Phase Field Modelling of Fast Crack Propagation

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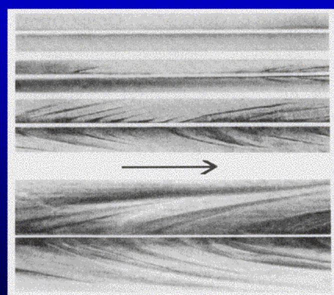
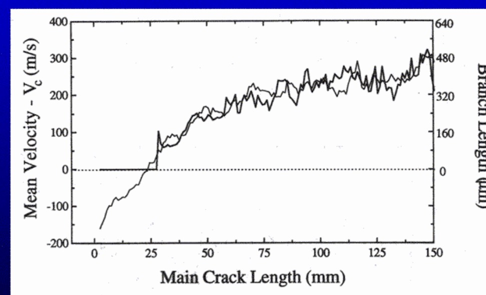
Contents

The Mystery of Fracture

- Why are cracks not always straight?
- How fast can cracks grow?
- Why do cracks split?
- What is happening in the tip region?

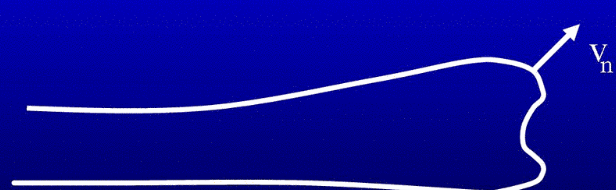




Can we develop a minimum theory of fracture?

A Macroscopic Theory of Fracture?

- Unavoidable ingredients: Elasticity + surface energy
- Linear elasticity: Tip blunting necessary
- Pattern formation: equation of motion for each interface point

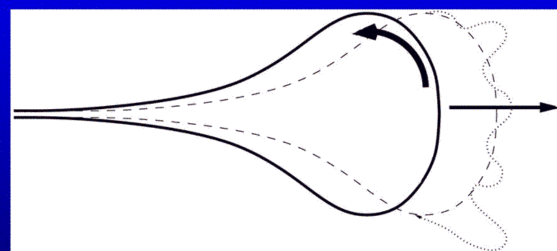


- Crack path prediction without assumptions!

Fast Crack Growth By Surface Diffusion

Only ingredients: Continuum theory

- Linear theory of dynamical elasticity
- Surface energy
- Surface diffusion

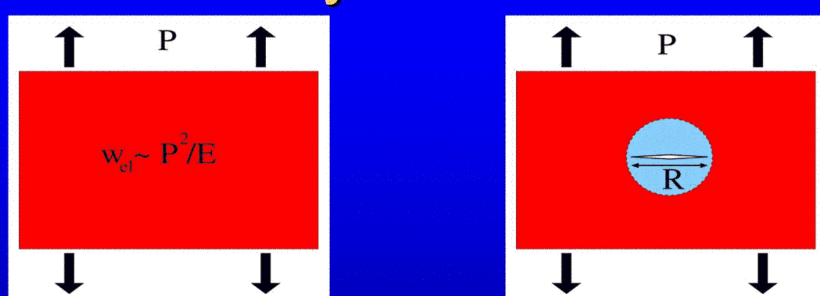


Predictions:

- Steady state velocity appreciably below Rayleigh speed
- Tip blunting
- Tip splitting instability

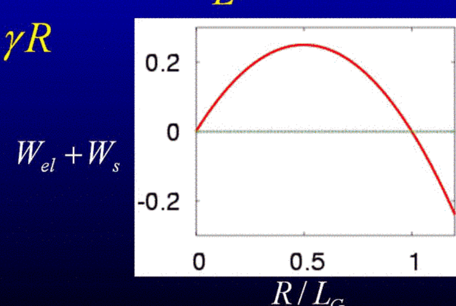
Simplification: Melting/crystallization instead of surface diffusion

