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25th Nordic Seminar on Computational Mechanics

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

+

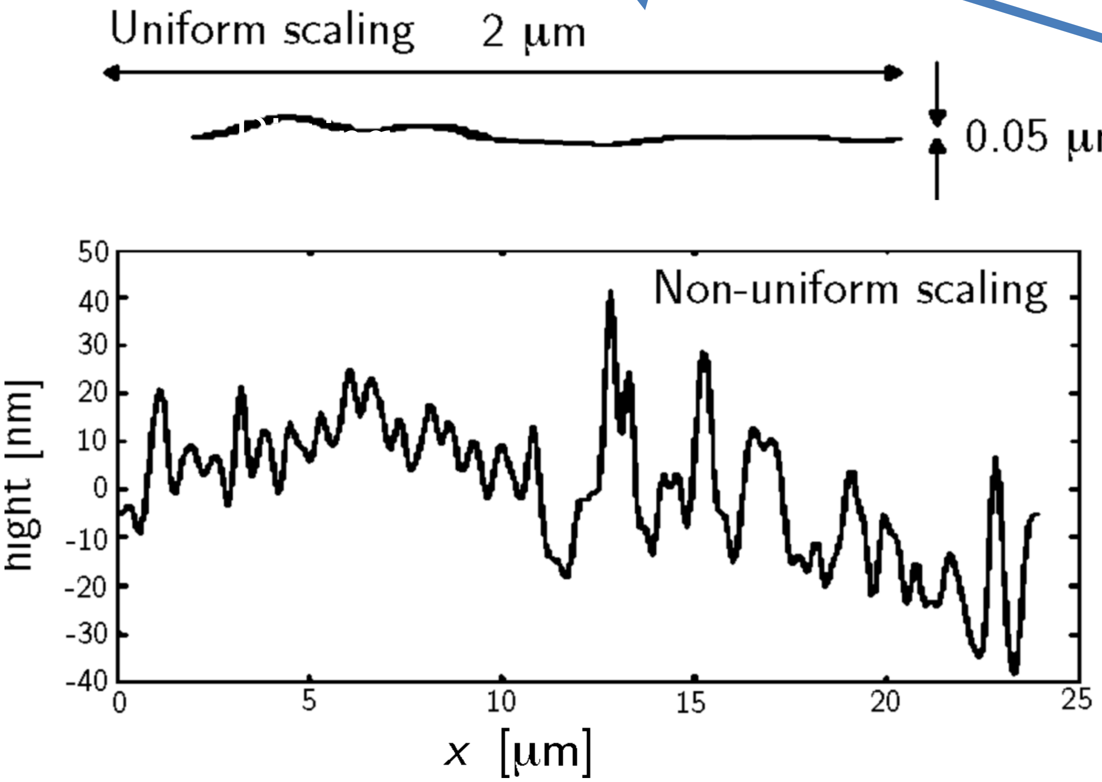
Corroding environment leads to:

