TOPOLOGICAL DEFECT MOTION AND DOMAIN COARSENING IN MESOPHASES

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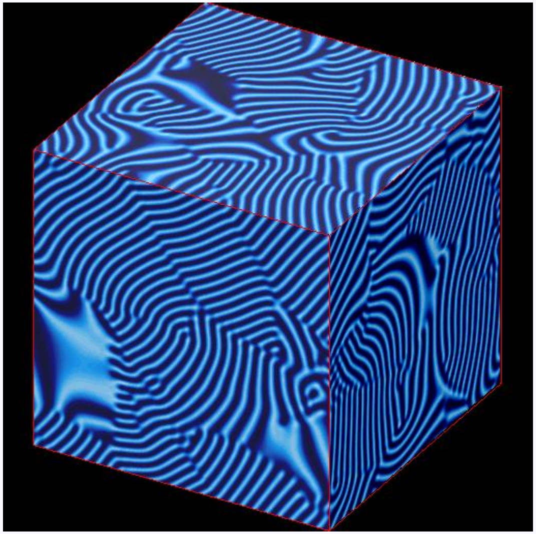
1. Topological defects in smectic and hexagonal mesophases.
2. Long wavelength description of defect motion.
3. Domain coarsening.
4. Non-adiabatic effects and pinning.
   - Supercritical bifurcation to a lamellar phase (smectic symmetry).
   - Subcritical bifurcation to a hexagonal phase (crystalline symmetry).



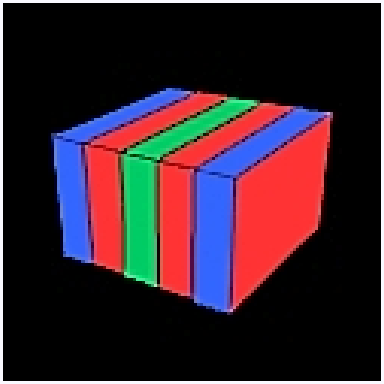
With Denis Boyer

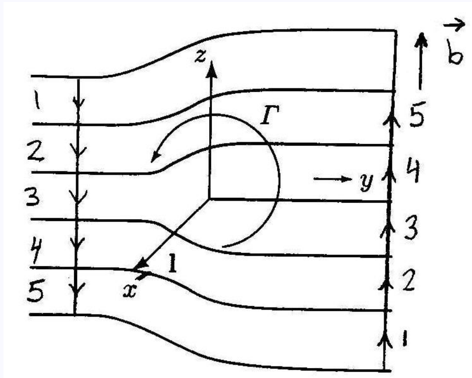
RELAXATION OF MESOPHASES

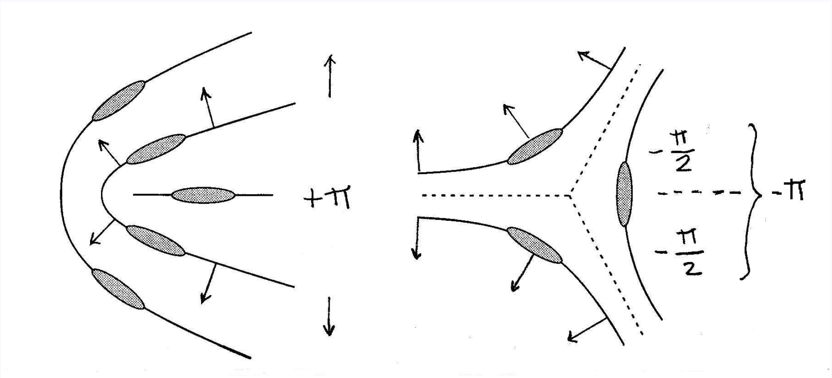
- Decay controlled by the relaxation of the longest lived modes - topological defects.
- Interaction and collective motion of topological defects (dislocations, disclinations, and grain boundaries) in macroscopically disordered structures.
- Long wavelength description of defect motion and microstructure coarsening.
  - In a block copolymer, only diffusive relaxation of monomer concentration (no chain dynamics).
- Absence of nonvariational terms (sufficiently close to threshold).
  - In a block copolymer, no flow.

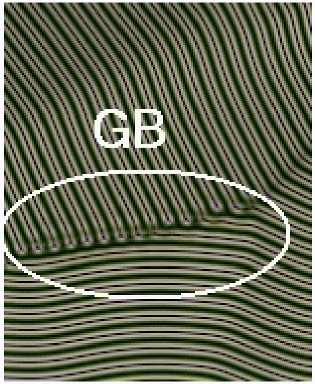
SMECTIC SYMMETRY

- Broken translational symmetry in only one direction.

