Phase Field Models

Elastic Stress Effects

T. A. Abinandanan

Department of Materials Engineering
Indian Institute of Science

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Outline

- **Elastic stress effects**
- **Phase field models**
- **Modulus mismatch: Rafting**
- **Modulus mismatch: Thin film instability**
- **Multiple domains: Anisotropic misfit**
- **Summary**

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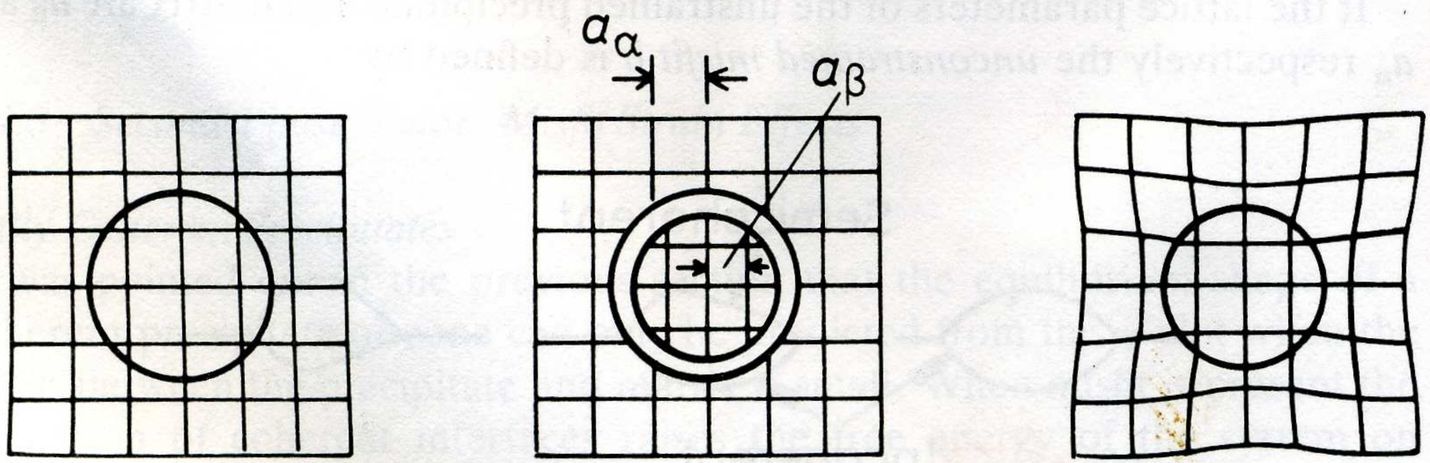
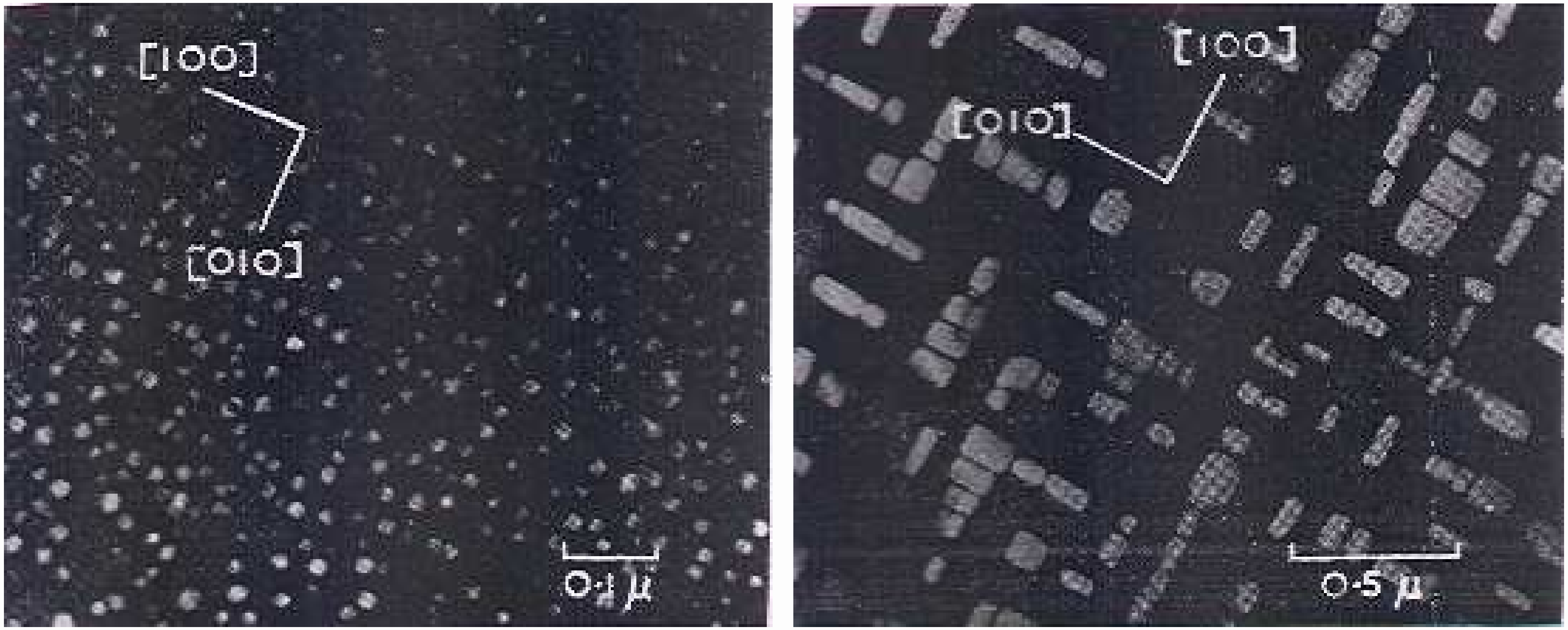
Origin of elastic stresses



Schematic from Porter and Easterling

1. **Misfit: Lattice parameter mismatch**
2. **Externally applied stress**
3. Interfacial stress
4. Thermal stresses

