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Modelling of stress driven material dissolution

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"Environmental Stress Cracking is one of the most common causes of unexpected brittle failure of thermoplastic polymers. Environmental stress cracking may account for around 15-30% of all plastic component failures in service."

H. F. Mark. Encyclopedia of Polymers Science and Technology – 3rd Ed., John Miley & Sons Inc. 2004

Accidental fracture of lid of a Thorens gramophone



+



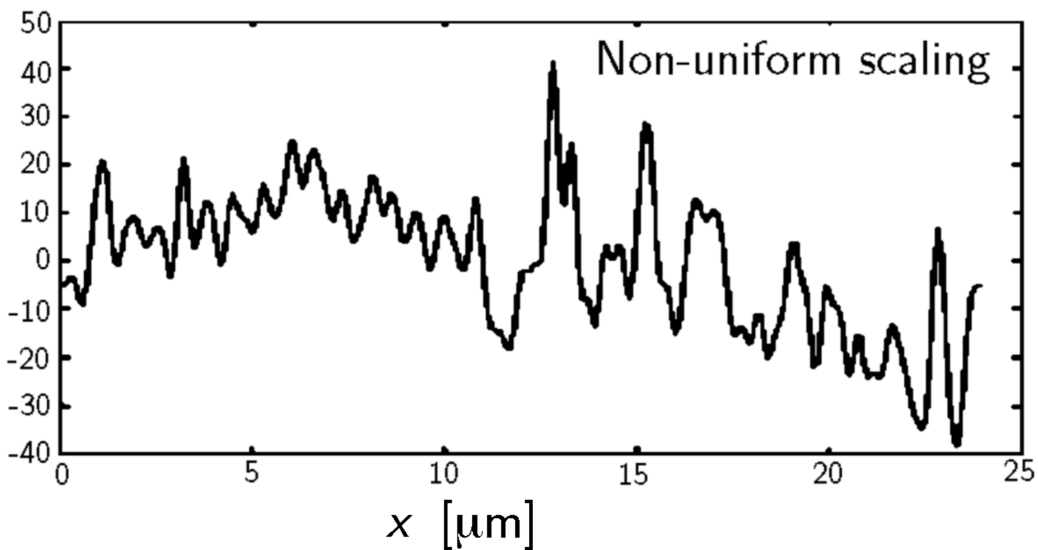
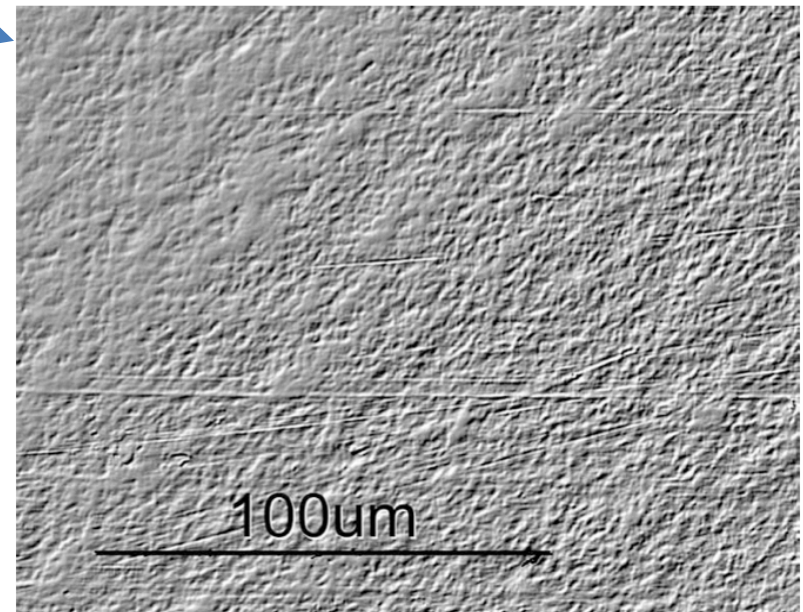
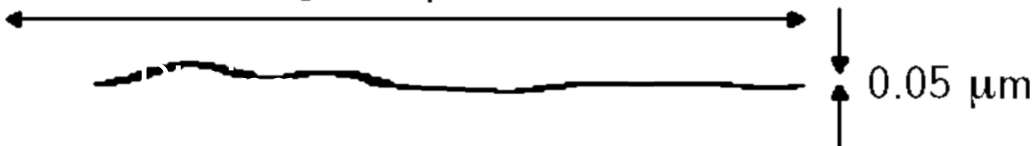
Corroding environment leads to:

1. Continuous loss of mass
2. Pitting
- ...and with mechanical stress present
3. Surface roughening

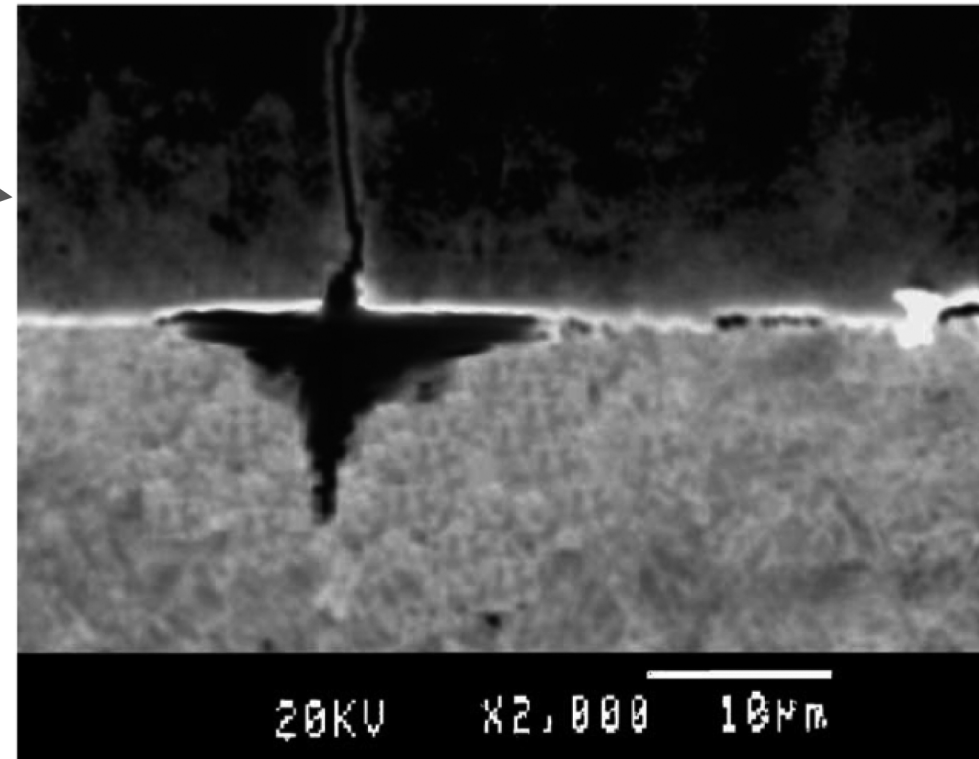


(from Kim *et al.* 2000)

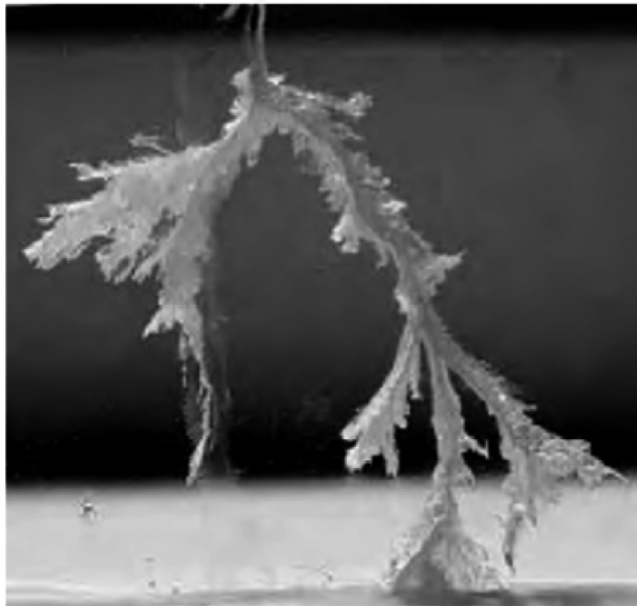
Uniform scaling 2 μm



4. Evolving pits
5. Formation of cracks
6. Crack growth
7. Crack branching



Cr/zon six charge related of land and groove substrate erosion through a micro-crack at the 12:00 bore origin. (Sopok *et al.* 2005) (Bjerkén Ortiz 2010)