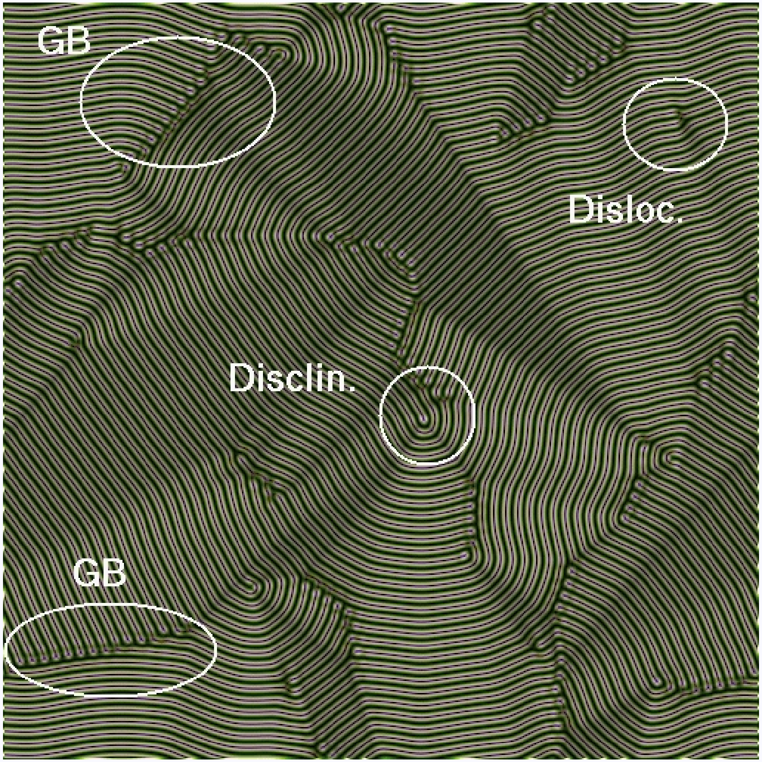






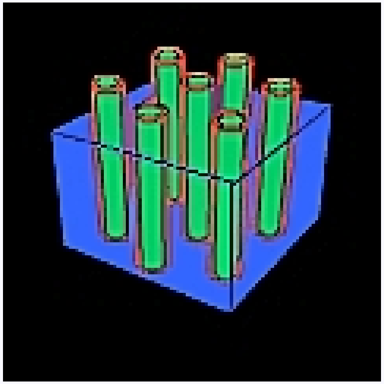
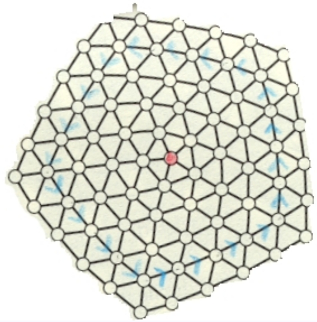
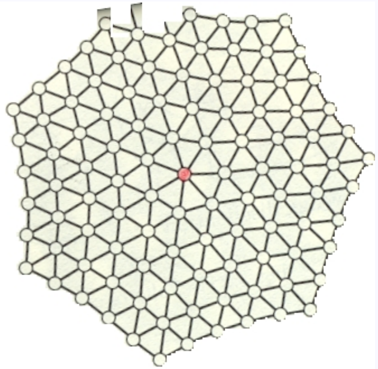
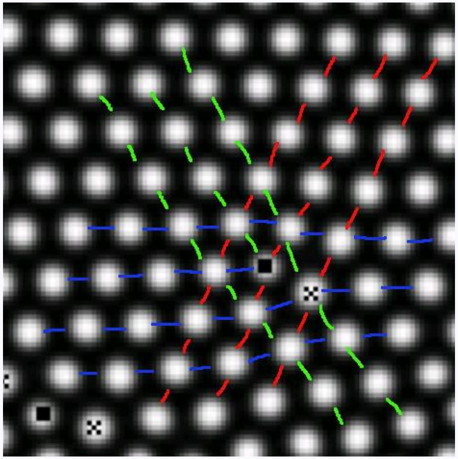
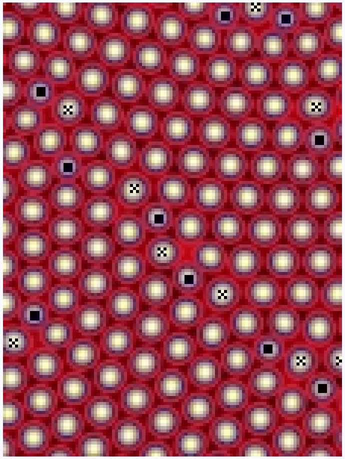


LAMELLAR PHASE

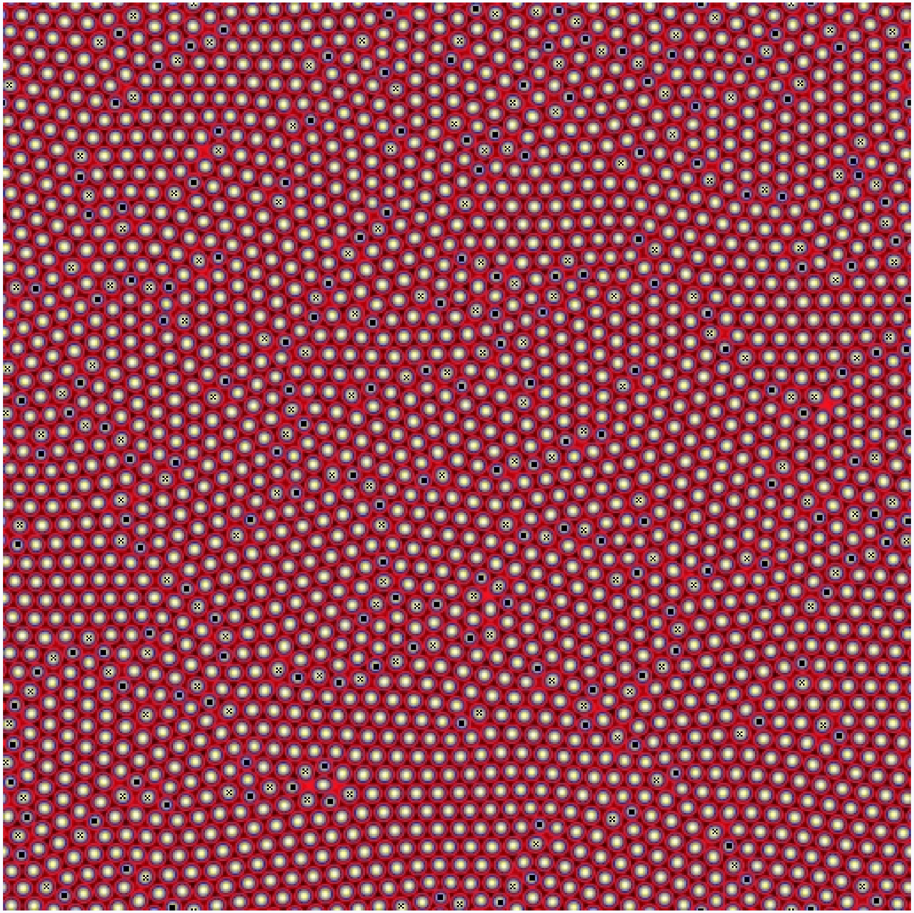


HEXAGONAL SYMMETRY

- Broken translational symmetry in two directions (2D crystal).

