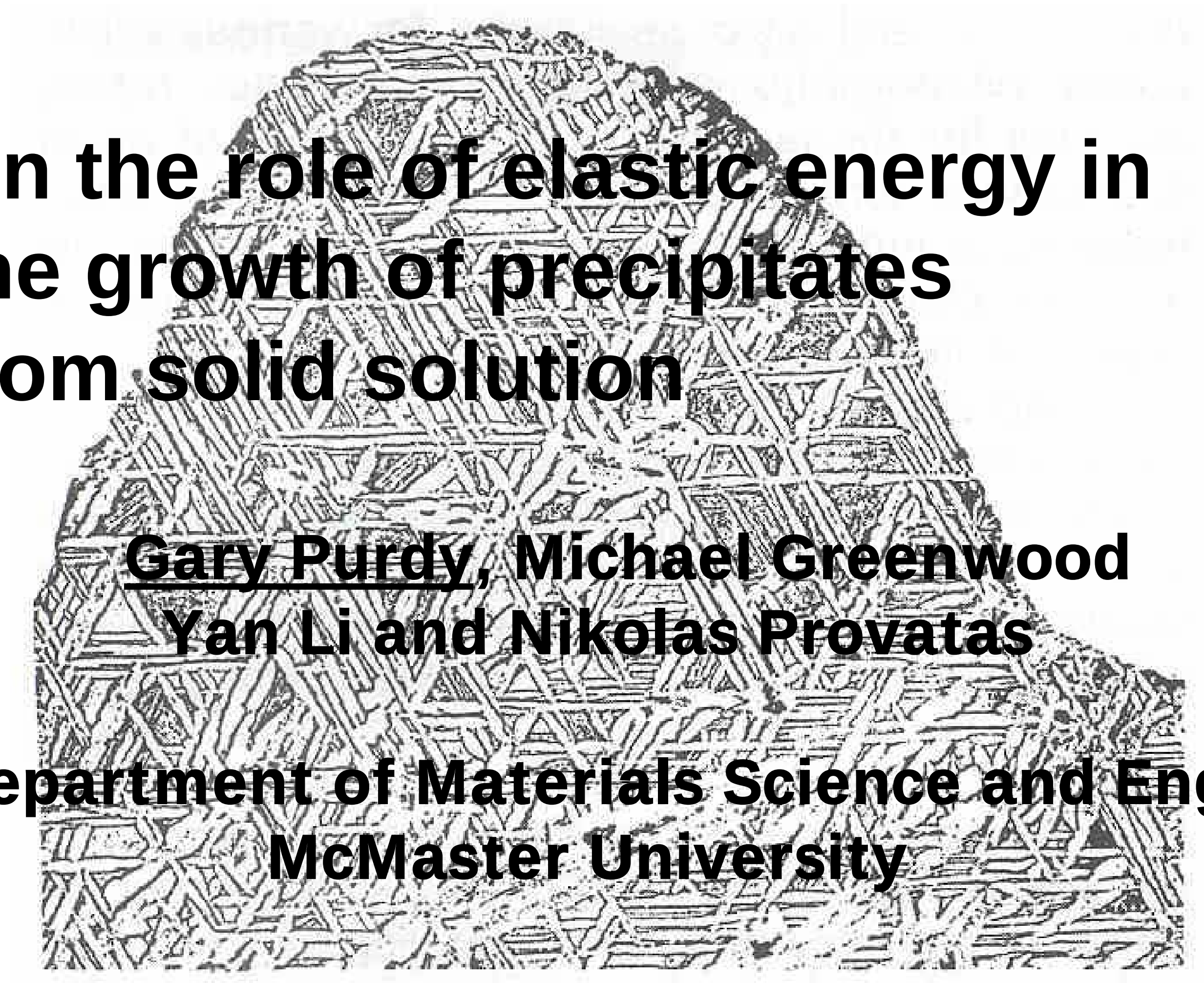
On the role of elastic energy in the growth of precipitates from solid solution



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Widmanstätten Project:

Acknowledgements:

Experiment and Classical Modeling

Yan Li

Marc Bletry

Phase-field Modeling

Nikolas Provatas

Michael Greenwood

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

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Outline:

Precipitation of θ' in α Al-Cu, γ in β–brass.

- Kinetics of precipitate lengthening
- The diffusion field
- <u>Roles of elastic energy</u>
- Classical force-balance analysis
- Solid state dendrites
- Phase field modeling; progress

Conclusion

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

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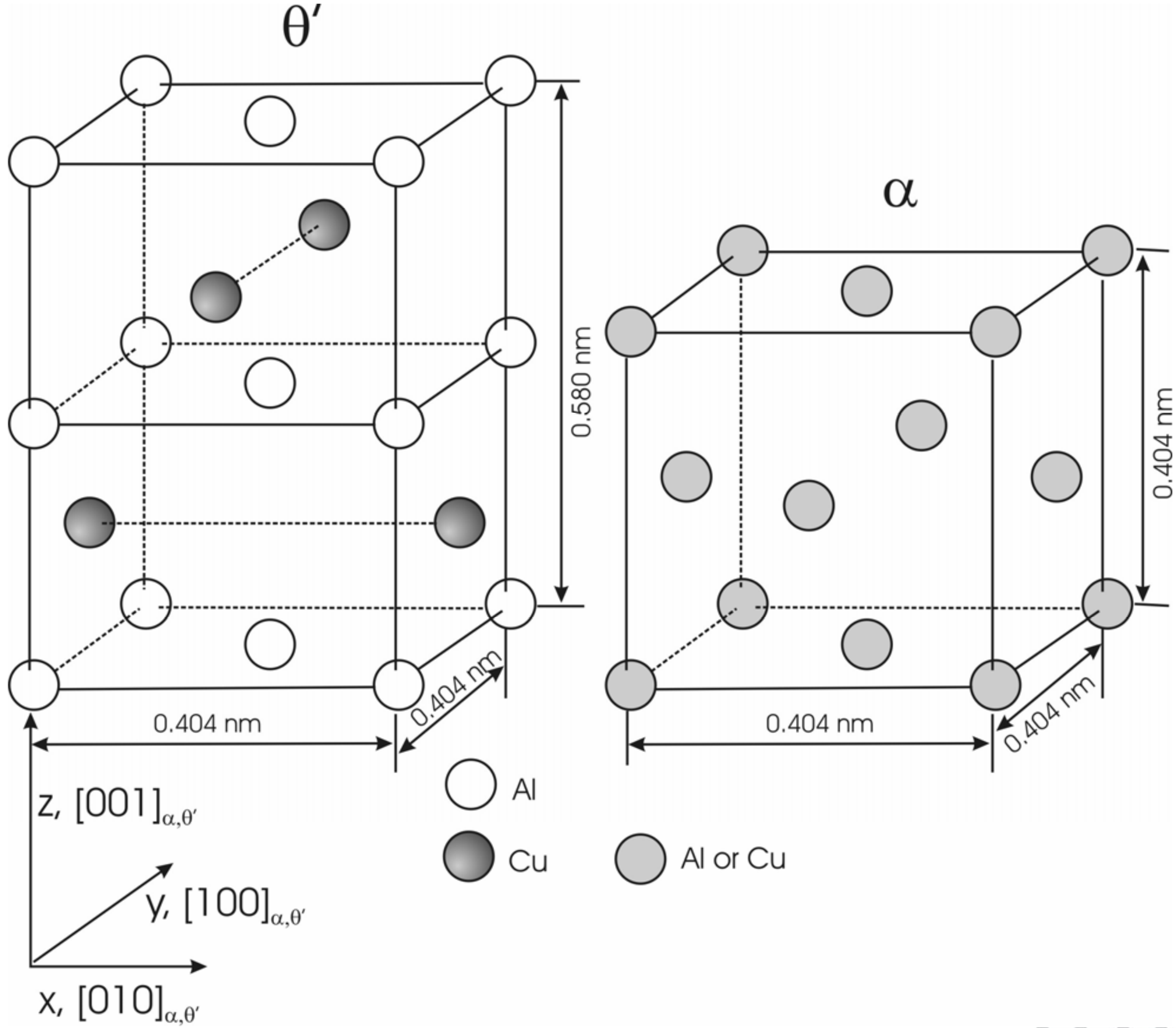
θ’ in α Al-Cu



