

Predicting γ/γ' Microstructure in Ni-Based Superalloys Using Phase Field Method

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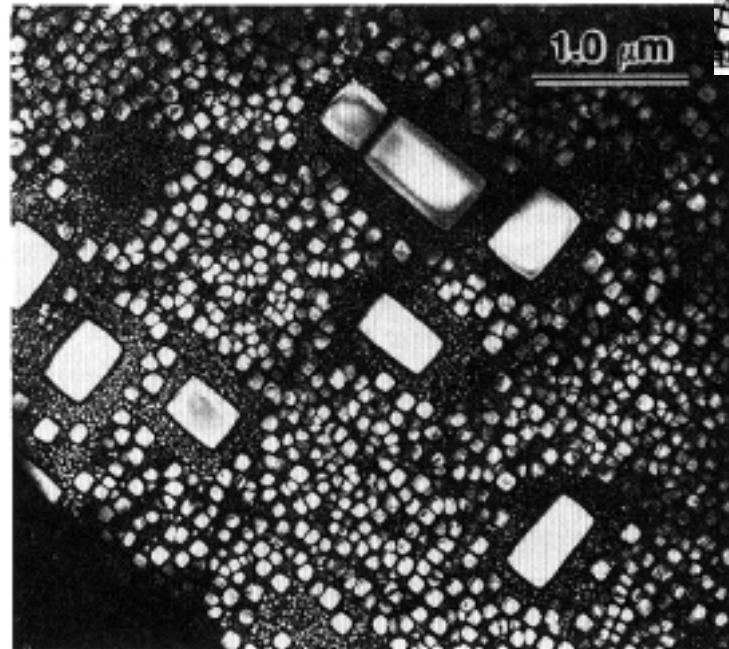
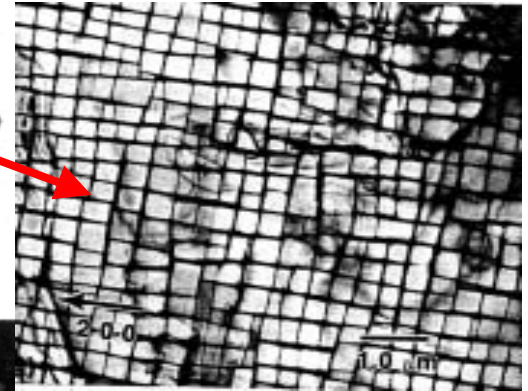
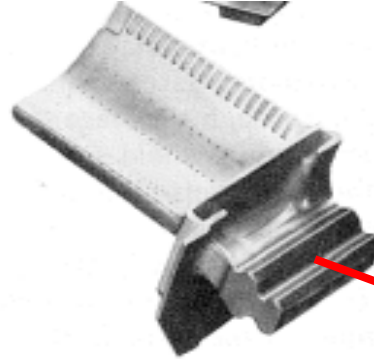
Outline

- Challenges for modeling γ/γ' microstructures
- Introduction to the phase field method
- Issues to be addressed to develop the phase field method into a useful engineering tool
 - concurrent nucleation, growth and coarsening
 - effect of elastic interaction on nucleation
 - linking to thermodynamic and diffusivity databases
- Summary

Complexity of γ/γ' Microstructure

Superalloy turbine blade materials

- very high volume fraction (>60%) of precipitates
- strong elastic interactions among precipitates
- non-spherical shape and strong spatial correlation
- bimodal distribution forms on continuous cooling

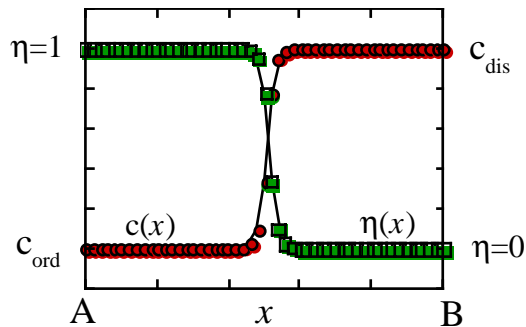
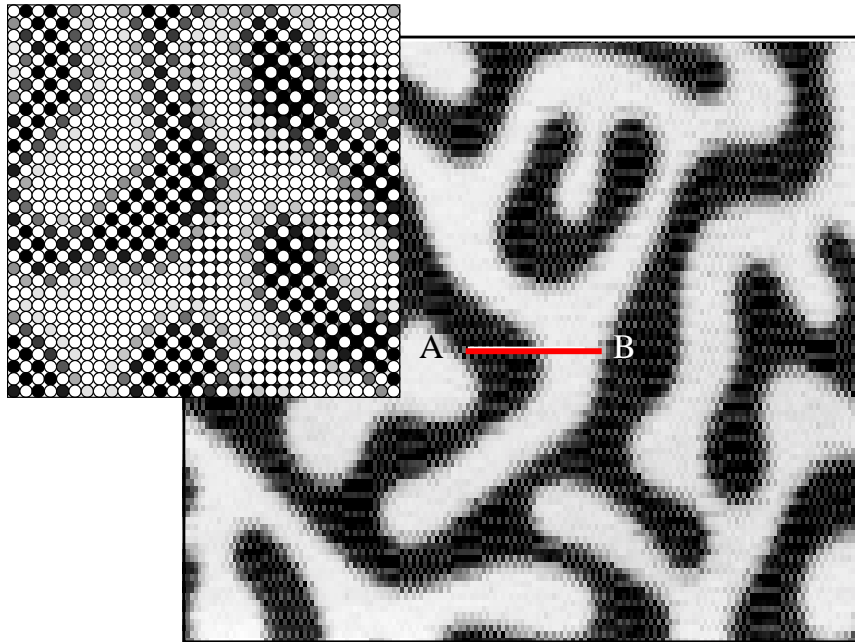


Requirements

Any useful engineering tools, capable of making quantitative prediction of the γ/γ' microstructures, should be able to deal with simultaneously the following:

- Large supersaturation, high volume fraction, arbitrary particle shape, strong spatial correlation, ordered precipitates.
- Non-isothermal processes - concurrent nucleation, growth and coarsening.
- Effect of elastic interactions on nucleation, growth and coarsening.
- Accurate treatment of multicomponent diffusion, boundary migration and alloy thermodynamics.
- Computational efficiency and robustness of models developed.

Phase Field Model



- Kinetic Equations

$$\frac{dX_i}{dt} = -L_i \frac{dF}{dX_i}, \quad \begin{aligned} X_i &= X_i(\mathbf{r}) \\ F &= F(X_1, X_2, \dots) \end{aligned}$$

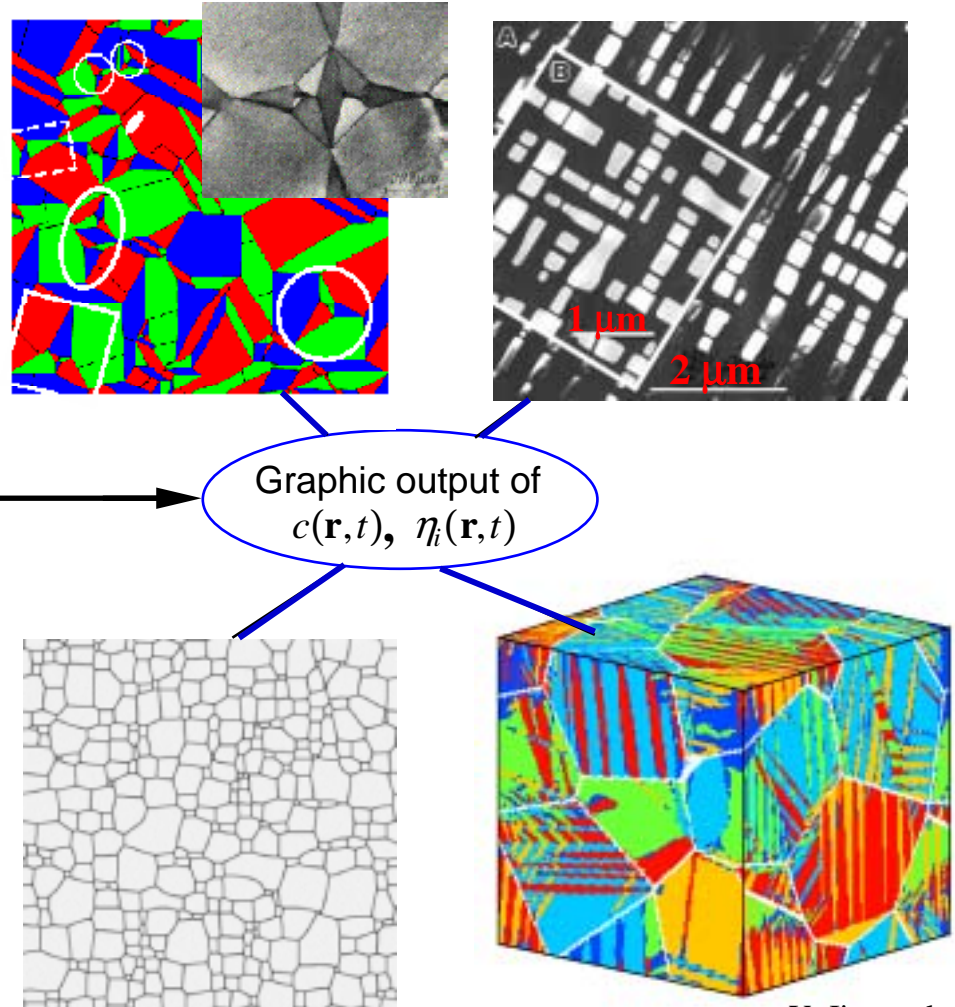
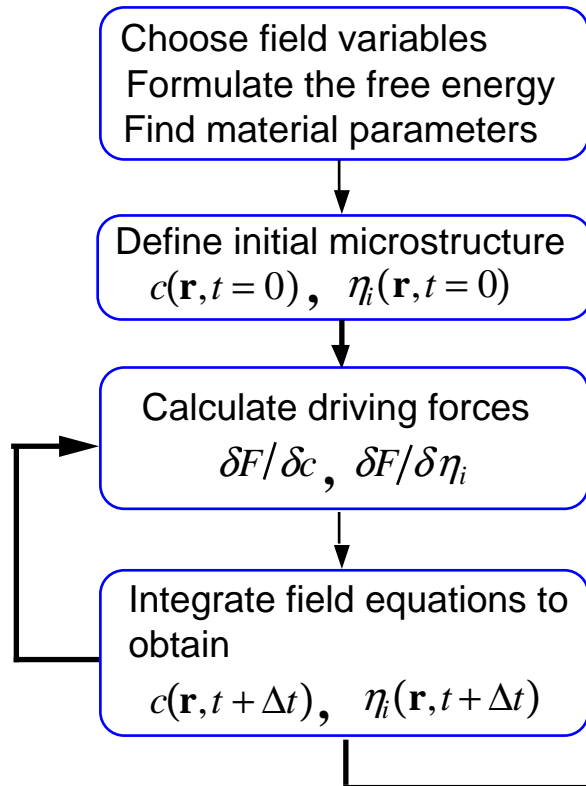
$$\frac{\partial c(\mathbf{r}, t)}{\partial t} = \nabla \cdot \left(M \nabla \frac{\delta F}{\delta c(\mathbf{r}, t)} \right) + \xi_c(\mathbf{r}, t)$$