Growing crack in a polycarbonate exposed to acetone (Hejman 2011)

Evolving Surface Morphology

Asaro-Tiller (1972), Grinfeld (1986, 1993), Srolovitz (1989), Freund (1995), Kim *et al.* (2000)

Gibb's free energy

$$\Phi = U_c + U_e$$

where

U_c is the free chemical energy and

U_e is the free elastic energy

The free chemical energy

$$U_c = -\gamma \frac{\partial^2 h}{\partial x^2}$$

where

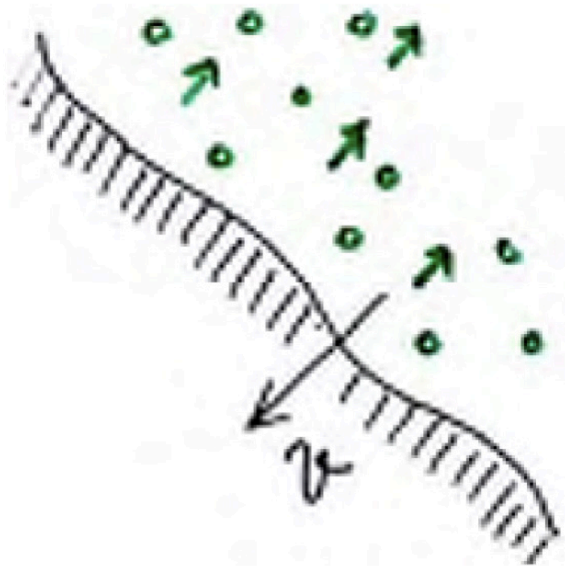
$h(x)$ gives the position of the surface

γ is the surface energy density

The free elastic energy (Cerutti)

$$U_e = \frac{1}{2} \sigma_{ij} \epsilon_{ij} \sim \frac{1}{2} \mu \frac{\partial h}{\partial x}$$

Evaporation-condensation



$$\frac{\partial h}{\partial t} = -L_1 \Phi$$

Surface diffusion



$$\frac{\partial h}{\partial t} = L_2 \frac{\partial^2 \Phi}{\partial x^2}$$

Governing equations:

Evaporation - condensation

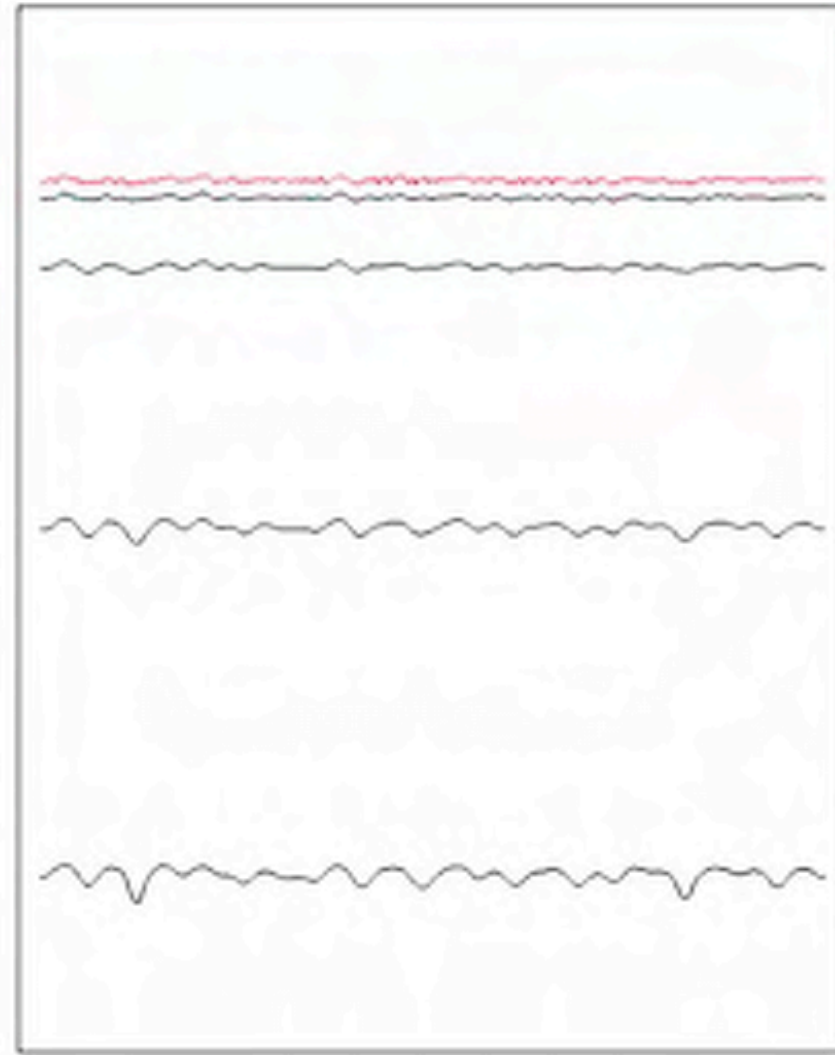
$$\frac{\partial h}{\partial t} = L_1 \left(\gamma \frac{\partial^2 h}{\partial x^2} - \frac{k}{2} \mu \frac{\partial h}{\partial x} \right)$$

or surface diffusion

$$\frac{\partial h}{\partial t} = L_2 \frac{\partial^2}{\partial x^2} \left(-\gamma \frac{\partial^2 h}{\partial x^2} + \frac{k}{2} \mu \frac{\partial h}{\partial x} \right)$$