Theory of Cracks I

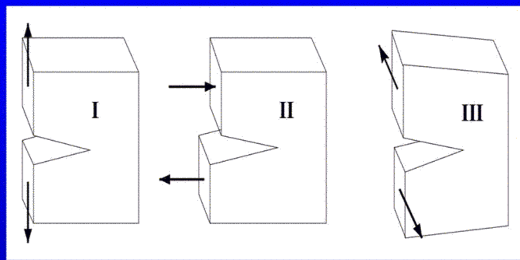


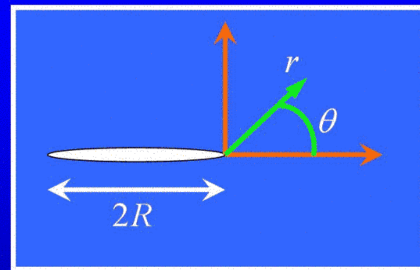
- Elastic relaxation in the area $\propto R^2$: $W_{el} \propto -\frac{P^2 R^2}{E}$
- Increase of surface energy: $W_s \propto \gamma R$
- Griffith length:

$$L_G \propto \frac{E\gamma}{P^2}$$



Theory of Cracks II





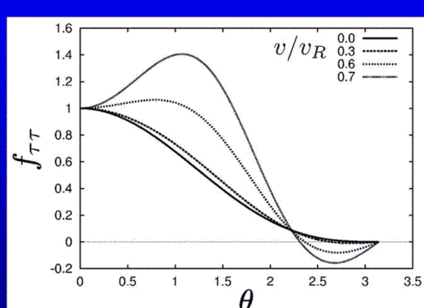
- Three modes of loading
- Stress distribution in the vicinity of the crack tip:

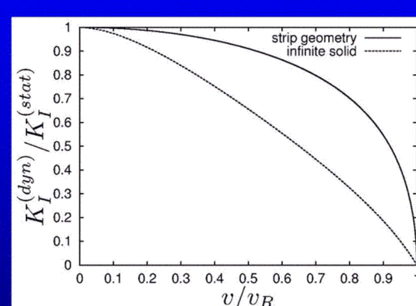
Static elasticity: $\sigma_{ij} = \frac{K}{r^{1/2}} f_{ij}(\theta)$

Dynamic elasticity: $\sigma_{ij} = \frac{K(v/v_R)}{r^{1/2}} f_{ij}(\theta, \frac{v}{v_R})$

Stress intensity factor: $K \propto PR^{1/2}$ Rayleigh speed: $v_R \propto (E/\rho)^{1/2}$

Dynamical Effects

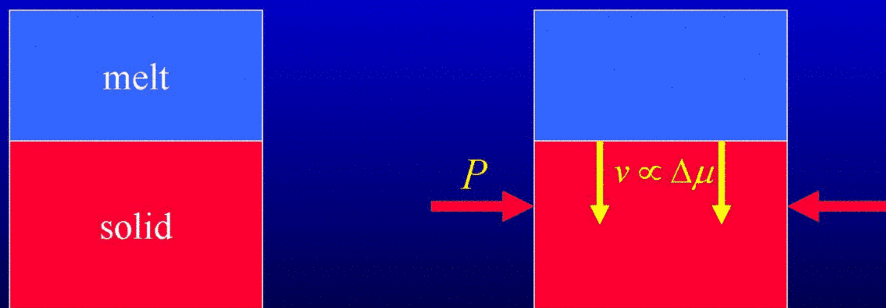




- Maximum stress not in forward direction for high crack speeds
- Cracks cannot be faster than Rayleigh speed

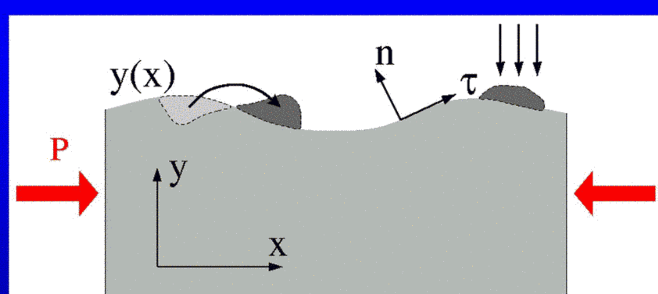
Elastic Effects on Phase Transitions

- Solid-liquid interface in thermal equilibrium: $\mu_{sol} = \mu_{liq}$
- Elastic stresses: $\Delta\mu = \Omega \frac{1}{2} \sigma_{ij} u_{ij}$