HEXAGONAL PHASE



ORDER PARAMETER MODEL

$$\tau_0 \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = \epsilon\psi - \frac{\xi_0^2}{4k_0^2}\left(k_0^2 + \nabla^2\right)^2 \psi + g_2\psi^2 - \psi^3$$

Stationary solution $g_2 = 0$

- $\epsilon < 0$: $\psi = 0$
- $\epsilon > 0$: $\psi(\vec{r}, t) = \epsilon^{1/2} A_0 \sin(\vec{k}_0 \cdot \vec{r}) + \mathcal{O}(\epsilon^{3/2})$.

Lamellar pattern oriented along an arbitrary $\vec{k}_0$. *Smectic phase*.

Stationary solution $g_2 \neq 0$

- $-|\epsilon_m(g_2)| < \epsilon < \epsilon_M(g_2)$: $\psi(\vec{r}, t) = \sum_{n=1}^{6} A_n e^{i\vec{k}_n \cdot \vec{x}} + \text{c.c.}$.

Hexagonal pattern. *Crystalline phase*.

WEAKLY NONLINEAR ANALYSIS

Consider slowly varying modulations around linearly unstable solution (for $g_2 = 0$),

$$\psi(\vec{r}, t) = A(\vec{r}, t)e^{ik_0 x} + c.c.,$$

$$\tau_0 \frac{\partial A(\vec{r}, t)}{\partial t} = \left[\epsilon + \xi_0^2 \left(\partial_x - \frac{i}{2k_0}\partial_y^2\right)^2 - 3|A|^2\right] A(\vec{r}, t)$$

(Ginzburg-Landau equation).

- This equation is a universal long wavelength description of a stationary, supercritical bifurcation.
- Rotational invariance of the underlying governing equations lost.

AMPLITUDE EQUATION DESCRIPTION OF DISLOCATION MOTION

(Siggia and Zippelius, 1981)

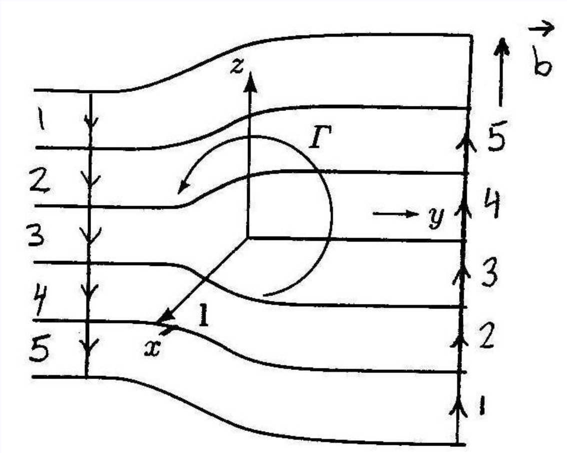
Point defect in the envelope field,

$$\psi = Ae^{i\vec{k}\cdot\vec{x}} = \rho(\vec{x})e^{i\theta(\vec{x})}e^{i\vec{k}\cdot\vec{x}}.$$

$$\oint \nabla\theta \cdot \vec{dl} = \pm 2\pi.$$

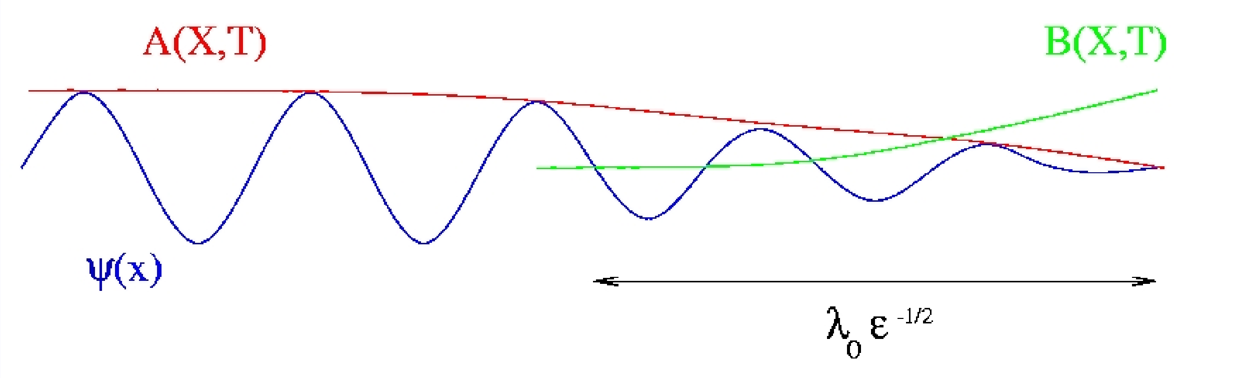
Climb velocity is found,

$$v \propto (k - k_0)^{3/2}.$$



Phase θ plays the role of the displacement field u.