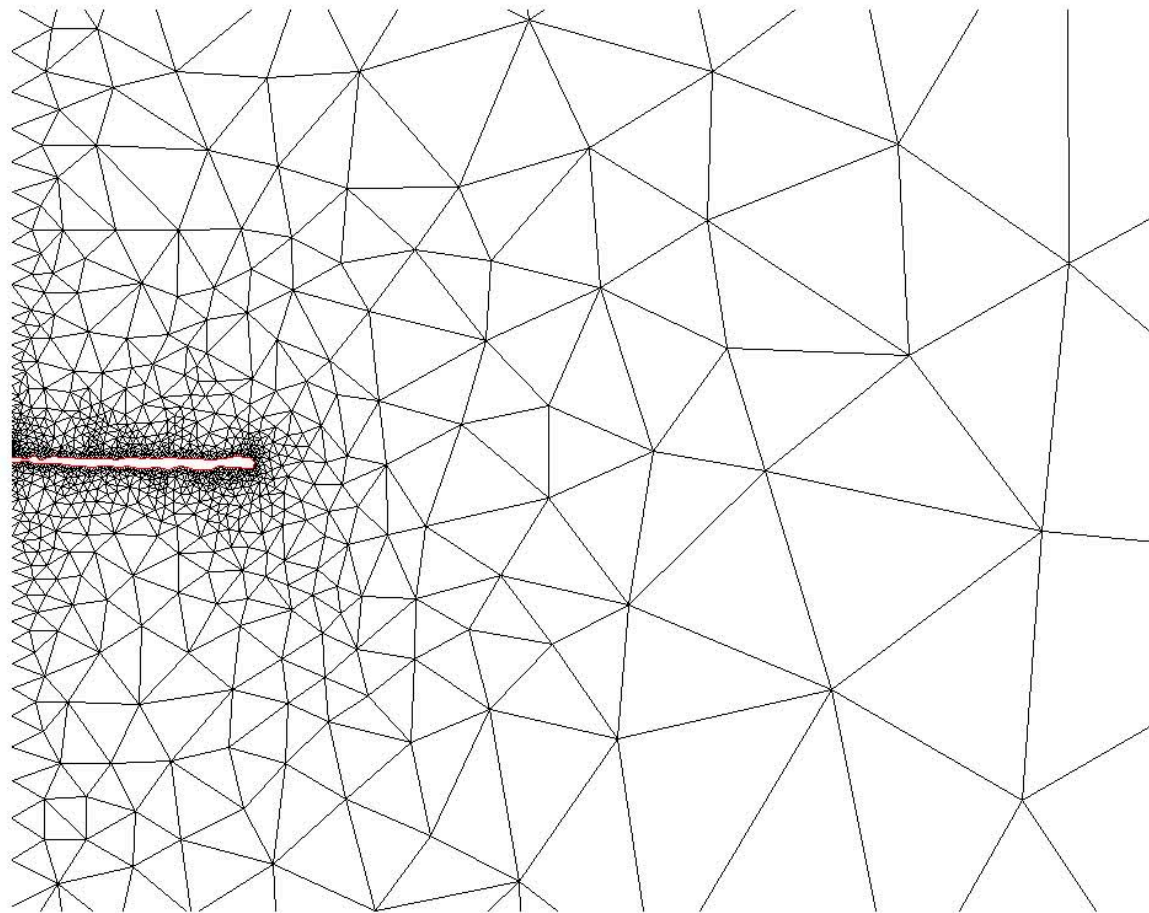
FEM calculation of an evolving surface

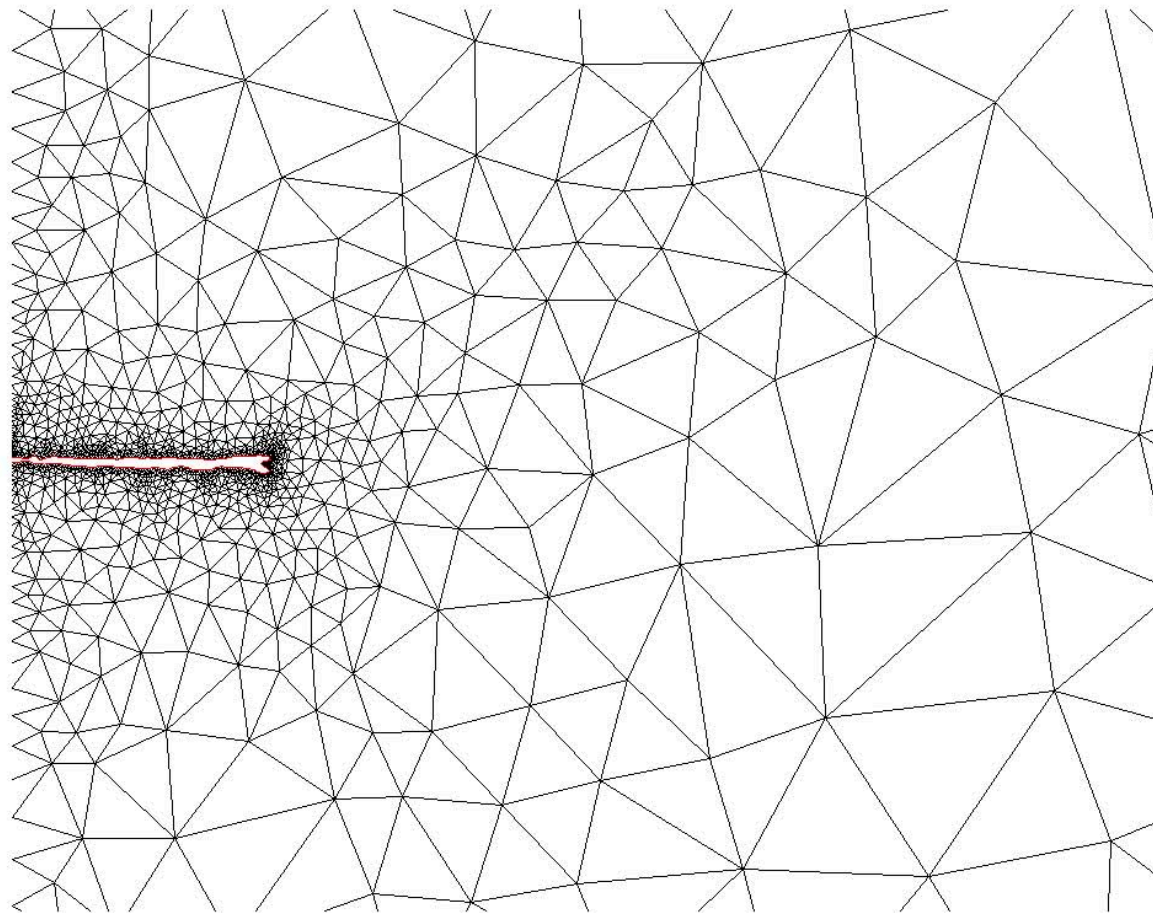
Increasing time
and depth

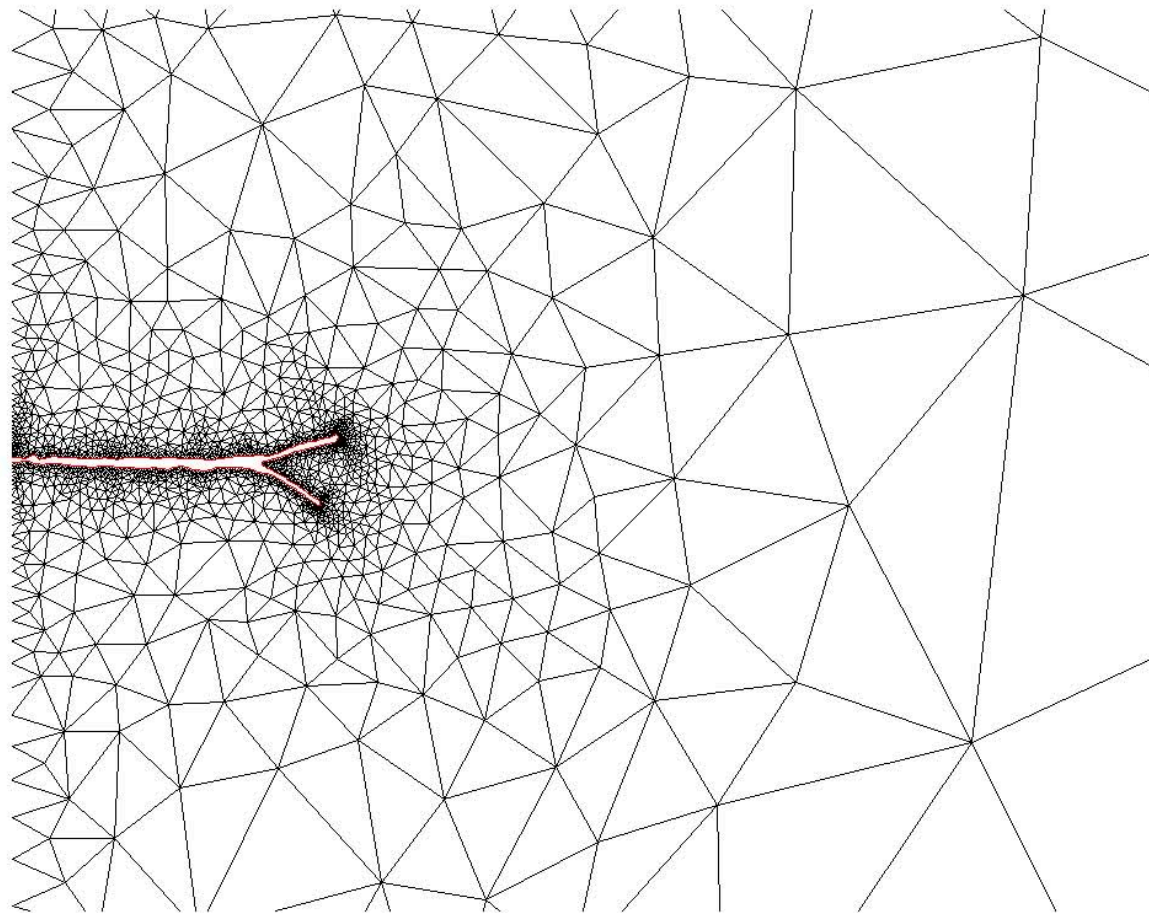


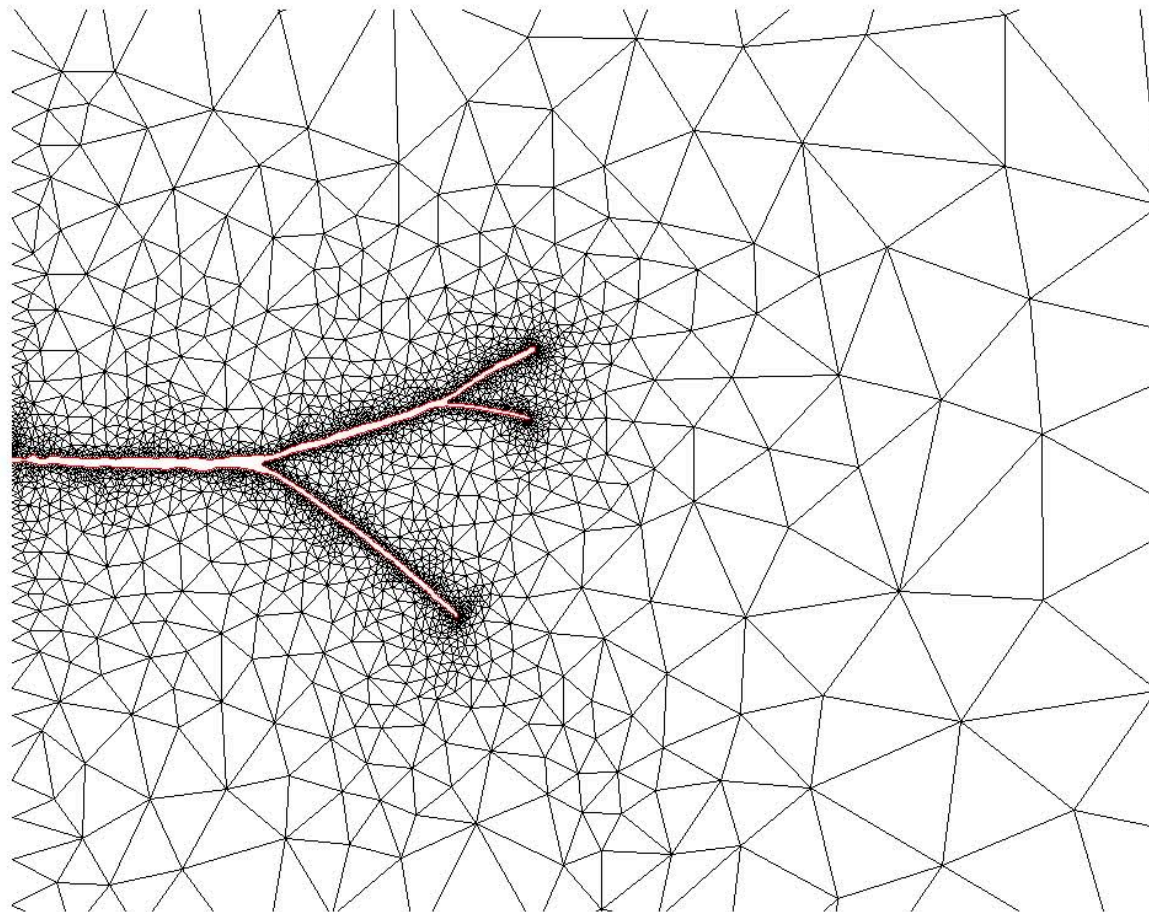