- The solid phase becomes less favorable

The Grinfeld Instability I



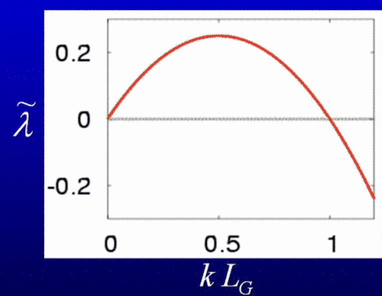
- Nonhydrostatic loading: $\sigma_{nn} \neq \sigma_{\tau\tau}$
- Morphological instability not due to elastic displacement
- Chemical potential at the surface: $\mu = \Omega\left(\frac{1}{2}\sigma_{ik}u_{ik} - \gamma\kappa\right)$
- Melting/crystallization: $v_n = \frac{D}{\gamma\Omega}\mu$

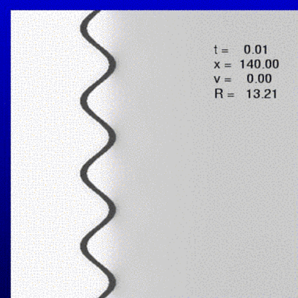
The Grinfeld Instability II

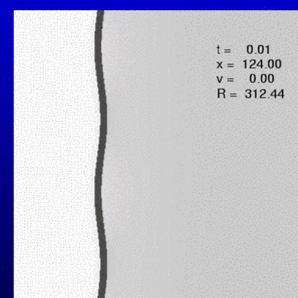
- Stability analysis of a flat surface (melting/crystallization):

$$\Delta y = y_0 \sin(kx)\exp(\lambda t)$$

$$\lambda = D\left[\frac{2P^2(1-\nu^2)}{E\gamma}|k| - k^2\right]$$

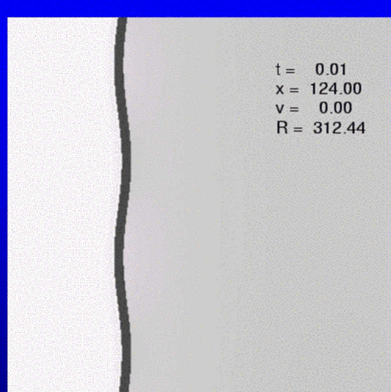


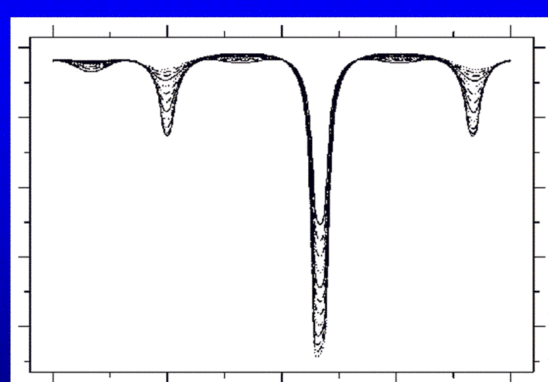




- Long wave modes are unstable
- Griffith length is the characteristic lengthscale: $L_G \propto E\gamma / P^2$

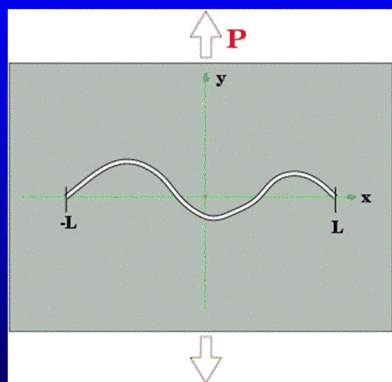
The Cusp Singularity





- Finite time singularity: Velocity and tip curvature diverge!
- Incomplete physical description!

Grinfeld Instability on Crack Surfaces



- Surface of a straight crack: $\sigma_{nn} \neq \sigma_{\tau\tau}$
- Long wave instability if $L > 5.18\, L_G$
- Surface diffusion (melting and crystallization) is slow!

