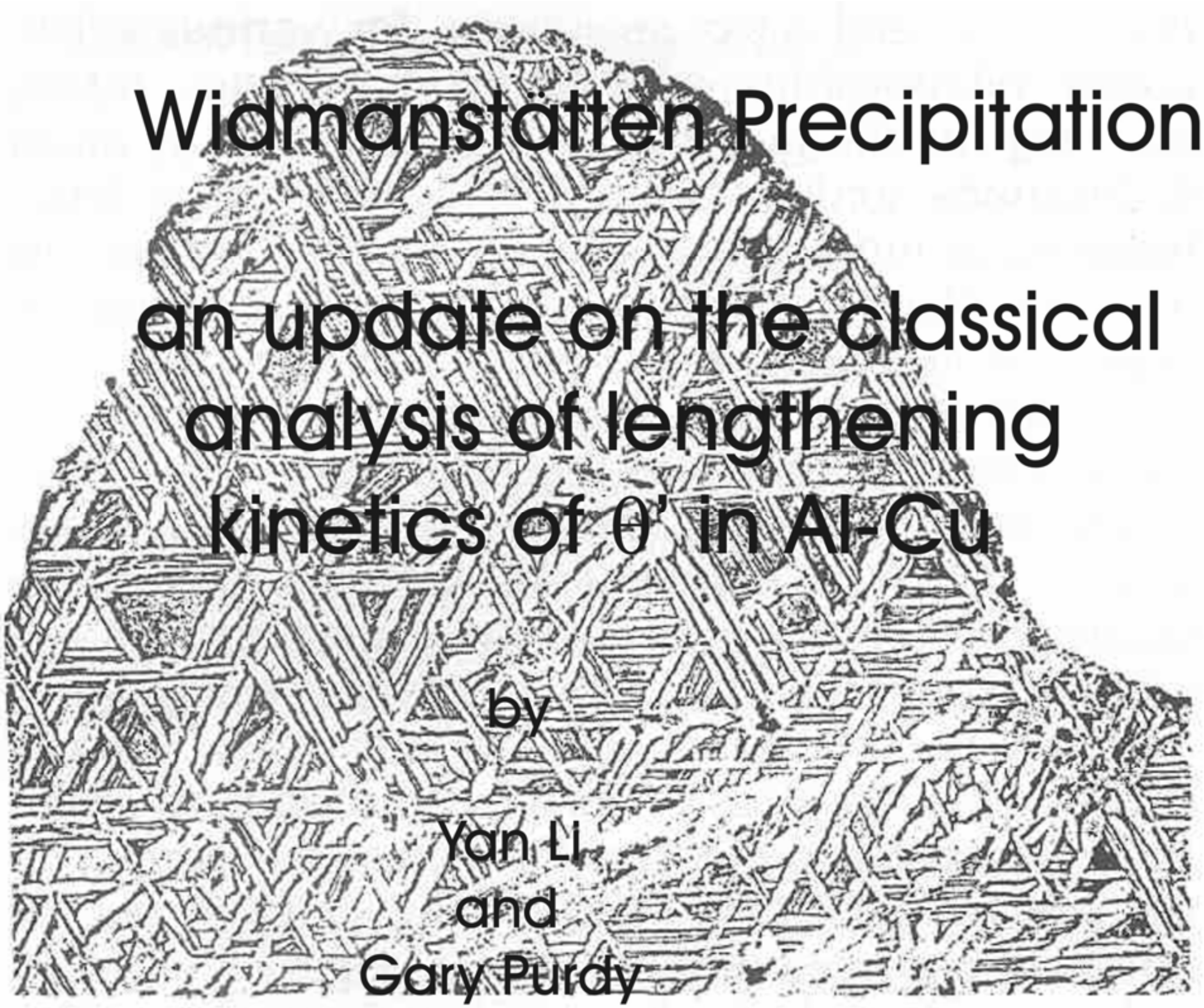


Widmanstätten Precipitation

an update on the classical analysis of lengthening kinetics of θ' in Al-Cu

by

Yan Li

and

Gary Purdy

Outline:

Precipitation of θ' in α Al-Cu

- Kinetics of precipitate lengthening
- The diffusion field
- Roles of elastic energy
- Classical force-balance analysis

Conclusion

McMaster University

Update; Widmanstätten Project:

(i.e. current status)