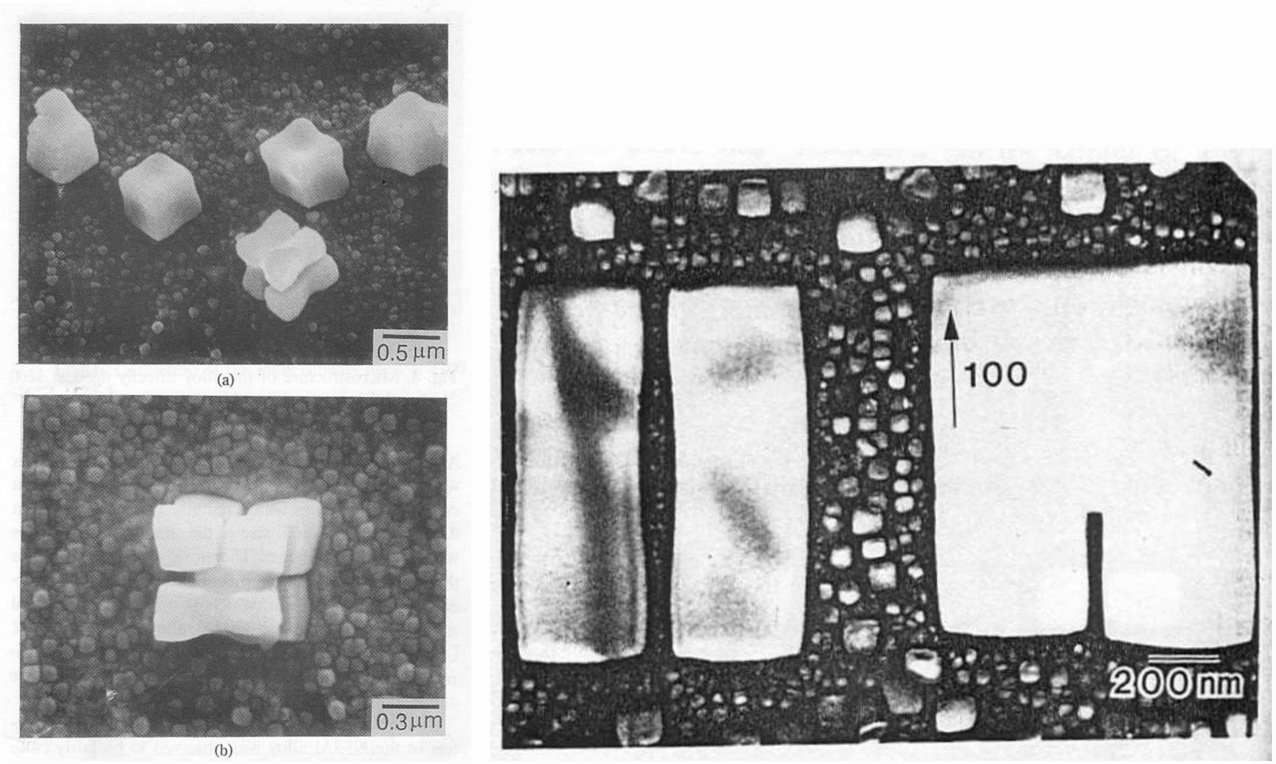
Long range interactions



(Ardell and Nicholson (Eshelby), 1966)

- Particle shape transitions
  Sphere → Cuboid → Plate
- Particle alignment

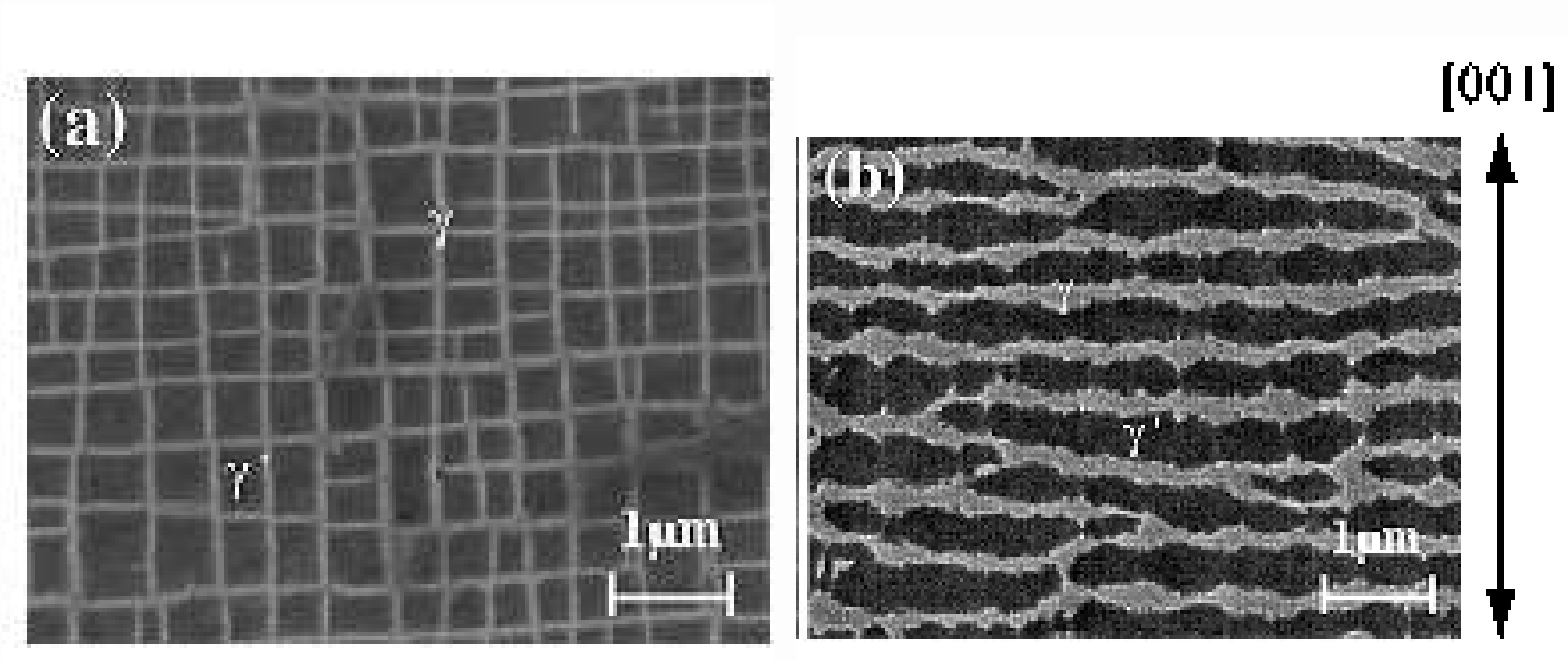
Stresses may overwhelm capillarity



(Yeon et al and Kaufmann et al - 1989)

