Problem and scales

Selection of the dendrite tip radius and arm spacing

Scales for tip selection

$d_0 = \Gamma / (\Delta S \Delta T_0)$ Capillary length **~ 10^{-9}m**

$L_{diff} = 2D/v_{tip}$ Diffusion length **~ 10^{-4}m**

Peclet number $\mathrm{Pe} = \rho_{tip} / L_{diff}$

Selection parameter $\sigma^* = d_0 V_{tip} / (2D\,\mathrm{Pe}^2)$

Anisotropy ε defines solution **$r_{tip} = [d_0 L_{diff}/\sigma^*(\varepsilon)]^{1/2}$ ~ µm**

More scales in directional solidification of alloys:

$L_t = \Delta T_0 / G$ Solidification length **~ cm**

Primary arm spacing selection

$\lambda \sim (L_t \rho_{tip})^{1/2} \sim 100\ \rho_{tip}$

Phase-field equations

Evolution equation for the phase field

$$\frac{\partial \phi_s}{\partial t} = \mu\left[\sigma(\mathbf{n})\left(\nabla^2\phi_s + \frac{\pi^2}{2\eta^2}(\phi_s - \phi_l)\right) + \frac{\pi}{\eta}\sqrt{\phi_s\phi_l}\,\Delta G\right]$$

Evolution equation for the solute concentration

$$\partial_t c + \nabla\cdot(\mathbf{U}\phi_l c_l) = \nabla\left[D_l\phi_l\nabla c_l\right] + \nabla\cdot\left[\frac{\eta}{\pi}(c_s - c_l)\partial_t\phi_s\mathbf{n}\right]$$

antitrapping current

Driving force

$$\Delta G = \Delta S(T_m - m_l c_l - T)$$

$\eta -$ interface thickness

Interface energy

$$\sigma(\mathbf{n}) = \sigma_0\left(1 - \frac{3}{2}\varepsilon + \frac{5}{2}\varepsilon\left(n_x^4 + n_y^4 + n_z^4\right)\right)$$

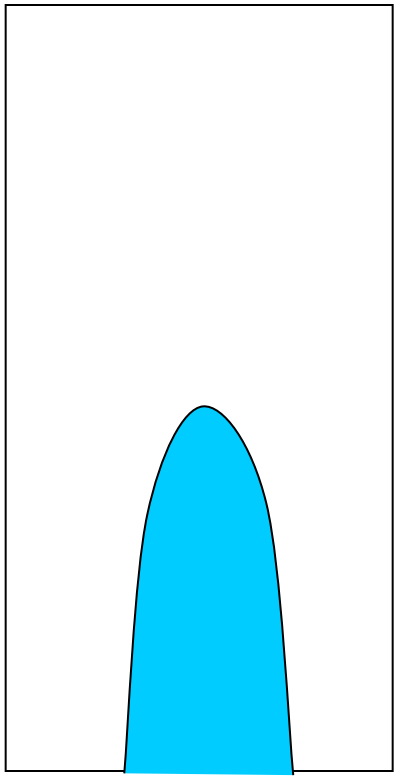
$$c_s = k c_l$$

$$\mathbf{n} = \nabla\phi_s / |\nabla\phi_s|$$

Material and simulation data

Material data of AlCu		Benchmark
Melting point Al	T_m	933.6 K
Liquidus slope	m_l	$2.6\ K/\%$
Partition coefficient	k	0.14
Liquid diffusivity	D_l	$3\times10^{-9}\ m^2/s$
Interface energy	σ_0	$0.24\ J/m^2$
Interface anisotropy	ε	0.3
Entropy of fusion	ΔS	$10^6\ J/\left(m^3K\right)$
Grid spacing	Δx	$0.4-1.5\ \mu m$
Interface thickness	η	$1.6-9\ \mu m$
Temperature gradient	$\partial T/\partial z$	$10^4\ K/m$
Cooling rate	$\partial T/\partial t$	$0.4\ K/s$

Effect of the grid spacing



Domain size: $L_X = L_Y = 100\ \mu m$

$L_z = 270\ \mu m$

Grid spacing: 0.4,0.5,0.6,0.8,...1.5 μm

Dendrite length: 120 μm

Growth velocity: $V_g = \frac{\partial T / \partial t}{\partial T / \partial z} = 40\ \frac{\mu m}{s}$