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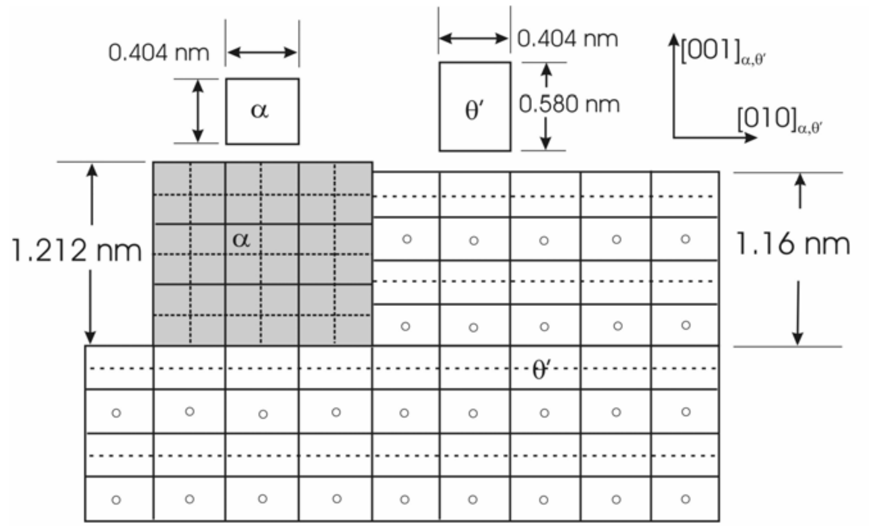
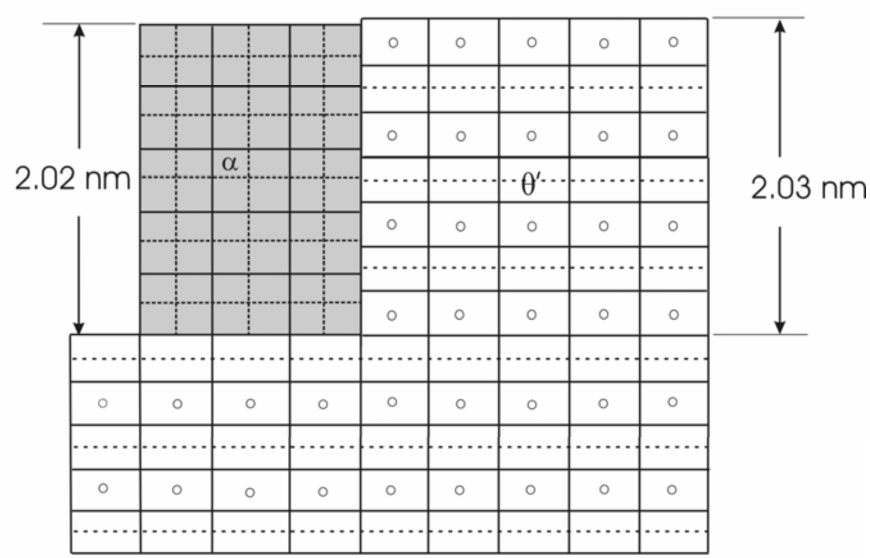


Type A: (-4.3% misfit)



Type B: (+0.45% misfit)

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

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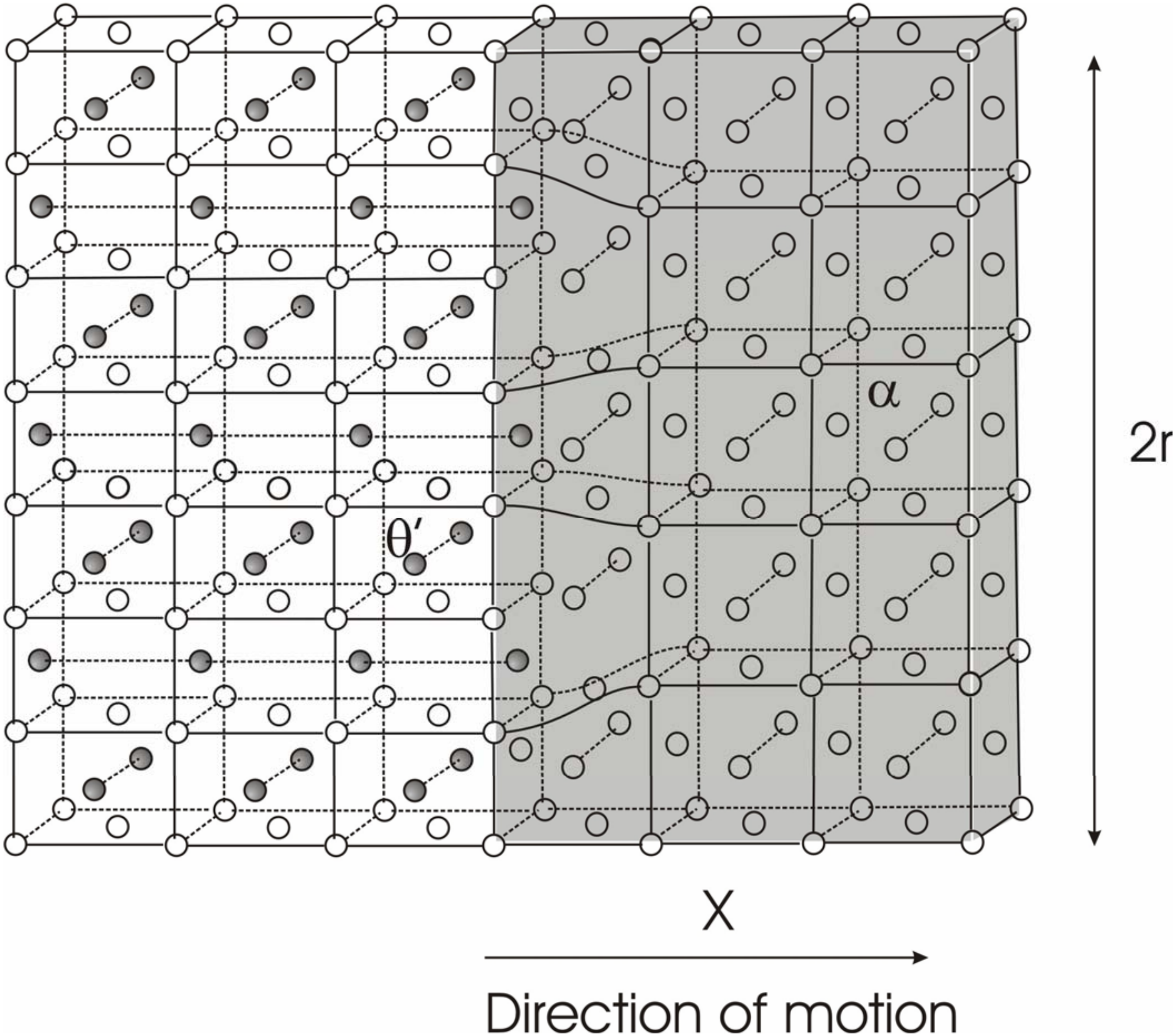