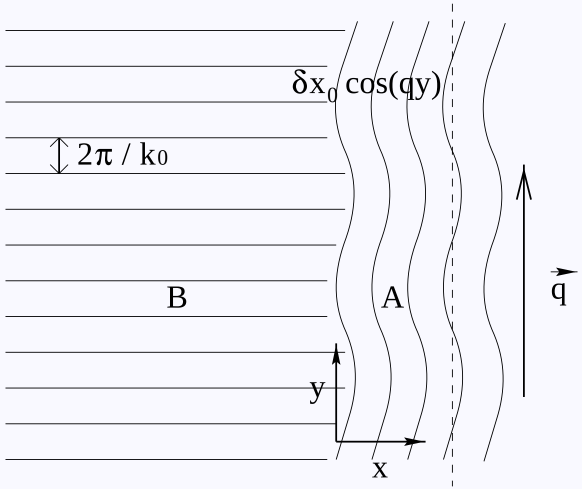
AMPLITUDE EQUATION DESCRIPTION OF A GRAIN BOUNDARY



$$\frac{\partial A}{\partial t} = \epsilon A + \xi_0^2 \left(\partial_x - \frac{i}{2k_0} \partial_y^2 \right)^2 A - 3|A|^2 A - 6|B|^2 A,$$

$$\frac{\partial B}{\partial t} = \epsilon B + \xi_0^2 \left(\partial_y - \frac{i}{2k_0} \partial_x^2 \right)^2 B - 3|B|^2 B - 6|A|^2 B.$$

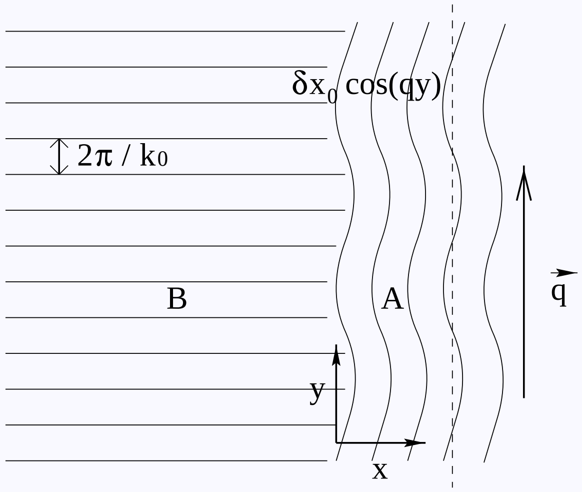
GRAIN BOUNDARY MOTION



$$F = \int d\vec{r} \Big\{ -\epsilon(|A|^2 + |B|^2) + \frac{3}{2}(|A|^4 + |B|^4) + 6|A|^2|B|^2 +$$

$$\xi_0^2 |(\partial_x - \frac{i}{2k_0}\partial_y^2)A|^2 + \xi_0^2|(\partial_y - \frac{i}{2k_0}\partial_x^2)B|^2 \Big\}$$

GRAIN BOUNDARY MOTION



- Linear relaxation rate $\sigma \propto q^4$.
- Nonlinear uniform translation mode,

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

$$v_{gb}(t) = \frac{\text{Time dependent driving force}}{\text{Mobility}}$$

DOMAIN COARSENING

- A time dependent length $\overline{R}(t)$ (characteristic domain size) emerges, to which all other lengths scale.
- As $t \to \infty$, $\overline{R}(t) \to \infty$, and all other scales of microscopic origin become irrelevant (cf. correlation length divergence near a critical point).
- Scaling functions are introduced. For example for the domain size distribution,

$$p(R,t) = \mathcal{G}\left(\frac{R}{t^x}\right) \quad \overline{R}(t) \sim t^x.$$

- Universality classes have been introduced according to the value of x.
  - Purely relaxational dynamics, $x = 1/2$.
  - Relaxational dynamics with global conservation law, $x = 1/3$.
  - Binary fluids (non-variational modes), $x = 1$.
  - Smectic phases, $x = 1/3$.

COARSENING MECHANISM IN SMECTICS

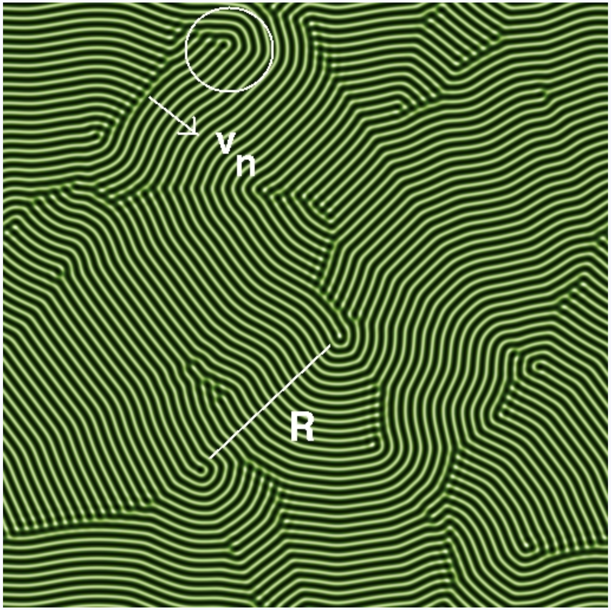
- Grain boundary velocity,

$$v_n \propto \kappa^2 \sim R^{-2}$$

with the scale R set by the distribution of disclinations.