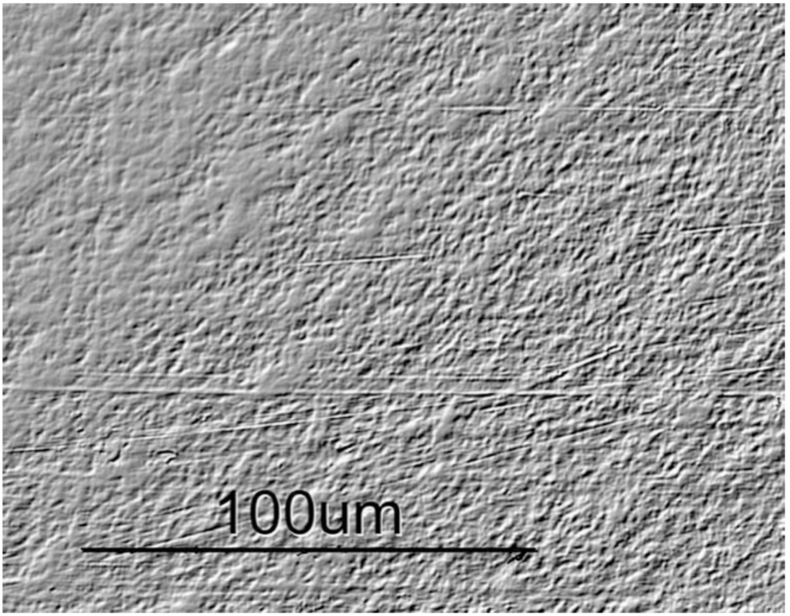
1. Continuous loss of mass
2. Pitting

...and with mechanical stress present

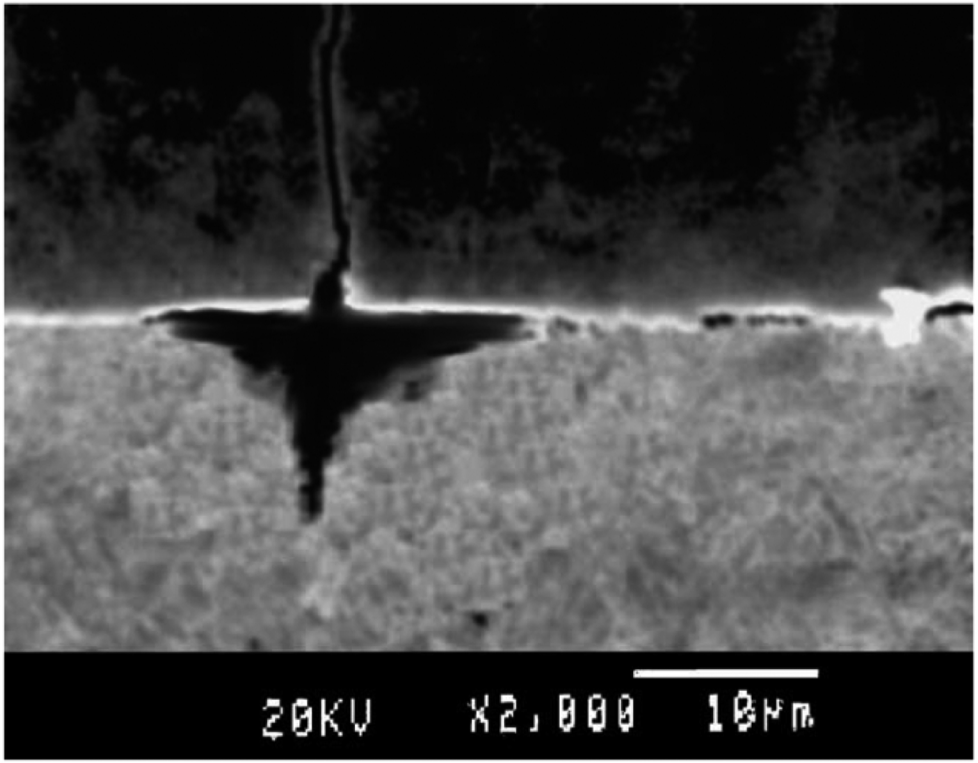
3. Surface roughening

(from Kim *et al.* 2000)