=2.02nm

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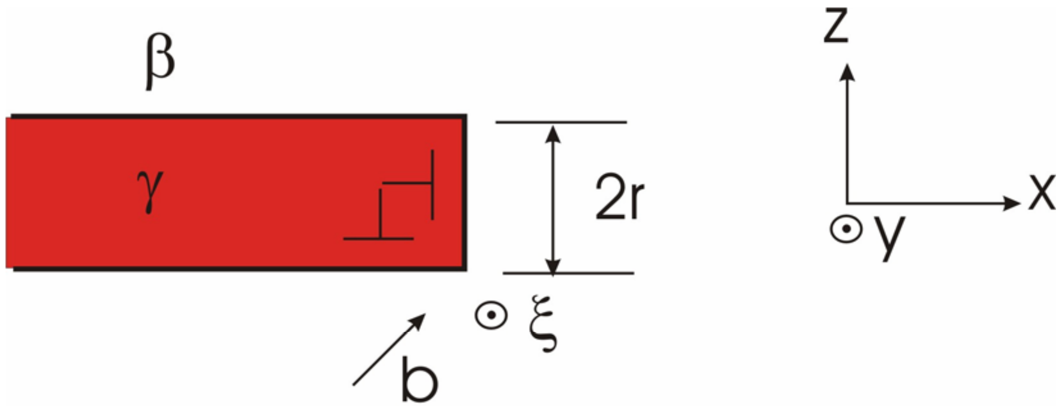
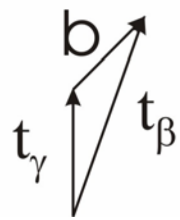
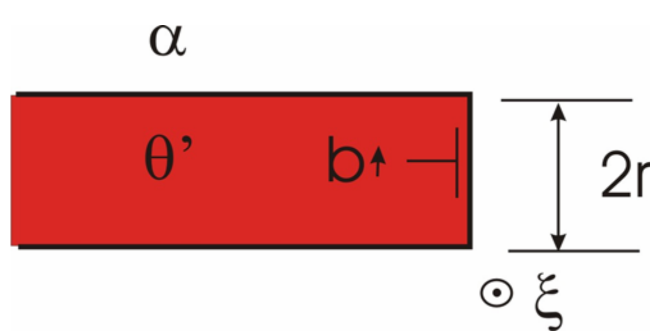
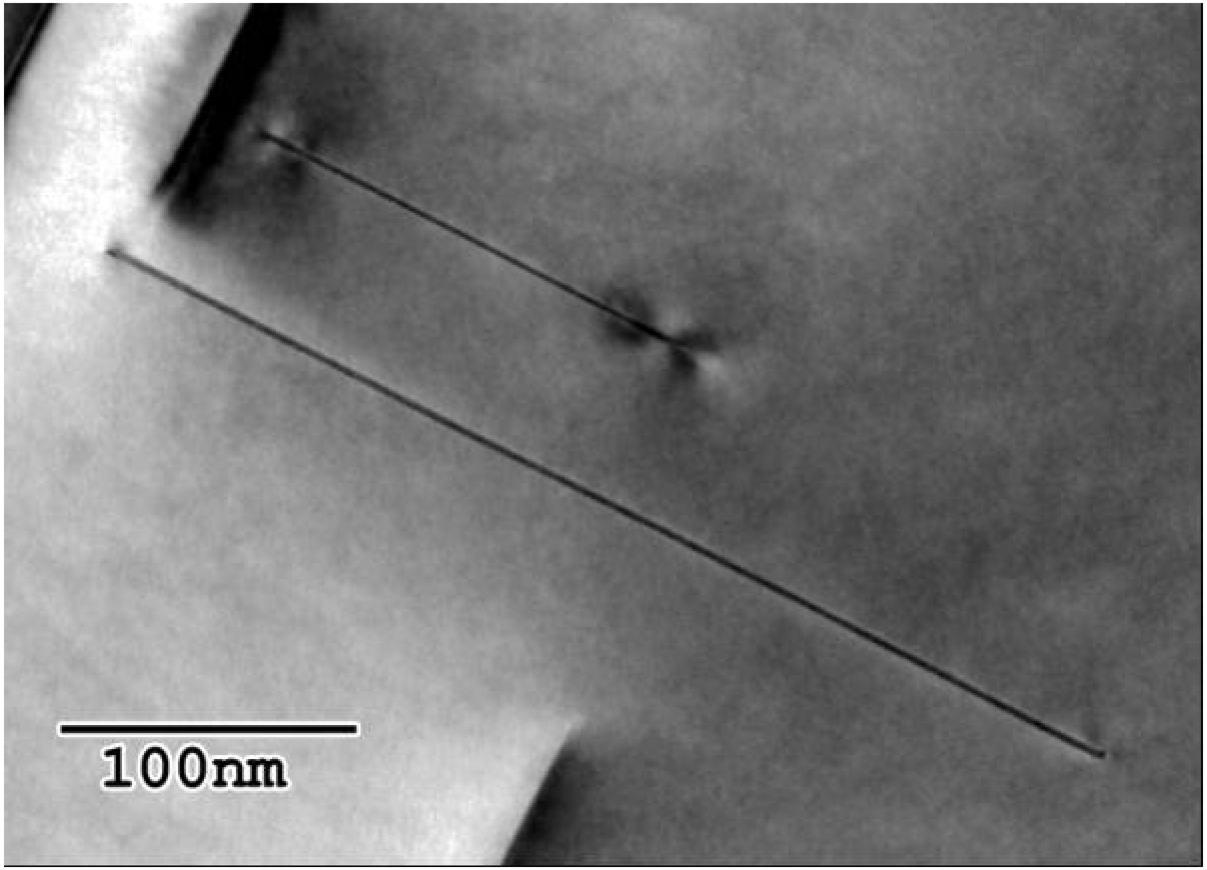


General case,
Plate-like ppt.





The specific case of θ' in α Al-Cu



1.2 and 2.0 nm thick precipitates, 20 min., 230°C.

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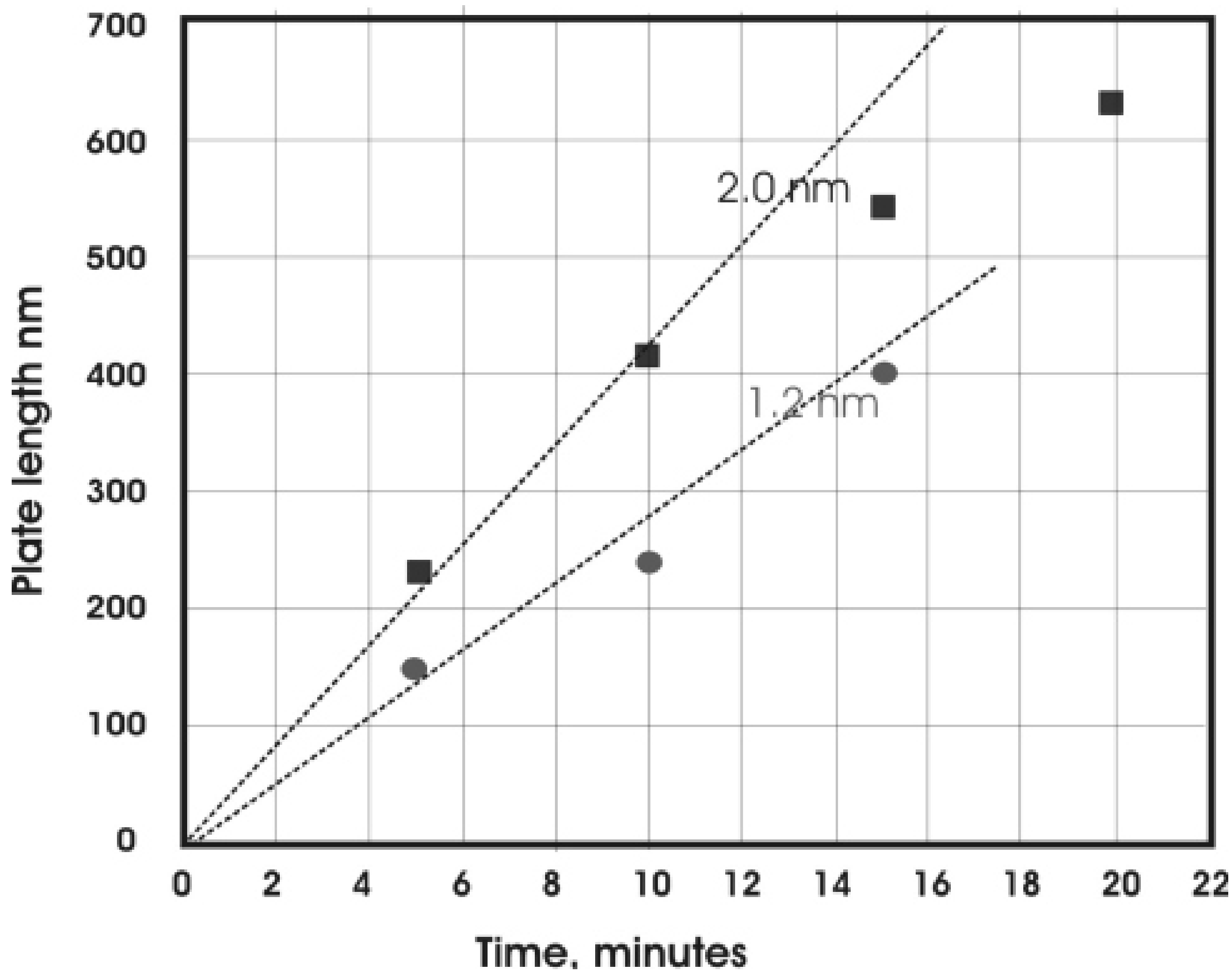

700
600
500
400
300
200
100
0
Plate length nm
2.0 nm
1.2 nm
0
2
4
6
8
10
12
14
16
18
20
22
Time, minutes

Growth kinetics; classical approach.

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

A local force balance is employed to relate velocity $\boldsymbol{v}$ to a set of forces:

- Intrinsic drag, $\boldsymbol{P_i}$ related to interfacial structure, mobility $\boldsymbol{M}$
- A thermodynamic driving force, $P_{th} = \Delta G_{int}/V_m$
- A capillary force P_σ due to interfacial curvature,
- 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.

