Phase Field Solidification Modeling

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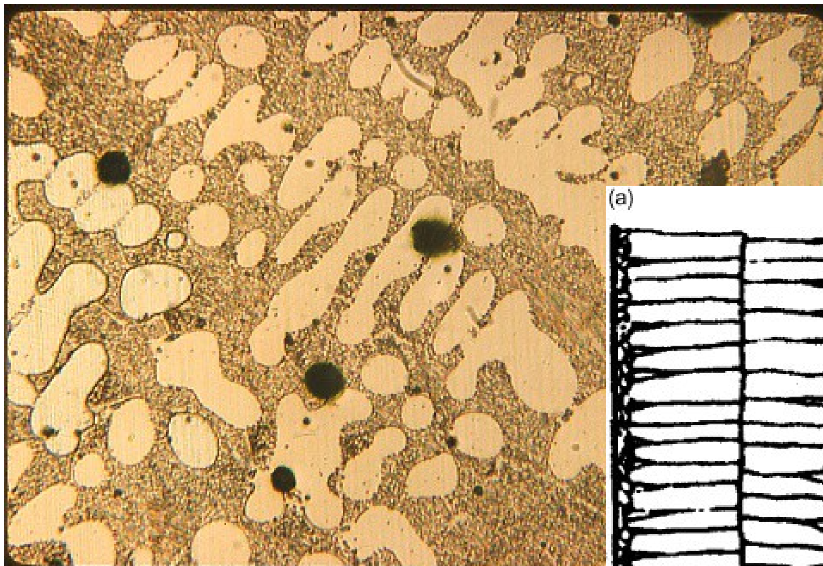
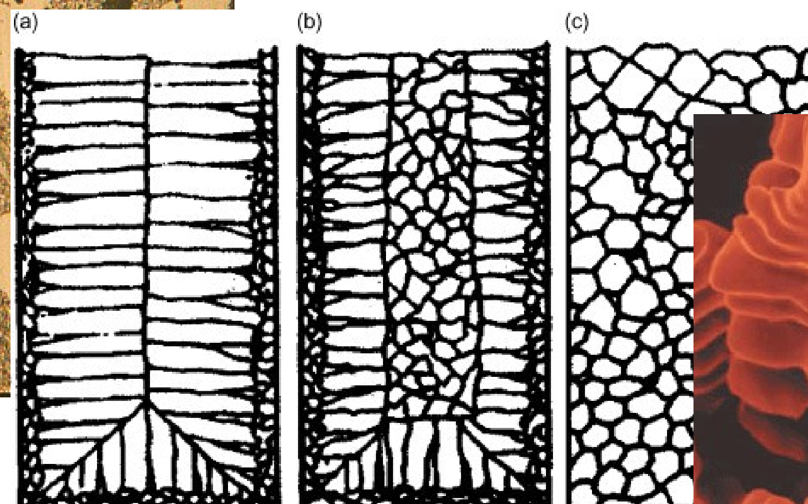
Solidification

- Casting, welding
- Consider:
  - Nucleation and growth (hetero/homogeneous)
  - Thermal and constitutional undercooling
  - Solute segregation
  - Cellular and dendritic growth
  - Multi-phase systems, decomposition

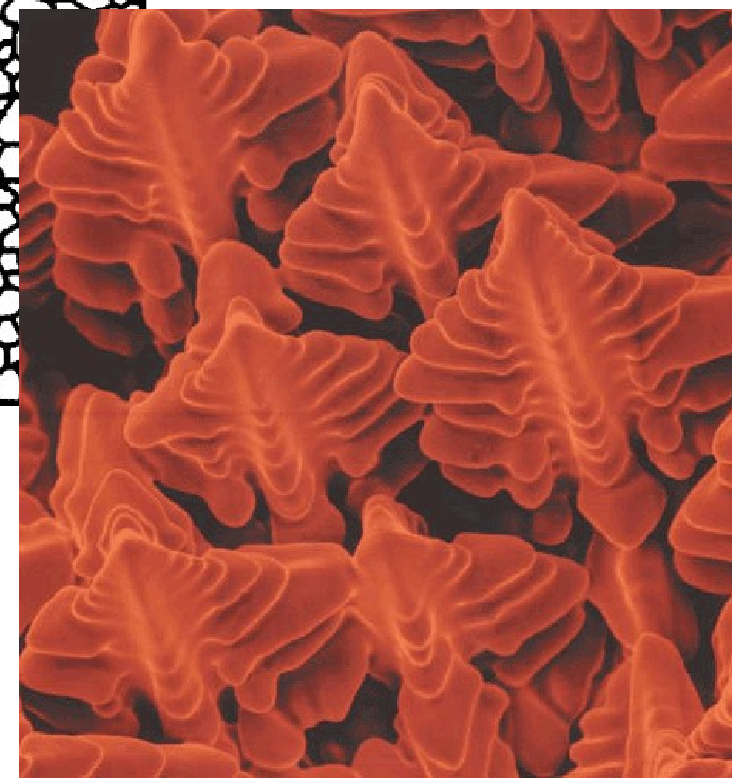
Solidification Microstructures



Eutectic in cast Cu
George Langford, MIT



Classic Casting microstructures
Kelton and Greer (2010)