- Coarsening law,

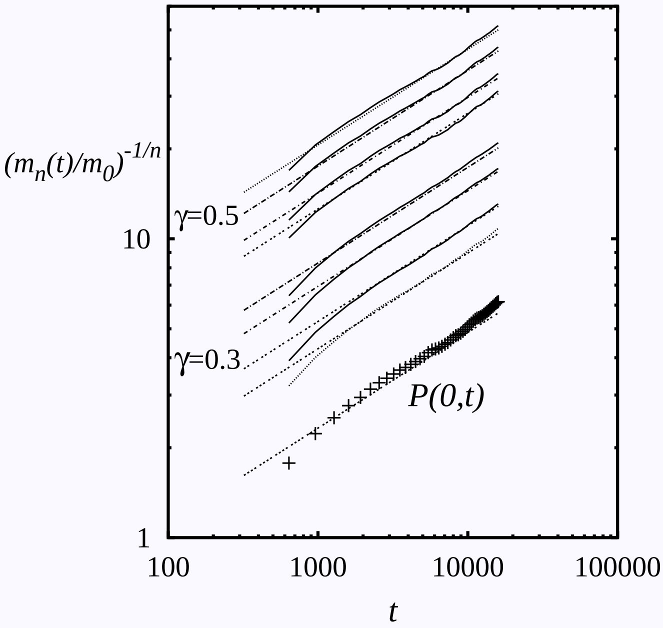
$$R(t) \sim t^{1/3}$$



DOMAIN COARSENING

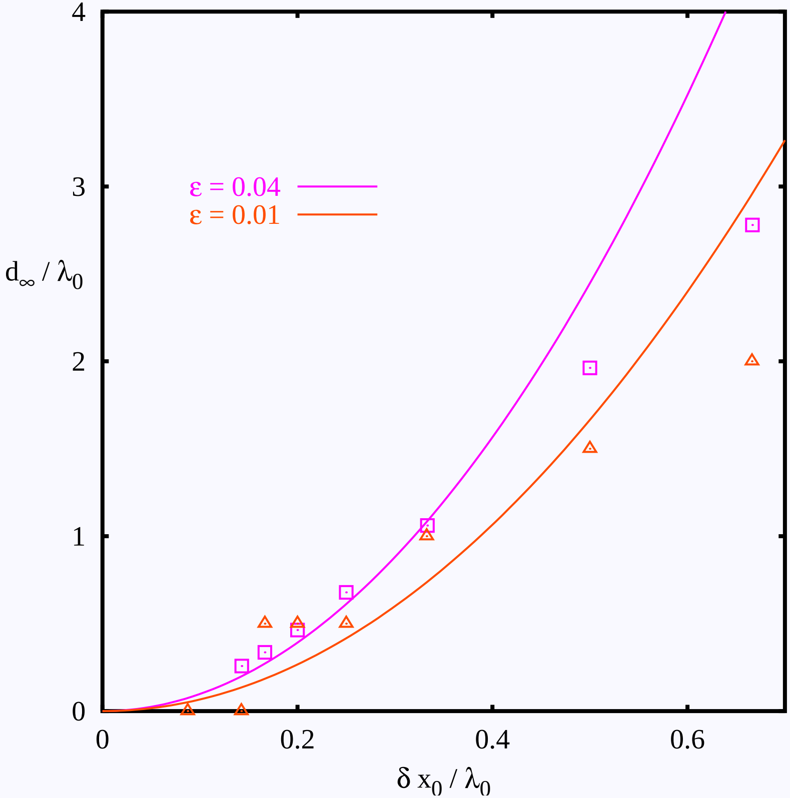
Moments of the distribution of domain curvatures,

$$m_n(t) = \int_0^{\kappa_c(t)} d\kappa\ \kappa^n P(\kappa, t) \quad P(\kappa, t) = t^{1/z} f(\kappa t^{1/z})$$

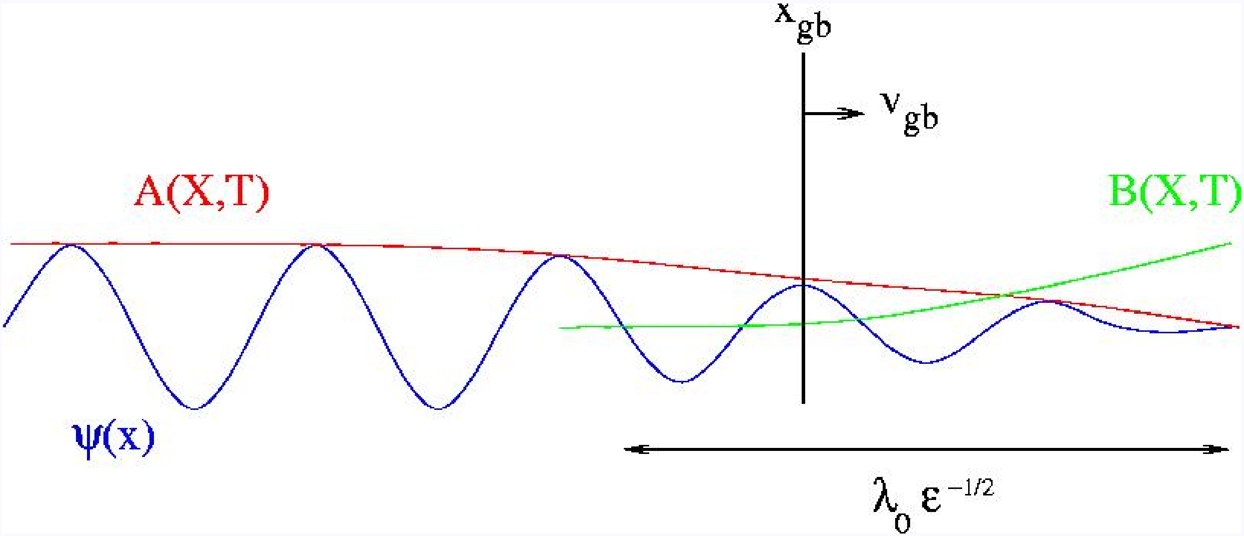


NON-ADIABATIC MOTION

For small $\epsilon \sim 0.1$, the decoupling between slowly varying amplitudes and the phase of the lamellae already breaks down.



NON-ADIABATIC EFFECTS AND PINNING



For a grain boundary, we find,

$$v_{gb} = \frac{\epsilon}{3k_0^2 D(\epsilon)}\kappa^2 - \frac{p(\epsilon)}{D(\epsilon)}\cos(2k_0 x_{gb} + \phi) + \tilde{\eta},$$

with $\langle \tilde{\eta}(t)\tilde{\eta}(t') = (k_B T / D(\epsilon) L_{gb})\delta(t - t')$.