Experiment and Classical Modeling

Yan Li

Phase-field Modeling

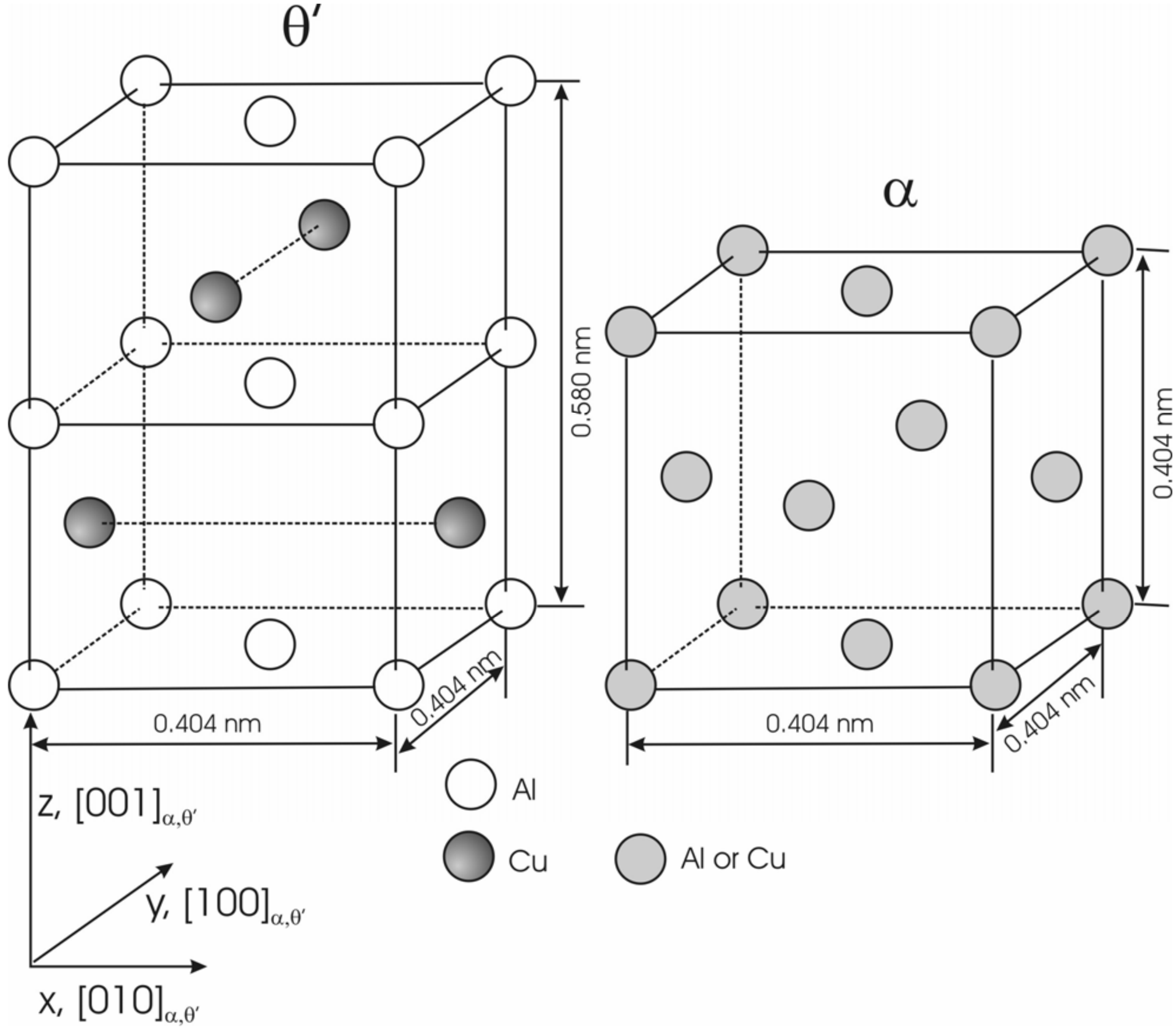
Michael Greenwood

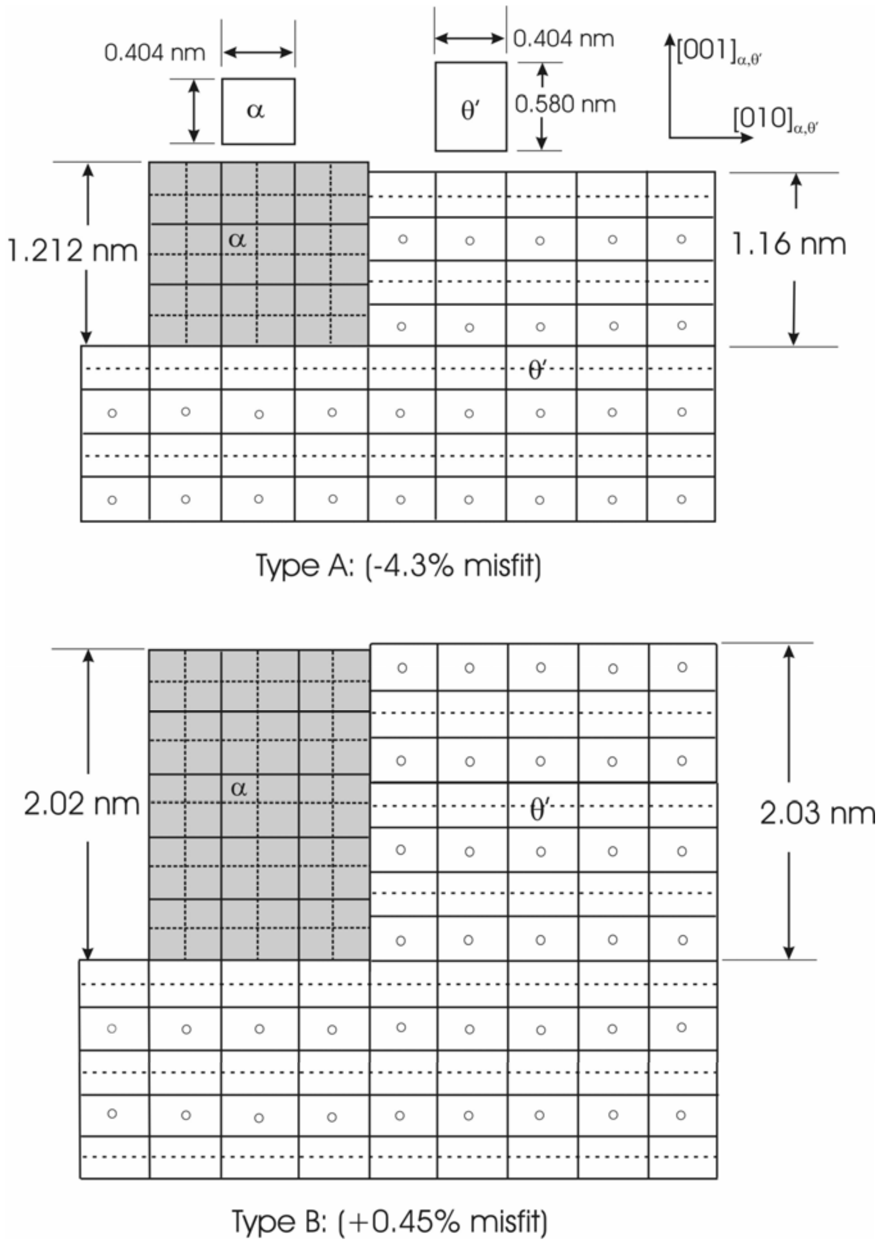
Objective: "evaluation of the roles of interfacial energy, elastic energy, diffusion and interface mobility in the formation of Widmanstätten precipitates."