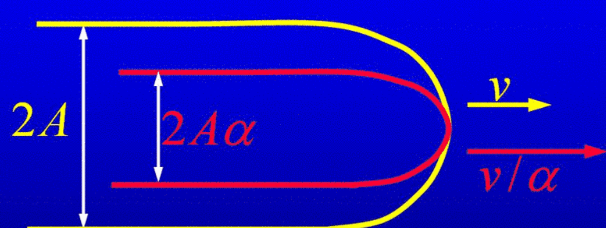
Cracks can deform (slowly!) even behind the tip!

Steady State Motion I

Claim: Steady state motion is impossible with *static* elasticity

Proof: Step 1. The scaling invariance

Assume that we found a solution.



Construction of a rescaled solution: $length \rightarrow \alpha \cdot length$

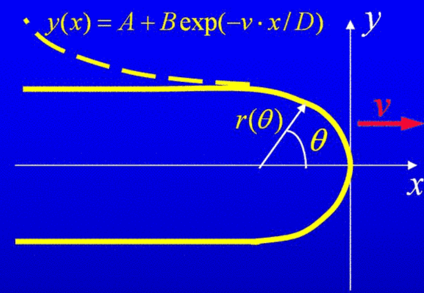
$$\mu = \Omega\left(\frac{1}{2}\sigma_{ik}u_{ik} - \gamma\kappa\right) \propto \alpha^{-1} \qquad v_n = \frac{D}{\gamma\Omega}\mu \propto \alpha^{-1}$$

$$v \rightarrow v/\alpha$$

Notice: Only with static elasticity, since σ does not depend on v!

Steady State Motion II

Proof: Step 2. The tail behavior



- Equation of motion: $v_n = \frac{D}{\gamma\Omega}\mu$
- Steady state: $\frac{\partial y}{\partial t} = -vy'$

➢ Shape equation: $\kappa = \frac{\sigma_{ik}u_{ik}}{2\gamma} + \frac{vy'}{D\left(1+y'^2\right)^{1/2}}$

Start integration at the tip: $y(0) = 0, \quad r'(\theta = 0) = 0$ (origin + symmetry)

Tail: v is the only parameter: $y = y(x, v)$

- No stresses in the tail region: $-v \cdot y' = Dy''$

  $\Rightarrow y(x) = A + B\exp(-v \cdot x / D) \qquad \left(A = A(v), B = B(v)\right)$

- Boundary condition: $B(v) = 0$ selects v ?
- Rescaling: $A \propto B \propto 1/v \quad \Rightarrow v \to \infty$ ➢ Selection impossible!

Steady State Motion III

- Static Elasticity: Only the combination vA/D appears in the shape equation

➢ Steady state solution does not exist

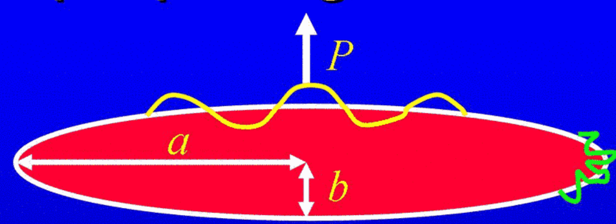
- *Dynamic* elasticity: Velocity appears in the two combinations vA/D and v/v_R

➢ No rescaling possible

➢ Two independent parameters: complete selection

➢ Steady state solution does exist

Tip Splitting Instability



- Elliptical crack can be solved analytically, $a >> b$
- Long wave instability if $a \propto E\gamma / P^2$
- Stresses at the tip: $\sigma_{\tau\tau}^{(tip)} \propto Pa / b \to \infty$
- Grinfeld length at the tip: $L_G^{(tip)} \propto E\gamma / {\sigma_{\tau\tau}^{(tip)}}^2$
- Instability if $L_G^{(tip)}$ fits into the tip radius $r^{(tip)} = b^2 / a$

$$a \propto E\gamma / P^2 \propto L_G$$

Phase Field Simulations: Basics

Sharp interface:

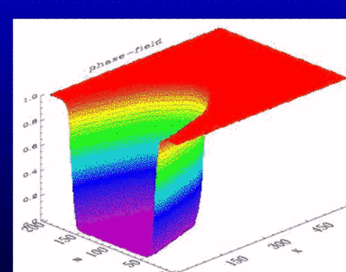
- Chemical potential: $\mu = \Omega\left(\frac{1}{2}\sigma_{ik}u_{ik} - \gamma\kappa\right)$
- Normal velocity: $v_n = \frac{D}{\gamma\Omega}\mu$

Phase field: $\phi = 0$ liquid, $\phi = 1$ solid

- Interface width ε
- Equation of motion for the phase field:

$$\frac{\partial\phi(x,y,t)}{\partial t} = -\frac{D}{3\gamma\varepsilon}\frac{\delta F}{\delta\phi}$$

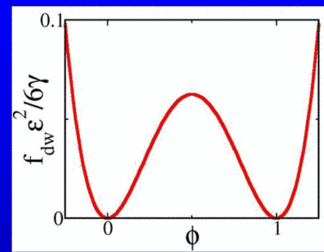
- Find proper free energy F!



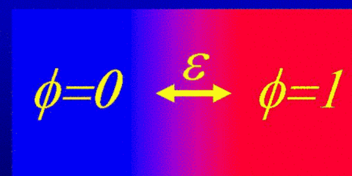
Phase Field Simulations: Surface Energy

Goal: Correct sharp interface limit $\varepsilon \to 0$

$$F[\phi] = \int dV \left(f_s + f_{dw} \right)$$

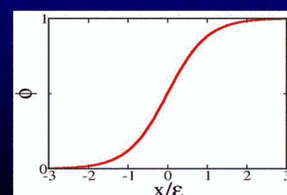


- Double well potential: $f_{dw} = \frac{6\gamma}{\varepsilon^2}\phi^2(1-\phi)^2$
- Interfacial energy: $f_s = \frac{3\gamma\varepsilon}{2}(\nabla\phi)^2$



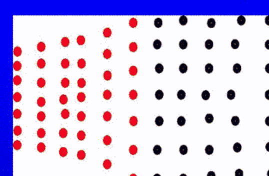
Straight, static interface: $\frac{\delta F}{\delta \phi} = 0$

$$\phi(x) = \frac{1}{2}\left(1 + \tanh\frac{x}{\varepsilon}\right)$$



Phase Field Simulations: Elasticity

- Dynamical elasticity
- Two solid phases with different elastic constants
- Coherent interface (continuous displacement)
- Equal mass density



Elastic energy density: $f_{el} = \mu(\phi)u_{ij}^2 + \lambda(\phi)u_{ii}^2$

Free energy: $F[\phi, u_i] = \int dV \left(f_s + f_{dw} + f_{el} \right)$

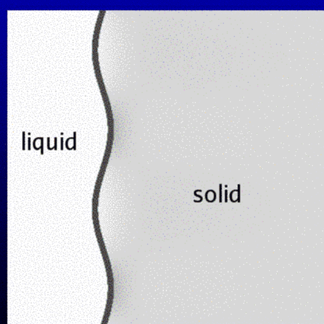
Phase field dynamics: $\frac{\partial \phi}{\partial t} = -\frac{D}{3\gamma\varepsilon}\frac{\delta F}{\delta \phi}$

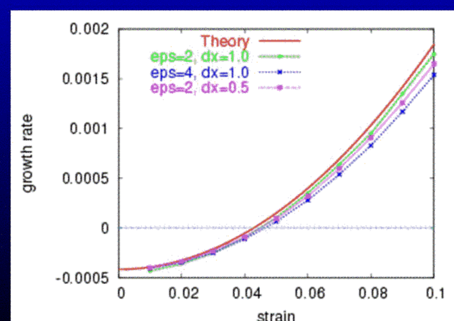
Elastodynamics: $\rho \ddot{u}_i = -\frac{\delta F}{\delta u_i}$

Leads to the correct sharp interface limit!