The function $D(\epsilon)$ is a friction coefficient, and

$$p(\epsilon) \sim \epsilon^2 e^{-\alpha/\sqrt{\epsilon}}.$$

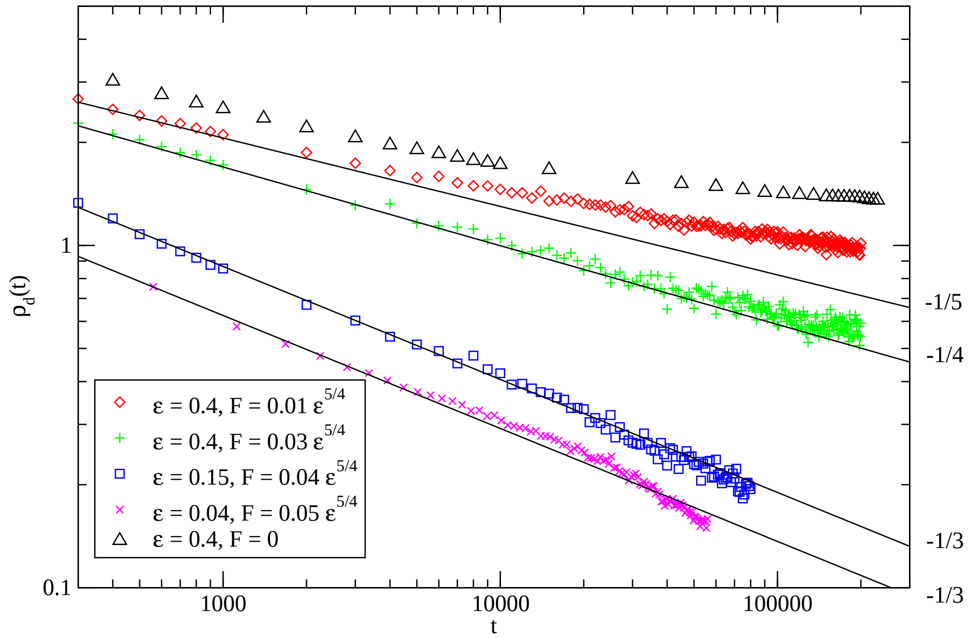
NON-ADIABATIC EFFECTS AND PINNING

- Grain boundary located at potential minima - decoupling between grain boundary location and lamellar phase lost.
- Continuous motion only in the limit $\epsilon \longrightarrow 0$.
- Effective coarsening exponents when ϵ is not sufficiently small.
- Effective exponents change when random fluctuations added to equations of motion (unlike phase ordering systems).
- Glassy states at some ϵ.

EFFECTIVE COARSENING EXPONENTS

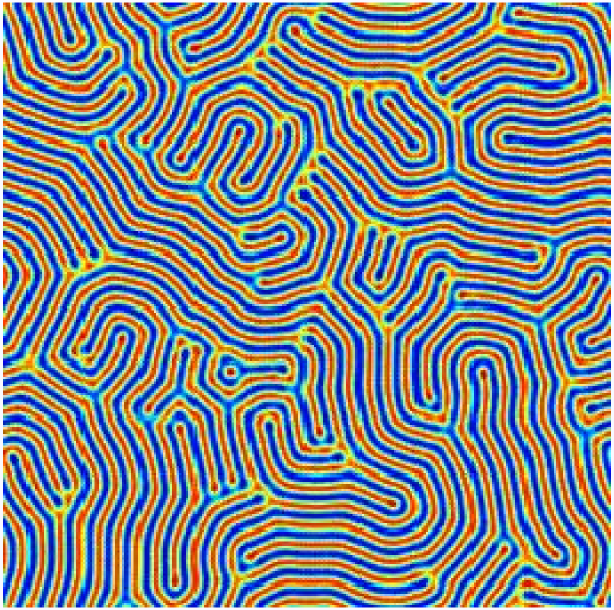
- Elder, Viñals, and Grant, 1992.
  - Structure factor: $x = 1/5$ (no noise), $x = 1/4$ (noise).
  - Lamellar relaxation $x = 1/4$ crossing over to $x = 1/2$.
- Cross and Meiron, 1995.
  - Structure factor (no noise): $x = 1/5$.
  - Structure factor (non-gradient model and no noise): $x = 1/5$.
- Hou, Sasa, and Goldenfeld, 1997.
  - Structure factor: $x = 1/5$ (no noise), $x = 1/4$ (noise)
  - Domain wall density: $x = 1/4$ (no noise), $x = 0.3$ (noise)
- Christensen and Bray, 1998.
  - Structure factor: $x = 1/5$ (no noise), $x = 1/4$ (noise)
  - Local director correlation function: $x = 1/4$ (no noise), $x = 0.3$ (noise).