McMaster University

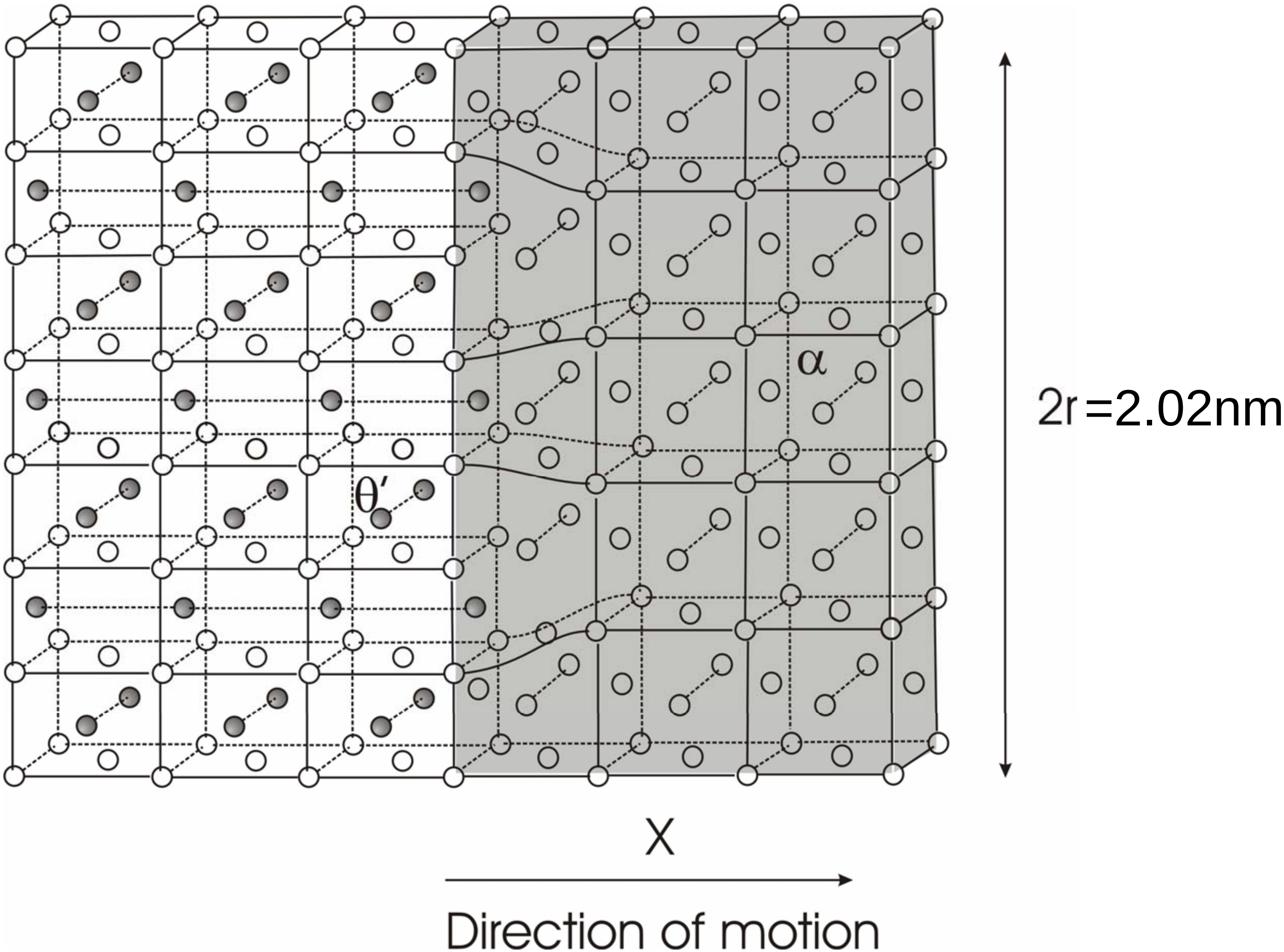
Lengthening of θ' precipitates in an Al-2.75 mass% Cu monocrystal