$$\frac{\partial \eta_p(\mathbf{r}, t)}{\partial t} = -L \frac{\delta F}{\delta \eta_p(\mathbf{r}, t)} + \xi_p(\mathbf{r}, t)$$

$$F = F_{chem} + E_{el}$$

Phase Field Model

- Basic Procedures



Y. Jin et. al.

Focusing on superalloys, phase field handles well high volume fraction, non-spherical particle shape and elastic interactions between particles.

Limitations

Current phase field models are

- qualitative in nature
- limited to isothermal conditions with site-saturation approximation for nucleation
- most work done on model systems without material-specific inputs.
- computationally intensive

In order to develop the phase field method into a quantitative engineering tool for γ/γ' microstructure prediction, we must:

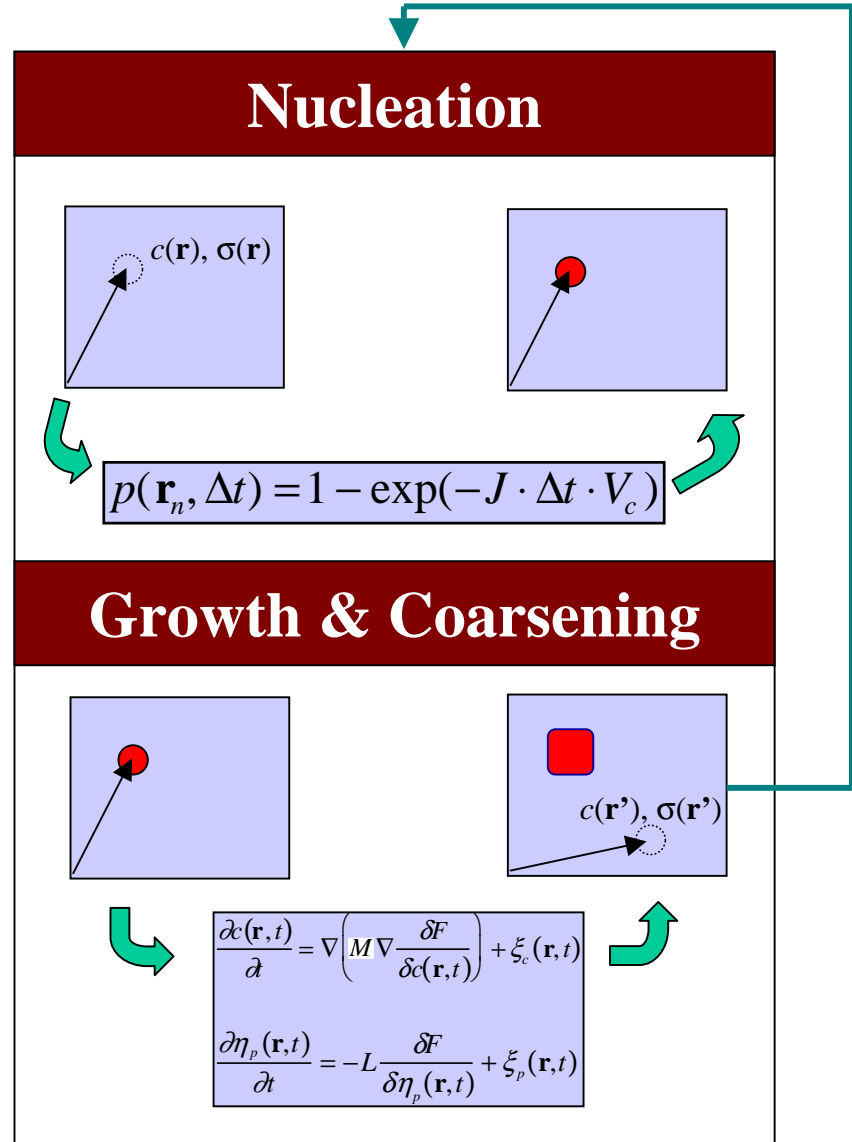
- incorporate explicitly nucleation to deal with non-isothermal processes - concurrent nucleation, growth and coarsening
- account for elastic interaction during nucleation
- link to multicomponent diffusion and alloy thermodynamic databases for material-specific parameters (Asta, Hoyt & Kama, Wolverton & Chen, Grafe & Bottger, Asta, Chang, Wilkins and Wang, ...)
- develop more efficient algorithms and/or establish constitutive relations

Explicit Nucleation Algorithm

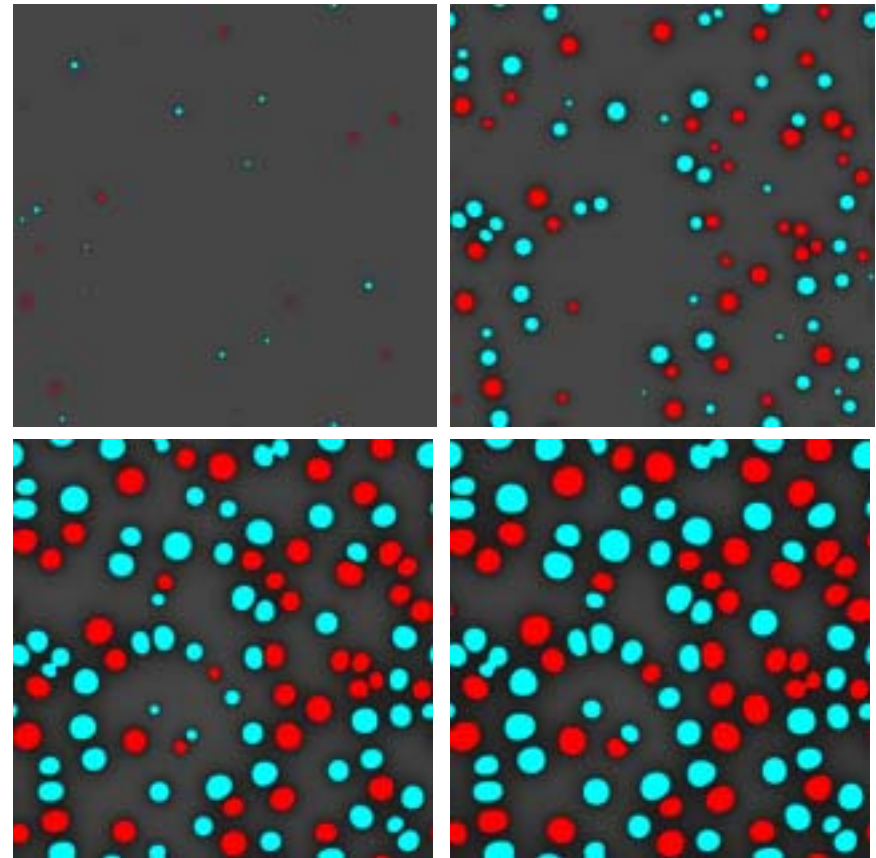
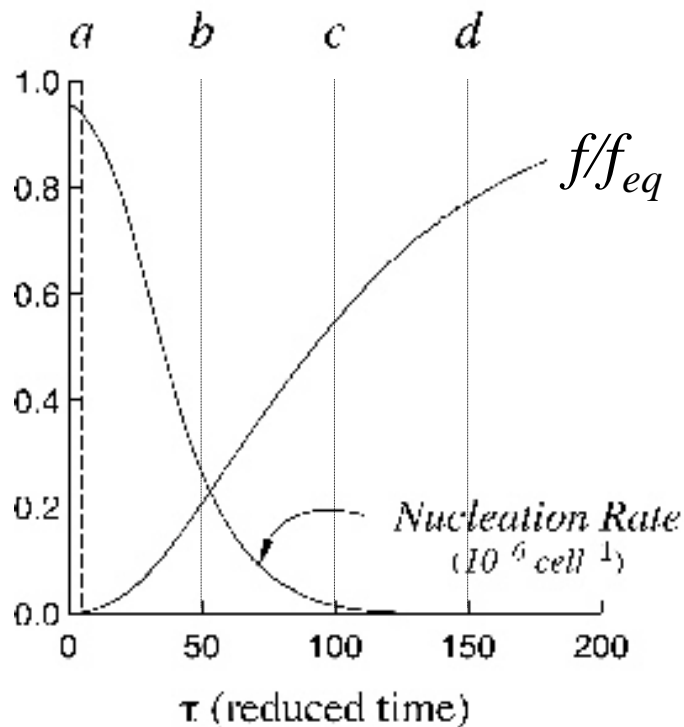
Determination of Nucleation Rate as a Function of Supersaturation and Stress