EFFECTIVE COARSENING EXPONENTS



GLASSY CONFIGURATIONS

Characteristic pinning scale: $R_{gl} \sim \lambda_0 \epsilon^{-1/2} e^{\alpha/(2\sqrt{\epsilon})}$



$\epsilon = 0.5$

RANDOM FLUCTUATIONS

- Approximate equation of grain boundary motion,

$$\dot{x}_{gb} = \left(\frac{k_0 F_0}{2D}\right) R_{gl}\kappa^2 - \left(\frac{k_0 F_0}{2D}\right)\frac{1}{R_{gl}}\cos(2k_0 x_{gb}+\phi) + \frac{1}{\sqrt{2D}}\left(\frac{F}{R_{gb}}\right)^{1/2}\xi$$

$$\text{with} \quad F_0 = \frac{2\epsilon}{3k_0^3 R_{gl}}$$

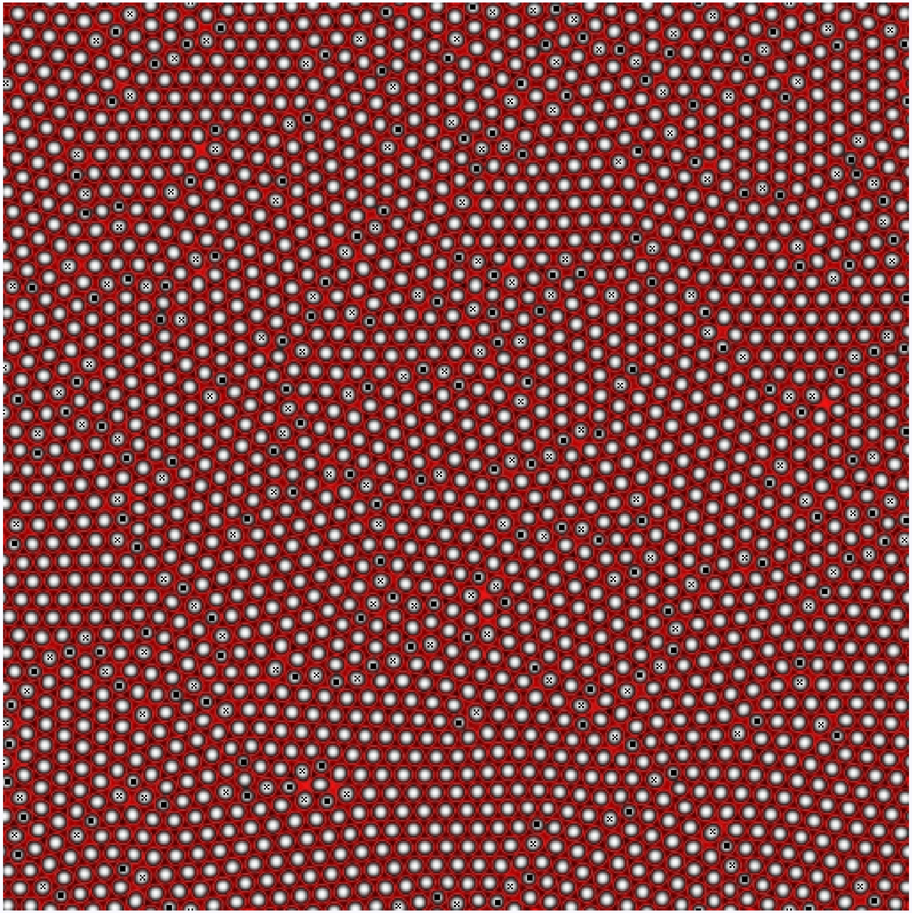
- Escape over a barrier. The Kramers rate of escape is,

$$r \sim \exp\left(-\frac{F_0}{F}\frac{R_{gb}}{R_{gl}}\right).$$

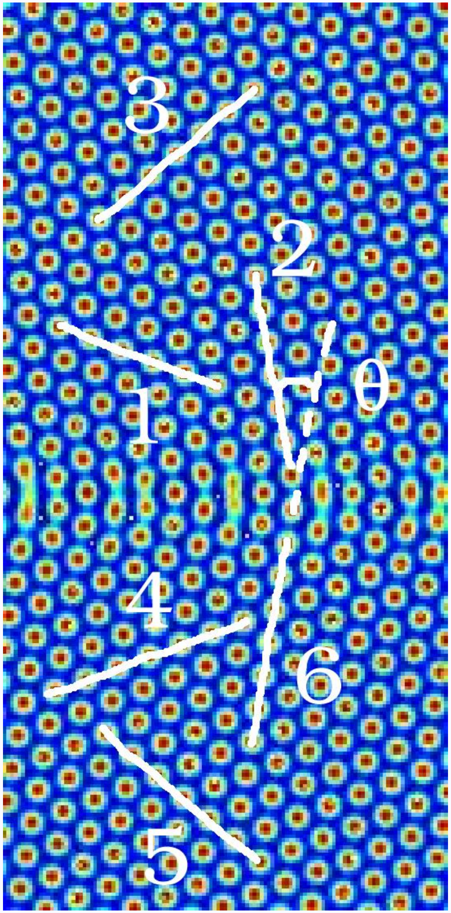
- The noise intensity to unpin a boundary of perimeter R_{gb},

$$F = R_{gb}\frac{F_0}{R_{gl}} \sim \frac{R_{gb}\epsilon^2}{k_0} e^{-\alpha/\sqrt{\epsilon}}.$$