θ' in α Al-Cu

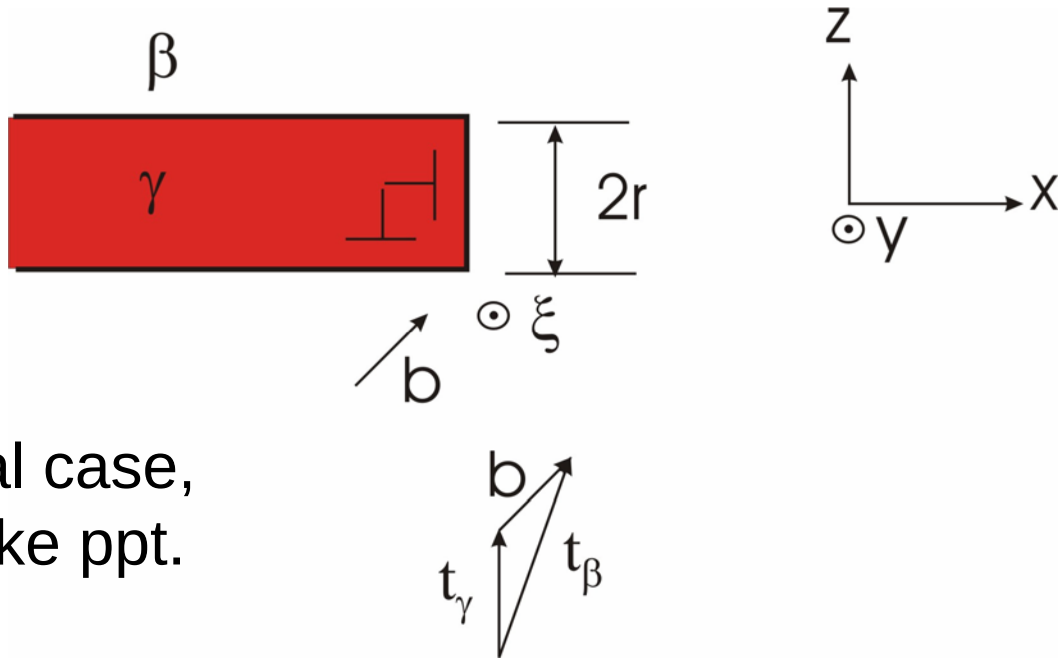




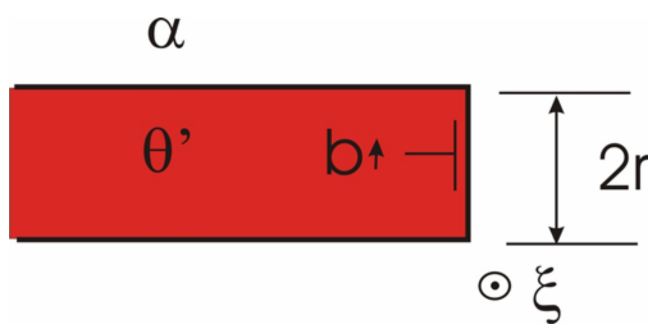
Purdy and Hirth
Phil. Mag., let.,
2006, **86**, 147



