A MESOSCOPIC DESCRIPTION OF DEFECT MOTION

Jorge Viñals

School of Physics and Astronomy
University of Minnesota

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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.
Consider a mesoscopic model with periodic ("lattice") solutions (broken symmetry). Asymptotic analysis of defect motion, and coupling between "lattice" and continuum description.

- Extension of continuum model with lattice dependent degrees of freedom.
COARSE GRAINED MODEL

- Time dependent Ginzburg-Landau equation:

\[
\frac{\partial \psi}{\partial t} = -\Lambda \frac{\delta F}{\delta \psi}
\]

\(\psi \propto \rho_a - \rho_b\) order parameter.

- For symmetric diblock melts (lamellar phase)
  - (Ohta-Kawasaki (with \(\Lambda = -M\nabla^2\))

\[
F[\psi] = \int dr \left( \frac{-\tau}{2} \psi^2 + \frac{u}{4} \psi^4 + \frac{K}{2} (\nabla \psi)^2 \right) + \frac{B}{2} \int drdr' \psi(r) G(r-r') \psi(r')
\]

with \(\nabla^2 G(r-r') = -\delta(r-r')\).

  - (Leibler/Swift-Hohenberg in weak segregation limit)

\[
\frac{\partial \psi}{\partial t} = \left[ \epsilon - (\nabla^2 + q_0^2)^2 \right] \psi - \psi^3
\]

\(\epsilon\) distance from the order-disorder threshold, \(q_0\) lamellar spacing.
PHASE DIAGRAM (DIBLOCK)

[K. Yamada, M. Nonomura, and T. Ohta, Macromolecules 37, 5762 (2004)]
ASYMPTOTIC THEORY, $\epsilon \to 0$

- Assume weak distortion,

$$\psi = \epsilon^{1/2} A(X, Y, T)e^{iq_0 x} + \text{c.c.}$$

- Ginzburg-Landau equation for envelope $A$ (in original variables),

$$\tau_0 \frac{\partial A}{\partial t} = \epsilon A + \xi_0^2 \left( \partial_x - \frac{i}{2q_0} \partial_y \right)^2 A - g_0 |A|^2 A,$$

- Which can be derived from a free energy

$$F = \frac{1}{2} \int dx \left[ -\epsilon |A|^2 + \xi_0^2 \left| \left( \partial_x - \frac{i}{2q_0} \partial_y \right) A \right|^2 + \frac{g_0}{2} |A|^4 \right]$$

$$\tau_0 \frac{\partial A}{\partial t} = -\frac{\delta F}{\delta A^*}$$
NONEQUILIBRIUM MICROSTRUCTURE
DEFECTS IN COLUMNAR PHASES

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

Solutions for $\psi$ around defects are regular. Envelope equation is on the other hand

$$\psi(x, t) = A(X, T) e^{i q \cdot x} = \rho(X, T) e^{i \theta(X, T)} e^{i q \cdot x}.$$

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

For $\epsilon \to 0$, climb velocity is,

$$v \propto (q - q_0)^{3/2}.$$

[Siggia and Zippelius, 1981]

Phase $\theta$ plays the role of the displacement field $u$. 

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Order parameter expanded in slowly varying amplitudes:

\[ \psi = A e^{i k_0 x} + B e^{i k_0 z} + \text{c.c.} \]

where

\[ A = A(\epsilon^{1/2} x, \epsilon^{1/4} y, \epsilon^{1/4} z, \epsilon t) \]
\[ B = B(\epsilon^{1/4} x, \epsilon^{1/4} y, \epsilon^{1/2} z, \epsilon t) \]
ENVELOPE DESCRIPTION OF A GRAIN BOUNDARY

\[ \frac{\partial A}{\partial t} = \epsilon A + \xi_0^2 \left( \partial_x - \frac{i}{2q_0} \partial_y \right)^2 A - 3|A|^2 A - 6|B|^2 A, \]

\[ \frac{\partial B}{\partial t} = \epsilon B + \xi_0^2 \left( \partial_y - \frac{i}{2q_0} \partial_x \right)^2 B - 3|B|^2 B - 6|A|^2 B. \]
ENVELOPE DESCRIPTION OF A GRAIN BOUNDARY

Linear relaxation rate $\sigma \propto q^4$.