- Theory
- Experiment
- Simulations

$J(c, \sigma)$

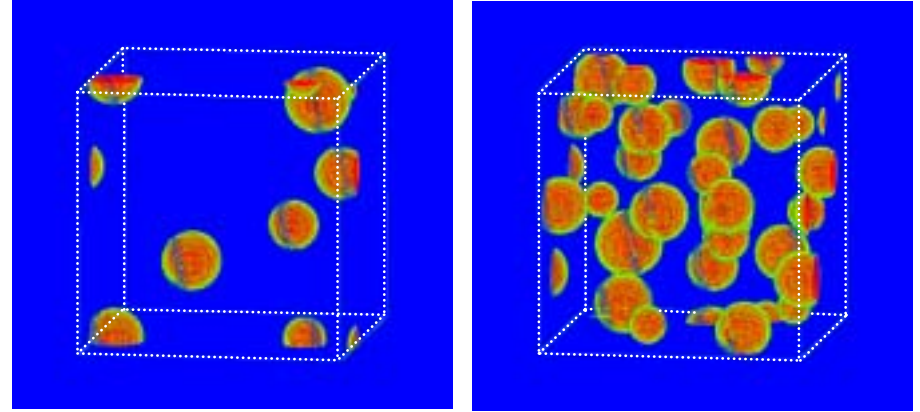
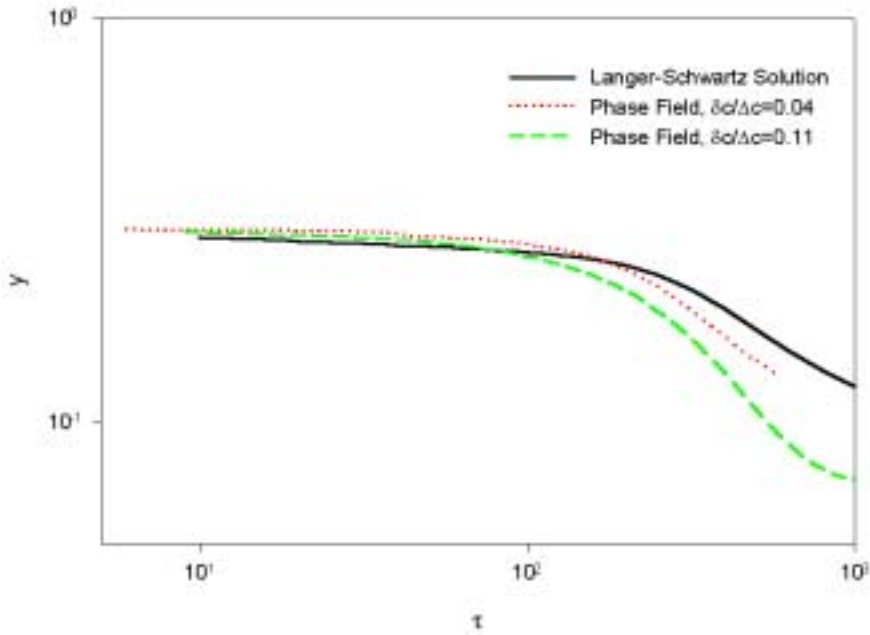


Concurrent Nucleation, Growth and Coarsening under Isothermal Conditions



a|b
c|d

Comparison with Langer-Schwartz Model



LS model: close form, computationally efficient.

• **Limitations:**

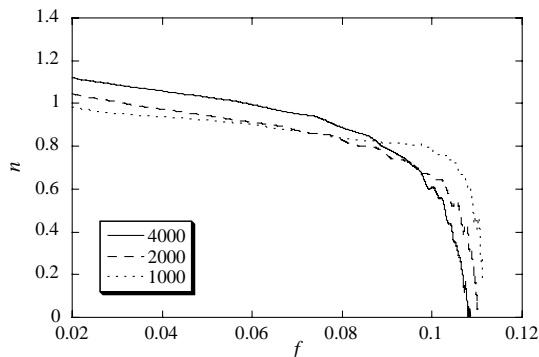
- no microstructural details, no elastic interactions, spherical particles with small and uniform supersaturation, no particle coalescence.
- linear capillarity and simple size distribution function (relaxed by Kampmann and Wagner later on).
- linearized free energy model ($f'' = \text{constant}$, independent of composition)
- constant diffusivity.

Overall Transformation Kinetics

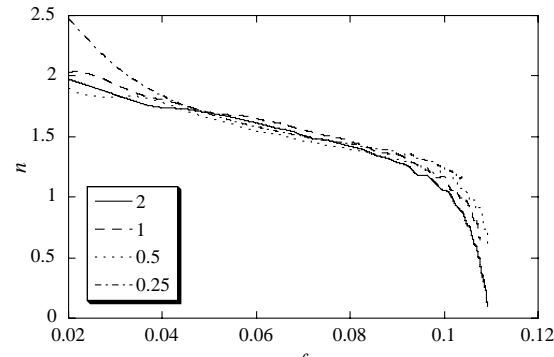
- Johnson-Mehl-Avrami- Kolmogorov (JMAK) Theory
 - Point nuclei form randomly in infinite media
 - Grow isotropically with constant rate, cease when impinges (hard impingement)

$$f = 1 - \exp(-f_{xt}) = 1 - \exp(-\alpha t^n)$$

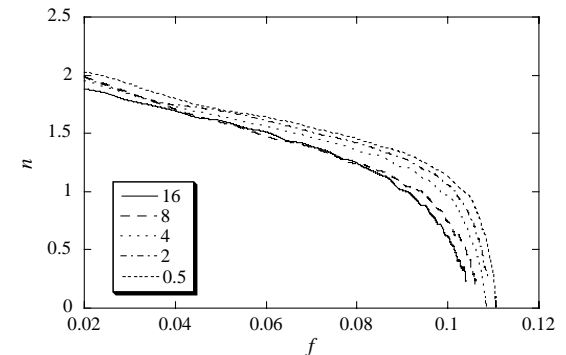
- Phase Field Predictions (2-D):
n values extracted from phase field simulations



site-saturation: $n=1$

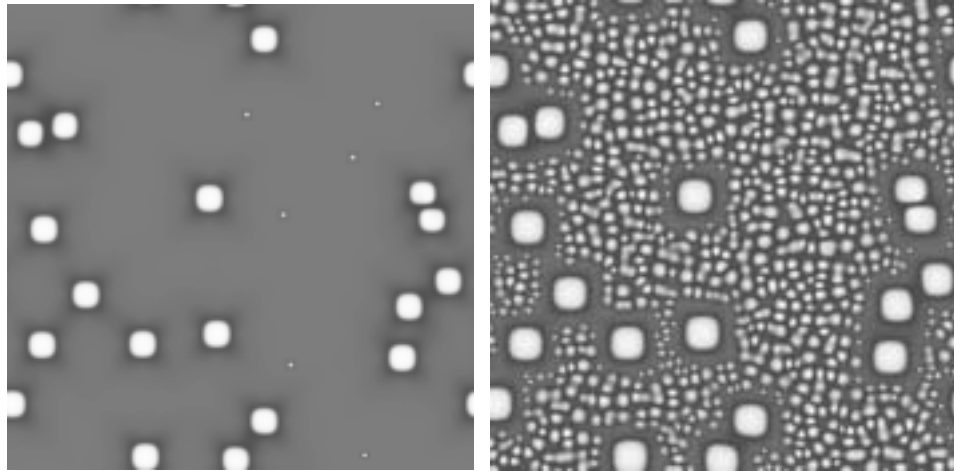


constant nucleation rate: $n=2$



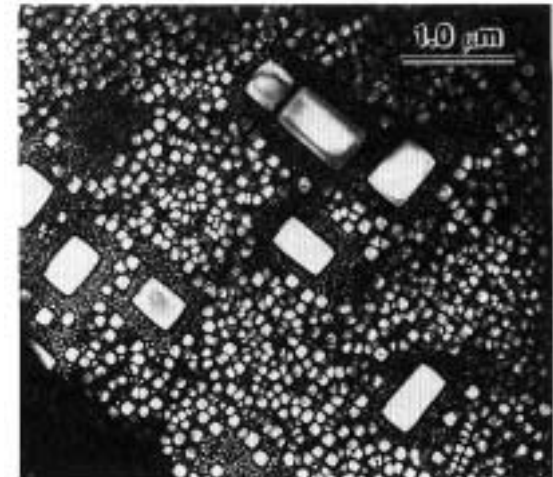
concurrent nucleation and growth: $1 < n < 2$