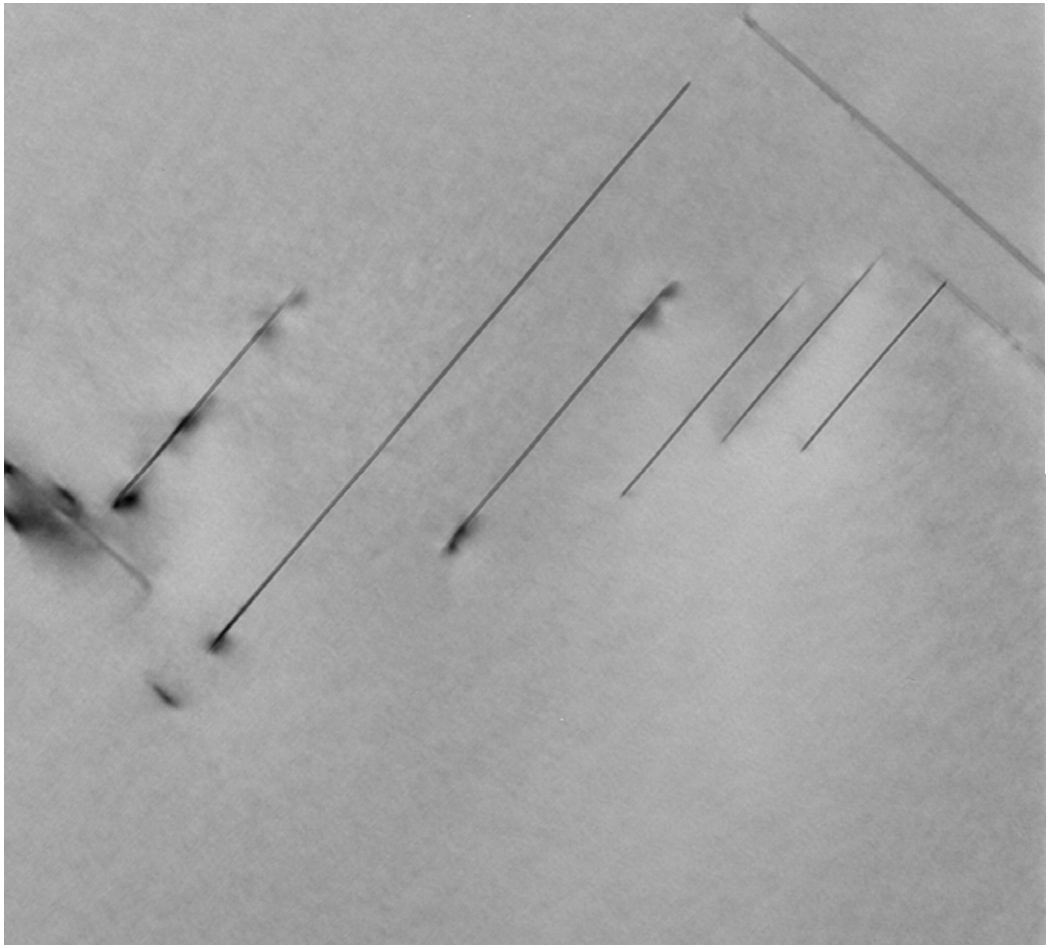
θ′
α
2r =2.02nm
X
Direction of motion



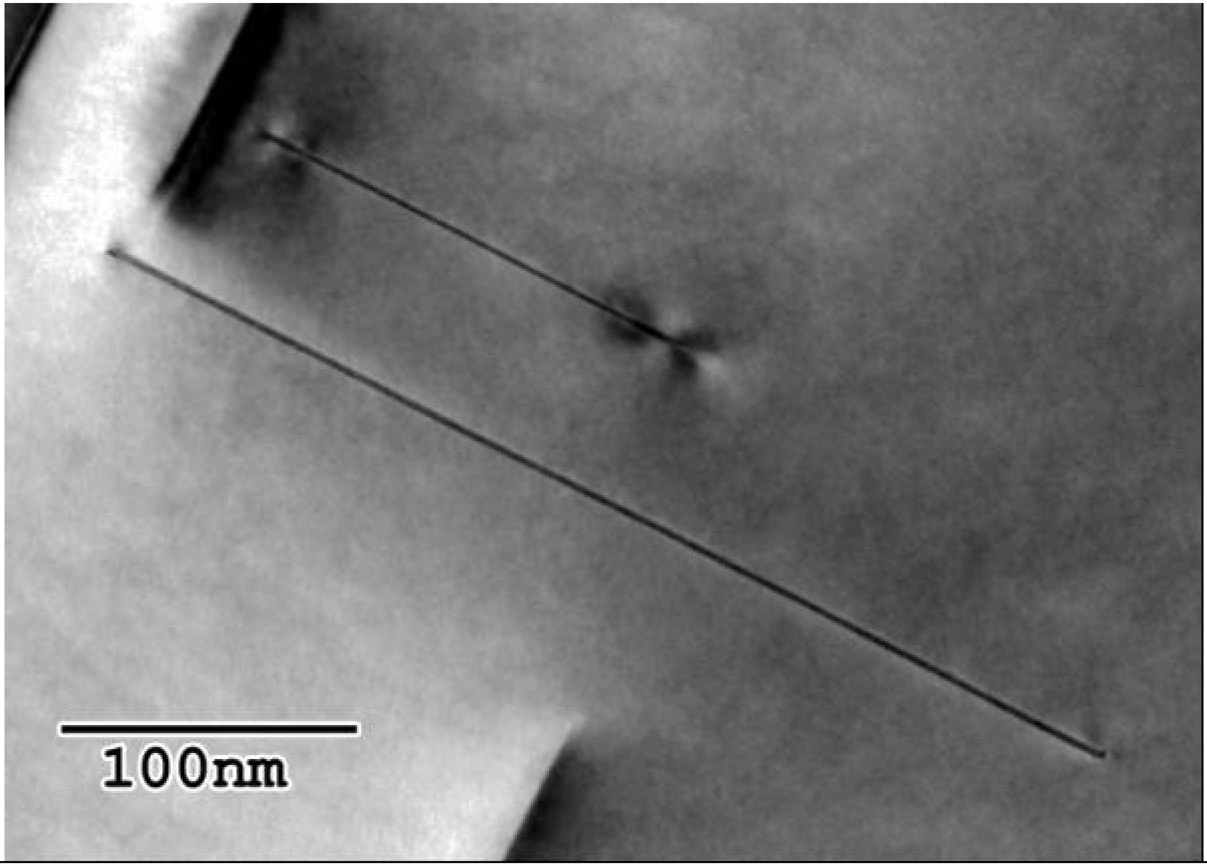
General case,
Plate-like ppt.



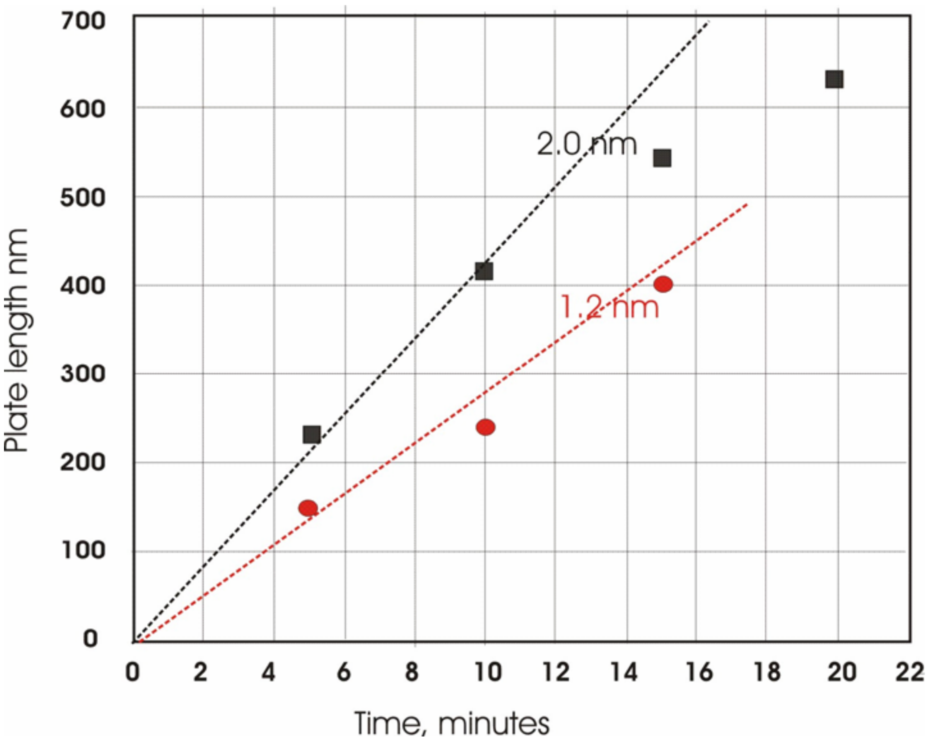
The specific case of θ' in α Al-Cu



Early stages of θ’ growth in Al-2.75Cu



1.2 and 2.0 nm thick precipitates, 20 min., 230^{o}C.