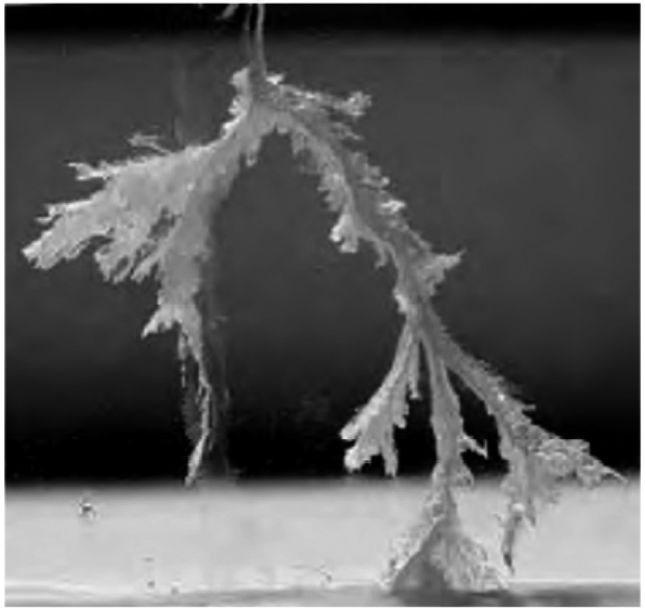




4. Evolving pits
5. Formation of cracks
6. Crack growth
7. Crack branching



Cr/zone 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

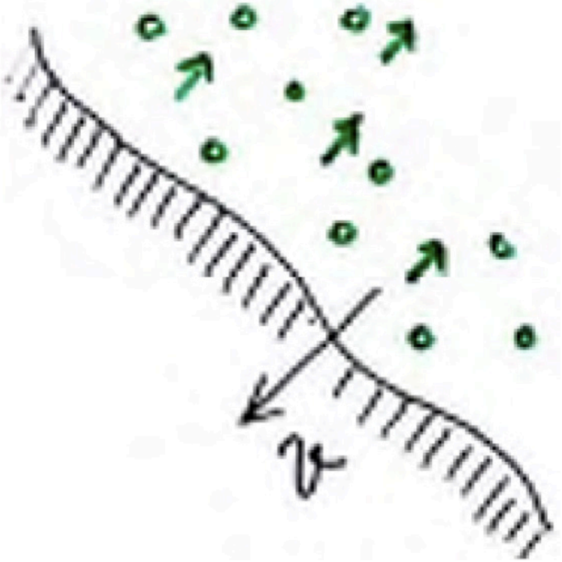
$h(x)$ gives the position of the surface

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

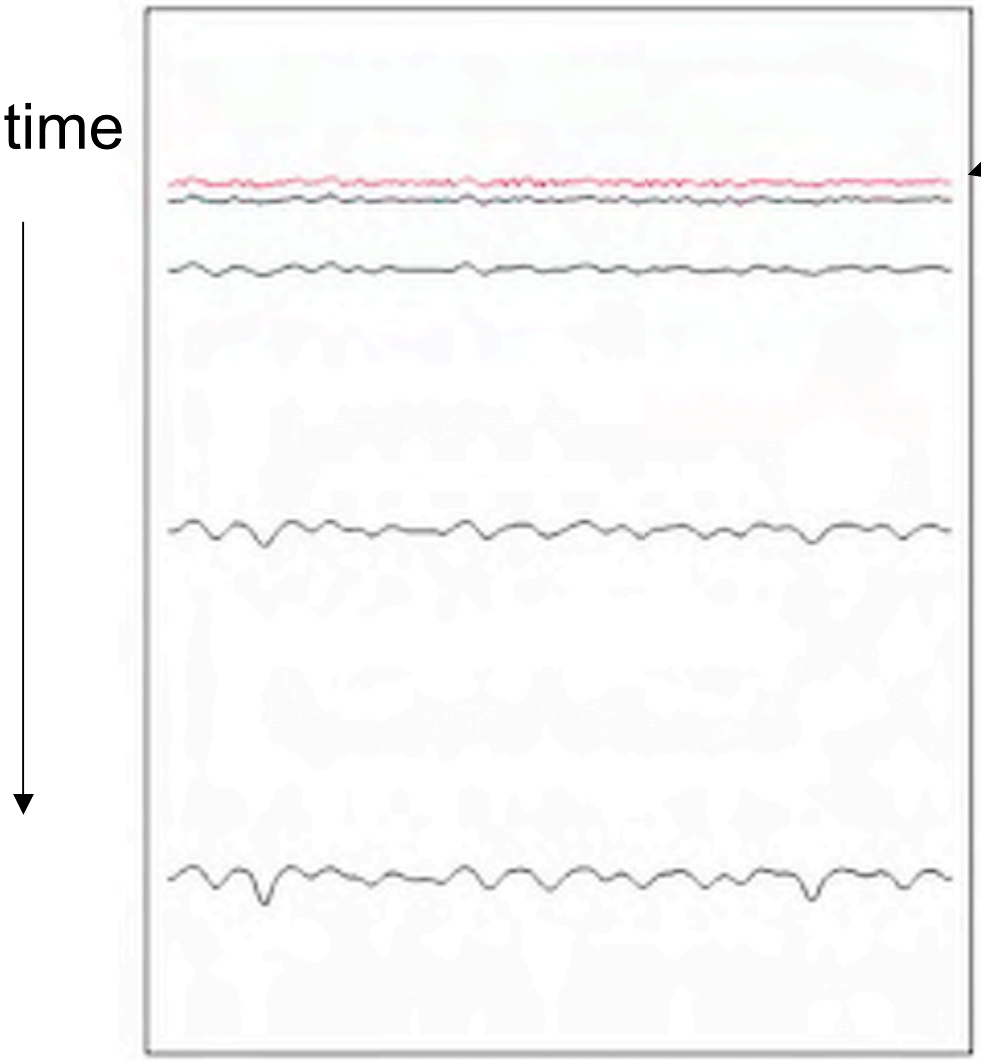
$$\frac{\partial h}{\partial t} = L_1 \left(\gamma \frac{\partial^2 h}{\partial x^2} \text{ - } \frac{k}{2} \mu \frac{\partial h}{\partial x} \right)$$