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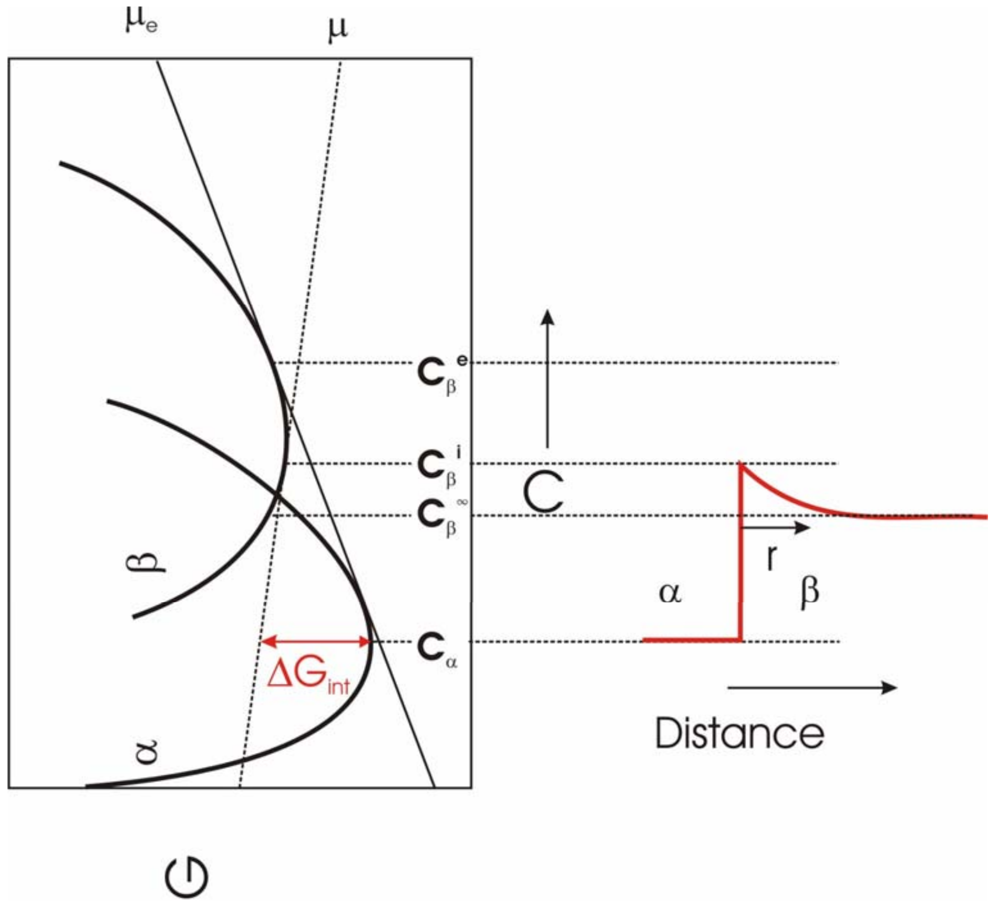

$$f_{th} = \frac{\Delta G_{\text{int}} \cdot 2r}{V_m};$$

Thermodynamic force
(per unit length);

$$v \approx \frac{D_\beta}{r} \frac{C_\beta^i - C_\beta^\infty}{C_\beta^i - C_\alpha}$$

Zener-Hillert analysis
of steady plate lengthening

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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 very 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.

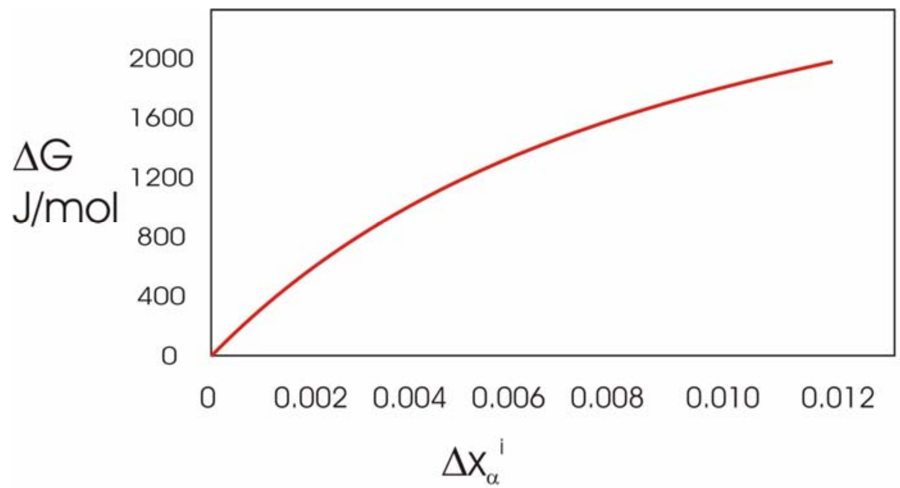
The metastable solubility is obtained from a measurement of the fraction of θ' in long time equilibrated samples (no other phases present) at 230^{o}C.

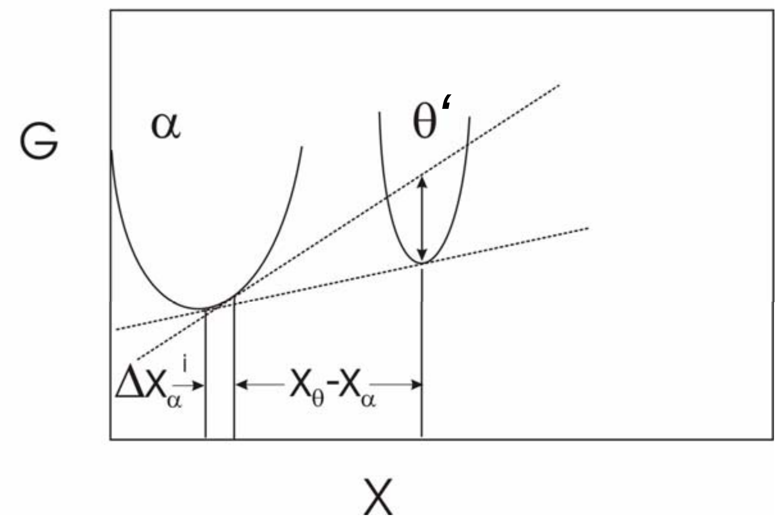
The result, obtained via measurement of images from 20 areas in [100] ZA:

0.26 (+/- 0.025) at.% Cu

(note approximation for discs in plane of foil.)

Thermodynamic driving force, P_{th}





Self strain energy:

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

Khachaturyan; particularized to a [100] disc:

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

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

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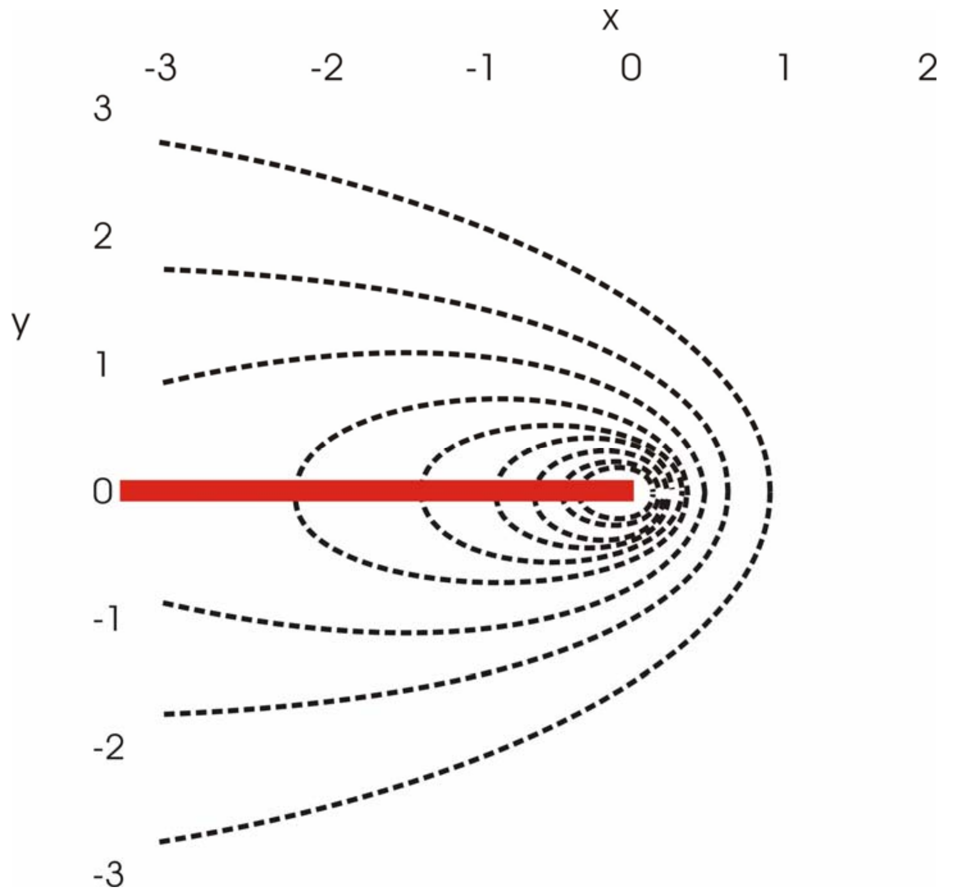
Solute Field (Vegard's) strain



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

Force/unit length on a migrating θ' disconnection/edge due to Vegard's strain from 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