- Particle splitting

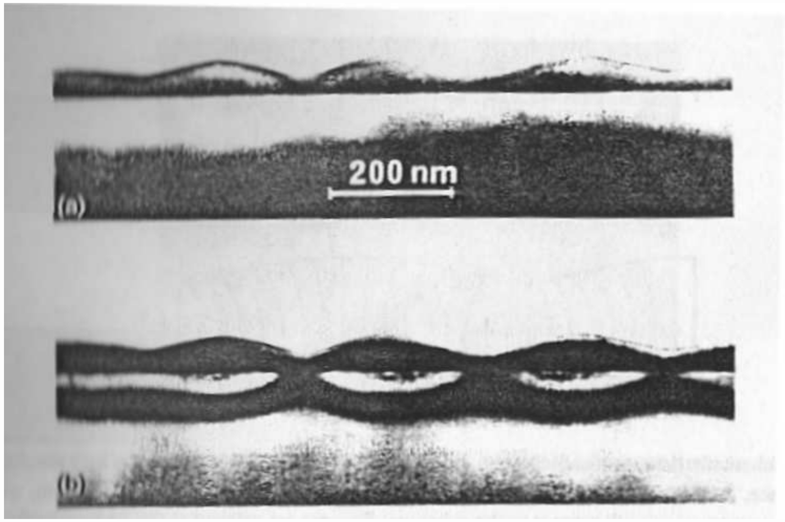
Coupling with an applied stress



(Ichitsubo et al, 2003)

- Rafting or directional coarsening
- When misfit is isotropic, rafting is possible only when elastic moduli are different.

Stresses could break thin films



(Cullis et al, 1992: 40 nm Si$_{0.79}$Ge$_{0.21}$ on (001) Si)

- Asaro-Tiller-Grinfeld instabilities

Elastic stress effects

- Misfit
- Elastic moduli
- Mismatch in elastic moduli
- Applied stresses

Effects can be highly anisotropic due to anisotropy in misfit, moduli and applied stress.

Scaling arguments

Competition between surface and elastic energies

- Surface energy scales with interfacial Area
  Dominates at small sizes.
- Elastic energy scales with precipitate volume
  Becomes more important at large sizes.

For example, in nickel-base superalloys, small particles have compact shapes, transitioning at large sizes to cuboids or plates.

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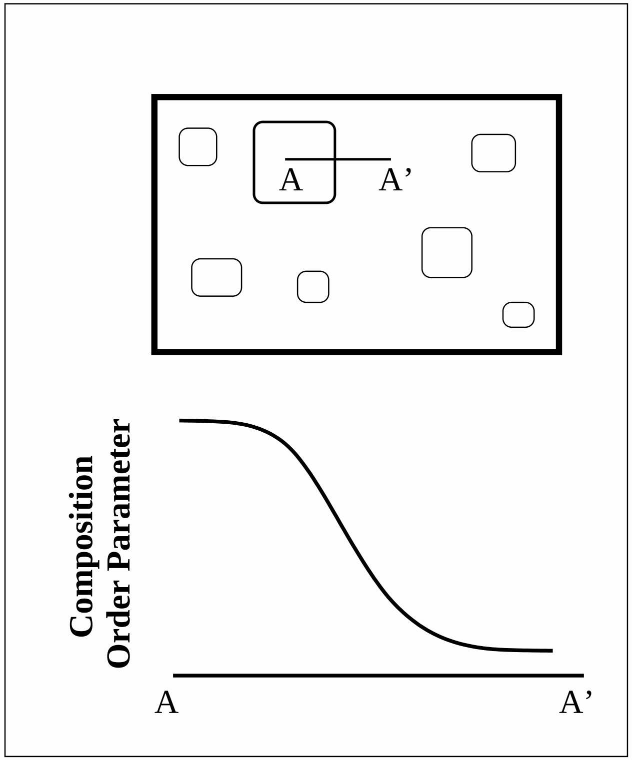
Phase field models

- Essentially, models of migrating interfaces.
  - Describe a configuration
  - Define the energy of a configuration
  - Define transition from one configuration to the next
- Complex geometries: there is no interface tracking.
- Versatile: easy to incorporate effects due to electric, magnetic and stress fields (multi-ferroics).
- Multiple levels of detail.
- Regimes beyond analytical theories.
  Thin film instability: from onset and growth all the way up to break up.

Phase field models: Configuration



- Field variables $c(\boldsymbol{r}, t)$ and $\eta_i(\boldsymbol{r}, t)$ change smoothly (continuously) from one phase (domain) to the other.
- Within a phase, c and η have little or no gradients.
- Interface is the region with large gradients in c and η.