Diffusion length: $L_{diff} = \frac{2D_l}{V_g} = 150\ \mu m$

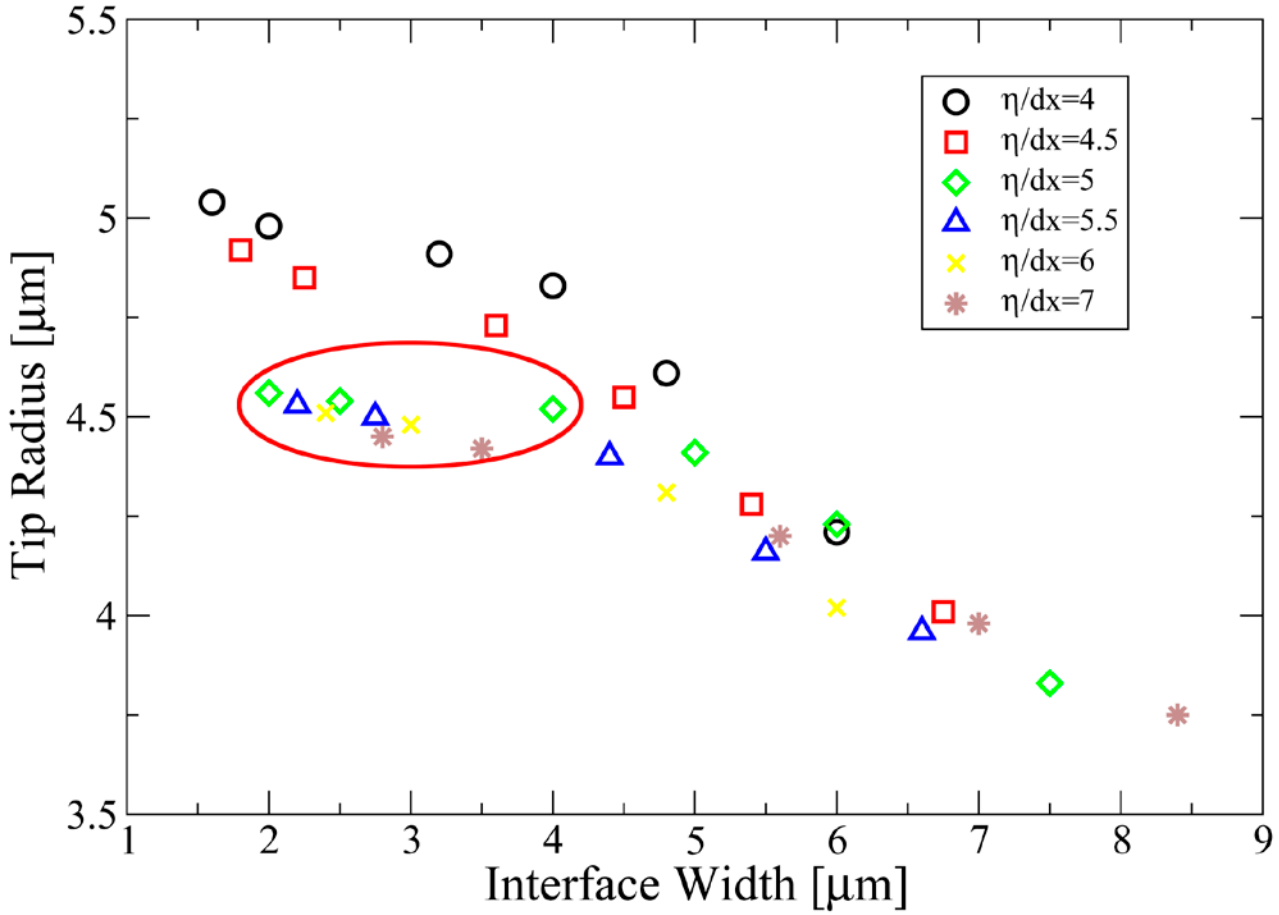
Boundary conditions:

Phase Field : Zero gradient

Concentration Field : Fixed 4% (top), zero gradient (others)