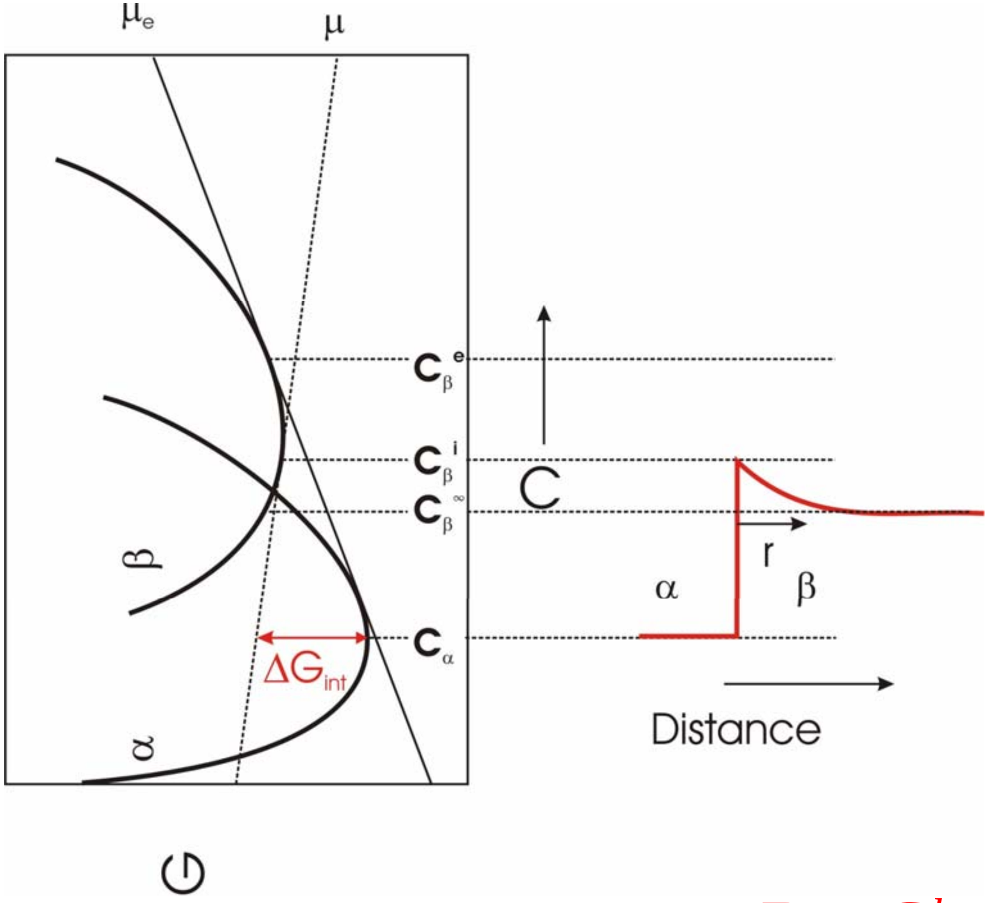
Lengths of the largest plates, 2.0 and 1.2 nm thickness;
(data derived from observations of many samples).

Growth kinetics; classical approach.

$$\frac{v}{M} = P_i = P_{th} + P_\sigma + P_{el} + P_{s.d.} + P_Z$$

A local force balance is employed to relate velocity v to a set of forces:

- Intrinsic drag, P_i related to interfacial structure, mobility M
- A thermodynamic driving force, $P_{th} = \Delta G_{int}/V_m$
- A capillary force P_σ due to interfacial energy,
- An elastic force, P_{el} due to coherency strains, misfit, interactions
- A solute drag force, P_{sd} due to solute diffusion within interface,
- A Zener drag, due to particle interactions with interface.



$$f_{th} = \frac{\Delta G_{\text{int}} \cdot 2r}{V_m};$$

Thermodynamic force
(per unit length);

$$v \approx \frac{D_\beta}{r} \frac{C^i_\beta - C^\infty_\beta}{C^i_\beta - C_\alpha}$$

Zener-Hillert analysis
of steady plate lengthening

For the analysis of lengthening kinetics, require:

- Diffusion data (extrapolated,very uncertain)
- Solubility of metastable phase (uncertain)
- Solution thermodynamics (OK)
- Elastic constants (OK)
- Vegard’s law slope (OK)
- Interfacial energy (low, but not well known)
- “Burgers vectors” of precipitates (OK)

To proceed, determine solubility of θ' in α, then compare rates of growth of 1.2 (strained) and 2 nm thick (essentially unstrained) precipitates.

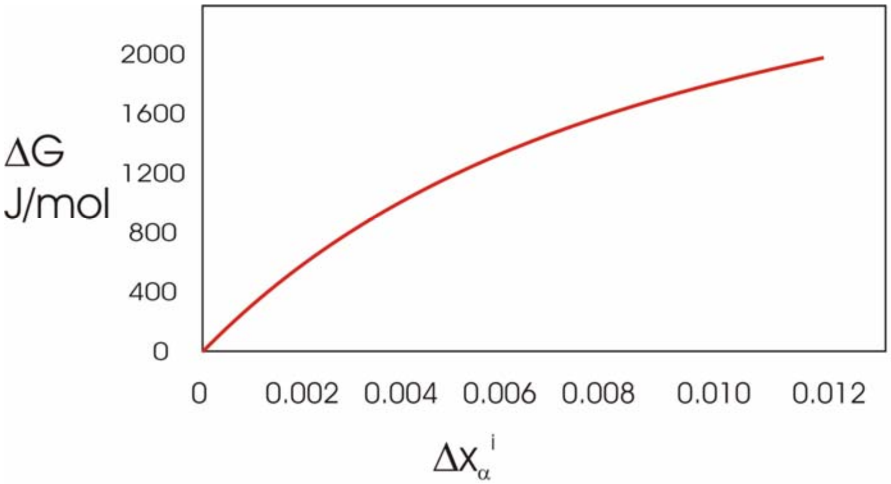
The metastable solubility is obtained from a measurement of the fraction of θ’ in long time equilibrated samples (no other phases present) at 230^{o}C.