Original surface



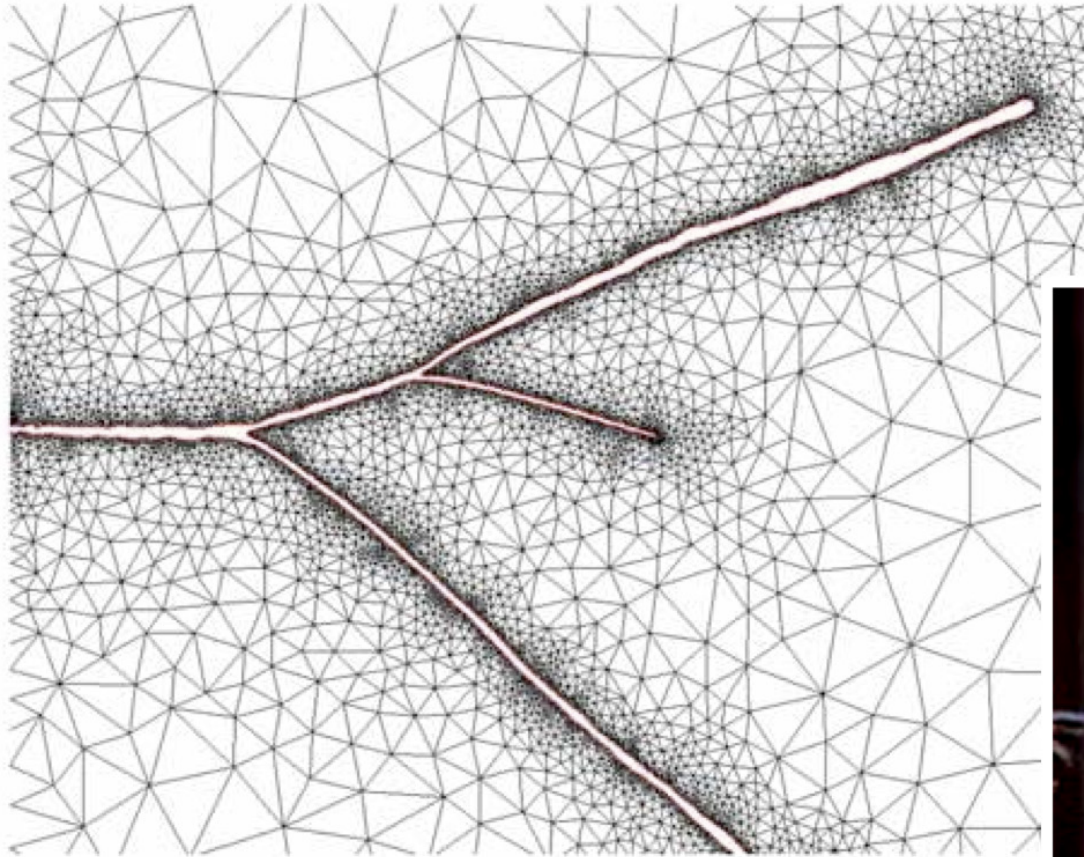








Branching



Landau potential:

$$\mathcal{F} = \mathcal{F}_c + \mathcal{F}_e + \mathcal{F}_{gr} ; \text{ Ginzburg, Landau (50)}$$