Phase field model: Energetics

Free energy:

$$F = F^{\text{chemical}} + F^{\text{elastic}}$$

$$F^{\text{chemical}} = \int \left[f_0(c) + \kappa_c (\nabla c)^2 + \kappa_i (\nabla \eta_i)^2 \right] dV$$

- κ_c and κ_i are gradient energy coefficients
- f_0 is the bulk free energy density (phase diagram)

Phase field model: Elastic energy

Elastic stress σ obeys equation of mechanical equilibrium:

$$\nabla \cdot \sigma = 0,$$

$$\sigma_{ij} = C_{ijkl}(u_{k,l} - \varepsilon^0_{kl})$$

$$F^{\text{elastic}} = \frac{1}{2}\int \sigma{:}\varepsilon^{el} dV$$

- Elastic strain: $\varepsilon^{el} = \varepsilon - \varepsilon^0$
- ε^0_{kl} - misfit strain

Phase field model: Elastic energy

- The misfit strain, ε^0_{kl}, depends on local composition or orderparameter or both.
- It can be:
  - Isotropic (modulus mismatch effects)
  - Anisotropic (multiple variant microstructures)

Phase field model: Kinetics

- Cahn-Hilliard equation:

$$\frac{\partial c}{\partial t} = \nabla \cdot M \nabla \frac{\delta \left\{ \frac{F}{N_V} \right\}}{\delta c}$$

- Cahn-Allen (Ginzburg-Landau) equation:

$$\frac{\partial \eta_i}{\partial t} = -L \frac{\delta \left\{ \frac{F}{N_V} \right\}}{\delta \eta_i}$$

- M = atomic mobility; L - relaxation coefficient.
- The variational derivative $(\delta F / \delta c)$ is the generalized chemical potential μ (whose gradient drives diffusion)

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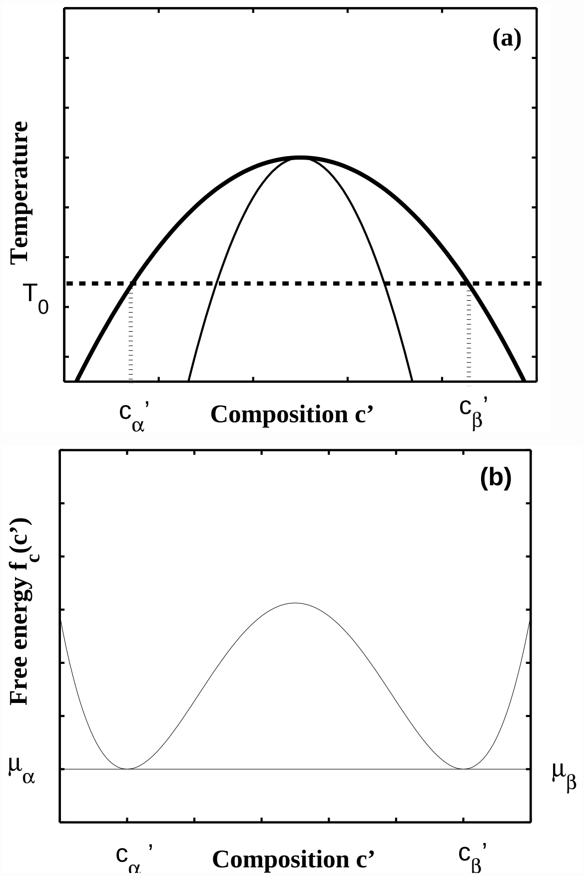
Elastic inhomogeneity

- If we assume elastic homogeneity (same elastic moduli in the two phases) we can explain:
  - Shape changes
  - Particle alignment
- However, elastic inhomogeneity is essential for explaining
  - Rafting (dilatational misfit)
  - Morphological instabilities in thin films

Phase field model: Model system



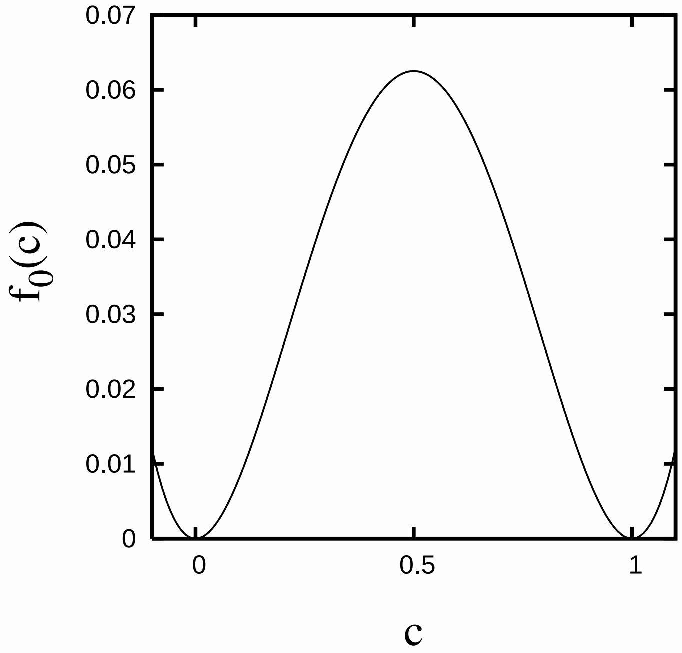
Phase separation and Spinodal Decomposition

- Binary A-B alloy system
- Miscibility gap at low temperatures
- Phase separation

Phase field model: Energetics

$$f_0(c) = Ac^2(1-c)^2$$

A sets the free energy barrier between the p and m phases



Single particle rafting

Uniaxial stress

(a) Tensile along x (b) Compressive along y

Single particle rafting

- Directions of elongation consistent with those of Schmidt and Gross.
- Inhomogeneity effect: Hard particles prefer compact shapes, while soft particles prefer plate-like shapes.
- Stress effect: Same sign of stress and eigenstrain favours the particle phase.
- Conclusion: Inhomogeneity determines extent of elongation, while sign of stress (vis a vis that of eigenstrain) determines growth rate.

Multi-particle: Rafting

$c_0 = 0.34$; $A_Z = 3$; $\delta = 0.5$; Uniaxial stress

(a) Tensile along x (b) Compresive along y

- Direction of rafting is the same as in single particles.
- Coalescence and particle migration also contribute to rafting.