Continuous Cooling

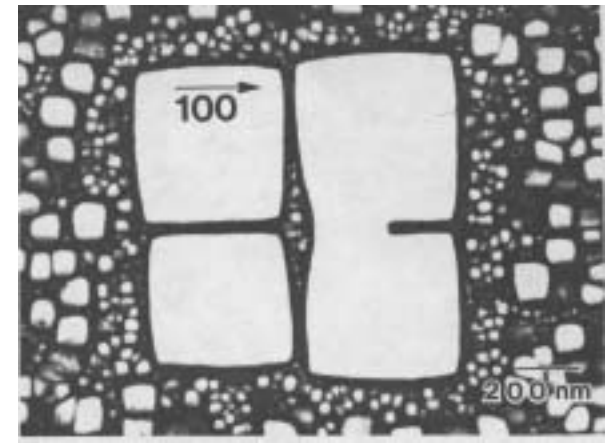
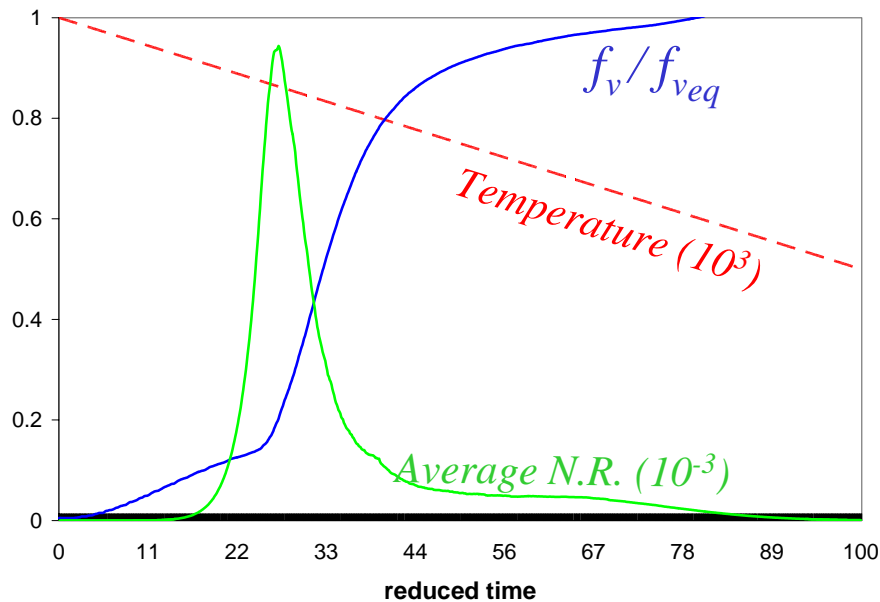


$\tau=25$

$\tau=100$

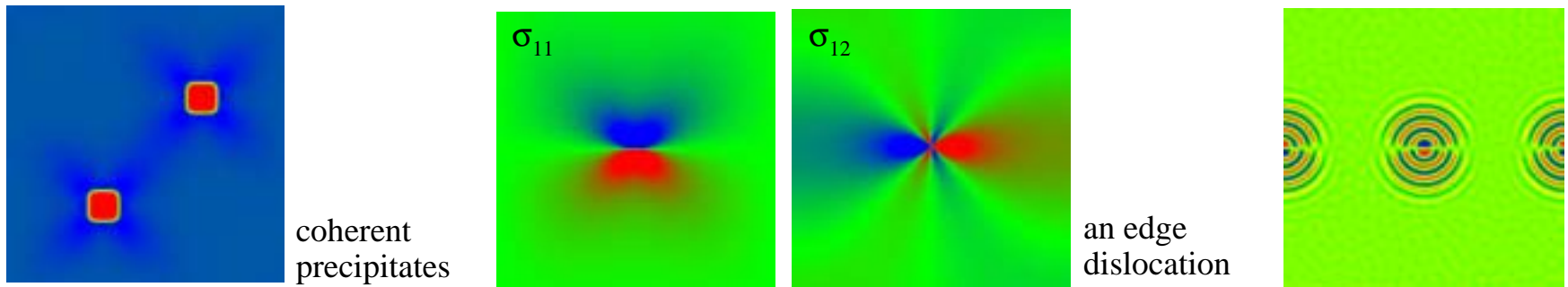


M. E. Gurtin and P. W. Voorhees.

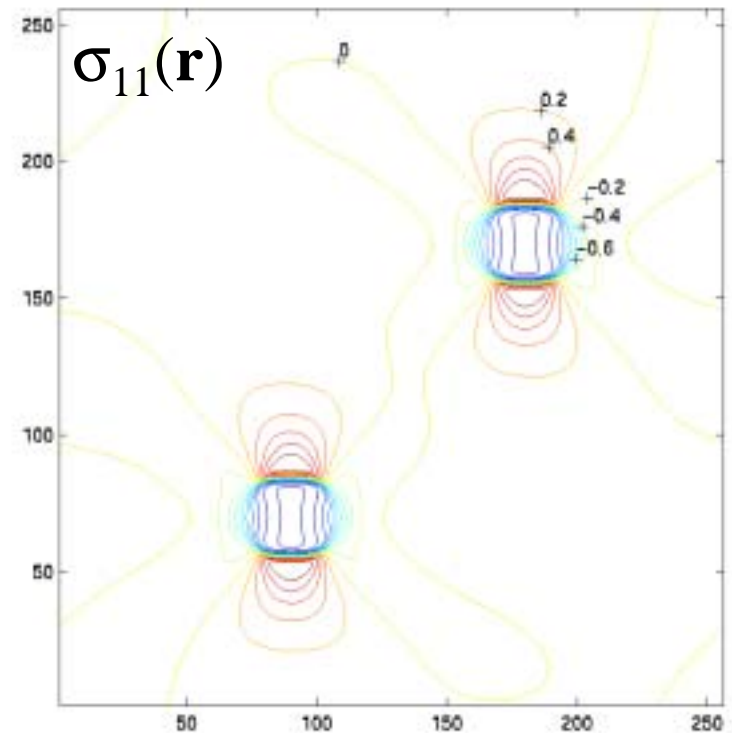
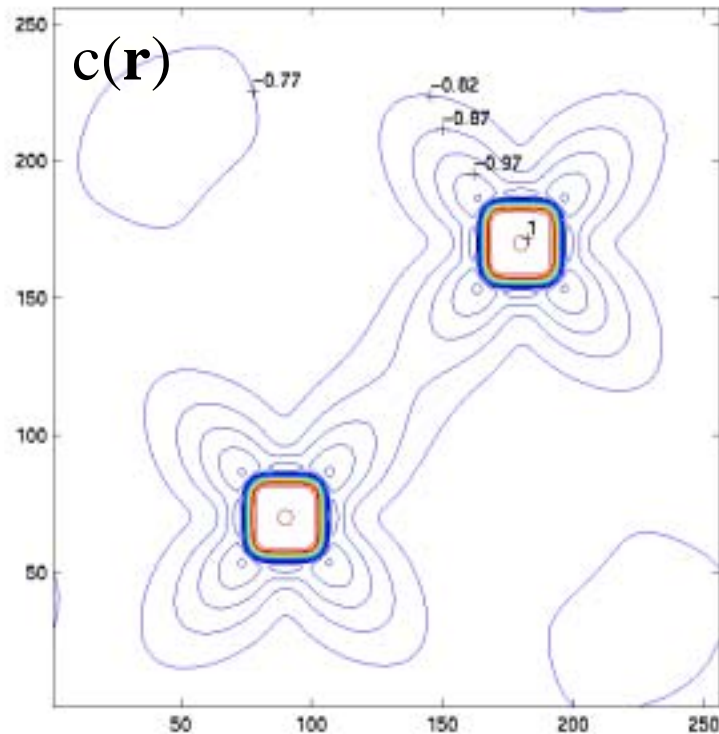


M. J. Kaufman et al.

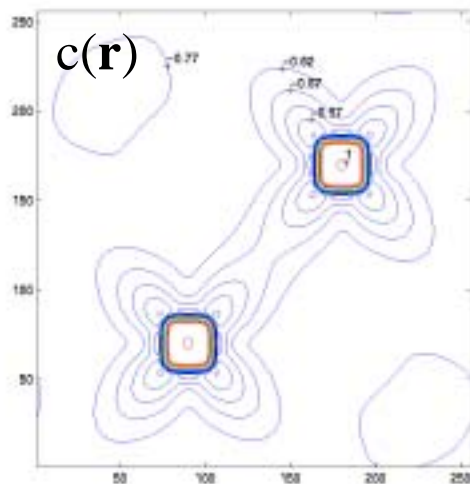
Nucleation in the Stress Field of Existing Particles