with

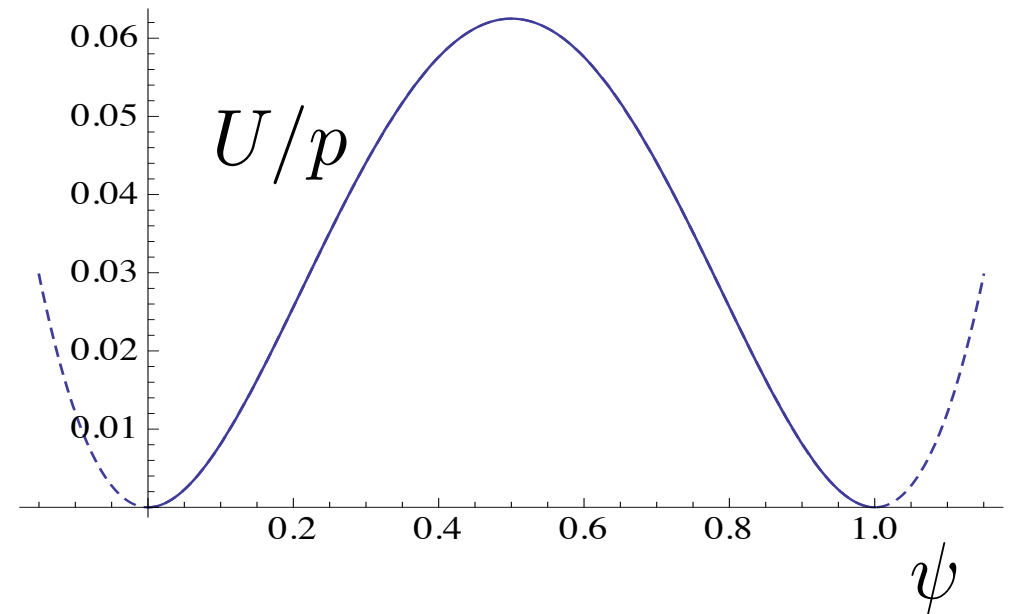
$$\mathcal{F}_e = \int \frac{G(\psi)}{2} (\nabla w)^2 dV$$

$$\mathcal{F}_c = \int U(\psi) dV$$

$$\mathcal{F}_{gr} = \int \frac{g_b}{2} (\nabla \psi)^2 dV$$

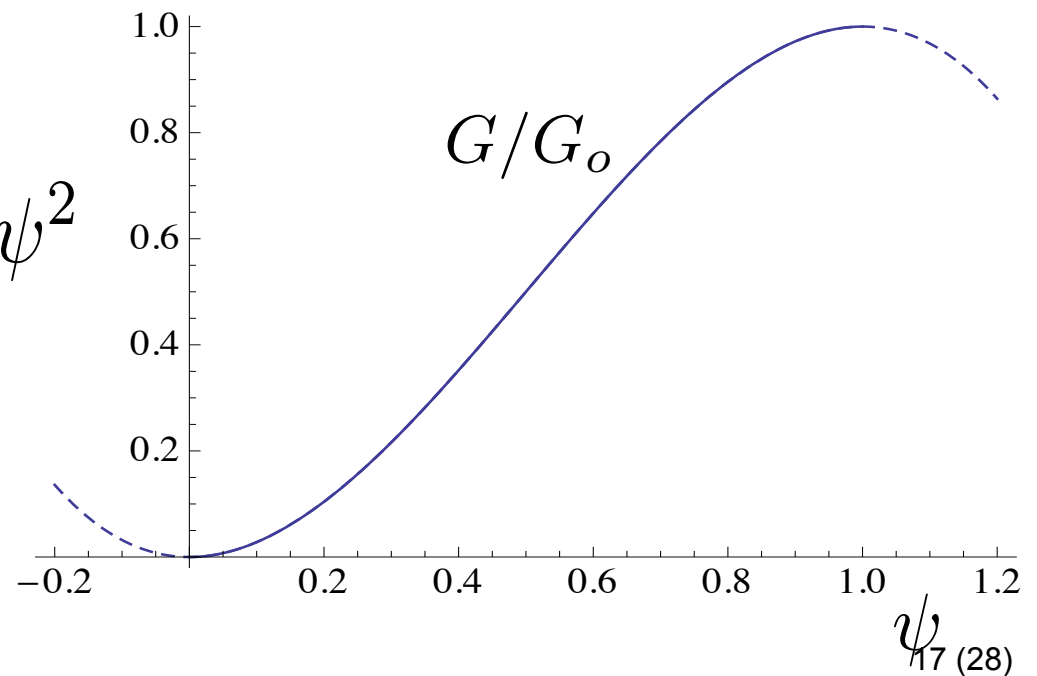
Double-well chemical potential

$$U(\psi) = p \psi^2 (1 - \psi)^2$$



Shear modulus

$$G(\psi) = G_o(\psi)(-2\psi + 3)\psi^2$$



Antiplane deformation \Rightarrow Two free variables

Displacements w and phase (density) ψ

$$\frac{\partial \psi}{\partial t} = -L_{\psi} \frac{\delta \mathcal{F}}{\delta \psi} , \quad \frac{\partial w}{\partial t} = -L_w \frac{\delta \mathcal{F}}{\delta w}$$

Ginzburg, Landau (50)

Evolution of the phase

$$\frac{\partial \psi}{\partial t} = -L_\psi \left[\frac{1}{2} G'(\psi) (\nabla w)^2 + p\psi(\psi^2 - 1) - g_b \Delta \psi \right]$$

Evolution of the displacements

$$\frac{\partial w}{\partial t} = L_w \nabla \cdot [G(\psi) \nabla w]$$

At equilibrium: $\nabla \cdot [G(\psi) \nabla w] = 0$

One dimension (Ginzburg, Landau)

$$g_b \psi_o'' - p \psi_o (\psi_o^2 - 1) = 0$$

solution

$$\psi_o = \tanh(x / \sqrt{2g_b})$$

With mechanical loading

$$g_b \psi'' - p \psi (\psi^2 - 1) + \kappa p (\psi^2 - 1) - \frac{c}{L_\psi} \psi' = 0$$

Seek perturbation solution:

$$\psi(x) = \psi_o(x) + \omega f(x) \quad \text{as} \quad \omega = c / L_\psi G_o (\nabla w)^2 \sqrt{p g_b} \rightarrow 0$$

The result

$$\psi'_o = \psi_o^2 - 1 = \frac{1}{\sqrt{2g_b}} \operatorname{sech}^2(x/\sqrt{2g_b}) \quad ,$$

gives

$$\left(\kappa - \frac{c}{L_\psi}\right) \frac{p}{\sqrt{2g_b}} \operatorname{sech}^2(x/\sqrt{2g_b}) = 0 \quad ,$$

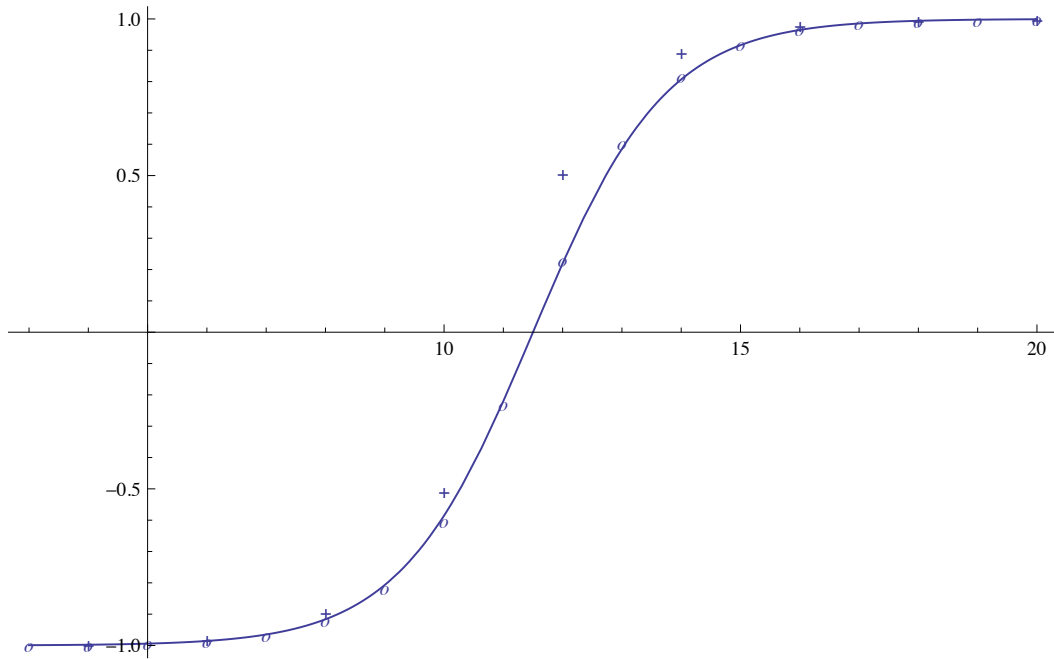
i.e. the speed of the corroding edge

$$c = L_\psi \kappa = \frac{3}{4} p L_\psi G_o (\nabla w)^2 \sqrt{\frac{2g_b}{p}} \quad .$$