or surface diffusion

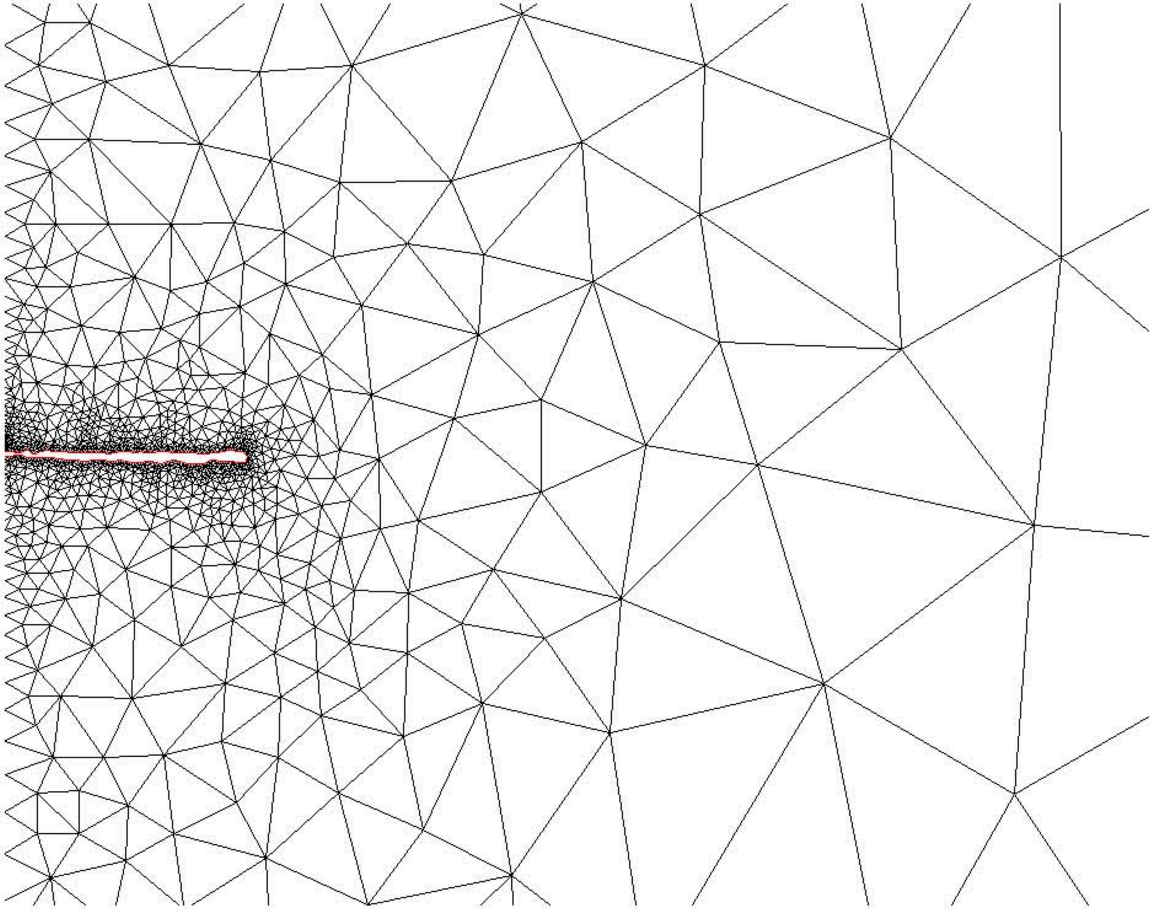
$$\frac{\partial h}{\partial t} = L_2 \frac{\partial^2}{\partial x^2} \left(-\gamma \frac{\partial^2 h}{\partial x^2} + \frac{k}{2} \mu \frac{\partial h}{\partial x} \right)$$