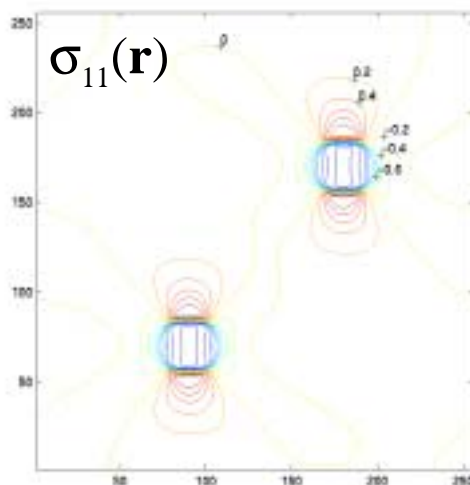
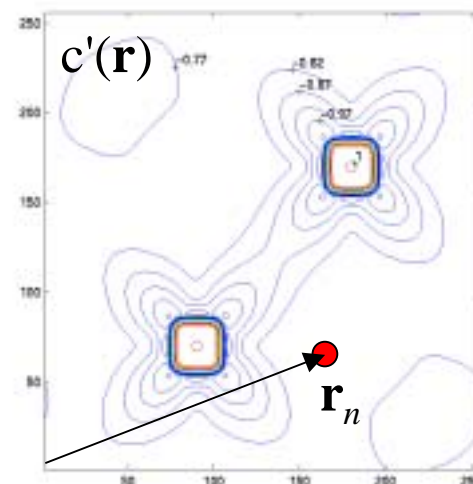
Focusing on coherent precipitates



Free Energy Change

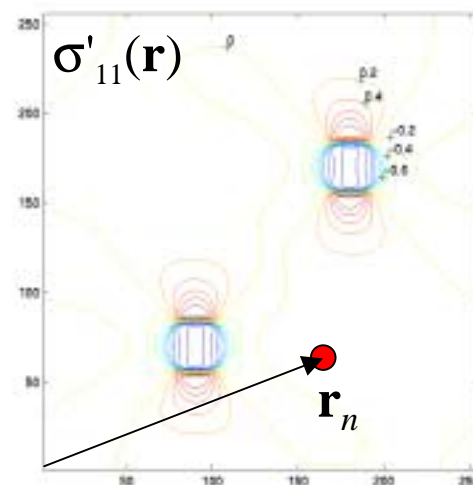


$$\Delta F = \Delta F_{chem} + \Delta E_{el}$$



$$\Delta F_{chem} = F'_{chem} - F_{chem}$$

$$\Delta E_{el} = E'_{el} - E_{el}$$



before the nucleation event

$$F = F_{chem} + E_{el}$$

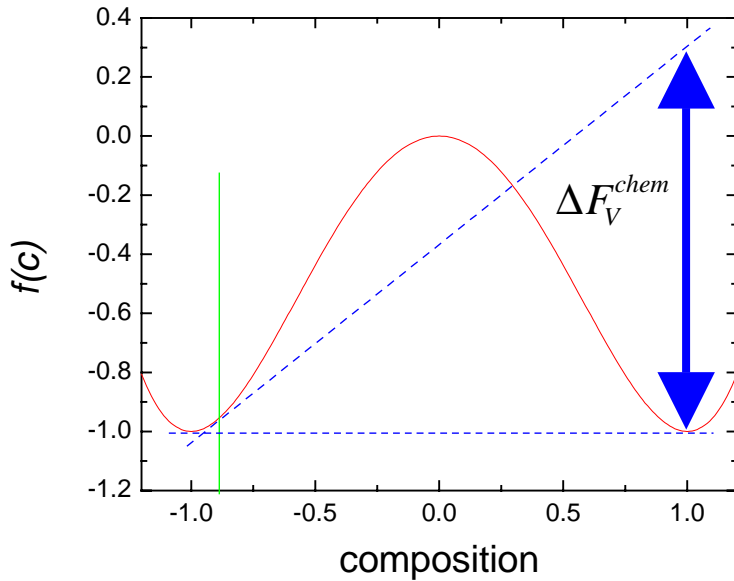
after the nucleation event

$$F' = F'_{chem} + E'_{el}$$

Free Energy Change

Chemical Free Energy Change

$$f(c) = -2c^2 + c^4$$



Elastic Energy Change

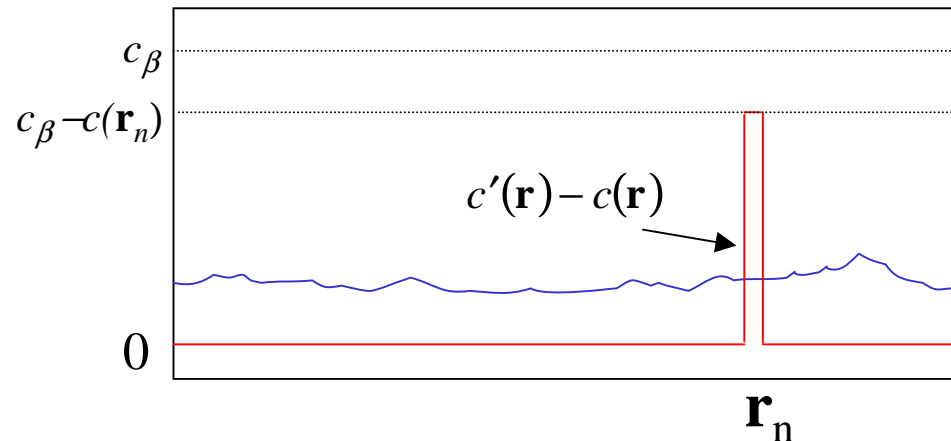
$$E^{el} = \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} B(\mathbf{n}) \tilde{c}(\mathbf{k}) \tilde{c}^*(\mathbf{k})$$

$$\Delta E_{el} = E'_{el} - E_{el}$$

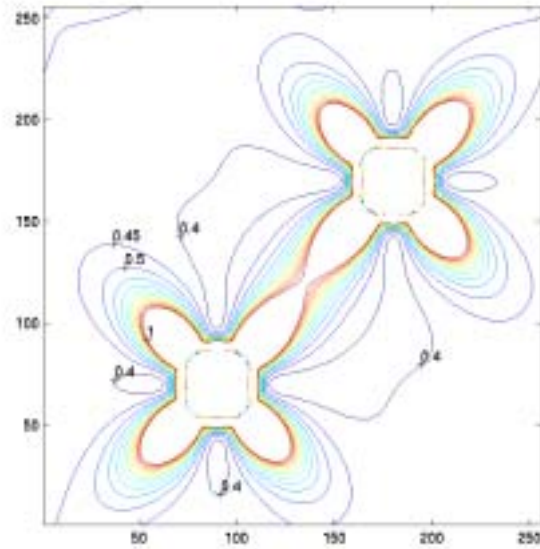
$$= \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} B(\mathbf{n}) [(\tilde{c} + \Delta\tilde{c})(\tilde{c}^* + \Delta\tilde{c}^*) - \tilde{c} \cdot \tilde{c}^*]$$

$$\Delta\tilde{c}(\mathbf{k}) = \{c'(\mathbf{r}) - c(\mathbf{r})\}_k \cong [c_\beta - c(\mathbf{r}_n)] \Delta V_n e^{i\mathbf{k} \cdot \mathbf{r}_n}$$

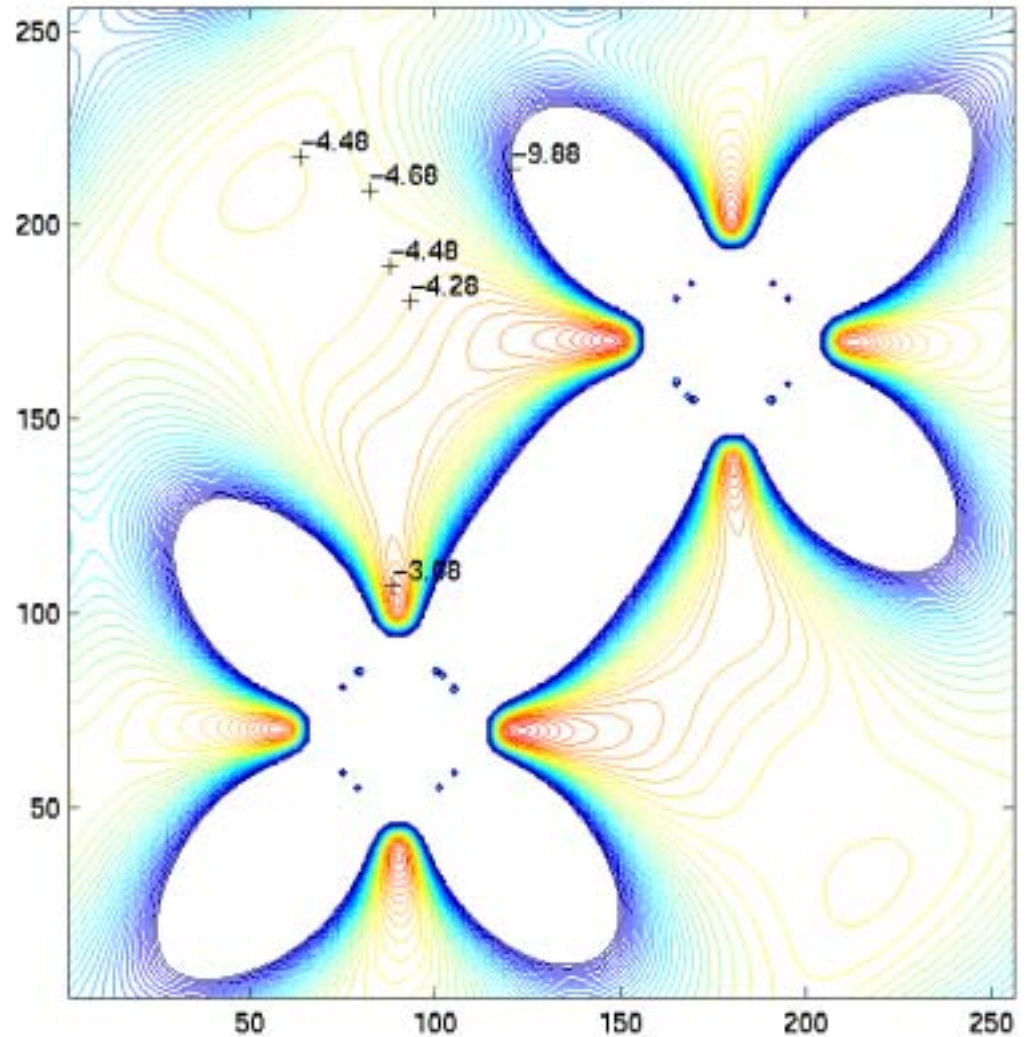
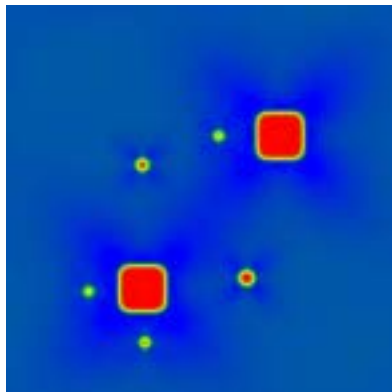
$$\Delta E_V^{el}(\mathbf{r}_n) \cong \frac{\Delta E_{el}(\mathbf{r}_n)}{\Delta V_n}$$