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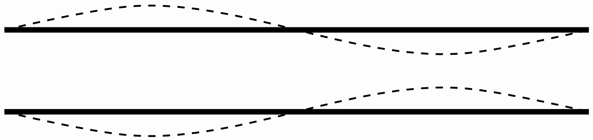
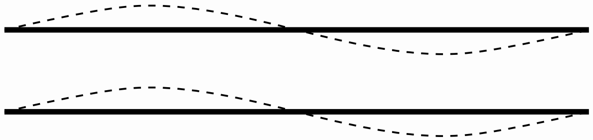
Thin film stability

- Hard film sandwiched between soft substrates; Isotropic elasticity (A_Z=1) and dilatational eigenstrain; Volume diffusion control.
- The hard (film) phase, which prefers compact shapes, is unstable.
- Types of break-up:



Symmetric



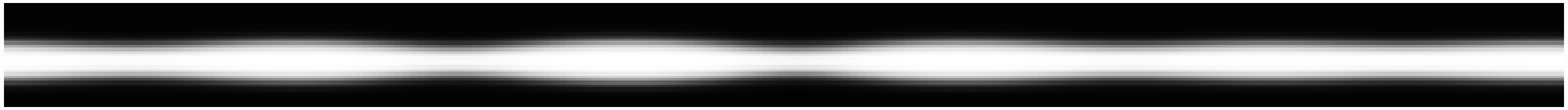
Antisymmetric

- Depends on θ, the ratio of interfacial and elastic energies, and δ. The break-up is antisymmetric for higher δ.

Symmetric onset ($\delta = 2$)

- For the fastest growing wave, $\lambda_{theory} = 97$ and $\lambda_{sim} = 102$.

Onset (t=115000)



Break-up (t=122000)

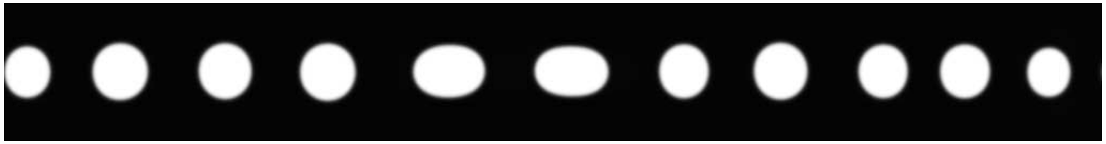
Late-stage (t=143000)

Antisymmetric onset ($\delta = 4$)

Onset (t=20000)

Break-up (t=25000)

Late-stage (t=34000)



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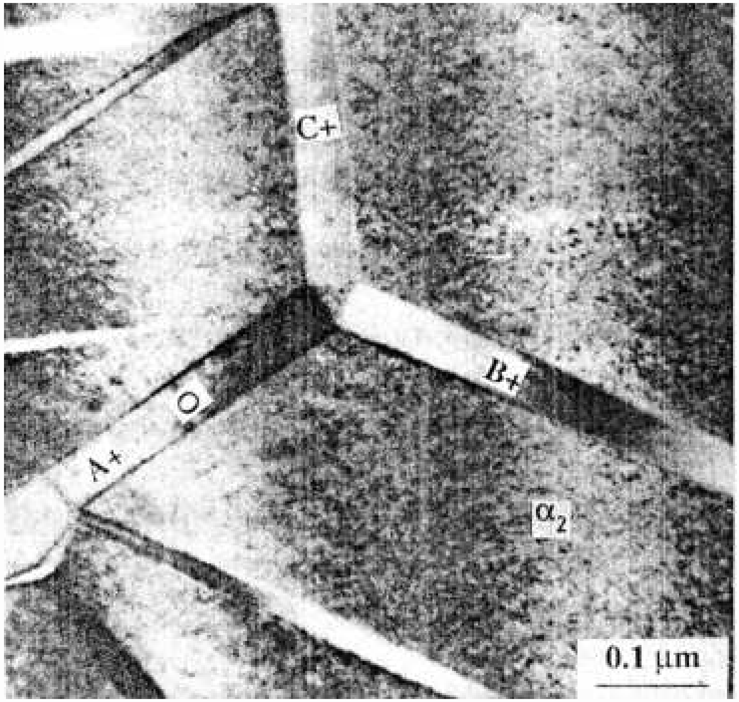
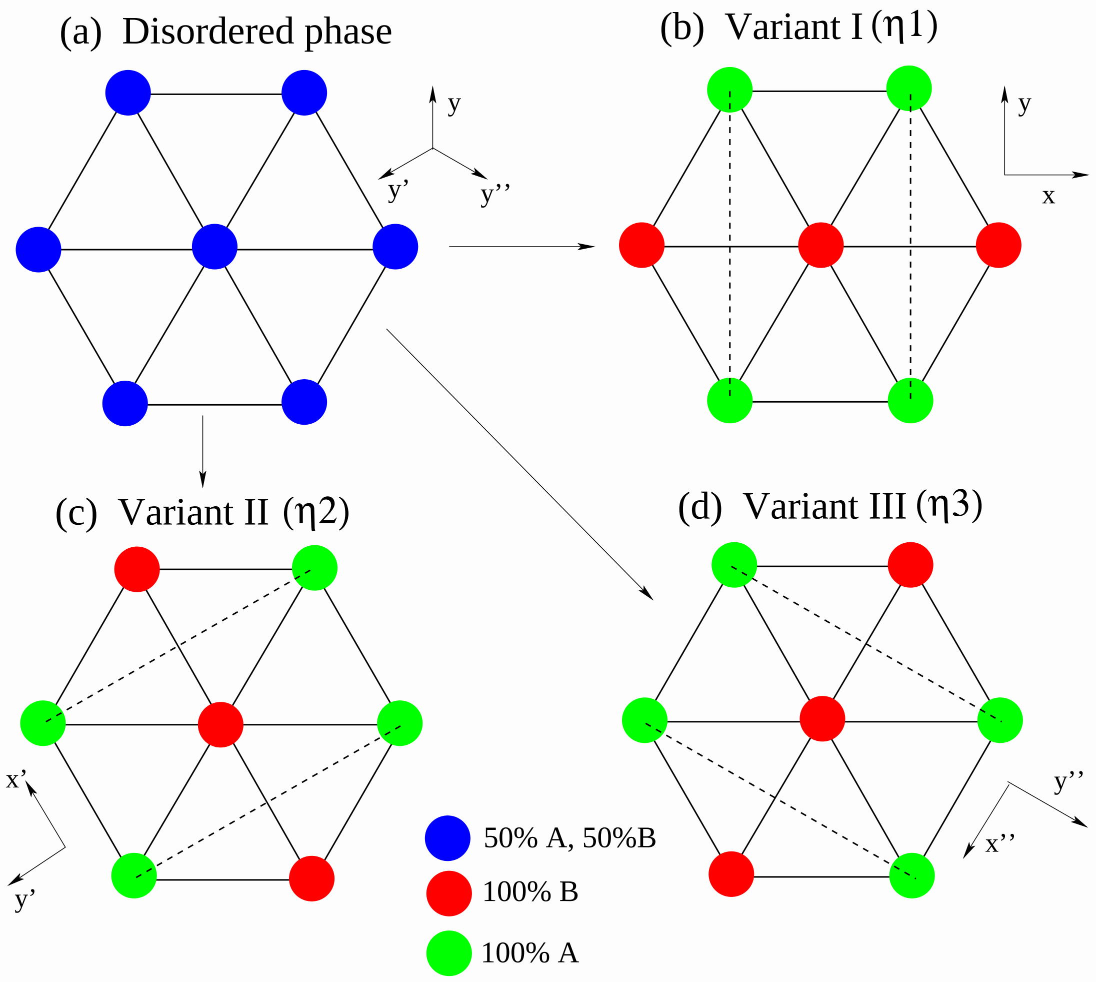
Multiple variants