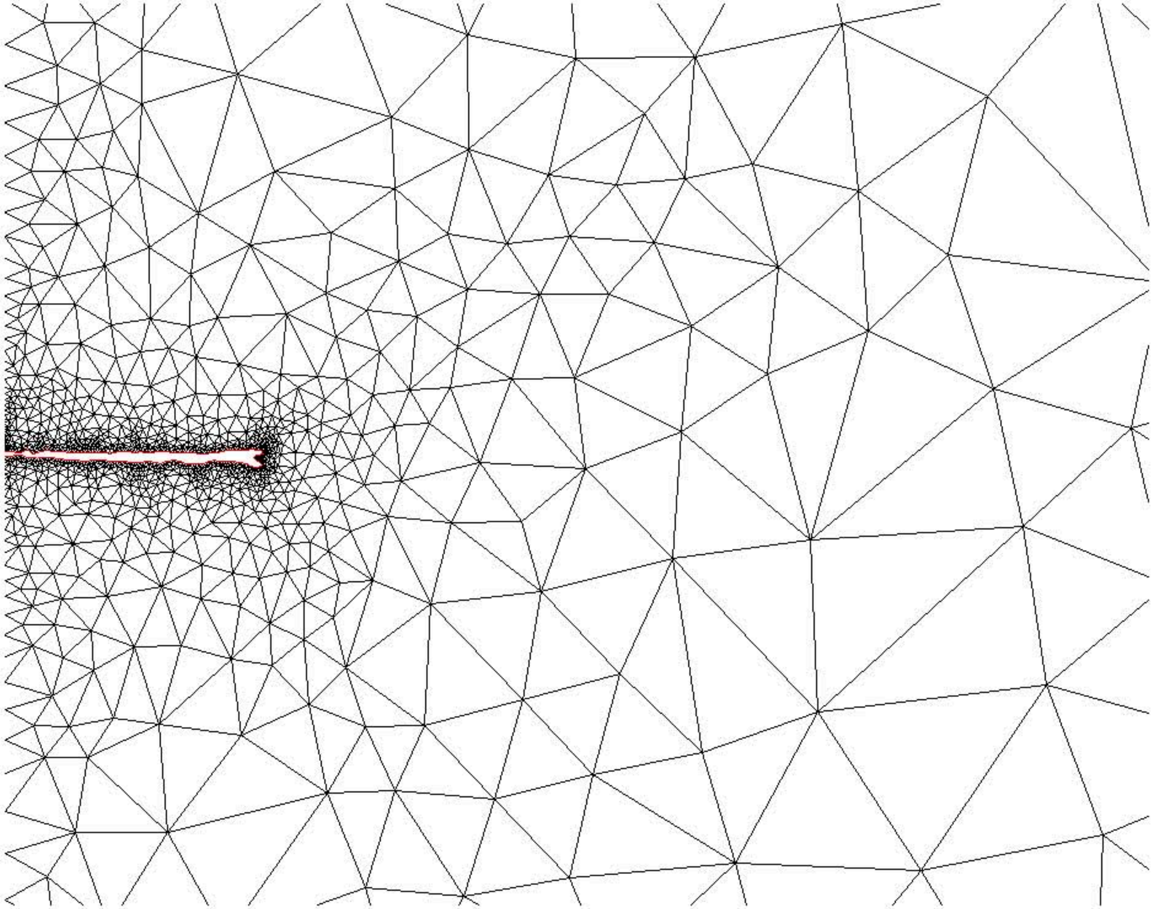
FEM calculation of an evolving surface