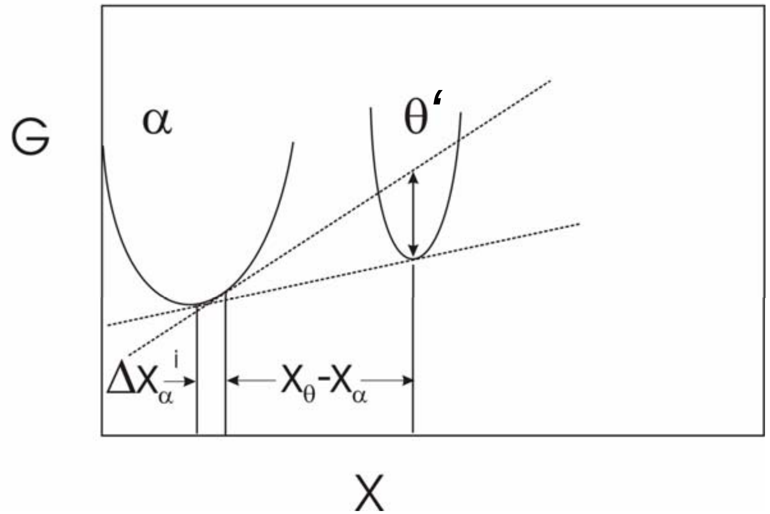
The result, obtained via measurement of images from 20 areas in [100] ZA:

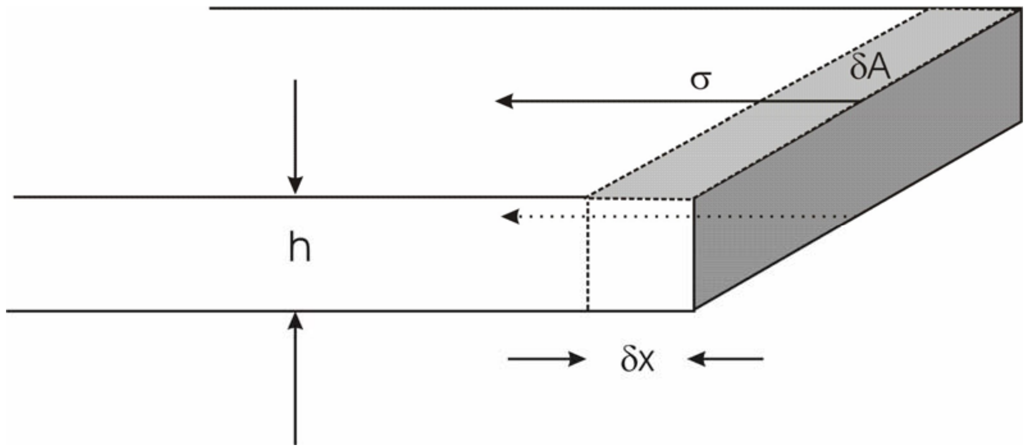
0.26 (+/- 0.025) at.% Cu

(note approximation for discs in plane of foil.)

Thermodynamic driving force, P_{th}







$$P_{\sigma}=2\sigma/h$$

Self strain energy:

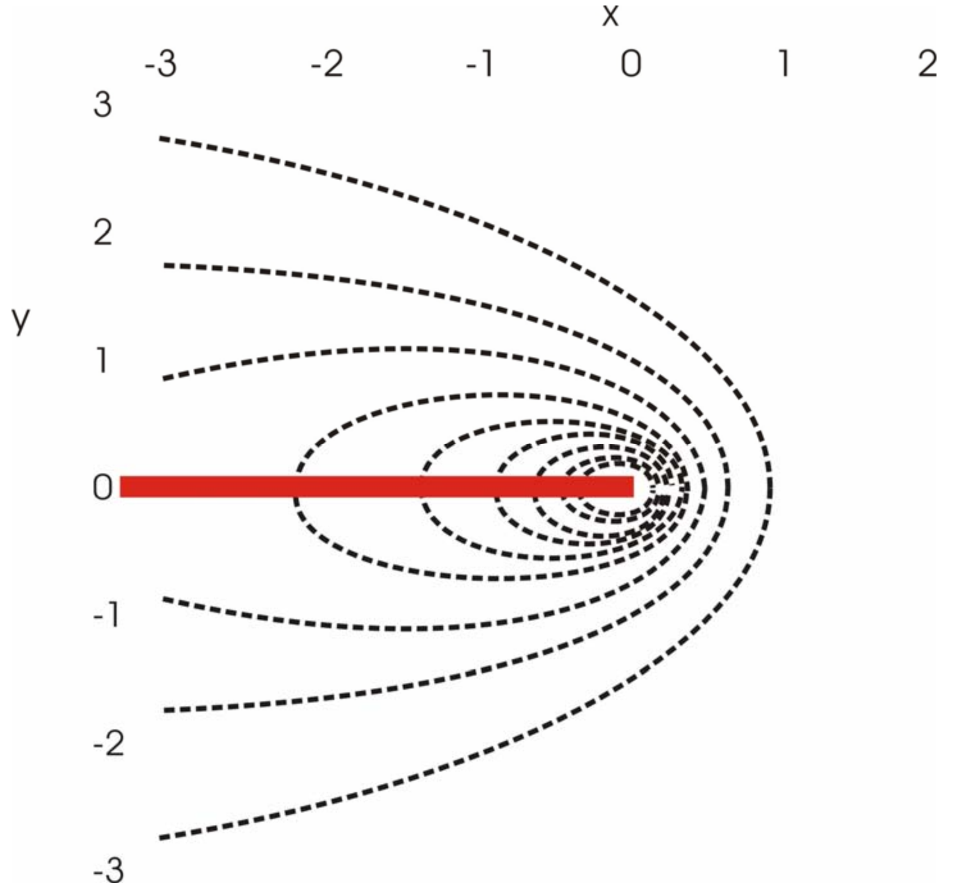
$$E_{el}{}^{self} = \frac{1}{2}\varepsilon_{ij}\int_{v}\sigma_{ij}dv$$