Ti-28.5Al-13Nb: three-sided star with **O** phase variants in α_2 phase (Muraleedharan et al., 1994)

Orientational variants



Misfit strain tensor

For the first variant:

$$\epsilon_{ij} = \epsilon \begin{pmatrix} 1 & 0 \\ 0 & t \end{pmatrix}$$

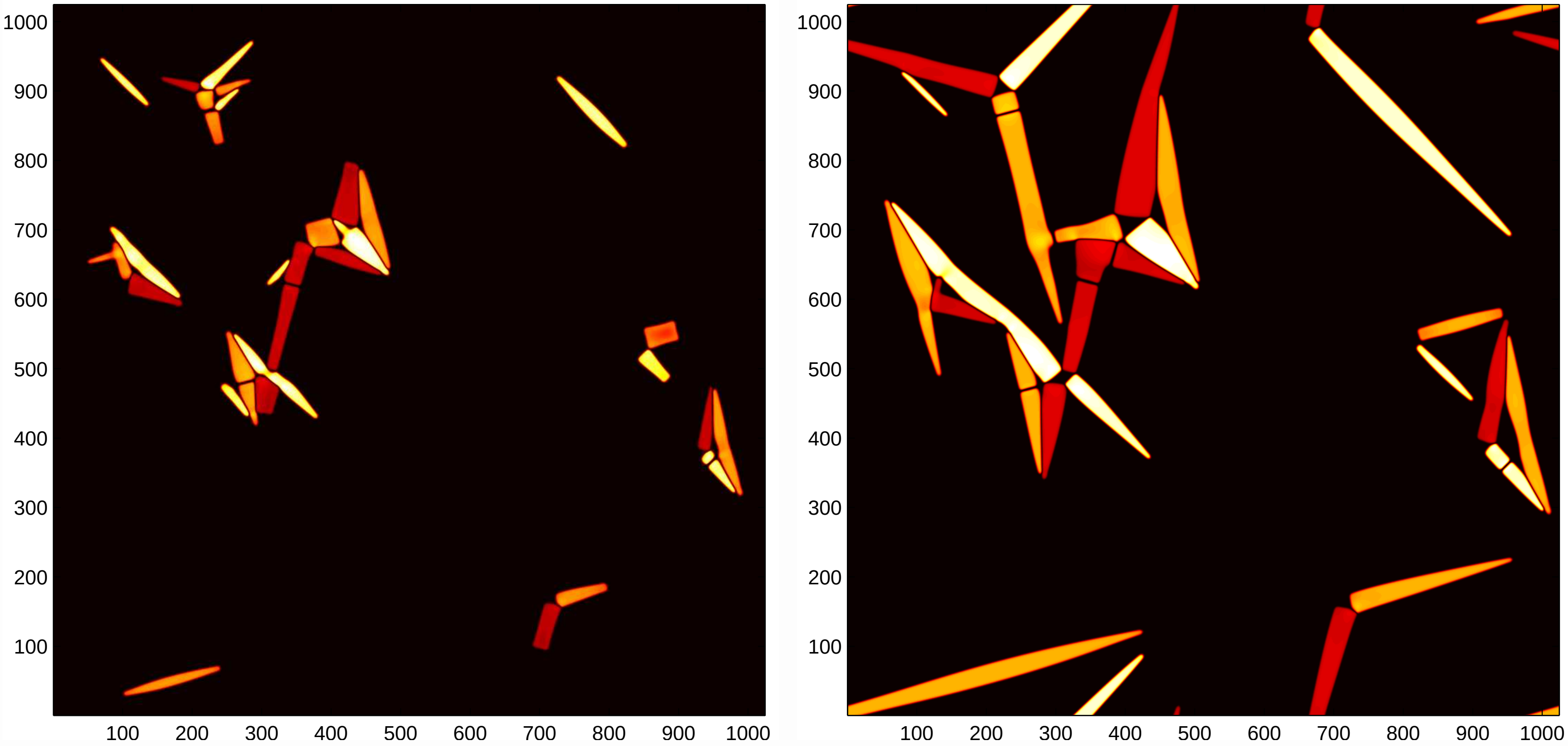
- Magnitude of misfit: ϵ
- Anisotropy in misfit: $\epsilon_{xx} \neq \epsilon_{yy}$; $-1 \leq t \leq 1$

  Isotropy when $t = 1$.
- Misfit tensors for the other variants are obtained by rotating this tensor by 120° and 240°.