Activation Energy and Nucleation Rate

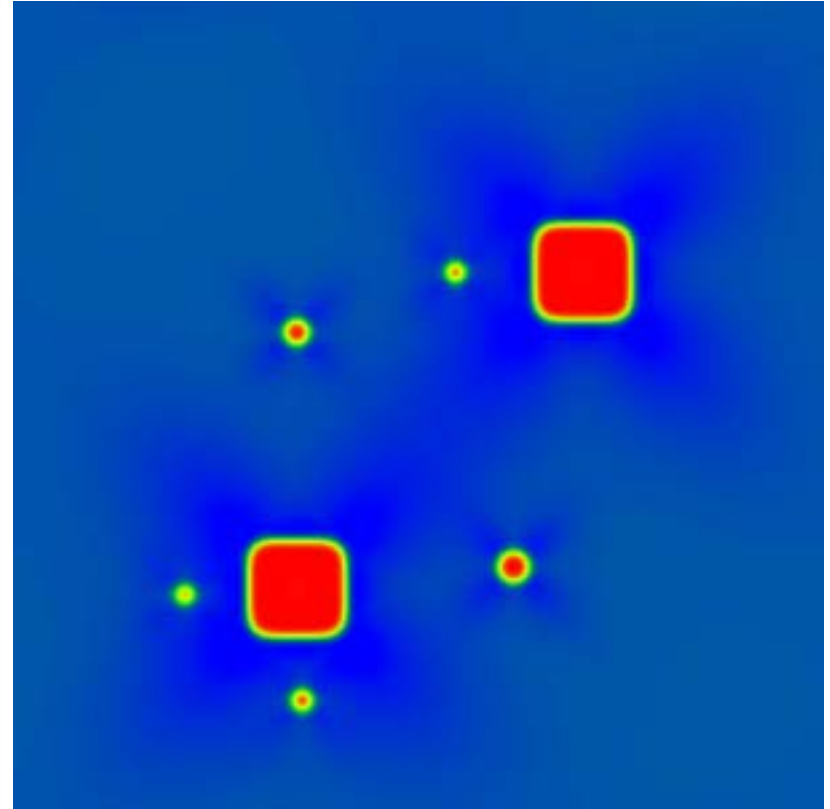
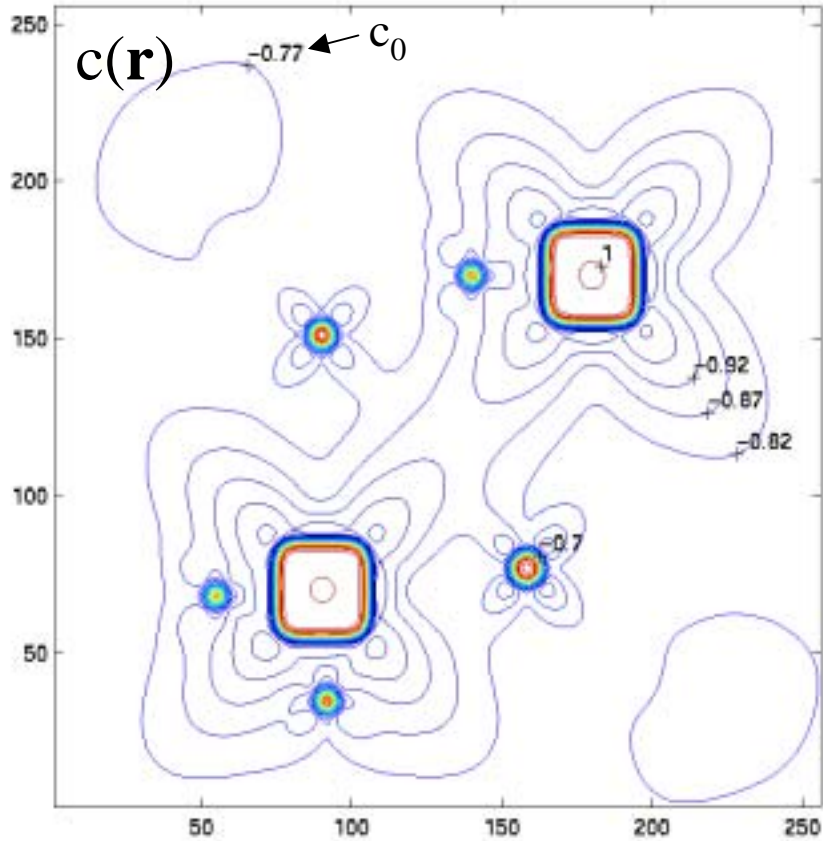


$$\Delta F_{2D}^* = \frac{\alpha \gamma^2}{\Delta F_V^{chem} + \Delta E_V^{el}}$$