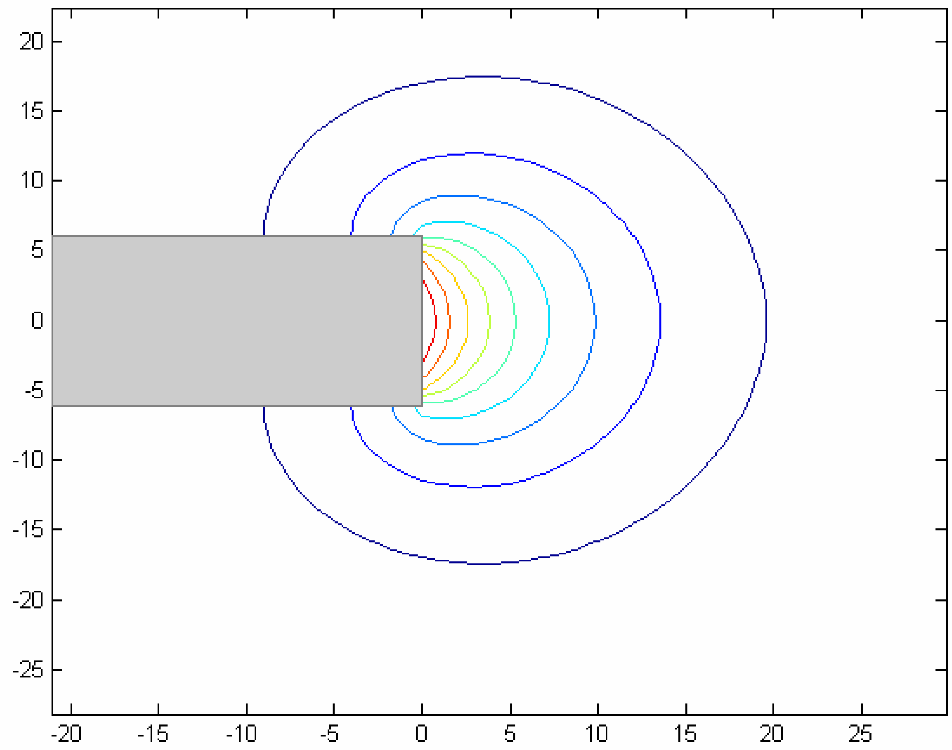
Using a balance of the estimated thermodynamic force, elastic (self) and elastic (diffusion field) forces, as well as the capillary term, the concentrations at the plate tips are found as:

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 relative rates of growth can now be estimated:

Diffusion field near the plate tip:



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

- Modelling, 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 classical modeling exercise for θ':

The dominant forces in migration are the thermodynamic driving force and the elastic (self-energy) resistive force.

The solute field (Vegard's Law) 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.

Progress in phase-field modeling of θ' precipitation; significance of elastic terms.

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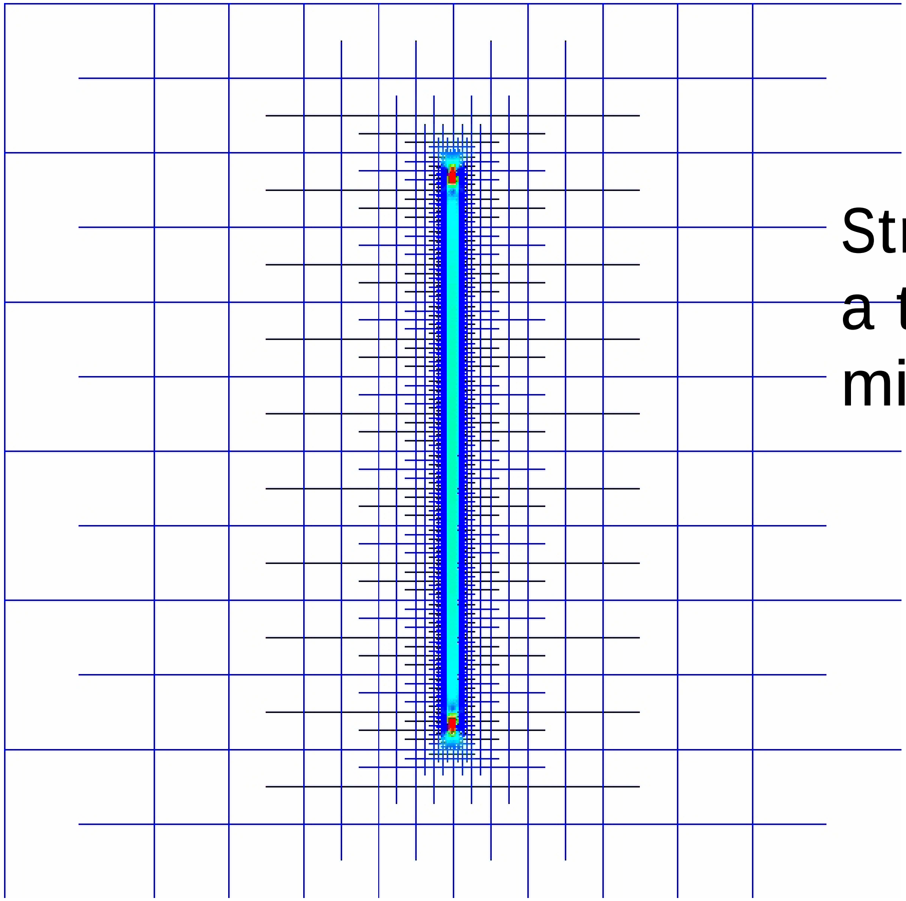
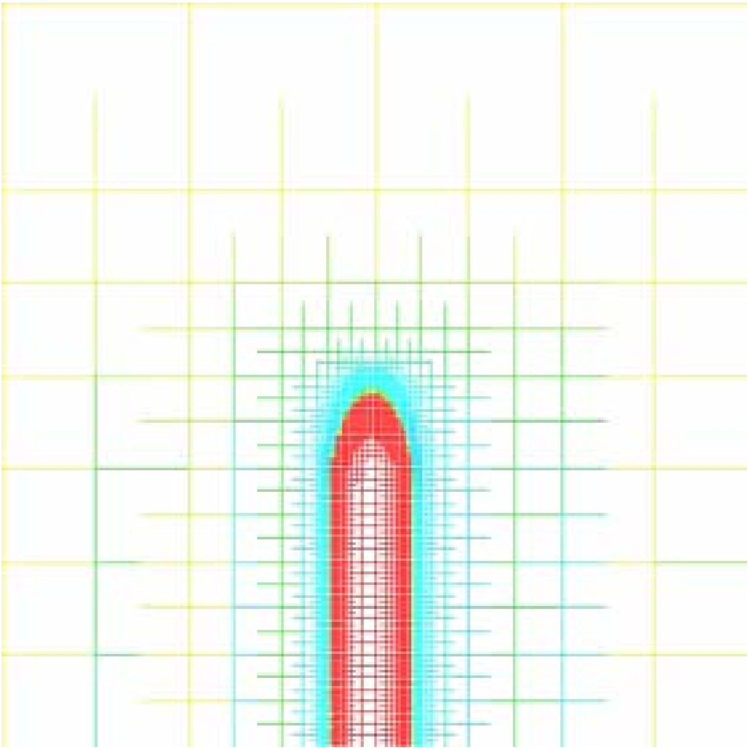


