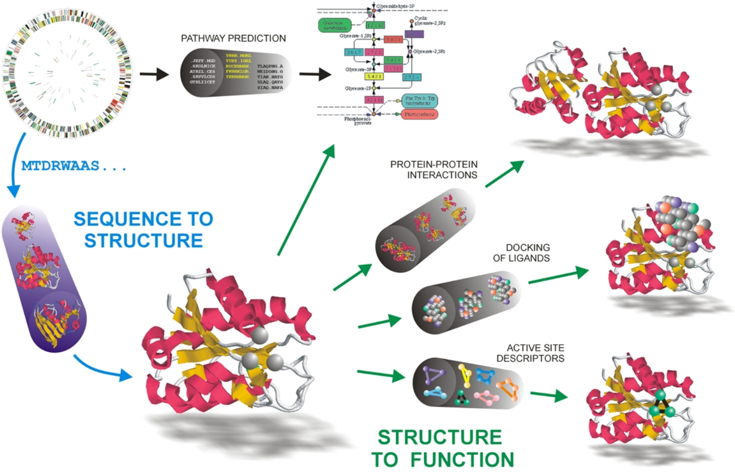
MATERIALS





[Materials Science and Engineering for the 1990s. National Research Council, 1989]

GENOMICS


PATHWAY PREDICTION
MTDRWAAS . . .
SEQUENCE TO
STRUCTURE
PROTEIN-PROTEIN
INTERACTIONS
DOCKING
OF LIGANDS
ACTIVE SITE
DESCRIPTORS
STRUCTURE
TO FUNCTION

THEMES

1. Nonequilibrium Phenomena

- Structure/properties depend on processing. Materials used under external, changing stresses.
- Nonlinearity.
- Phase diagrams, empirical correlations, etc. not sufficient. E.g., microstructure evolution.

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2. Multiple Scales

Science based on a collection of "Laws":

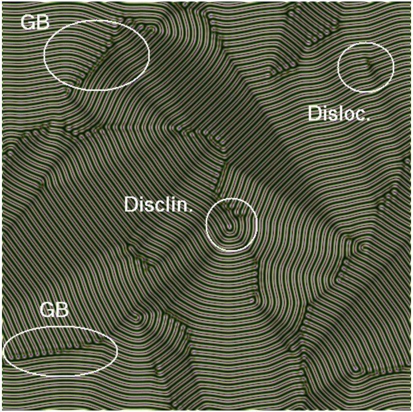
Microscopic Laws

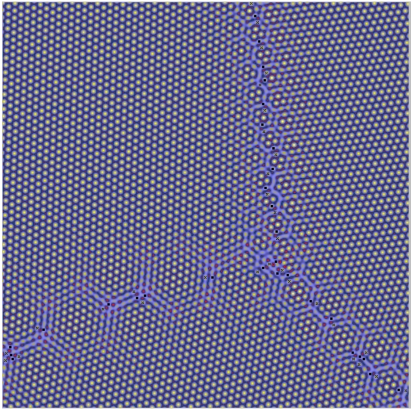
Mesoscopic Lawlessness
(cf. R. Laughlin)

Macroscopic Laws

Small but finite wavenumber and finite frequency ("mesoscale") response functions and transport coefficients are correlation functions.

MICROSTRUCTURE EVOLUTION



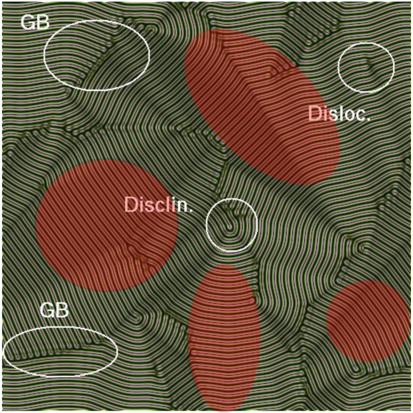


- Large gradients (locally) - not close to equilibrium, but very slow on a molecular scale.
- Large numbers of interacting defects: microstructure.
- Possible persistent dynamics.

ORDER PARAMETER DESCRIPTION

Non equilibrium configurations

- Multiple, locally ordered domains coexist
- Domains are degenerate by symmetry
- Complex boundary regions between domains: defects



Need:

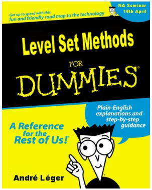
- a measure of local order,
- that is slowly varying in space,
- that accommodates boundary regions and defects.