$\log J^*(\mathbf{r})$

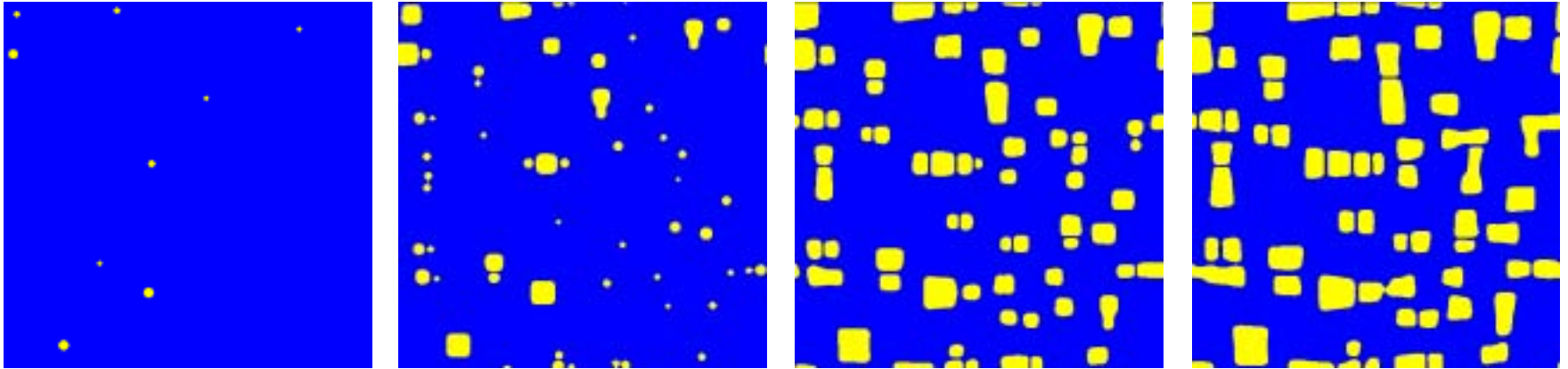
Simulation Results



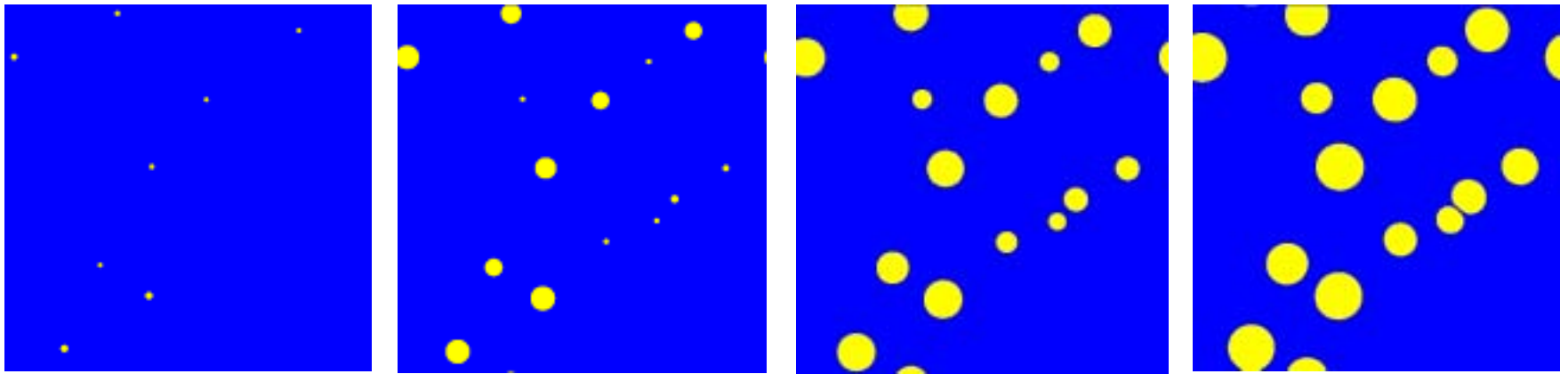
- Nucleation does not occur at the highest supersaturation locations
- Most of the nuclei appear along the elastically soft directions

Simulation Results

time evolution
→



misfitting particles

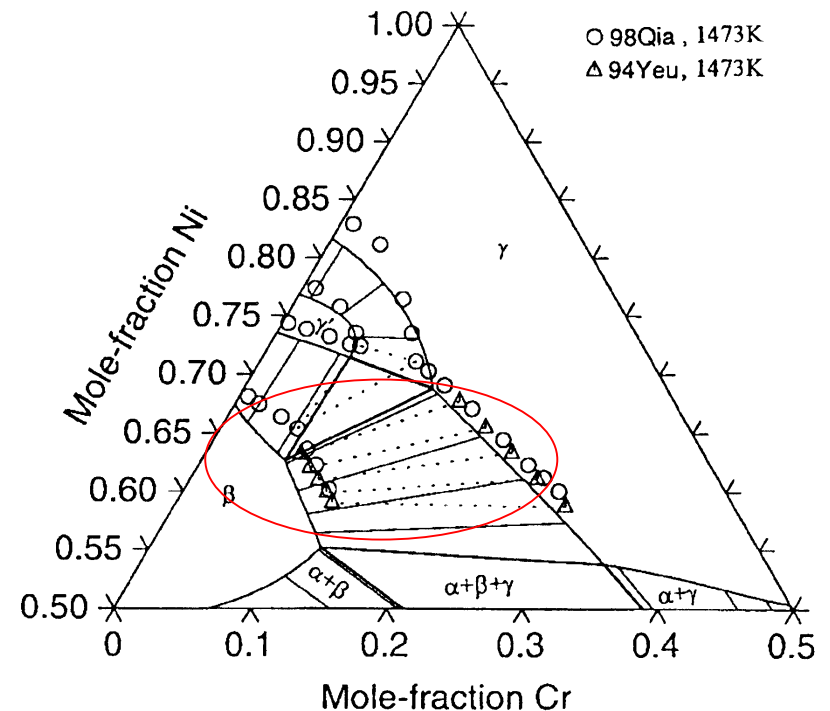
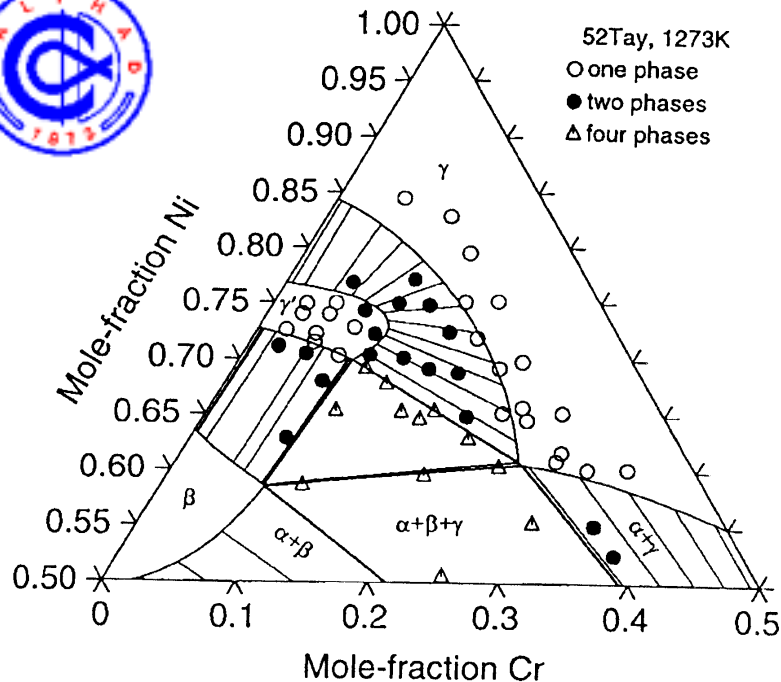


stress-free particles

Linking to CALPHAD Method

Ni-Al-Cr System: Thermodynamic Data

W. Huang and Y.A.Chang



Linking to CALPHAD Method

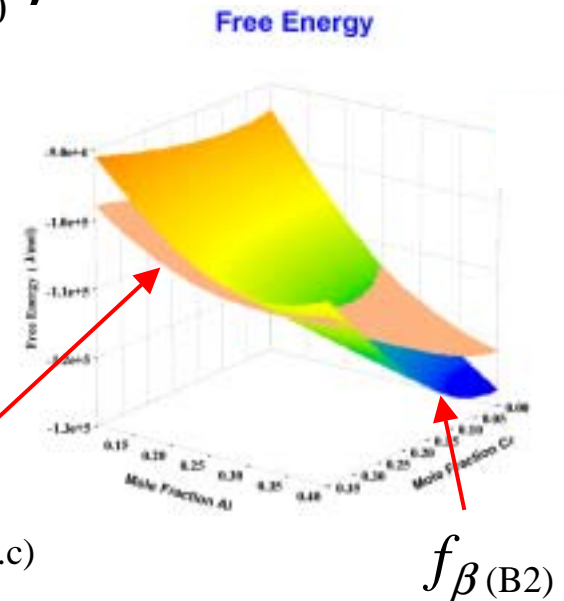
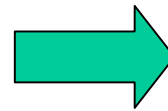
Ni-Al-Cr system

$$f(X_{Cr}, X_{Al}, \eta) = f^\gamma(X_{Cr}, X_{Al}) + f_1(X_{Cr}, X_{Al}, \eta)$$