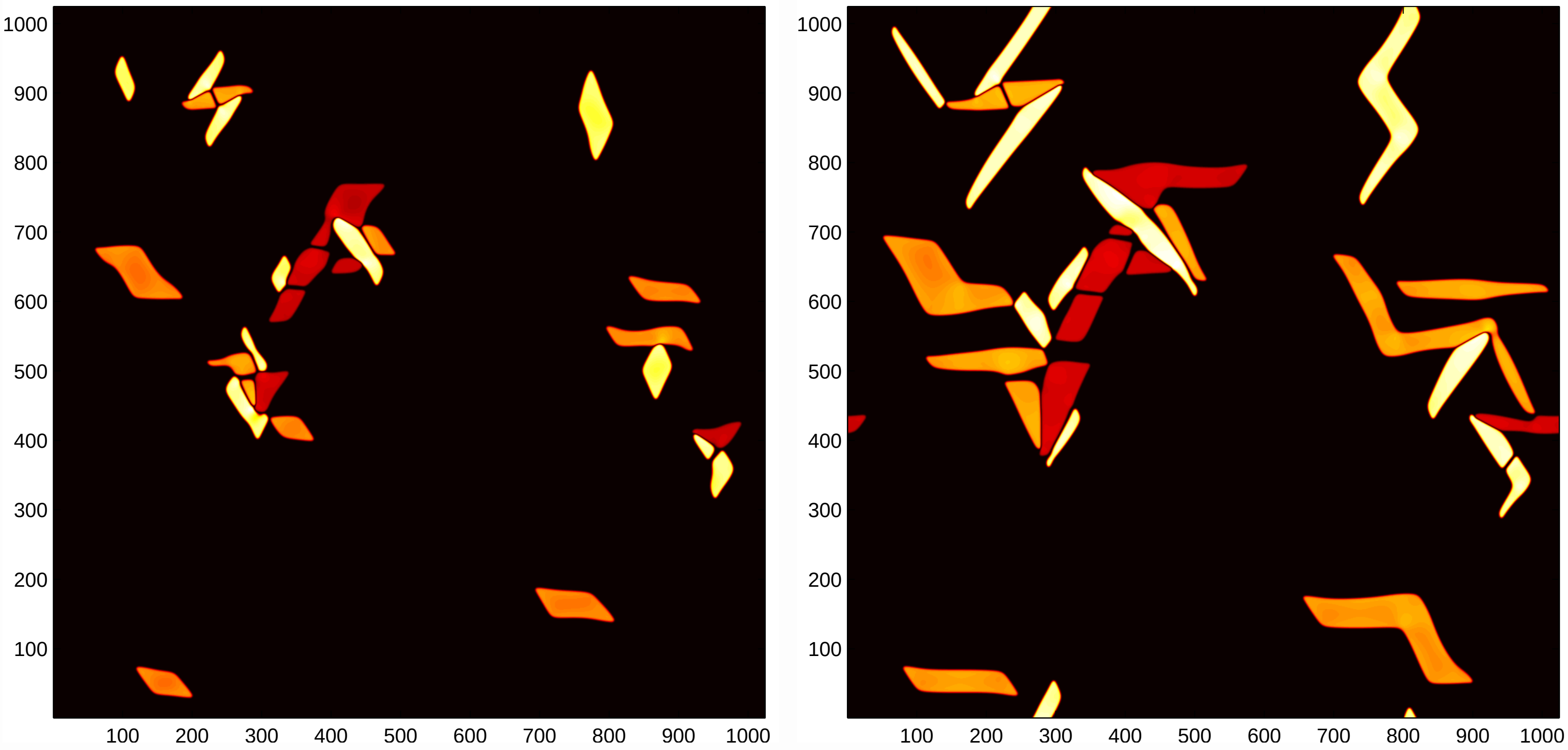
Special anisotropy: $t = -1$

- When $t = -1$ (the two principal misfits are equal and opposite):
- Sum of the misfits from the three variants is zero!
- During nucleation, the three variants can be formed in close proximity so as to minimize the elastic strain energy.