Nonlinear uniform translation mode,

$$v_{gb}(t) = \left( \frac{\xi_0^2}{4q_0^2} q^4 \right) \frac{(\epsilon/4)[q_0\delta x(t)]^2}{\int_{-\infty}^{\infty} dx \left[ (\partial_x A_0)^2 + (\partial_x B_0)^2 \right]} \sim \frac{\delta x(t)^2 q^4}{\sqrt{\epsilon}} \propto \frac{\kappa^2}{\sqrt{\epsilon}}$$

$v_{gb}(t) = \text{Mobility } \times \text{ Time dependent driving force}$
MULTIPLE SCALE COUPLING
“NON ADIABATIC EFFECTS”

Reconsider standard multiple scale expansion,

$$\psi = \epsilon^{1/2}\psi_{1/2} + \epsilon^{3/2}\psi_{3/2} + \ldots$$

At leading order

$$\psi_{1/2} = A(X_A, Y_A, T)e^{iq_0x} + B(X_B, Y_B, T)e^{iq_0y} + c.c.$$ 

Amplitude equation arises from a solvability condition at $O(\epsilon^{3/2})$,

$$\int_{x}^{x+\lambda_0} dx' \frac{d}{\lambda_0} \int_{y}^{y+\lambda_0} dy' \frac{d}{\lambda_0} \left( L\psi_{1/2} - \psi_{1/2}^3 \right) e^{-iq_0x'} = 0,$$

As $\epsilon \to 0$, fast and slow scales separate, and $(x, y, t)$ independent of $(X, Y, T)$. Only resonant terms with $e^{iq_0x}$ contribute to the solvability relation.
As $\epsilon \to 0$, interface width $\xi_0/\epsilon^{1/2} \gg \lambda_0$.

If $\epsilon$ is small but finite, terms like

$$\int_{x}^{x+\lambda_0} dx' A^3 e^{2i q_0 x'}$$

in the solvability condition may not integrate to zero.
Allowing this possibility, the lowest order envelope equations are

\[
\frac{\partial A}{\partial t} = \epsilon A + \xi_0^2 \left( \partial_x - \frac{i}{2q_0} \partial_y^2 \right)^2 A - 3|A|^2 A - 6|B|^2 A
\]
\[- \int_{x+\lambda_0}^{x'} dx' \frac{d}{\lambda_0} \left( A^3 e^{2iq_0x'} + A^* \right)^3 e^{-4iq_0x'} ,
\]

\[
\frac{\partial B}{\partial t} = \epsilon B + \xi_0^2 \left( \partial_y - \frac{i}{2q_0} \partial_x^2 \right)^2 B - 3|B|^2 B - 6|A|^2 B
\]
\[- 3 \int_{x+\lambda_0}^{x'} dx' \frac{d}{\lambda_0} \left( A^2 Be^{2iq_0x'} + A^* \right)^2 Be^{-2iq_0x'} .
\]

The new terms are exponential small in \(\epsilon\)

\[e^{-1/\sqrt{\epsilon}}\]
For a grain boundary, we find,

\[ v_{gb} = \frac{\epsilon}{3k_0^2D(\epsilon)\kappa^2} - \frac{p(\epsilon)}{D(\epsilon)} \cos(2k_0x_{gb} + \phi) \]

The function \( D(\epsilon) \) is a friction coefficient, and \( p(\epsilon) \) is a pinning force

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

\( p(\epsilon) \to 0 \) exponentially as \( \epsilon \to 0 \) (essential singularity). Grows quickly with \( \epsilon \).
DEFECT KINETICS (MESOSCALE)

\[ v_{gb}(t) = \frac{\Delta f}{D(\epsilon)} - \frac{p(\epsilon)}{D(\epsilon)} \sin [2q_0 x_{gb}(t) \sin(\theta/2)] , \]

with (Peierls stress)

\[ p \sim A_0^4 e^{-2a q_0 \sin(\theta/2) \xi}. \]