Strains around a tetragonally misfitting θ' plate



Computed diffusion field around a θ' plate tip

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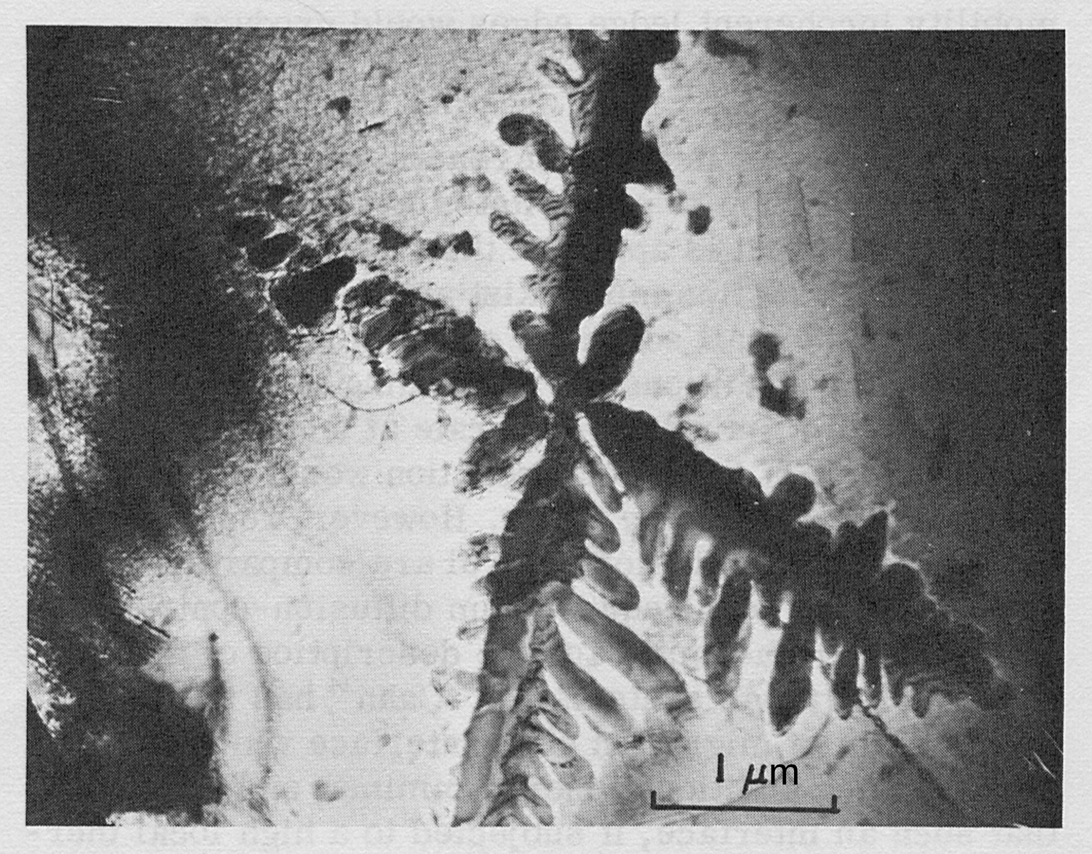
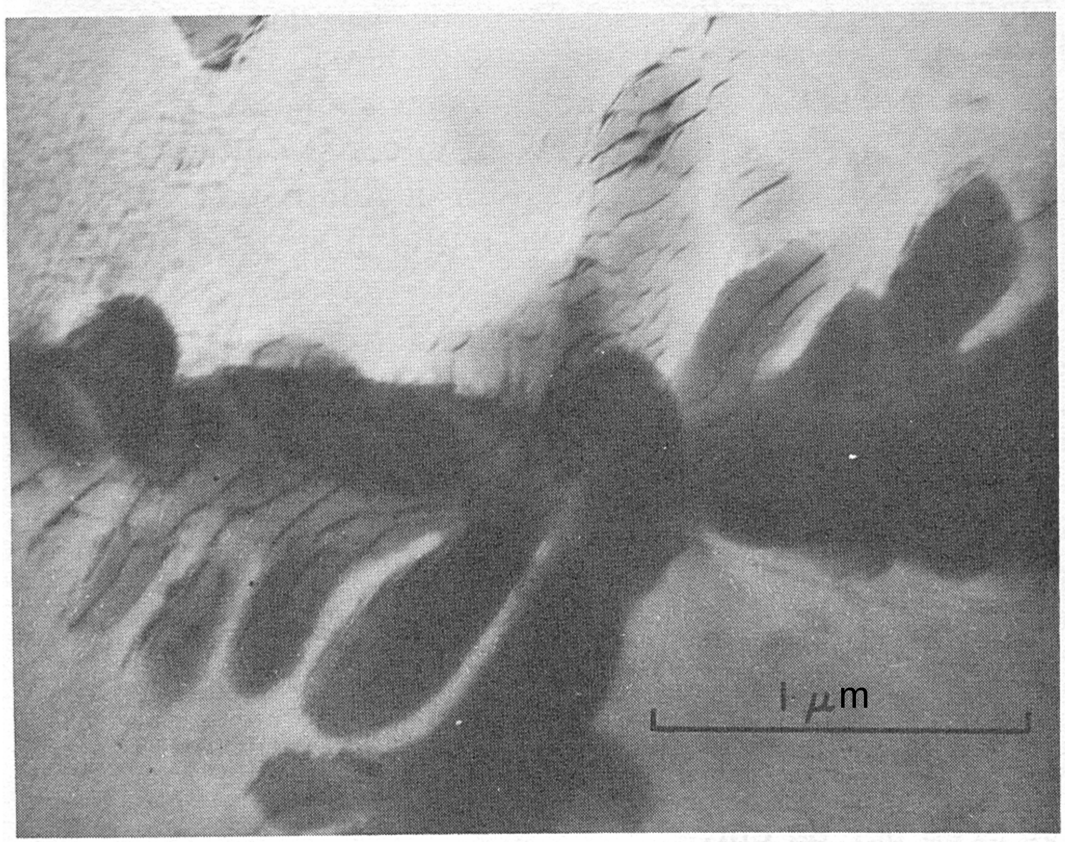
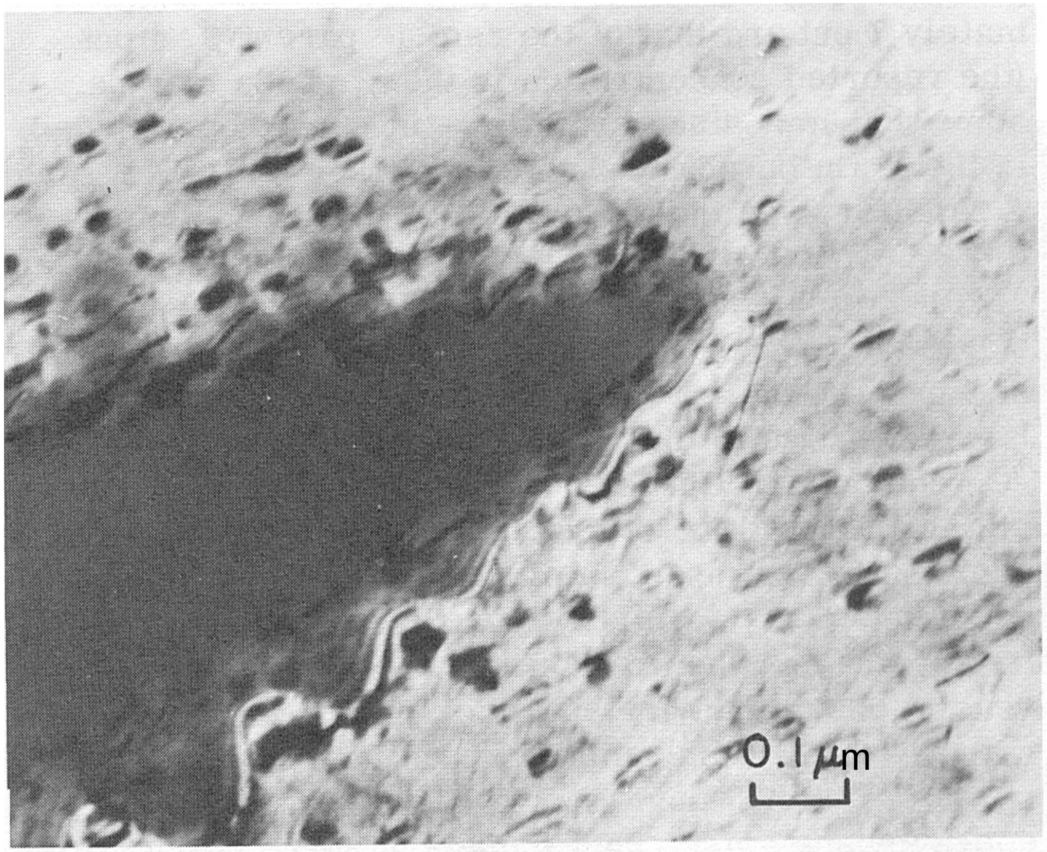
Precipitation of γ dendrites in β Cu-Zn



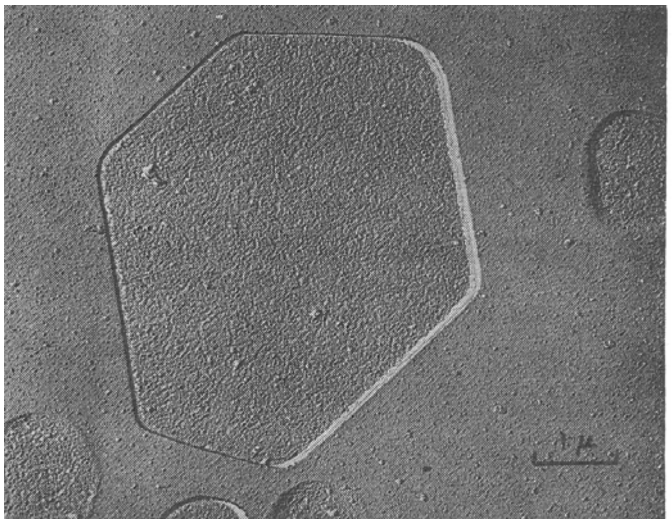
The preferred growth direction is <110>

The interfaces are semi-coherent





A dendrite tip shows early stages of side branching.