Special anisotropy: $t = -1$



$t = -0.5$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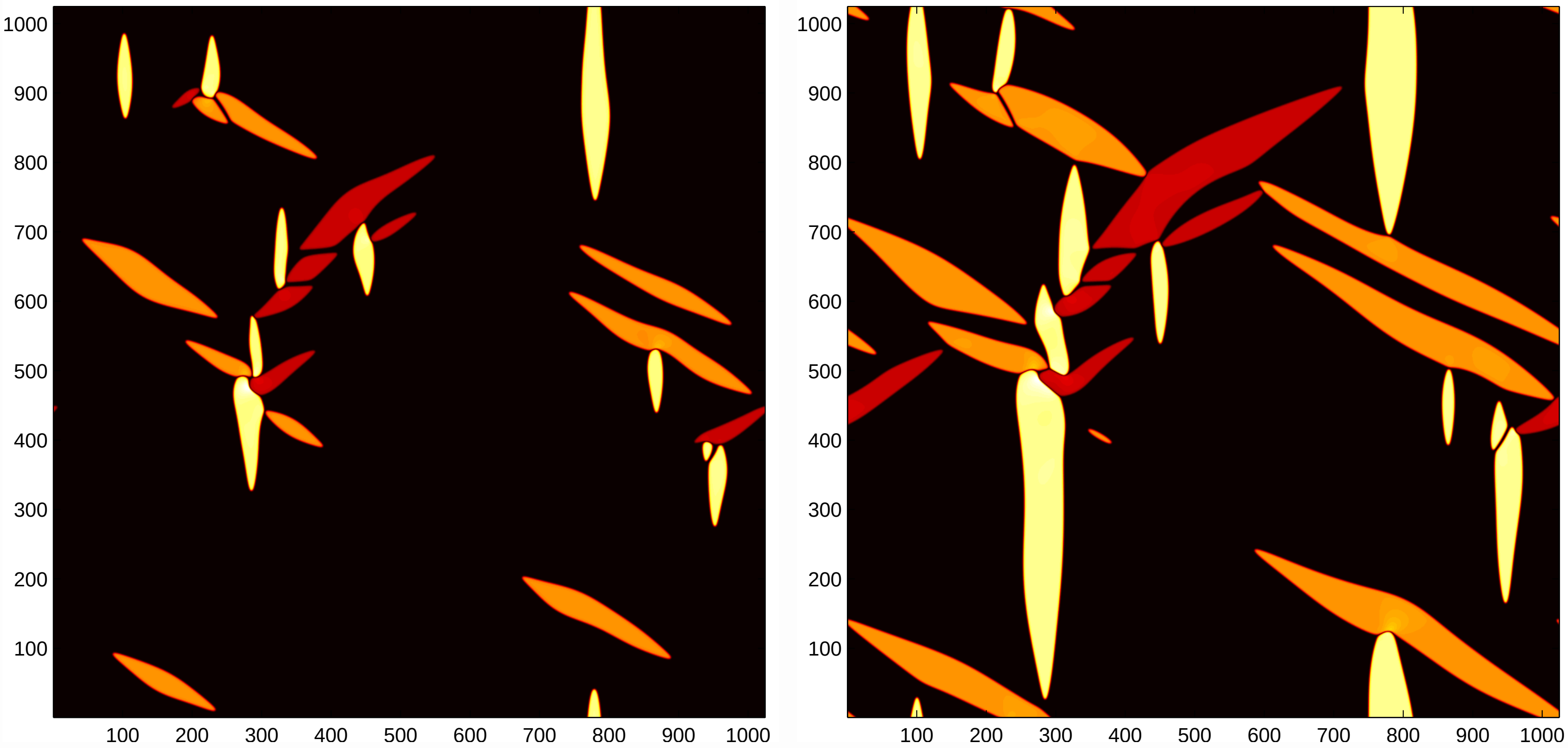
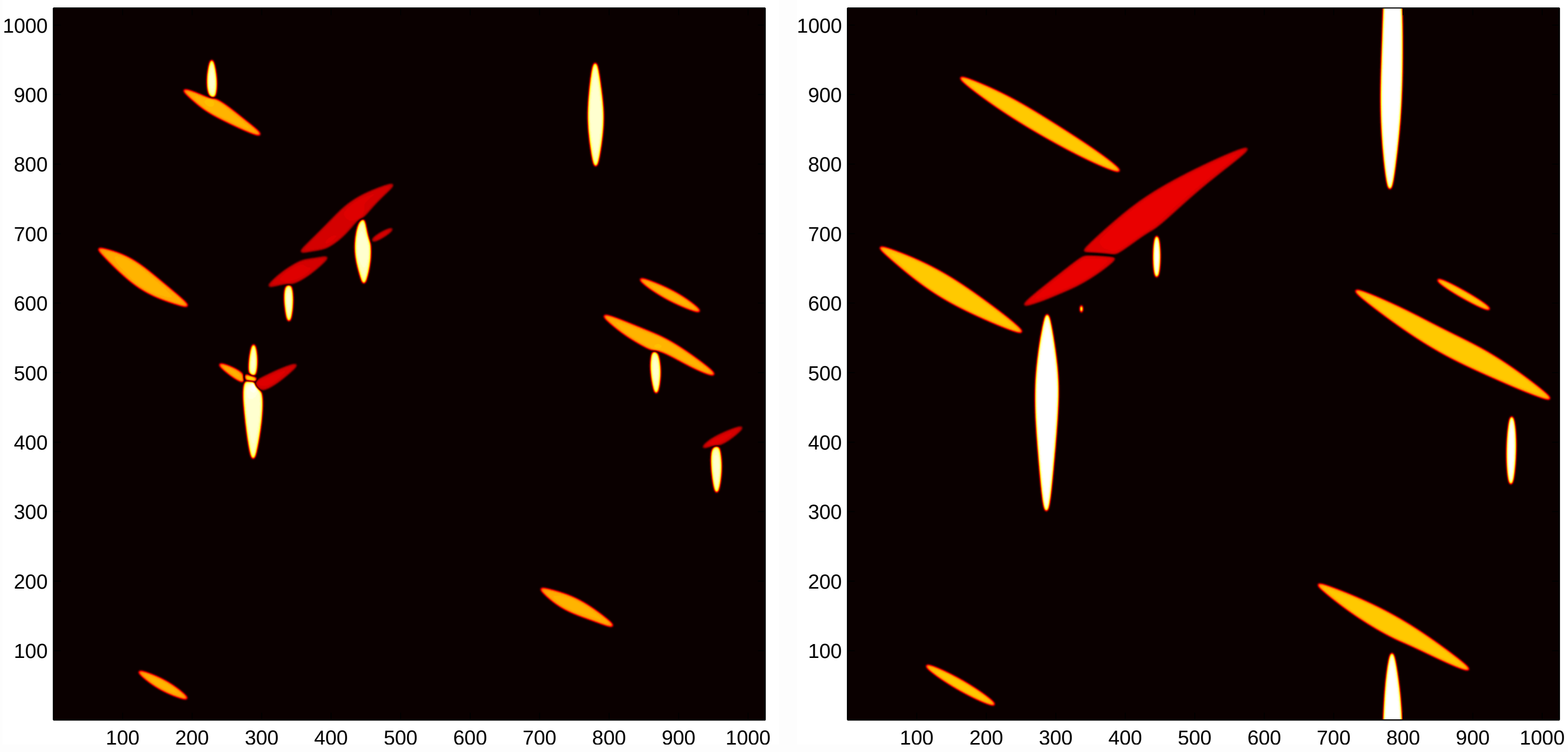
$t = 0$: Misfit along y is zero



$t = +0.5$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Summary

- Elastic stresses have a strong influence on microstructures.
- Phase field models as a tool for studying stress effects.
- Elastic modulus mismatch: Rafting (directional coarsening) under an uniaxial stress.
- Elastic modulus mismatch: Thin film instabilities.
- Microstructures with multiple variants.

Thank you!