Simulation results: convergence check

Convergence for different grid spacing and interface width



Simulation results: spacing selection

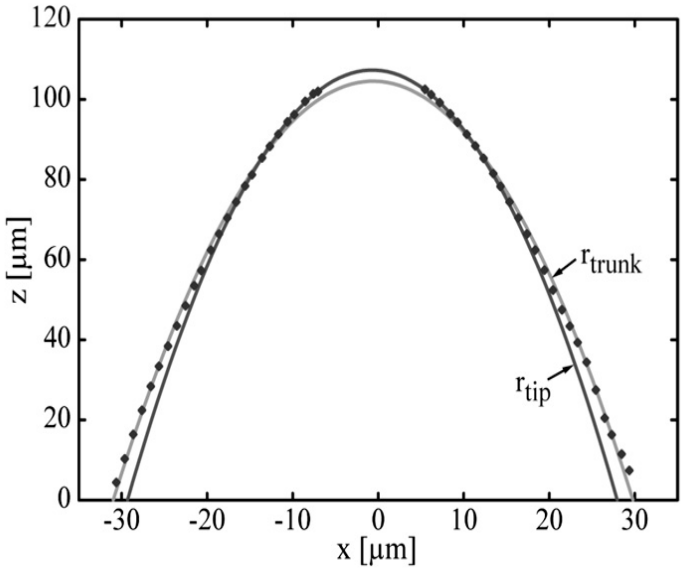
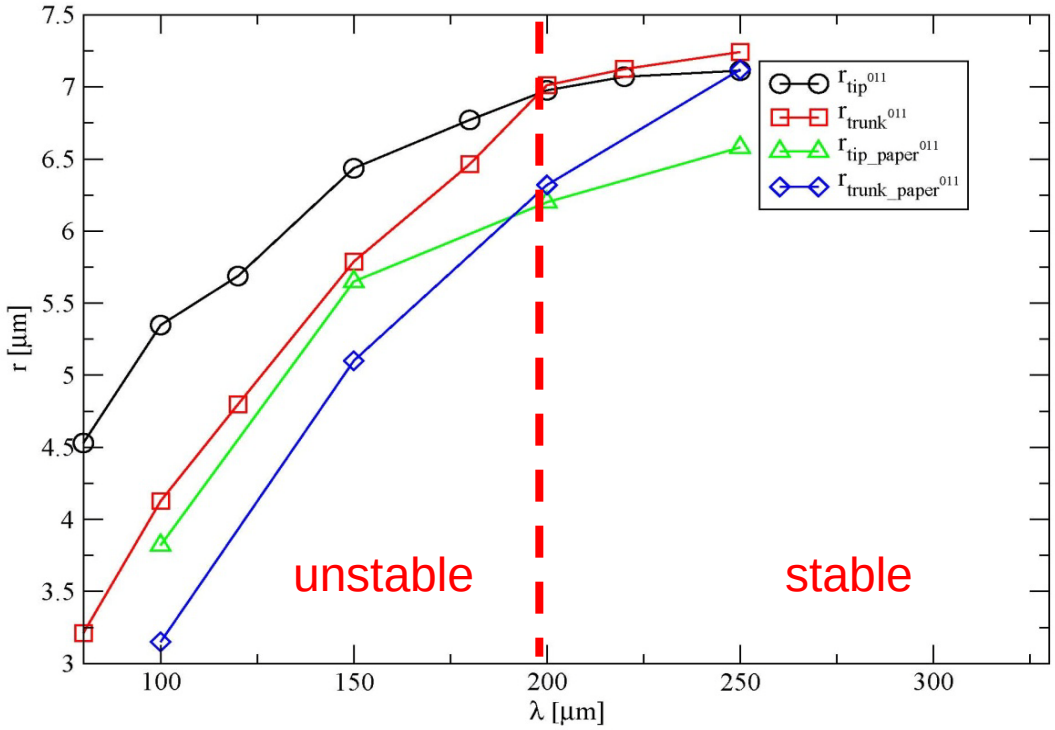


Fig. 6. Plot of the phase-field contour points with the fitted parabola r_{tip} and r_{trunk}. (Note the different scale on the x- and z-axes.).



Green & Blue lines are taken from "I.Steinbach. Acta Mat. 56 (2008)4965-4971"