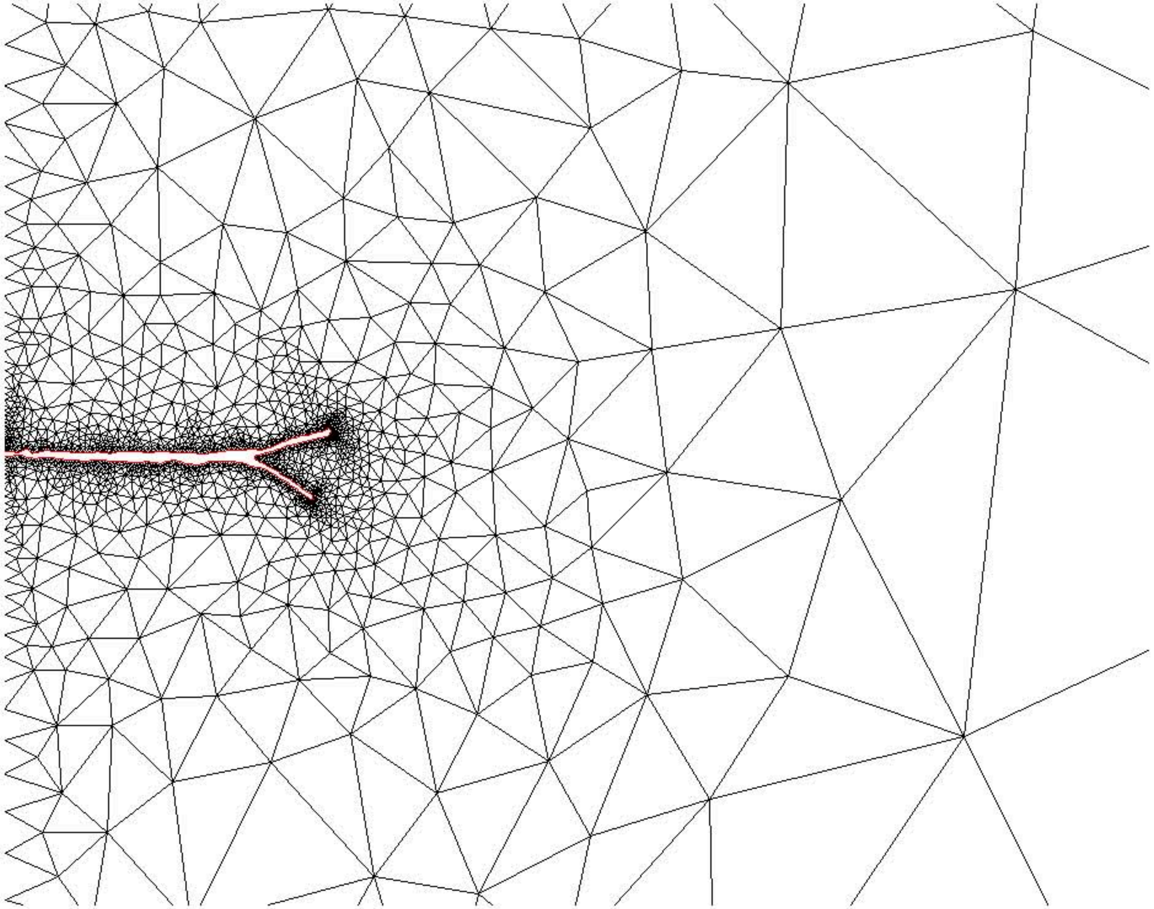
Increasing time
and depth

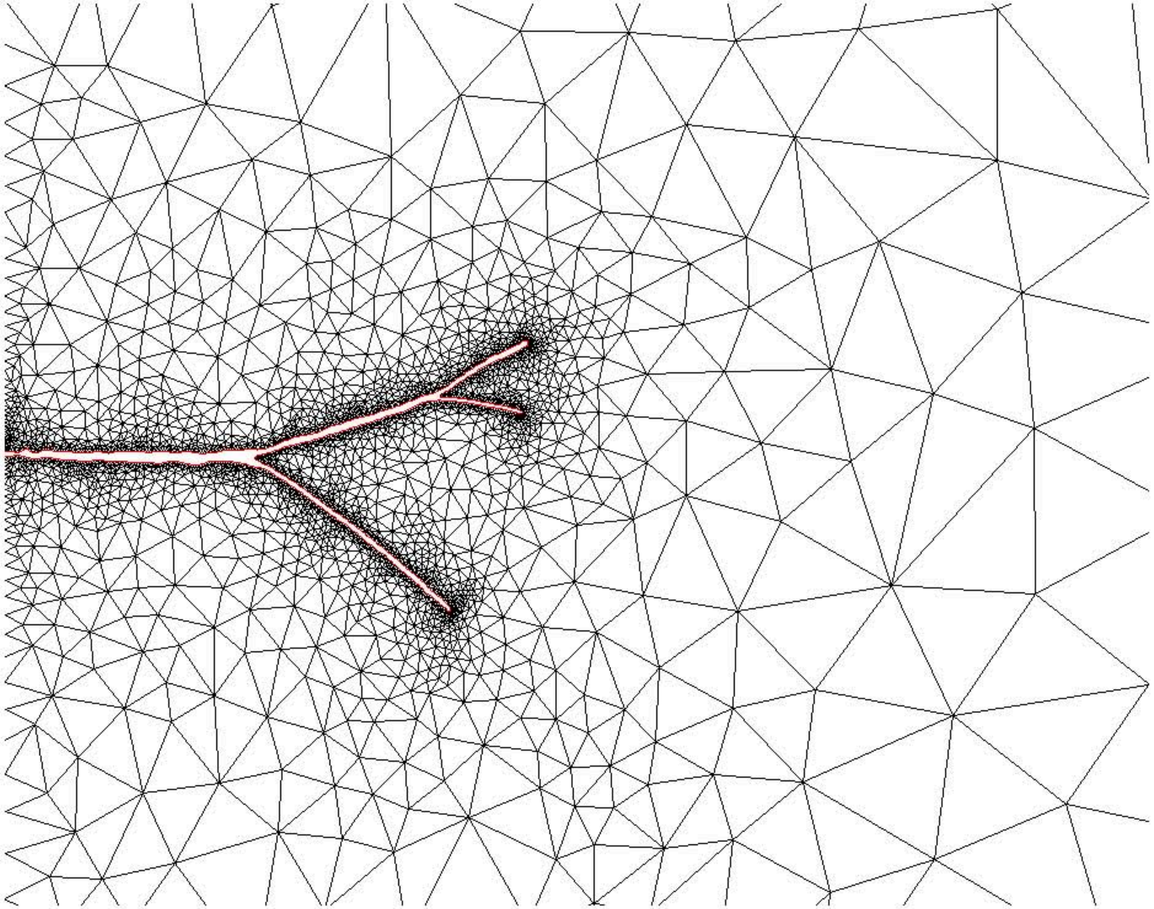