$\longrightarrow$ an indicator function or phase field.

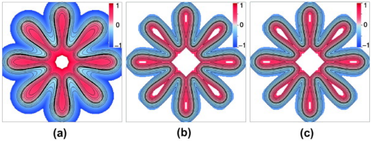
Physically: an order parameter.

Level Set methods

[S. Osher and J. Sethian, J. Comp. Phys. 79, 12 (1988)]



- Domain interfaces defined as a given value (level) of a continuous field defined everywhere.
- Equations of motion for the field

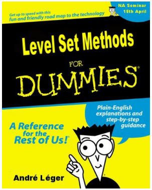


[D. Hartmann, M. Meinke, W. Schröder, J. Comp. Phys. 229, 1514 (2010)]

BOUNDARY TRACKING

Level Set methods

[S. Osher and J. Sethian, J. Comp. Phys. 79, 12 (1988)]



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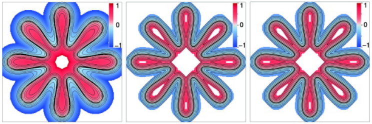


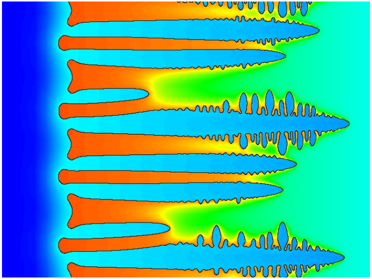
(a) (b) (c)

[D. Hartmann, M. Meinke, W. Schröder, J. Comp. Phys. 229, 1514 (2010)]

Phase field methods

[G. Caginalp and P. Fife, Phys. Rev. B 33, 7792 (1986)]

- Developed for solidification problems.
- A "phase" or indicator function labels domains occupied by either phase.
- Limit of small boundary thickness reduces to classical problem plus boundary conditions. Surface tension introduced into the phase field description



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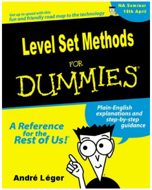

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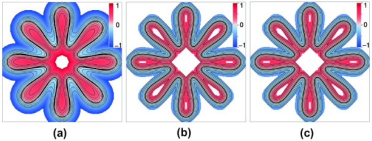

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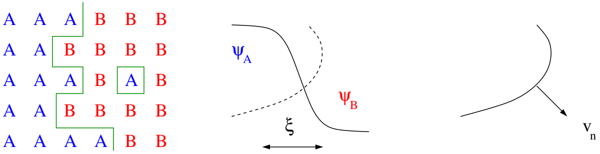
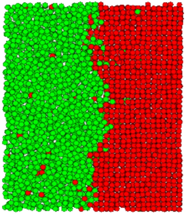
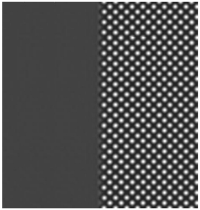
MESOSCALE DESCRIPTION



Microscopic Mesoscopic Macroscopic



[Peter Voorhees et al.]



[Ken Elder et al.]

- Microscopic (e.g., MD). Accurate to small time/length scales.
- Mesoscopic. Coarse grain down to (or above) thermal correlation length.
- Macroscopic. Linear thermodynamics, moving boundary problem.

COARSE GRAINING - TOP TO BOTTOM

Macroscopic - local equilibrium

- Local equilibrium, including order parameter ψ (symmetry breaking).
- Thermodynamics forces linear in gradients.
- Boundary conditions at dividing surfaces.

Moving boundary problem (e.g., grain growth)

Mesoscopic: density functionals with local gradients

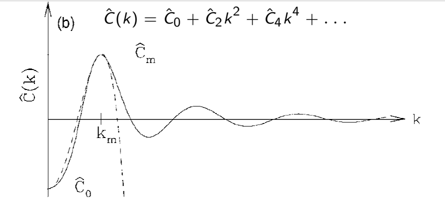
$$\beta F = \int d\mathbf{x} f\,[\psi, \nabla\psi]$$

Local equilibrium does not hold.