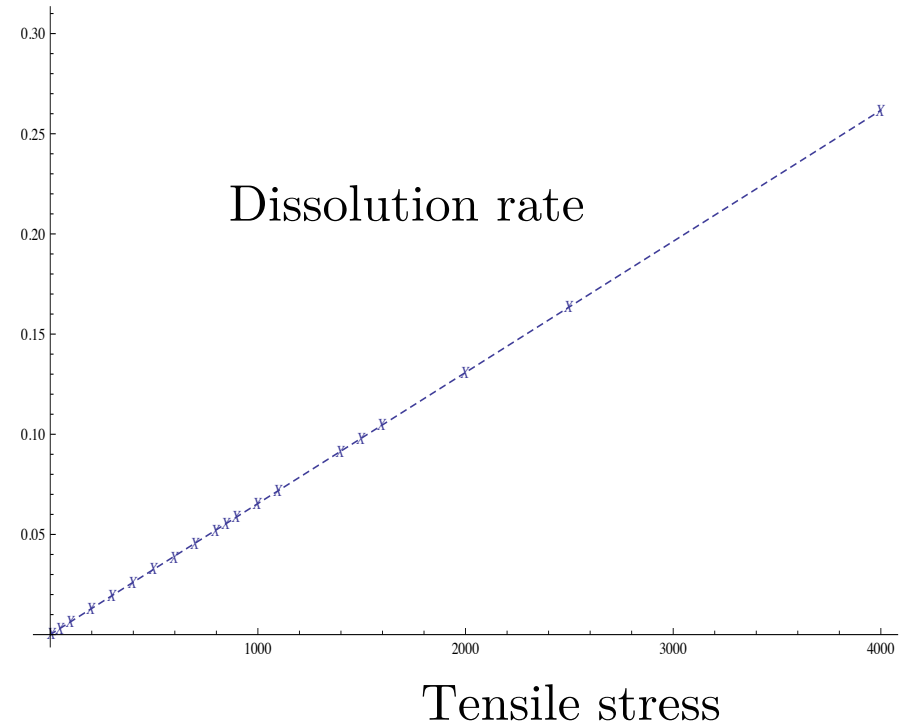
Steady state solution

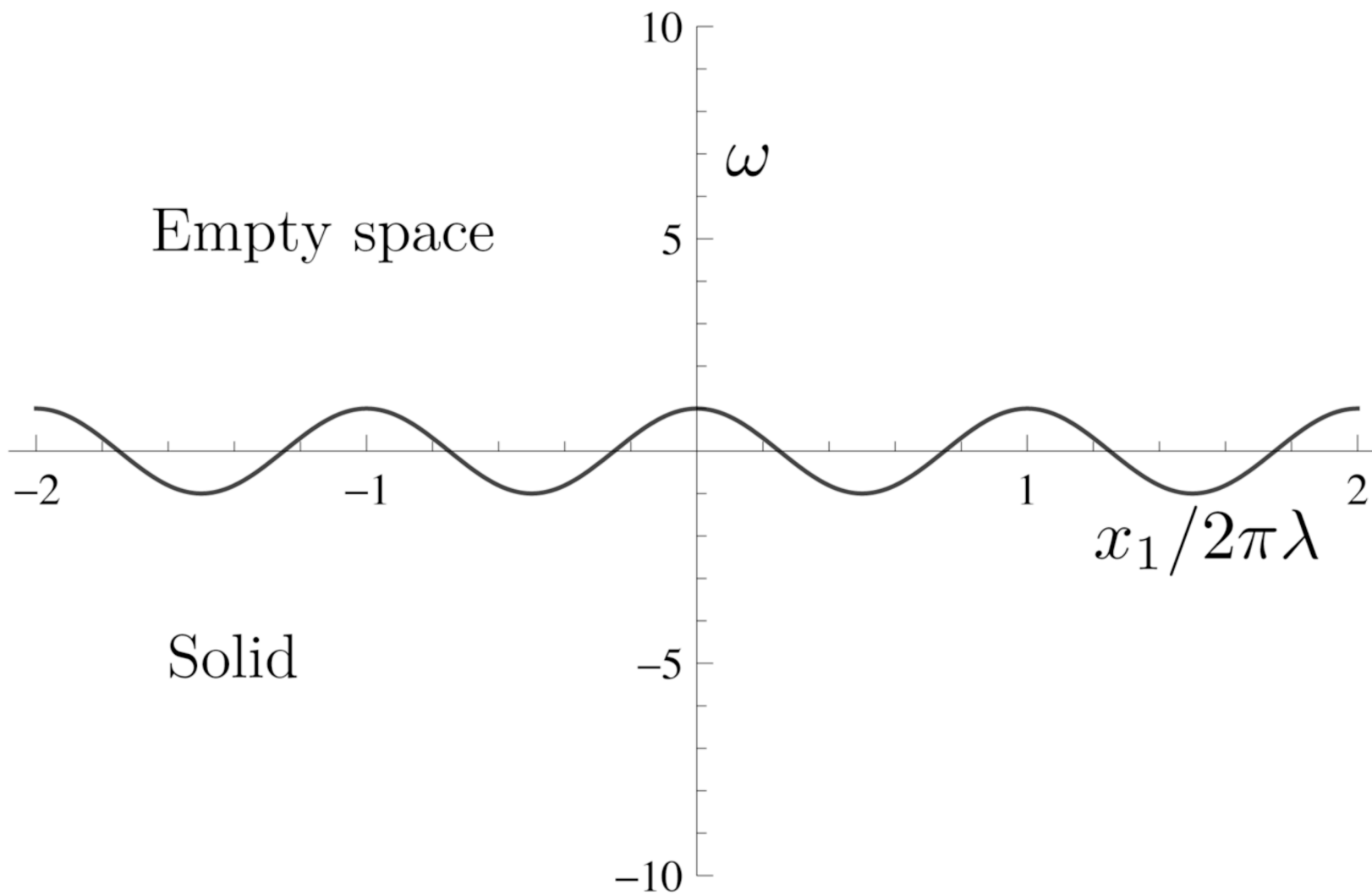
$$\psi = -\tanh\left(\sqrt{\frac{p}{2g_b}}x_2 + \frac{3}{4}L_\psi G_o(\nabla w)^2 \sqrt{\frac{2g_b}{p}}t\right)$$