Dendrites in Ni-based superalloy weld
David et al. (2003)

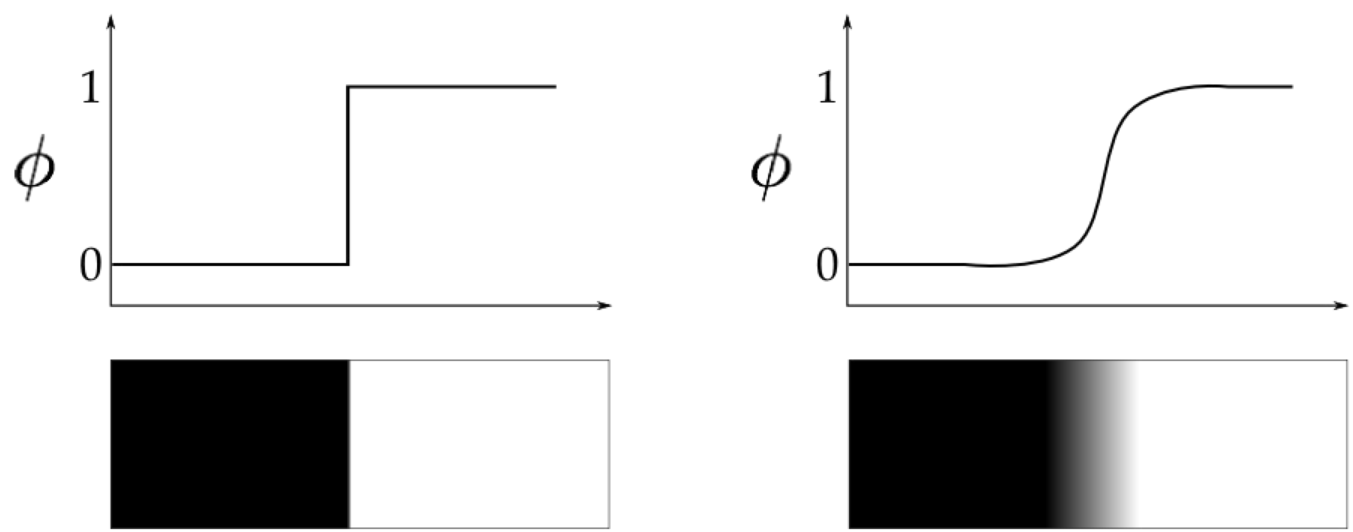
Serious impact on mechanical properties!

Modeling Solidification

- Option 1: "Sharp Interface Model"
  - Explicitly keep track of the interface
  - Conserve heat, mass in solid & liquid, couple with transport eqns. across boundary, add interfacial effects
  - **Very** computationally intensive for complex, realistic microstructures

Modeling Solidification

- Option 2: "Phase Field" (diffuse interface) model
  - Order parameter ϕ: a field that describes the phase:
    - Where $\phi = 1$, solid. Where $\phi = 0$, liquid.
    - Where $0 < \phi < 1$, "Interface"
  - Interface is not tracked, but ϕ is allowed to evolve



Governing Equations

"Gradient energy coefficient"

$$F = \int_V \left[f(\phi, T) + \frac{\varepsilon^2}{2} |\nabla \phi|^2 \right] dV$$

Contributions from pure phases

Only non-zero at interface

"Interface mobility"

$$\frac{\partial \phi}{\partial t} = M \left[\varepsilon^2 \nabla^2 \phi - \frac{\partial f(\phi, T)}{\partial \phi} \right]$$

$$\frac{\partial T}{\partial t} = D \nabla^2 u + \frac{1}{2} \frac{\partial \phi}{\partial t}$$

(for non-isothermal case)

$$f(\phi, T) = [1 - p(\phi)]\, f_S(T) + p(\phi) f_L(T) + Q g(\phi)$$

$$p(\phi) = \phi^3 \left(6\phi^2 - 15\phi + 10\right)$$

(interpolation)

$$g(\phi) = \phi^2 (1 - \phi)^2$$

(double well)