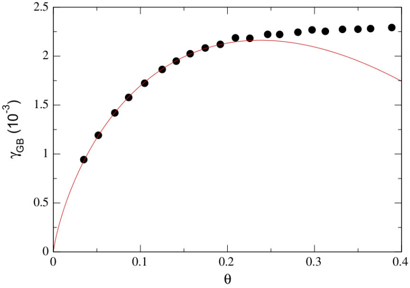
$df = \ldots + \xi_i d(\partial_i \psi)$

Mesoscopic: density functionals, correlation functions

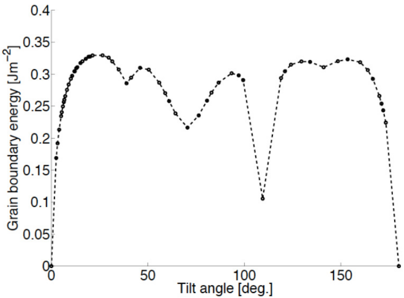
$$\beta F = \int d\mathbf{x} f\,[\psi] + \int d\mathbf{x} \int d\mathbf{x}' \psi(\mathbf{x}) C(\mathbf{x}, \mathbf{x}') \psi(\mathbf{x}')$$



DEFECT STRUCTURE AND ENERGETICS

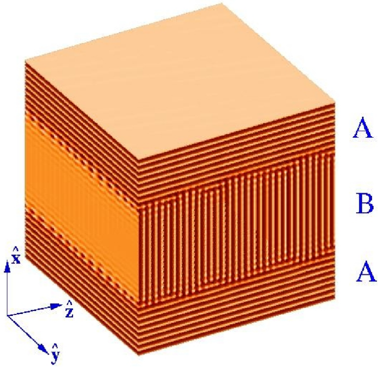


Comparison to Read-Shockley relation [K.-A. Wu and P. Voorhees. Acta mater. 60, 407 (2012)]



BCC Fe. [A. Jaatinen, V. Achim, K. Elder, and T. Ala-Nissila. Phys. Rev. E 80, 031602 (2009)]. Agrees well with MD simulations.

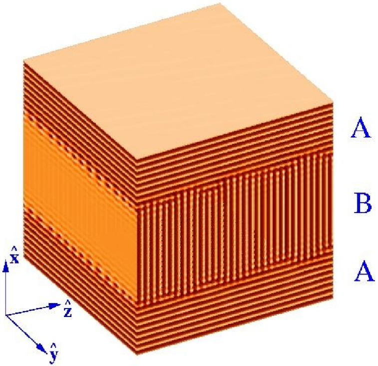
DEFECT KINETICS (MESO/MACRO)



$$\psi = Ae^{ik_0 x} + Be^{ik_0 z} + \mathrm{c.c.}$$

$$\frac{\partial A}{\partial t} = -\frac{\delta F[A,B]}{\delta A^*} \quad \frac{\partial B}{\partial t} = -\frac{\delta F[A,B]}{\delta B^*}$$

DEFECT KINETICS (MESO/MACRO)



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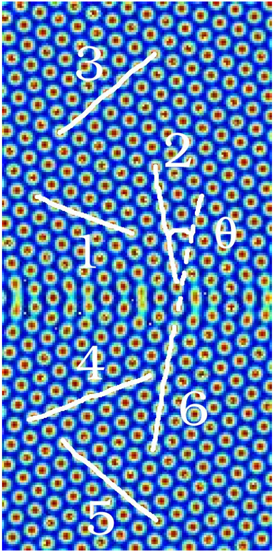
$$v_{gb}(t) = \left(\frac{\xi_0^2}{4k_0^2} q^4\right) \frac{(\epsilon/4)[k_0 \delta x_{gb}(t)]^2}{\int_{-\infty}^{\infty} dx\,[(\partial_x A_0)^2 + (\partial_x B_0)^2]}$$

$$v_{gb}(t) = \text{Mobility} \times \begin{matrix}\text{Time} & \text{dependent} \\ \text{driving} & \text{force}\end{matrix}$$

DEFECT KINETICS (MESO)



$$v_{gb}(t) = M\Delta f - \frac{p_{act}}{D} \sin\left[2k_0 x_{gb}(t) \sin(\theta/2)\right]$$

with (Peierls stress)

$$p_{act} \sim A_0^4 e^{-2ak_0 \sin(\theta/2)\xi}.$$

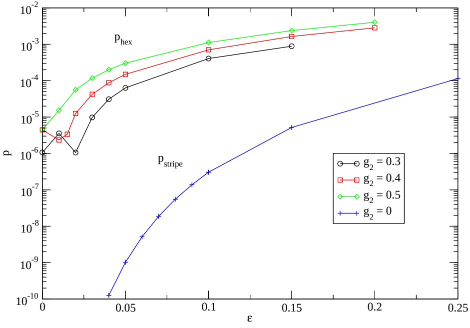
Supercritical (second order)