Grinfeld Instability: Phase Field Simulations

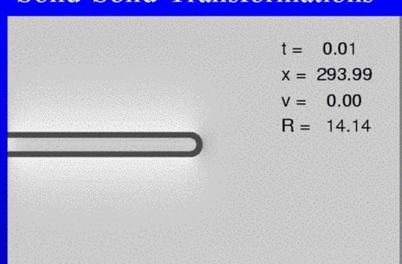
- Explicit phase field code
- Dynamical elasticity, explicit code
- Equations of motion derived from discretized variational principles
  - Numerical stability
  - Spatial and temporal symmetry
- Staggered grid





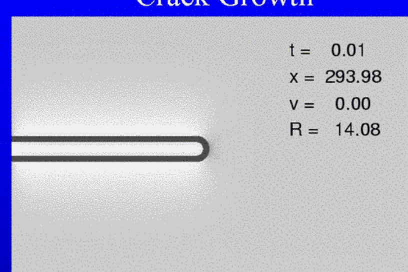
Phase Field Simulations

Solid-Solid-Transformations



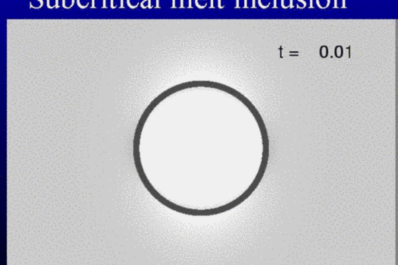
- Elastic properties: $\lambda_2 = 0.1\lambda_1$; $\mu_2 = 0.1\mu_1$
- Surface sound speed (hard phase): $v_R = 2.27$

Crack Growth

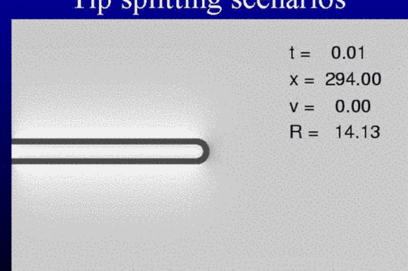


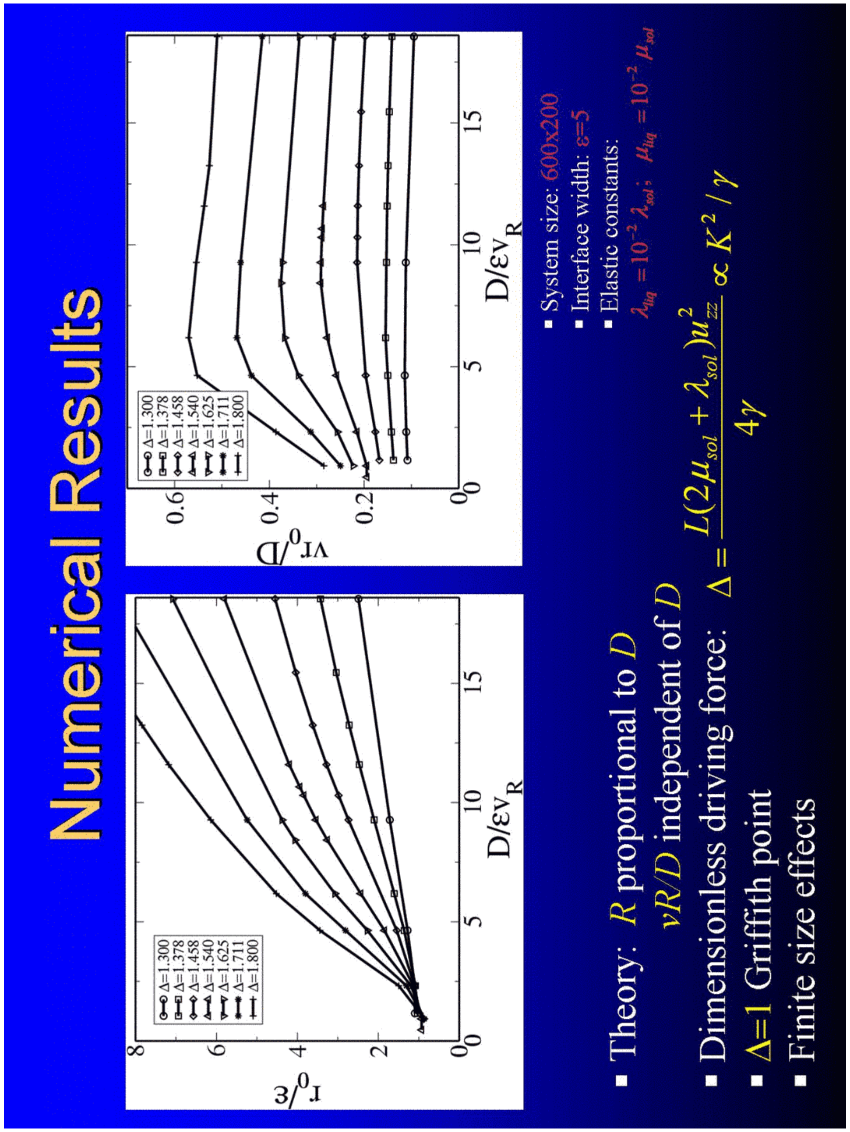
- Elastic properties: $\lambda_{liq} = 10^{-2}\,\lambda_{sol}$; $\mu_{liq} = 10^{-2}\,\mu_{sol}$
- Dilatational wave speed (soft phase): $v_d^{liq} = 0.49$