Transition Rate vs. Distance

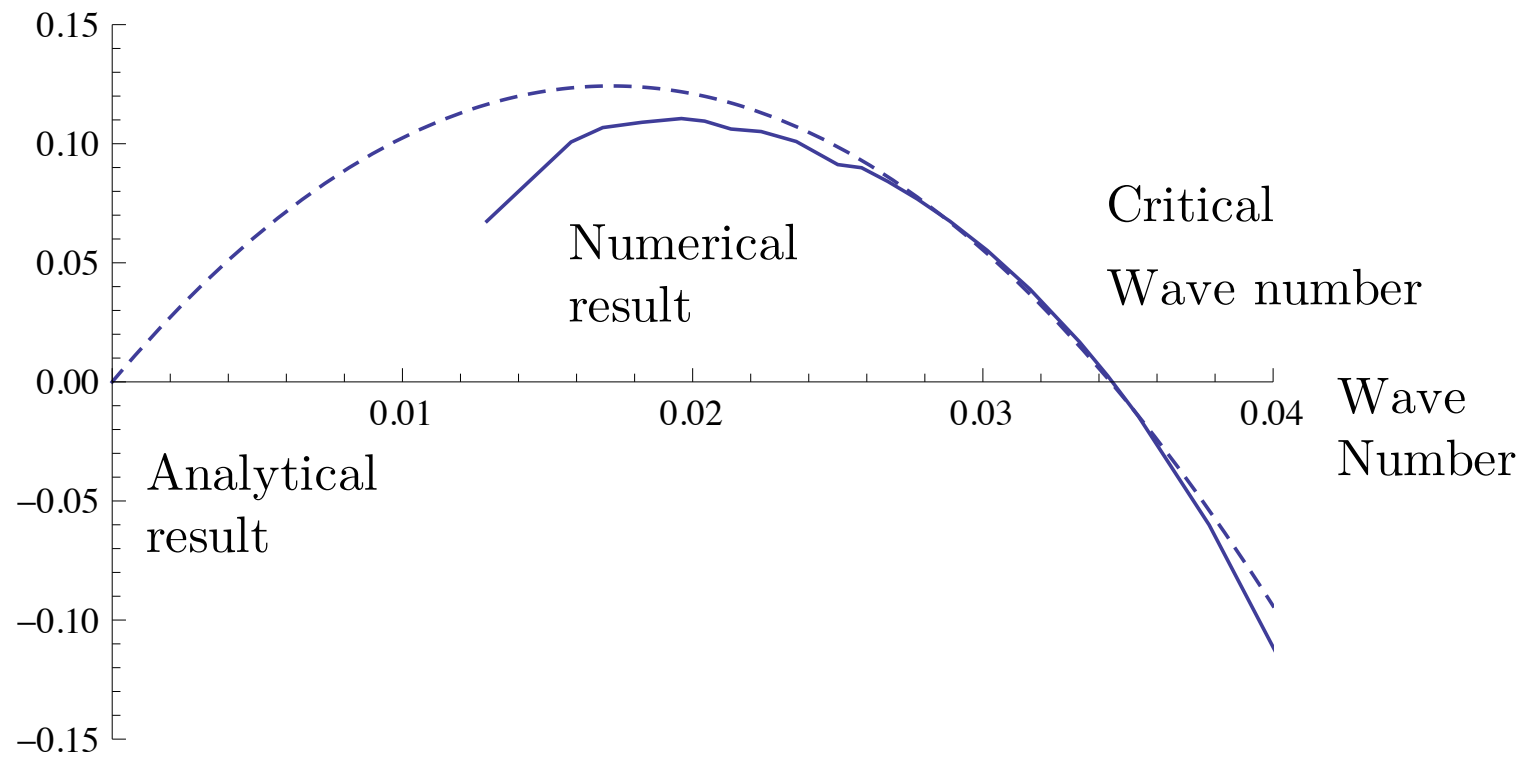


Dissolution Rate vs. Tensile Stress



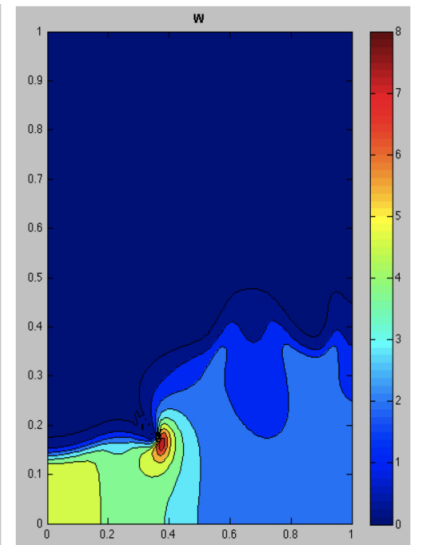
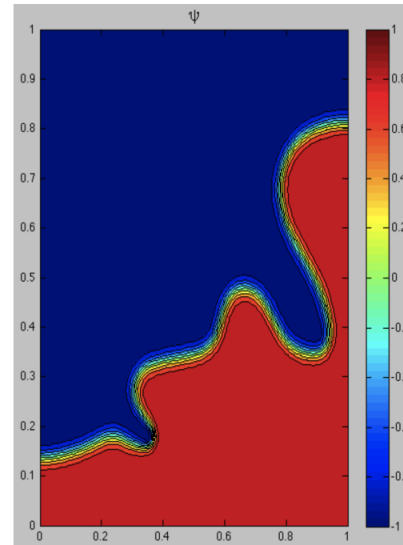
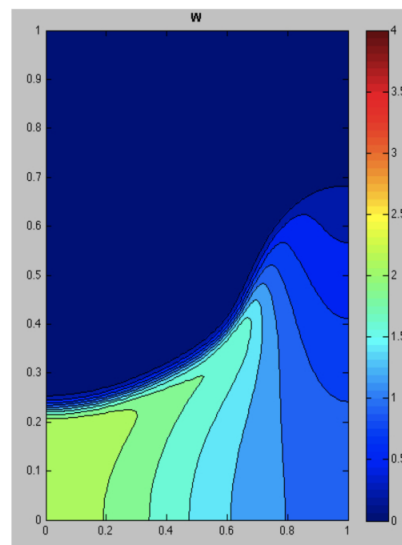
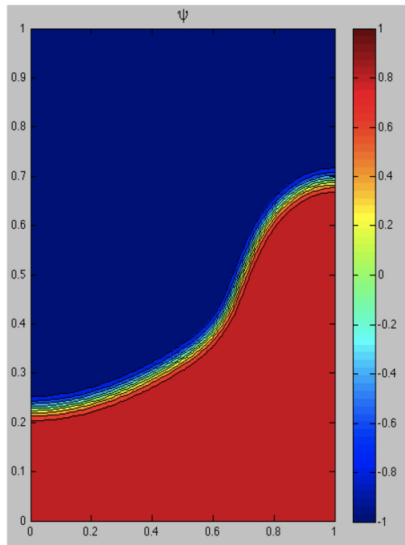
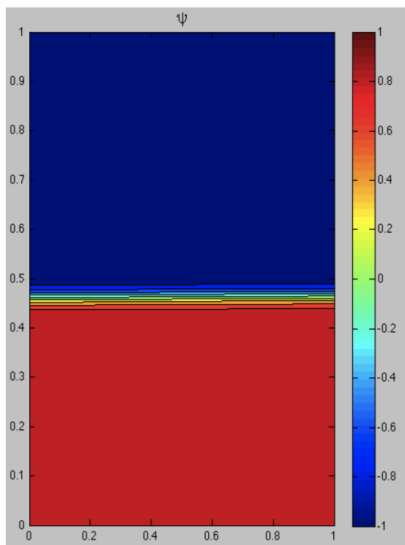
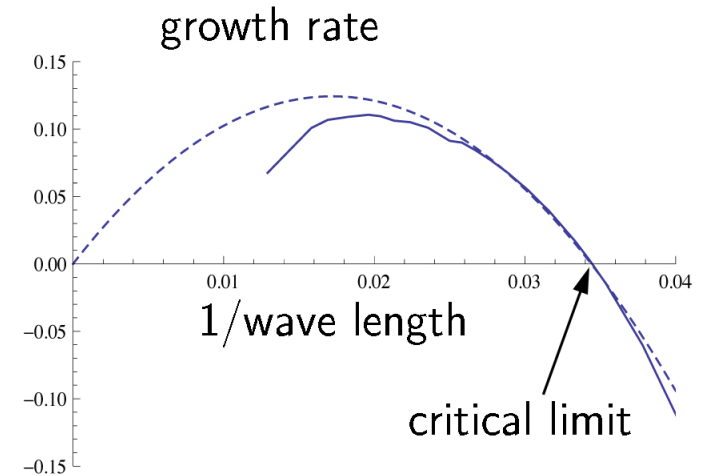