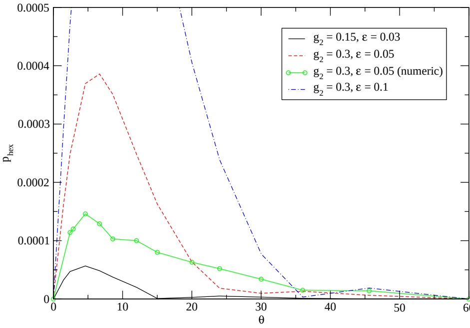
$$\xi \sim 1/\sqrt{\epsilon} \quad p_2 \sim e^{-1/\sqrt{\epsilon}} \rightarrow 0.$$

Subcritical (first order)

$$\xi \rightarrow \xi_0 = \frac{15\lambda_0}{8\sqrt{6}\pi g_2} \quad \text{finite.}$$

AMPLITUDE OF PINNING FORCE





Ferroelectric domain switching

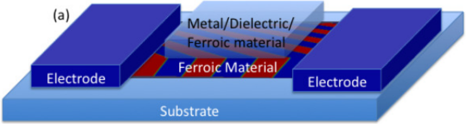
K. Ashraf and S. Salahuddin,

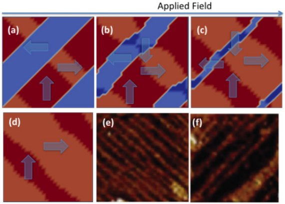
arXiv:1202.6116v1

Order parameters $\{\mathbf{P}, \epsilon_{ij}\}$, local polarization and strain field.

$$F = F\left[\mathbf{P}, \nabla \mathbf{P}, \epsilon_{ij}\right] - \mathbf{E} \cdot \mathbf{P}$$

$$\frac{\partial \mathbf{P}}{\partial t} = -\frac{\delta F}{\delta \mathbf{P}} + \xi(\mathbf{x}, t)$$





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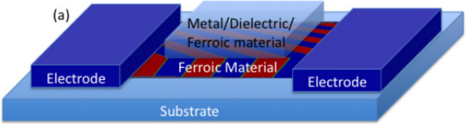
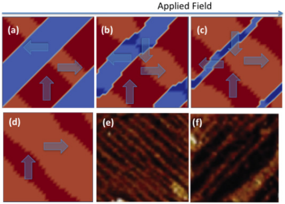


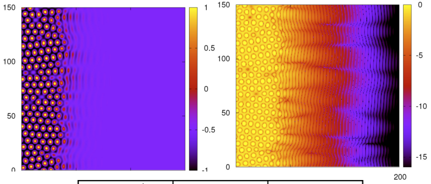


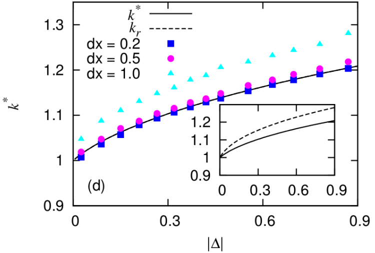
Wavelength selection in solidification

A. Archer, M. Robbins, U. Thiele, E. Knobloch, arXiv:1206.0902v1

Order parameter $\rho(\mathbf{x}, t)$, density.

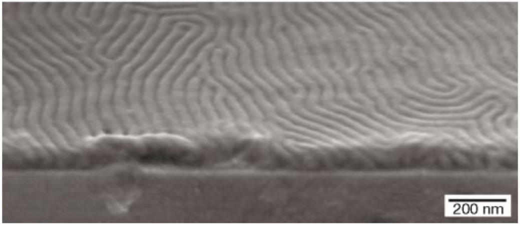
$$\frac{\partial \rho}{\partial t} = D\nabla^2\rho - \rho_0 D\nabla^2 \int d\mathbf{x}'\, C_2(|\mathbf{x}-\mathbf{x}'|)\rho(\mathbf{x}', t)$$