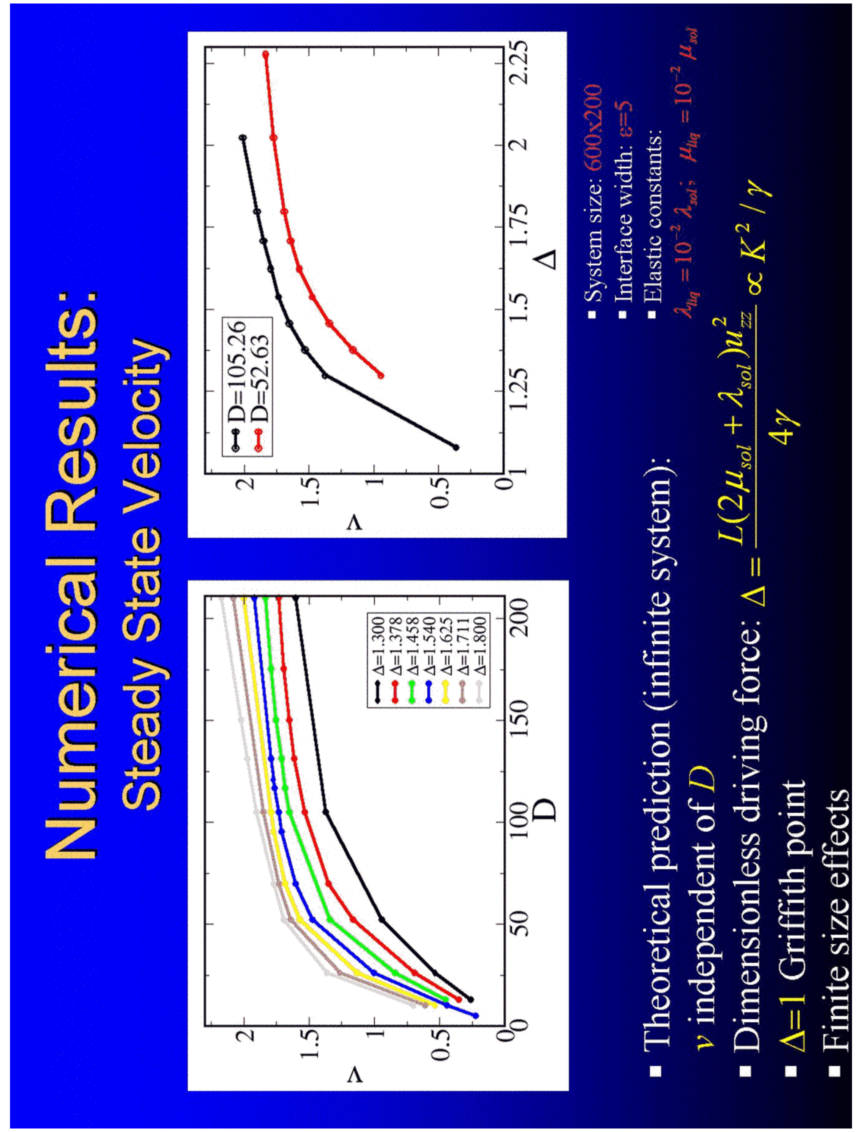
Subcritical melt inclusion



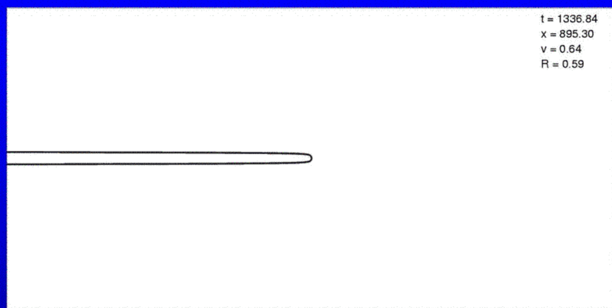
Tip splitting scenarios

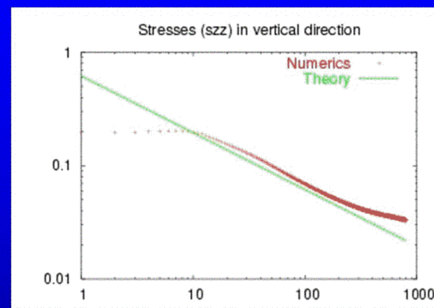


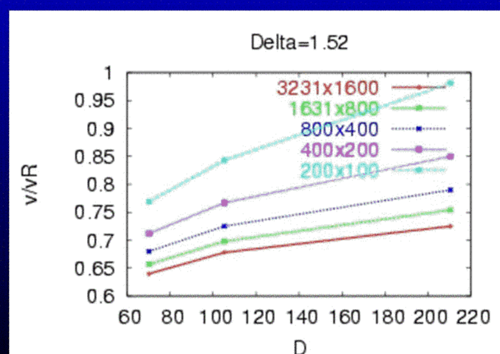

Numerical Results
Δ=1.300
Δ=1.378
Δ=1.458
Δ=1.540
Δ=1.625
Δ=1.711
Δ=1.800
r0/ε
D/εvR
vr0/D
D/εvR
System size: 600x200
Interface width: ε=5
Elastic constants:
$\lambda_{liq} = 10^{-2}\lambda_{sol}$; $\mu_{liq} = 10^{-2}\mu_{sol}$
Theory: R proportional to D
vR/D independent of D
Dimensionless driving force: $\Delta = \frac{L(2\mu_{sol}+\lambda_{sol})u_{zz}^2}{4\gamma} \propto K^2/\gamma$
Δ=1 Griffith point
Finite size effects


Numerical Results:
Steady State Velocity
Δ=1.300
Δ=1.378
Δ=1.458
Δ=1.540
Δ=1.625
Δ=1.711
Δ=1.800
v
D
D=105.26
D=52.63
v
Δ
System size: 600x200
Interface width: ε=5
Elastic constants:
$\lambda_{liq} = 10^{-2}\lambda_{sol}$; $\mu_{liq} = 10^{-2}\mu_{sol}$
Theoretical prediction (infinite system):
v independent of D
Dimensionless driving force: $\Delta = \frac{L(2\mu_{sol}+\lambda_{sol})u_{zz}^2}{4\gamma} \propto K^2/\gamma$
Δ=1 Griffith point
Finite size effects

Large Scale Simulations







Summary and Outlook

- Continuum model for crack growth by melting and crystallization
- Only ingredients:
  - Linear theory of elastodynamics
  - Surface energy
  - Melting/solidification (or surface diffusion)
- No finite time cusp singularity, steady state growth
- Fast propagation, velocity below Rayleigh speed
- Tip splitting through secondary Grinfeld instability
- Phase field simulations
- Universal curves: *v(Δ), R(Δ)*
- Solid-solid transformations
- Tip-splitting instability
- Surface diffusion: Sharp interface approach