Relative Growth Rate



$$\left(\frac{d}{dx_2} - 2\beta\right)(f' + f^2 - 1) = 0$$

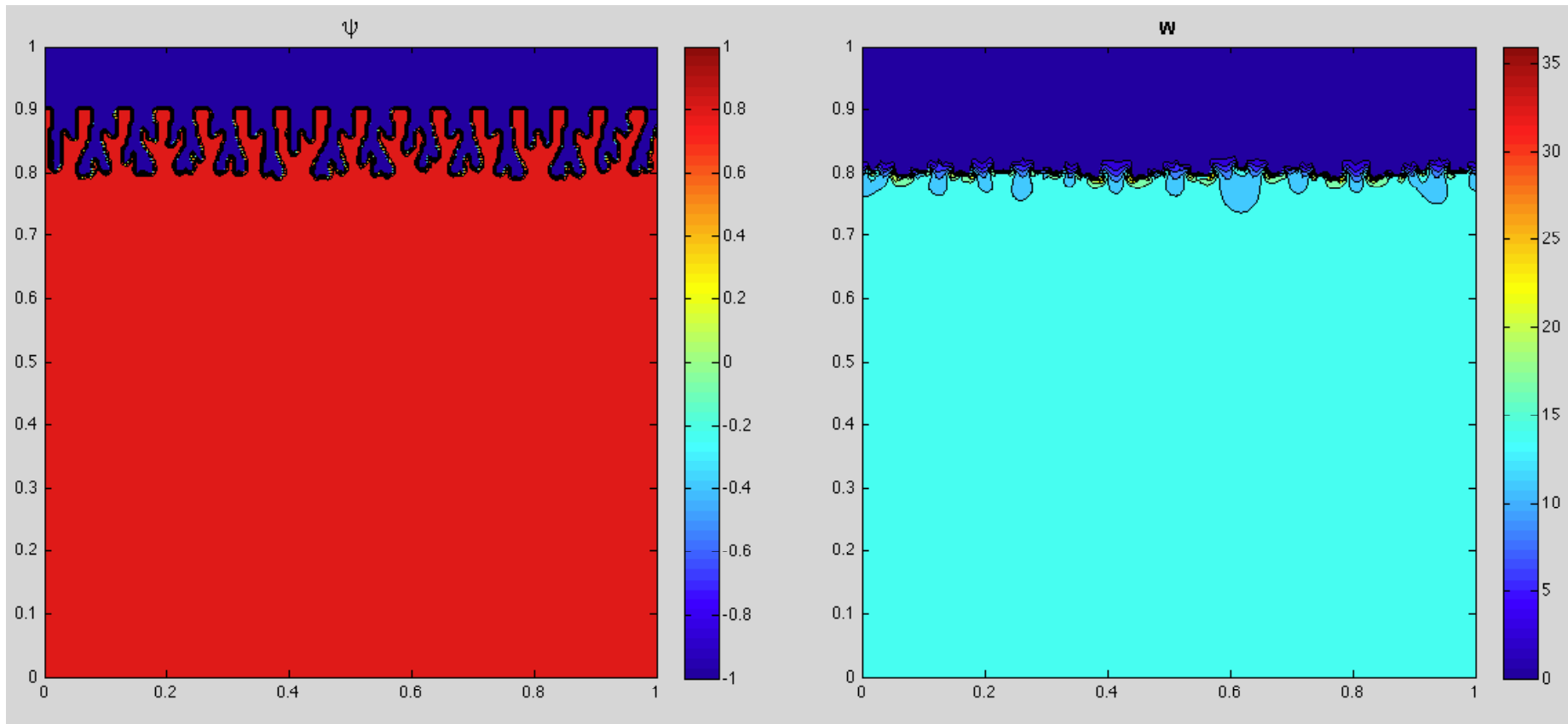
$$\psi = -\tanh\left(\sqrt{\frac{p}{2g_b}}x_2 + \frac{3}{4}L_\psi G_o(\nabla w)^2\sqrt{\frac{2g_b}{p}}t\right)$$



Red is remaining material

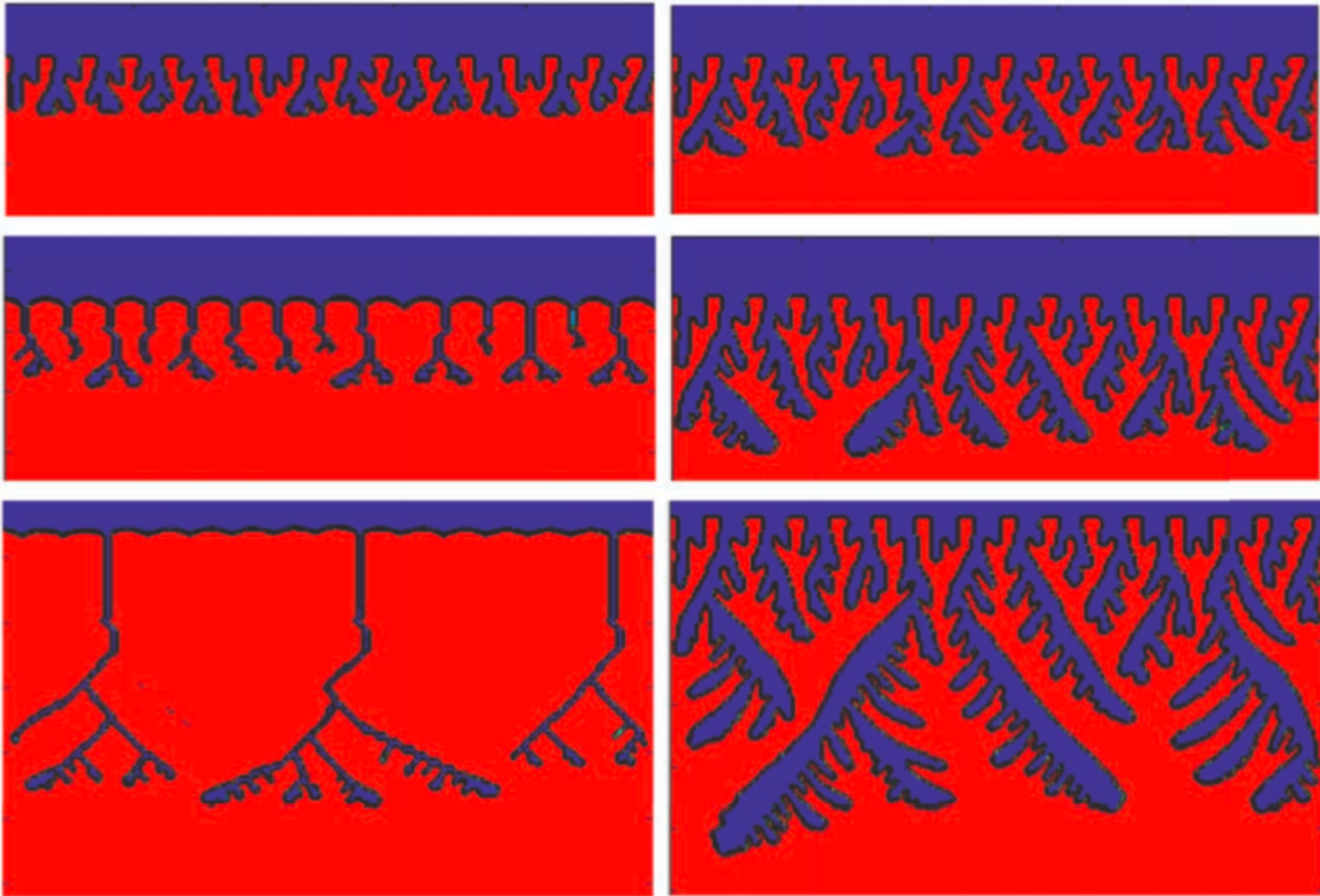
Effective Stress

Effective Stress



Red is remaining material

Effective stress



Without general corrosion

with general corrosion

Summary

- Stress corrosion cracking is modelled as a moving boundary problem
- Surface morphology, crack initiation and crack growth are captured
- Branching occurs when the crack front becomes unstable
- Solutions become semi-self similar