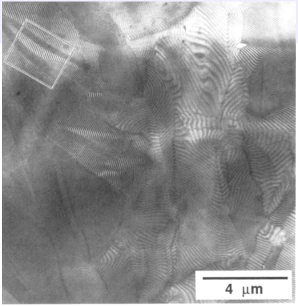


REVERSIBLE/HAMILTONIAN MODES

Block Copolymers

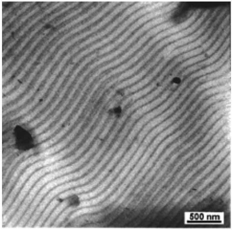


[Kim, ..., de Pablo, Nealy, 2003]



[Gido and Thomas, 1994]

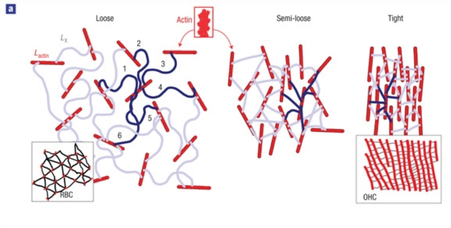
[Forster et al. 2001]



Amphiphilic systems

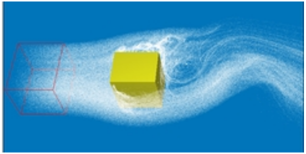
Liquid crystalline elastomers

[Dalhaimer, Discher, Lubensky, 2007]



MESOSCOPIC REVERSIBLE STRESSES

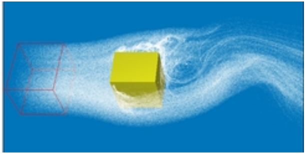
NORMAL FLUID



- Local equilibrium in the rest frame,
  $s = s(u, \rho) \quad T\frac{ds}{dt} = \frac{du}{dt} + p\frac{d1/\rho}{dt}$
- Conservation laws (e.g., momentum density $\mathbf{g} = \rho\mathbf{v}$)
  $$\partial_t g_i = -\partial_j \sigma_{ij}$$
- Reversible stress: $\sigma_{ij}^R = \rho v_i v_j + p\delta_{ij}$

MESOSCOPIC REVERSIBLE STRESSES

NORMAL FLUID



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CAHN-HILLIARD FLUID

[M. Gurtin, D. Polignone, JV, Math. Models and Meth. Appl. Sci. 6, 816 (1996)]

$$s = s(u, \rho, \psi, \partial_i \psi)$$

$$\sigma_{ij}^R = \rho v_i v_j + p\delta_{ij} - \frac{\partial s}{\partial(\partial_i \psi)} \partial_j \psi$$

needed so that advection of ψ does not cause entropy production.

GENERAL CASE

Reversible motion requires (Maxwell type relation)

$$\frac{\partial \dot{\psi}}{\partial v_i} = \frac{\partial \dot{g}_i}{\partial\left(\partial_j \xi_j\right)} \qquad \xi_j = \frac{\partial s}{\partial(\partial_j \psi)}$$

If ψ has a reversible current $\partial_t \psi + \mathbf{v} \cdot \nabla \psi = \ldots \ \frac{\partial \dot{\psi}}{\partial v_i} = -\partial_i \psi$ and non classical stresses result.

MESOSCOPIC DISSIPATIVE STRESSES

$$T\dot{S}_{prod} = \int d\vec{r} \left\{ -\left(J_i^{\psi} - v_i\psi\right)\partial_i\mu + \left(\sigma_{ij} - \sigma_{ij}^{R}\right)\partial_i v_j \right\}$$

Broken Symmetry incorporated in dissipative fluxes.

cf. [P. Martin, O. Parodi, P. Pershan, Phys. Rev. A 6, 2401 (1972)]

MESOSCOPIC DISSIPATIVE STRESSES

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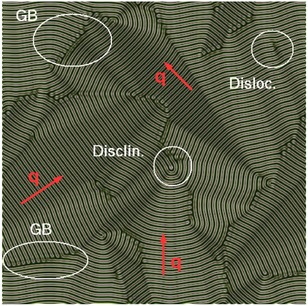