Khachaturyan; particularized to a [100] disc:

$$E_{el} = \frac{\left[\frac{1}{3}(C_{11}+2C_{12})(2\frac{C_{12}}{C_{11}}+1)\varepsilon - \frac{1}{3}(C_{11}-C_{12})(1-\frac{C_{12}}{C_{11}})\varepsilon\right]^{2}}{2C_{11}} \square V$$

$$P_{el}{}^{self} = \frac{\partial E_{el}}{\partial L}$$

Solute field strain



$$c(x,y)=\frac{c_\beta^i - c_\beta^e}{K_0\left(\frac{vb}{2D}\right)} e^{-vx/2D} K_0\left\{\frac{v}{2D}(x^2+y^2)^{1/2}\right\}$$

Force/unit length on a migrating θ' edge/ledge due to atomic misfit in the diffusion field

Purdy and Brechet 2005:

$$f_x = \frac{\partial^2 \Psi}{\partial x^2} \approx -2\mu\eta(c_\beta^i - c_\beta^\infty)\left\{1 + \frac{2.3}{K_0\left[\frac{vb}{2D}\right]}\right\}$$

μ: shear modulus of matrix

η: $= \frac{d \ln a}{dc}$

b: Burgers vector

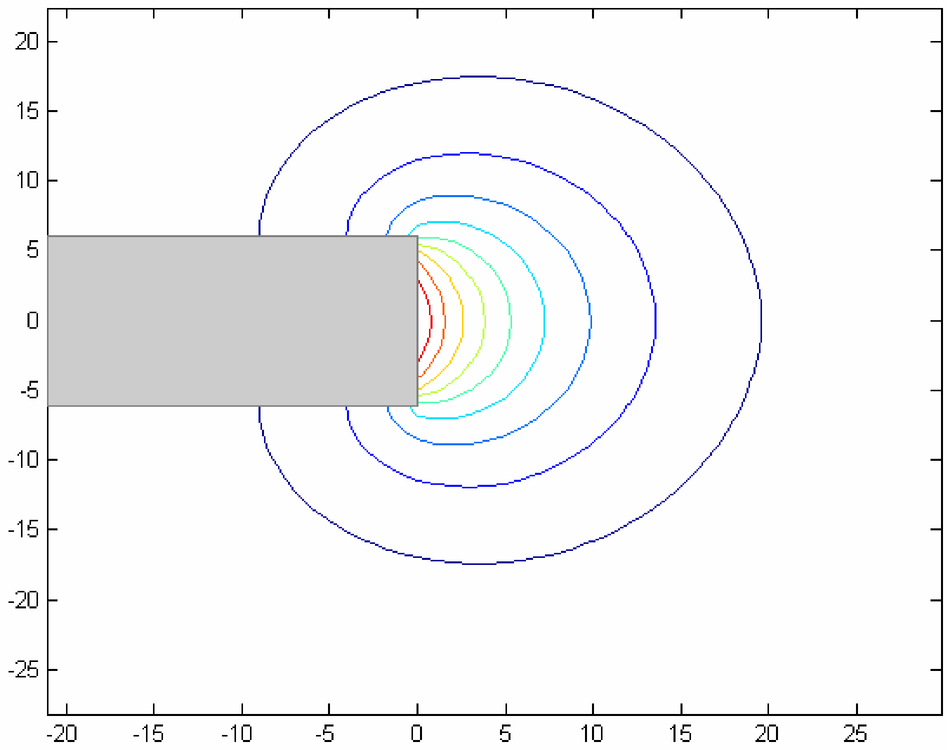
Using a balance of the estimated thermodynamic force, elastic (self) and elastic (diffusion field) forces, as well as the capillary term, the concentrations at the plate tips are estimated as:

For the 2 nm plates: $X_{\alpha}^{i} \approx 0.00265$

And for the 1.2 nm plates: $X_{\alpha}^{i} \approx 0.0088$

The <u>relative</u> rates of growth can now be estimated:

Diffusion field near the plate tip:



After Jones and Trivedi (1971):

$$\Gamma(x,y) = \frac{X_\alpha^0 - X(x,y)}{X_\alpha^0 - X_\alpha^i}$$

$$\nabla^2 \Gamma(x,y) + 2p \frac{\partial \Gamma}{\partial x} = 0$$

$$v = -\frac{D}{r} \Omega \frac{\partial \Gamma}{\partial x}\Big|_{x=0}$$

Yielding: $$\frac{v_{2nm}}{v_{1.2nm}} \approx 1.4$$

- Modeling, summary results:

  - Experimentally,

$$\frac{v_{2nm}}{v_{1.2nm}} = 1.5$$

  - A model that takes into account the elastic stresses, thermodynamic and capillary forces yields

$$\frac{v_{2nm}}{v_{1.2nm}} \approx 1.4$$

From the modeling exercise:

The dominant forces in migration are the thermodynamic driving force and the elastic (self-energy) resistive force. The results are very sensitive to the values of the input parameters.

The solute field elastic term is much smaller than the elastic self-energy term. This is due in part to the reduced gradient at the transformation front of the more highly strained precipitate.