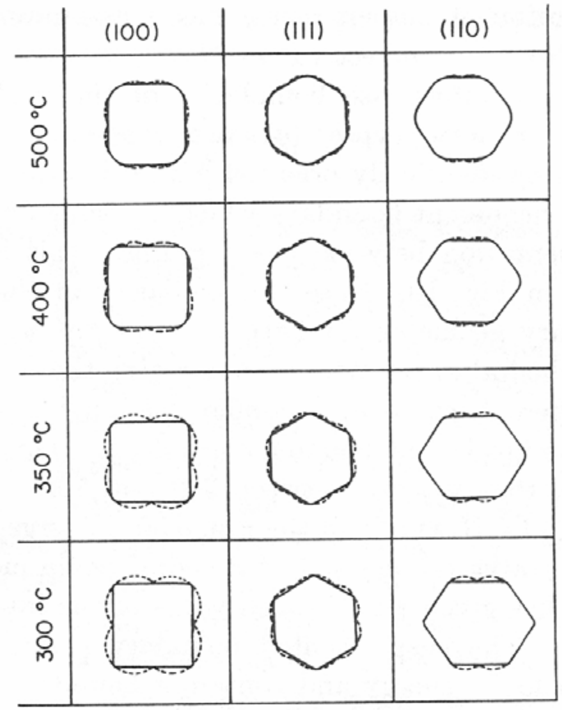


FIG. 8. The morphologies of the γ precipitates (solid curves) and the resulting Wulff Plots (dashed curves) for samples isothermally equilibrated for 500 hr at the temperatures designated.

Requirements for modeling of γ dendrite growth:

- Diffusion coefficient in parent β phase OK
- Phase equilibrium data OK
- Experimental lengthening kinetics OK
- Elastic terms, including anisotropy OK
- Interfacial energy terms, including anisotropy
- Vegard's Law coefficient; OK; small for Cu-Zn

In this case, we expect that the relative anisotropies of elastic and interfacial terms will determine precipitate habit.

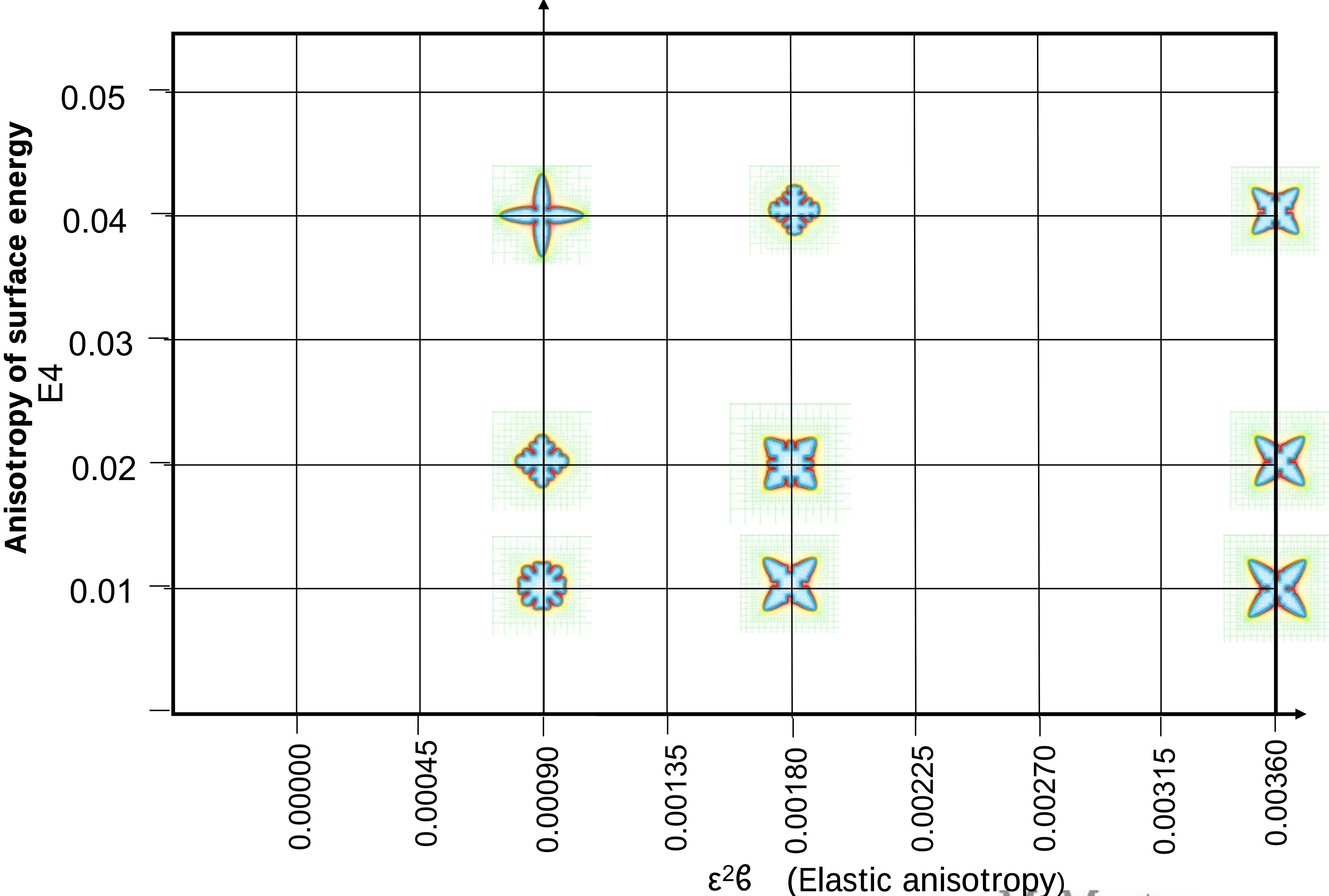
Previous analysis by Stephens and Purdy (Scripta Met., **8**, p323, 1974)

Compared lengthening of α rods and γ dendrites in similar β matrices.

Dendrite lengthening kinetics using Trivedi analysis, at supersaturations of $\Omega=0.2$ and 0.5 are consistent with a constant Interfacial resistance term (quantified by $\mu=0.08$ cm/s.

Phase field results:

These are two-dimensional simulations, which include the effects of anisotropy of interfacial energy and elasticity.



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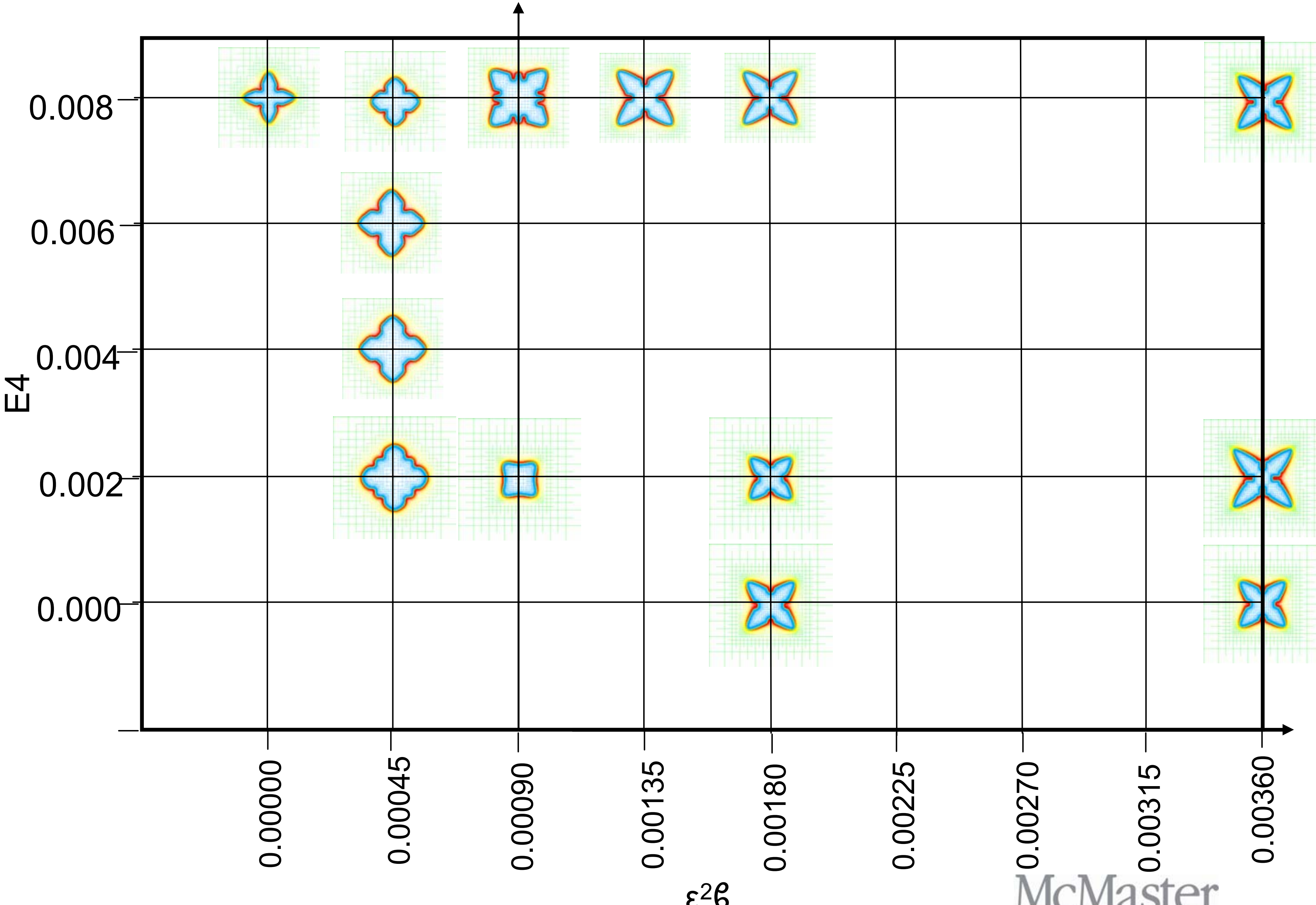