Lamellar phase: uniaxial fluid

$$\begin{aligned} J_i^{\psi\ D} &= -\left[\Lambda_L q_i q_j + \Lambda_T(\delta_{ij} - q_i q_j)\right]\partial_j\mu \\ \sigma_{ij}^{D} &= \alpha_1 q_i q_j q_k q_l D_{kl} + \alpha_4 D_{ij} \\ &\quad +\alpha_{56}\left(q_i D_{kj} + q_j D_{ki}\right) q_k \end{aligned}$$

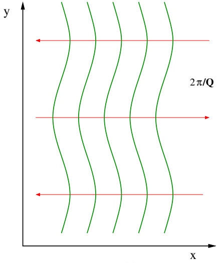
$$D_{ij} = \partial_i v_j + \partial_j v_i$$

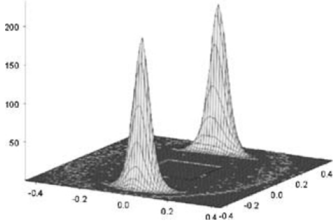
Cahn-Hilliard (isotropic) fluid

$$\begin{aligned} J_i^{\psi\ D} &= -\Lambda q^2 \partial_i\mu \\ \sigma_{ij}^{D} &= \alpha_4 D_{ij} \end{aligned}$$

TA

REVERSIBLE MODES AND LINEAR RESPONSE





[L. Wu, T. Lodge, F. Bates, J. Rheol. 49, 1231 (2005)]

Characteristic decay times determined by decay of transverse perturbations.

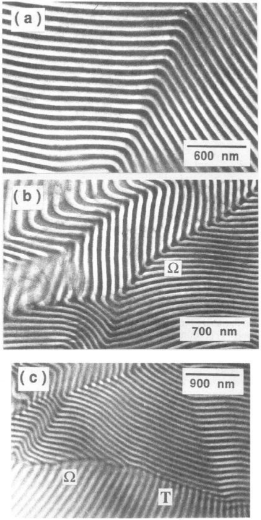
Transverse scattering intensity,

$$S(Q) = \frac{k_B T/\xi}{Q^4 + 2(Q/\lambda)^2}$$

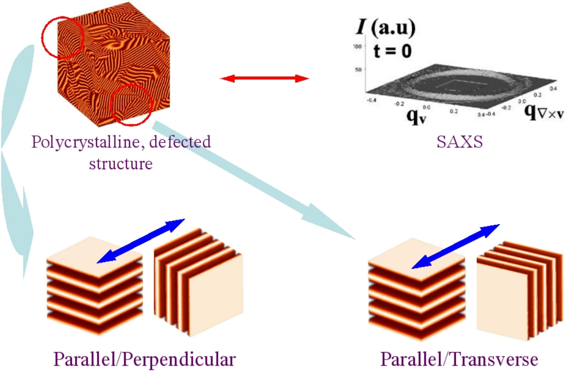
For a block copolymer in weak segregation,

$$\lambda \sim \frac{R_g N^{1/4}}{\sqrt{\epsilon}} \gg k_0^{-1}$$

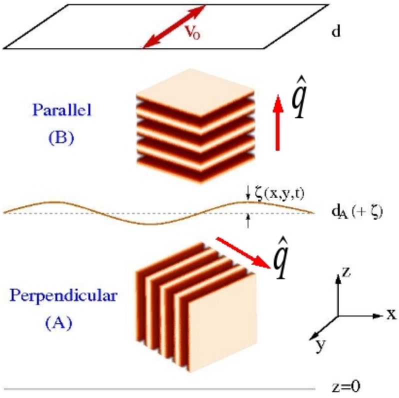
DOMAIN COARSENING AND ORIENTATION SELECTION



[S. Gido, E.L. Thomas, Macromolecules 27, 6137 (1994).]



RHEOLOGY AND ORIENTATION SELECTION



- In this low frequency formulation, both orientations are degenerate.

- Uniaxial form of dissipative stress leads to viscosity contrast. Hydrodynamic instability under shear.

- . Extended to uniaxial viscoelasticity. Hydrodynamic instability under shear when viscoelastic contrast is appreciable.

SUMMARY

1. Microscopic Laws

Mesoscopic Lawlessness
(cf. R. Laughlin)

Macroscopic Laws

2. Finite wavenumber and finite frequency response functions and transport coefficients are correlation functions.

3. Short scale energetics and kinetics entirely phenomenological. Nonlinearities also phenomenological.

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1. Naturally accommodates microstructure and evolution.

2. Quite efficient computationally.