Anisotropy

- To model, e.g., dendrites, need **anisotropic** (direction-dependent) crystal growth: use gradient energy coefficient

$$\hat{\boldsymbol{n}} = -\frac{\nabla\phi}{|\nabla\phi|}$$

$$\varepsilon^2(\hat{\boldsymbol{n}}) = \varepsilon_0^2(1-3\varepsilon_c)\left[1 + \frac{4\varepsilon_c}{1-3\varepsilon_c}\left(n_x^4 + n_y^4 + n_z^4\right)\right]$$

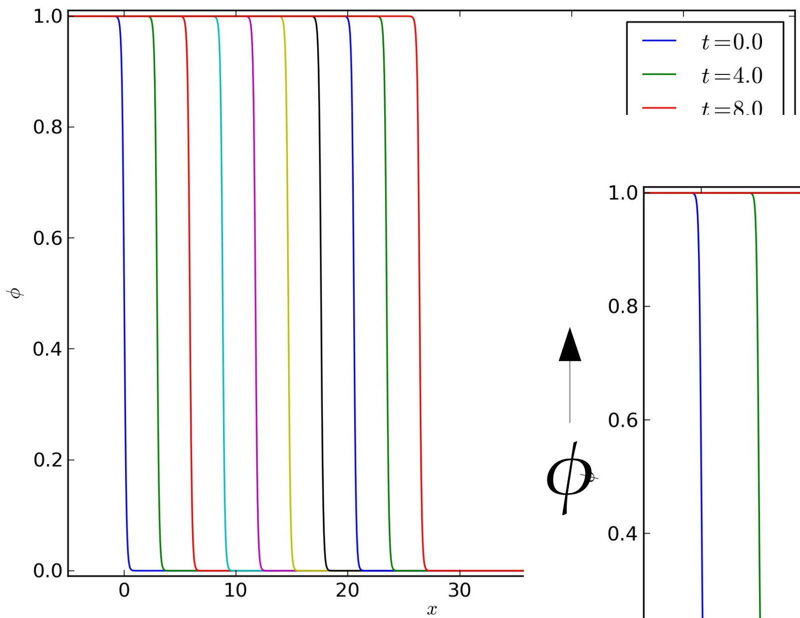
$$n_x^4 + n_y^4 + n_z^4 = \frac{(\partial\phi/\partial x)^4 + (\partial\phi/\partial y)^4 + (\partial\phi/\partial z)^4}{|\nabla\phi|^4}$$

2D phase field simulation of dendrites (not mine)
Furrer (2011)

This Work

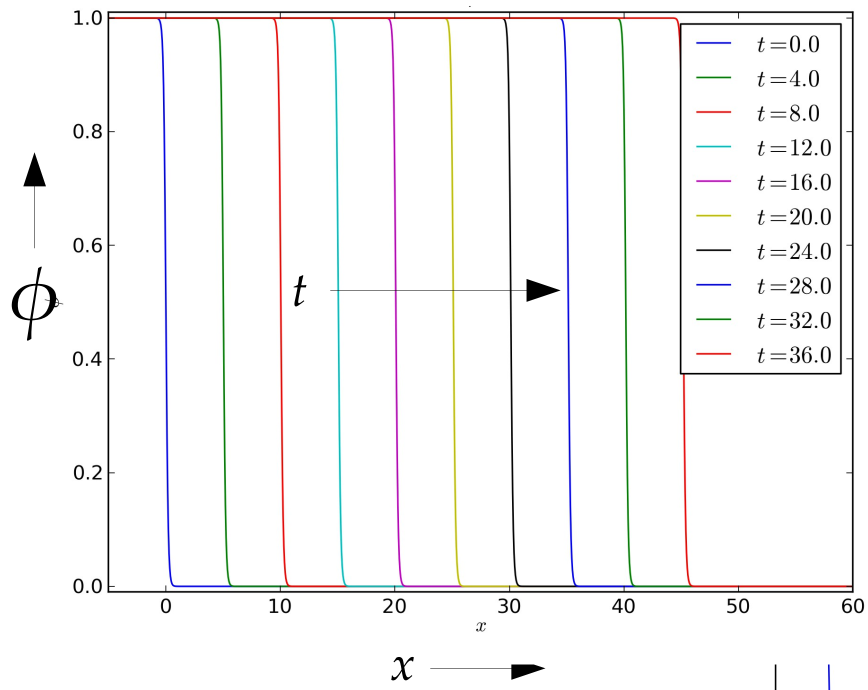
- Implemented single component 1-D phase field simulator for solidification
  - With clear hooks to extend to 2-D and binary systems
- Numerically integrated governing equations using implicit finite difference scheme
  - Explicit scheme required extremely small timesteps
  - Converted finite difference equations to matrix form, solve with LAPACK

1D Solidification of ~Ni



$\varepsilon = 1$
$M = 0.5$

$\varepsilon = 1$
$M = 1$



$\varepsilon = 2$
$M = 0.5$