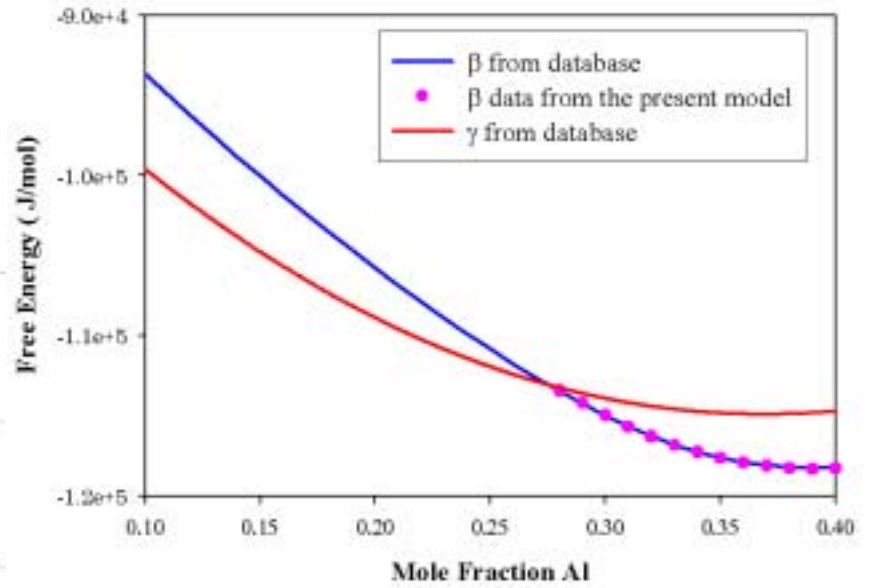
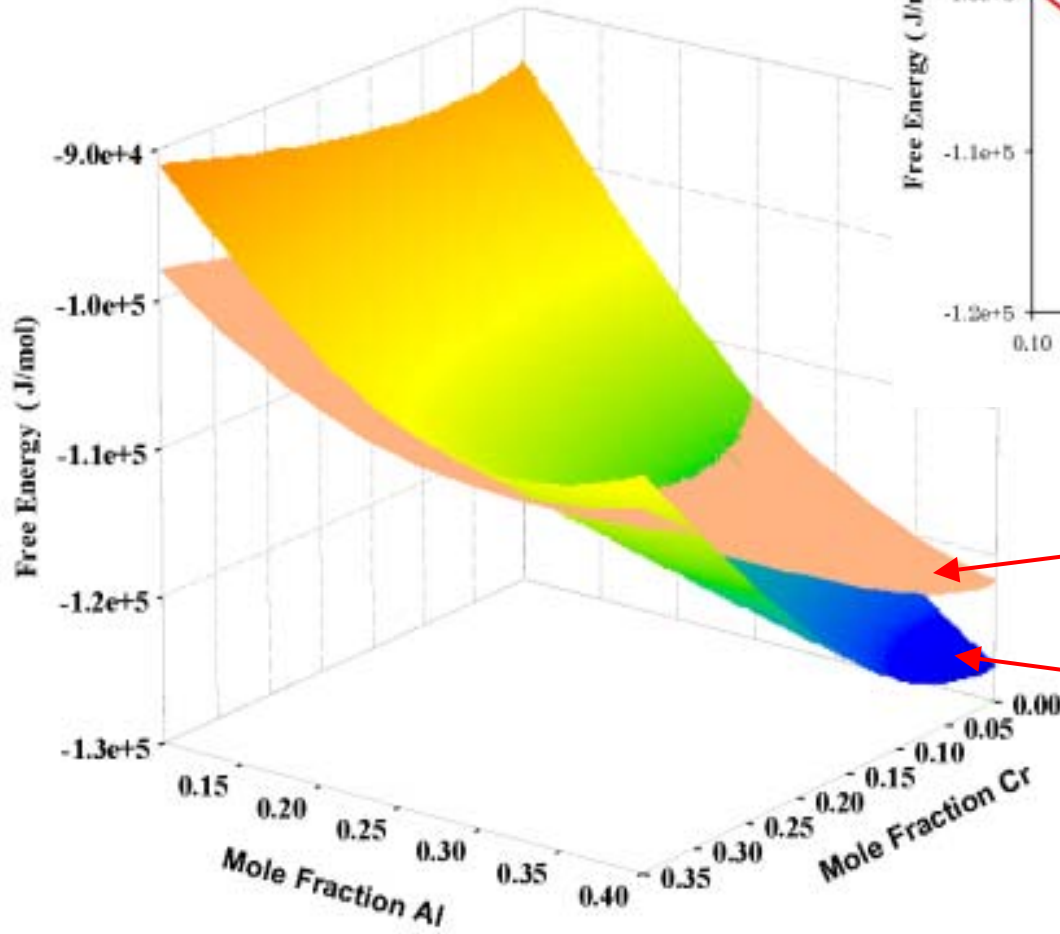
$$f_1(X_{Cr}, X_{Al}, \eta) = \frac{A(X_{Cr}, X_{Al})}{2} \eta^2 - \frac{A_2}{4} \eta^4 + \frac{A_3}{6} \eta^6$$

$$\frac{\partial f_1(X_{Cr}, X_{Al}, \eta)}{\partial \eta} = 0 \longrightarrow f_1(X_{Cr}, X_{Al}, \eta_0)$$

Ni-Al-Cr Database



Free Energy



$f_{\gamma(\text{f.c.c})}$

$f_{\beta(\text{B2})}$

Linking to Diffusivity Database

Ni-Al-Cr System

Atomic Mobility

$$\beta_B^\zeta = \frac{1}{RT} \exp\left(\frac{-\Delta G_B^*}{RT}\right) \quad B = \text{Cr, Al, or Ni}$$

$$\zeta = \gamma, \beta$$

$$\Delta G_B^* = X_{Cr} \Delta G_B^{*Cr} + X_{Al} \Delta G_B^{*Al} + X_{Ni} \Delta G_B^{*Ni}$$

$$+ X_{Cr} X_{Al} {}^0 \Delta G_B^{*Cr,Al} + X_{Cr} X_{Ni} {}^0 \Delta G_B^{*Cr,Ni} + X_{Al} X_{Ni} {}^0 \Delta G_B^{*Al,Ni}$$

Atomic Mobility

$$\beta_1^\zeta$$

Interdiffusivity

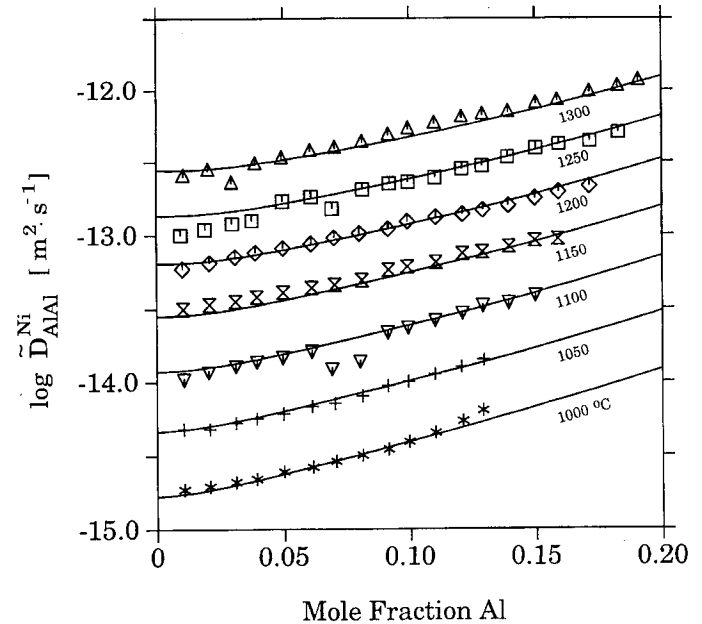
$$D_{ij}^\zeta$$



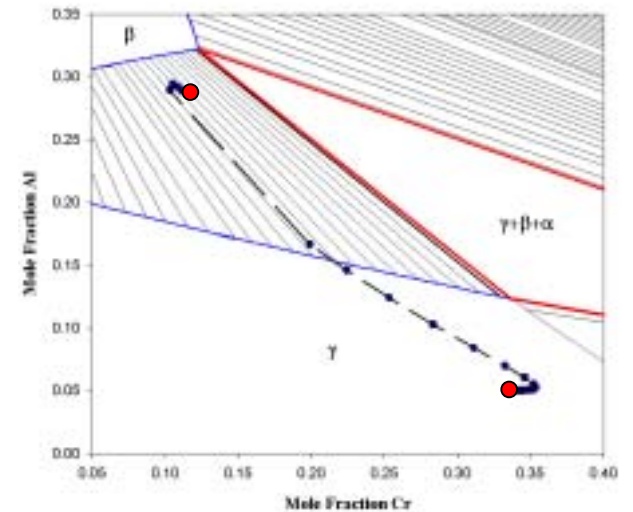
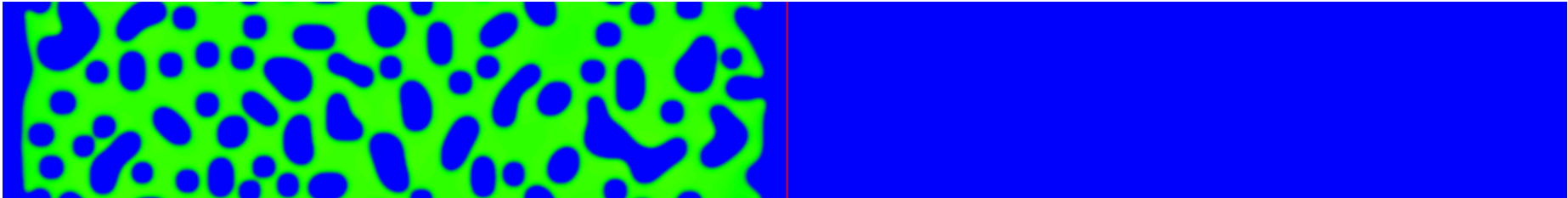
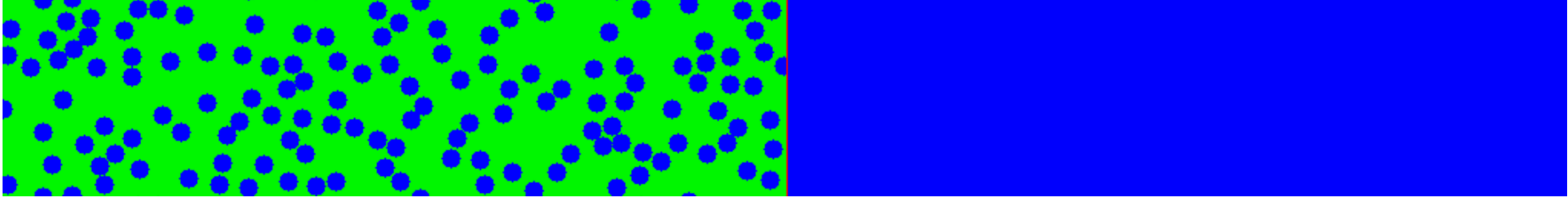
Chemical Mobility

$$M_{ij}^\zeta$$

A. Engström and J. Ågren



Ni-Al-Cr System: $\beta+\gamma/\gamma$ Couple



Summary

- The phase field method has a strong potential to handle the full complexity of γ/γ' microstructures in superalloys.
- Some of the issues related to the development of phase field method into an engineering model capable of making quantitative materials specific predictions are discussed.
- Encouraging progresses have been made to extend the phase field method to take into account the following:
 - concurrent nucleation, growth and coarsening
 - effect of elastic interaction on nucleation
 - linking to multicomponent diffusion and thermodynamic databases