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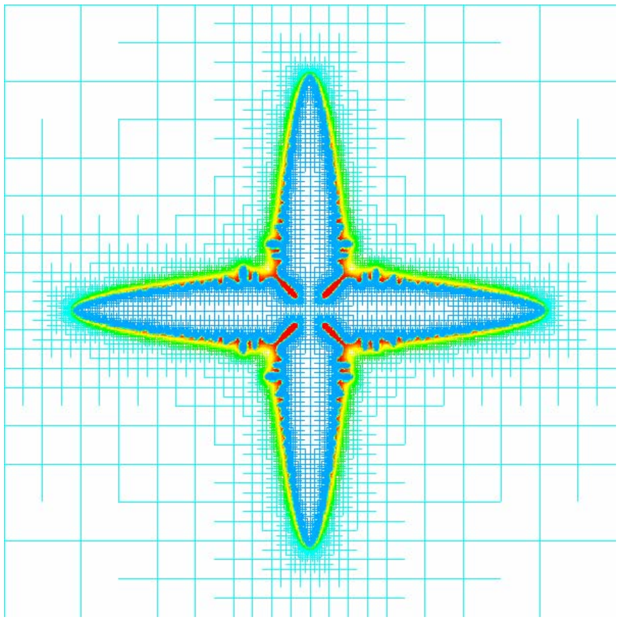
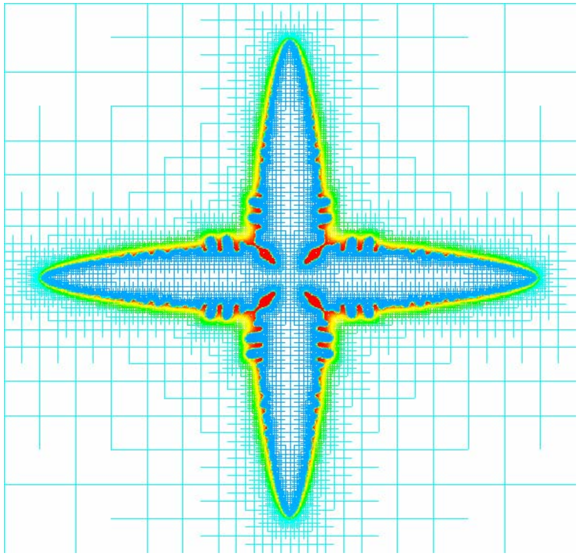
Surface anisotropy: E4 = 0.04

Increasing Elastic Anisotropy

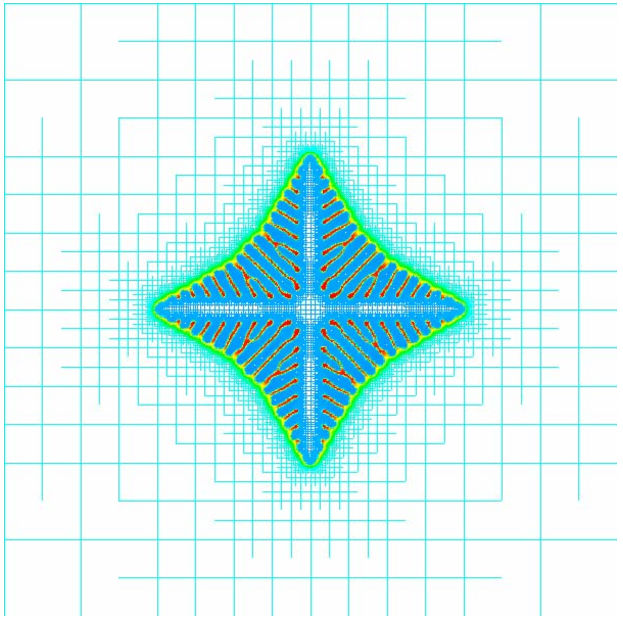
Elastic Anisotropy: Beta = 0.005



Elastic Anisotropy: Beta = 0.0075



Elastic Anisotropy: Beta = 0.01



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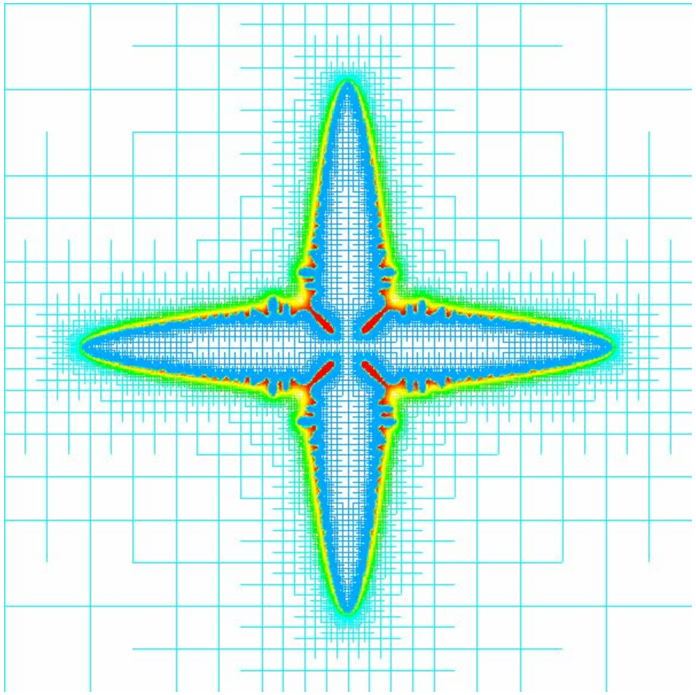
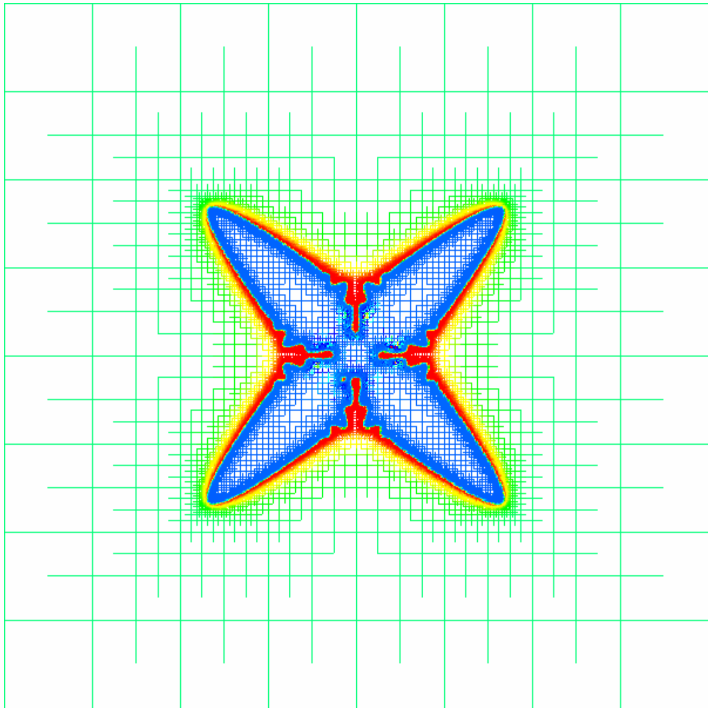
$\beta=0.005$



$\beta=0.020$



Conclusions:

Classical modeling of rod and disc growth is well advanced, and capable of accurately simulating precipitate growth from solid solution; it still relies on the availability of material parameters, such as interfacial energies and their anisotropies.

Phase field modeling of the same processes, while not entirely quantitative, yields new insights, and allows the exploration of parameter variations not accessible to experiment.

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