HEXAGONAL PHASE



SUBCRITICAL BIFURCATION TO A HEXAGONAL PHASE



$$Dv_{gb} = -p_{hex} \sin\left[2k_0 x_{gb} \sin(\theta/2)\right],$$

with (Peierls force),

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

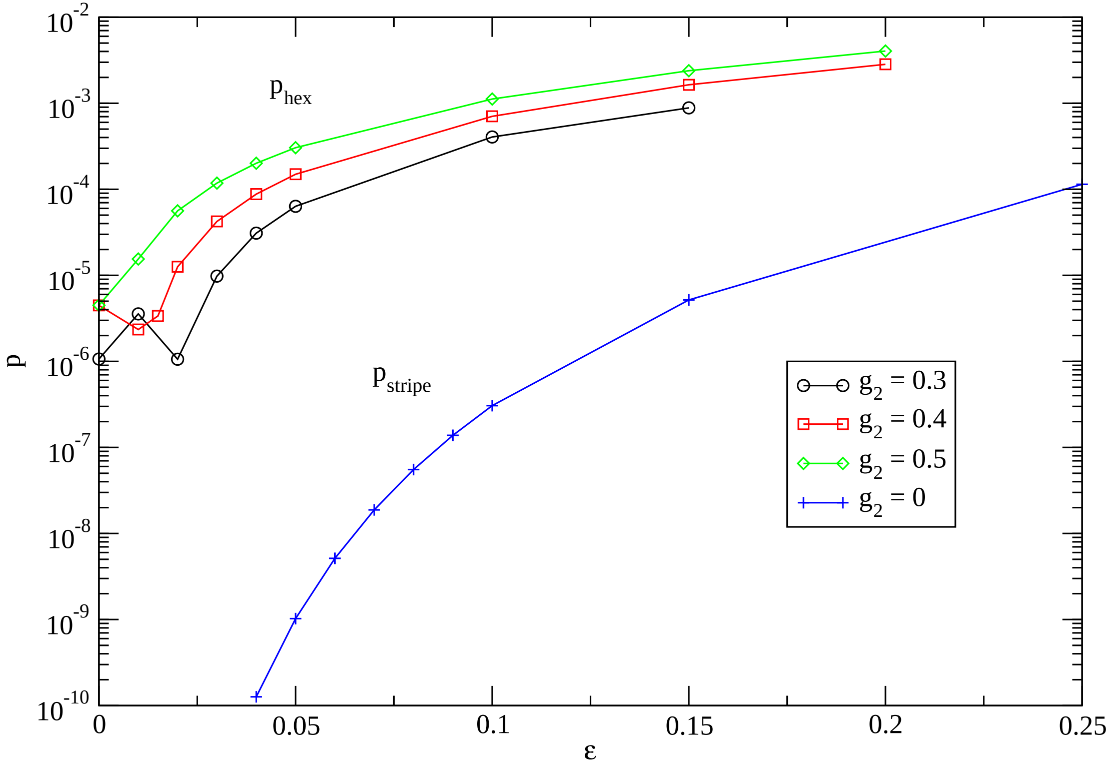
- Lamellar phase,

  $$\xi \sim 1/\sqrt{\epsilon} \quad p_{lam} \sim e^{-1/\sqrt{\epsilon}}.$$

- Hexagonal phase,

  $$\xi \to \xi_0 = \frac{15\lambda_0}{8\sqrt{6}\pi g_2}.$$

AMPLITUDE OF PINNING FORCE



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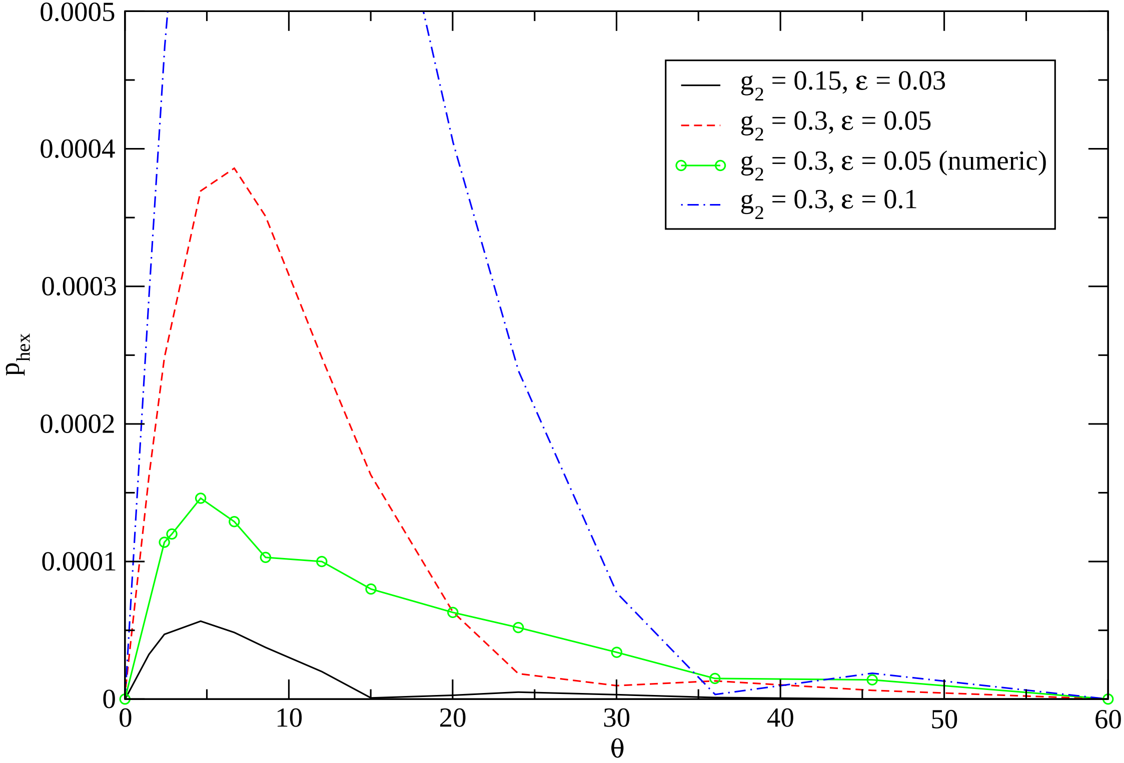

SUMMARY

- In the limit $\epsilon \to 0$, a lamellar microstructure coarsens in a self-similar fashion, with an exponent $x = 1/3$.
- At small but finite ϵ, non-adiabatic effects lead to pinning, to effective coarsening exponents, and to glassy behavior.
- At a subcritical bifurcation (e.g., hexagonal lattice), pinning effects cannot be avoided. The resulting Peierls force can be derived analytically from an order parameter model.
- Grain boundary mobility depends strongly on mis-orientation. The dependence in a hexagonal phase is qualitatively similar to that of a crystalline solid.