Supercritical (second order)

\[ \xi \sim 1/\sqrt{\epsilon} \quad p \sim e^{-1/\sqrt{\epsilon}} \to 0. \]

Subcritical (first order)

\[ \xi \to \xi_0 = \frac{15 \lambda_0}{8 \sqrt{6\pi} g_2} \text{ finite.} \]
AMPLITUDE OF PINNING FORCE

\[ g_2 = 0.3, \quad \varepsilon = 0.03 \]
\[ g_2 = 0.3, \quad \varepsilon = 0.05 \]
\[ g_2 = 0.3, \quad \varepsilon = 0.1 \]
Possible coarse grained variable to describe the state of a defected solid: dislocation density tensor $\alpha_{ik}(r)$. In $d = 2$, $b_i(r) = \alpha_{3i}(r)$, the Burger's vector density.

Defects lead to strain $u_{ij}$, and to energy in the medium (e.g., isotropic medium)

$$H = \frac{1}{2} \int \frac{d^2 q}{(2\pi)^2} \frac{q^2 \delta_{ij} - q_i q_j}{\alpha q^4} b_i(q)b_j(-q) + E_{\text{core}}$$

Defects lead to an antisymmetric part of $w_{ij}$: lattice rotation

$$w_{ij}(r) = u_{ij}(r) + \epsilon_{ij}\theta(r)$$

$$\theta(r) = -\frac{1}{2\pi} \int dr' \frac{b(r') \cdot (r - r')}{(r - r')^2}$$

$$\oint du_i = -b_i$$

$$w_{mk} = \partial_m u_k$$

$$\epsilon_{ilm} \partial_l w_{mk} = -\alpha_{ik}$$
Conservation of topological charge, and minimization of energy, leads to

\[ \partial_t b_j(r, t) = -\epsilon_{lm} B_{mjsi} \epsilon_{sb} \partial_l \partial_b \frac{\delta H}{\delta b_i(r, t)} \]

where kinetic coefficient \( B_{mjsi} \) depends on lattice symmetry.
Conservation of topological charge, and minimization of energy, leads to

$$\partial_t b_j(r, t) = -\epsilon_{lm} B_{mjsi} \epsilon_{sb} \partial_l \partial_b \frac{\delta H}{\delta b_i(r, t)}$$

where kinetic coefficient $B_{mjsi}$ depends on lattice symmetry.

- Is a kinetic coefficient all that is necessary from the underlying lattice?
- Defects do not move along the direction that minimizes $H$; they move along slip planes.
- Slip planes are locally rotated in a defected system.
Decompose Burger’s vector density along slip systems,

\[ \mathbf{b}(\mathbf{r}) = \sum_s b^{(s)}(\mathbf{r}) \hat{\theta}^{(s)}(\mathbf{r}) \]

(possible as long as there are no unbound disclinations).

Define a coarse grained defect mobility that distinguishes glide and climb in the locally rotated frame,

\[ D_{kj}^{(i)} = D_g \theta^{(i)}_k \theta^{(i)}_j + D_c \left( \delta_{kj} - \theta^{(i)}_k \theta^{(i)}_j \right) \]

Kinetic equation (square symmetry)

\[ \partial_t b_k = \sum_i \theta^{(i)}_k D^{(i)}_{nm} \theta^{(i)}_l \left( \partial_n \partial_m \frac{\delta H}{\delta b_l} \right) \]

with \( \hat{\theta}^{(s)}(\mathbf{r}) \) calculated self-consistently.
EXAMPLE: TWO EDGE DISLOCATIONS

- At $t = 0$, two edge disclinations separated by $x(0) = 10, y(0) = 0$:
- Only glide (no climb).
EXAMPLE: TWO EDGE DISLOCATIONS

At \( t = 0 \), two edge disclinations separated by \( x(0) = 10, y(0) = 0 \):

- Glide and climb.
1. In multiple scale problems, separation of disparate scales is not necessarily possible.

2. When the smallest scale is periodic, exponentially small terms appear that do not arise in nonlinear perturbative expansions.

3. Exponential terms lead to scale coupling: pinning and orientation dependences in the slow scales (amplitudes or envelopes).