Original surface

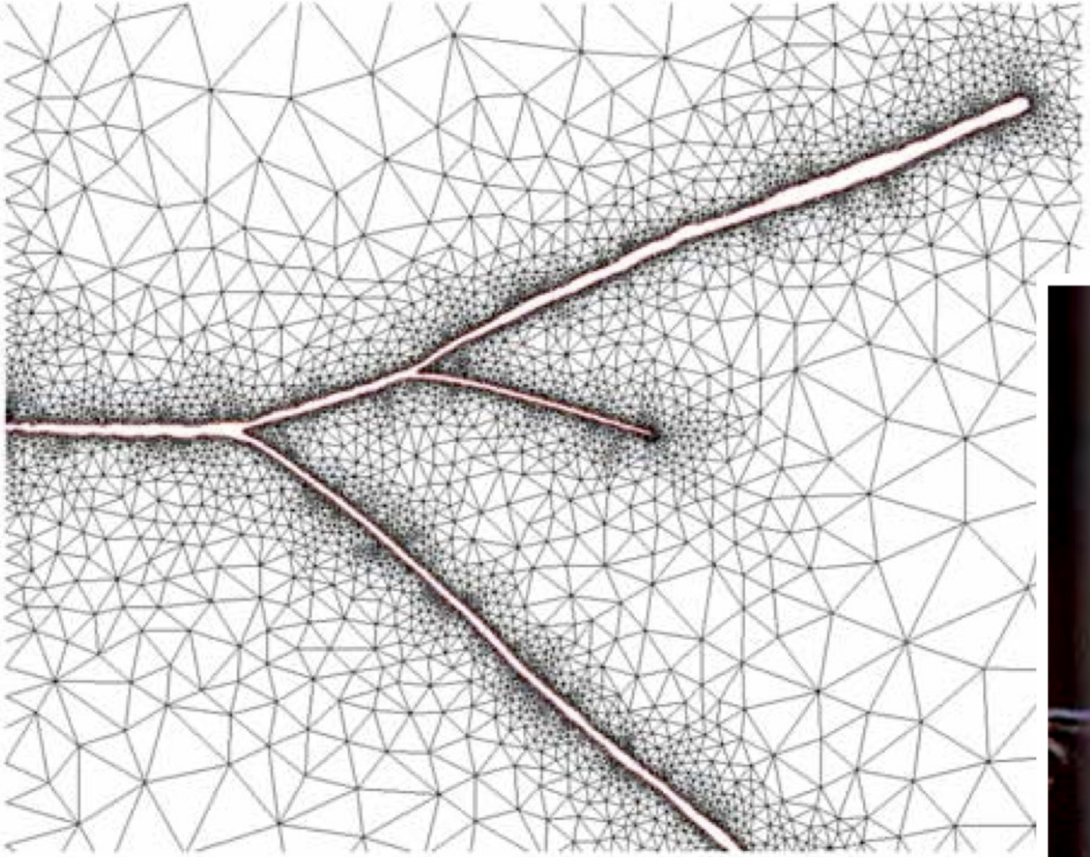


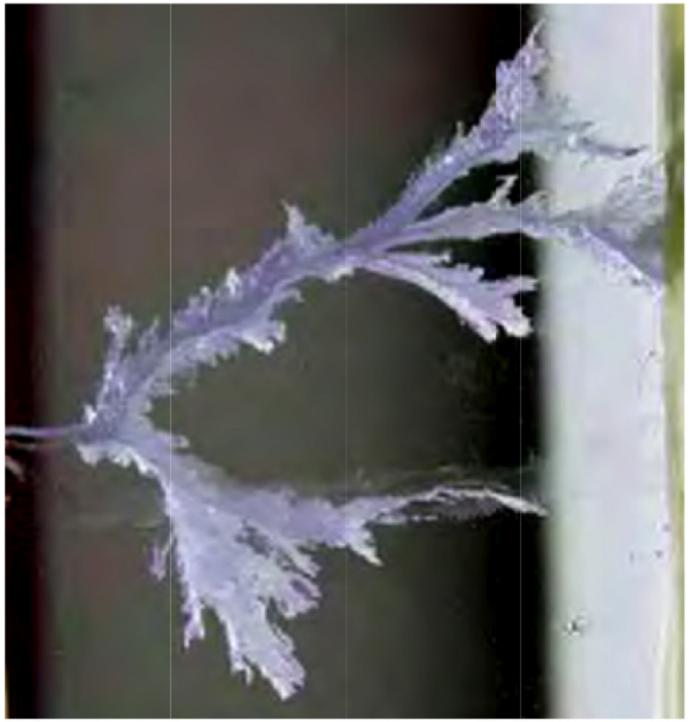






Branching





Landau potential:

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

with

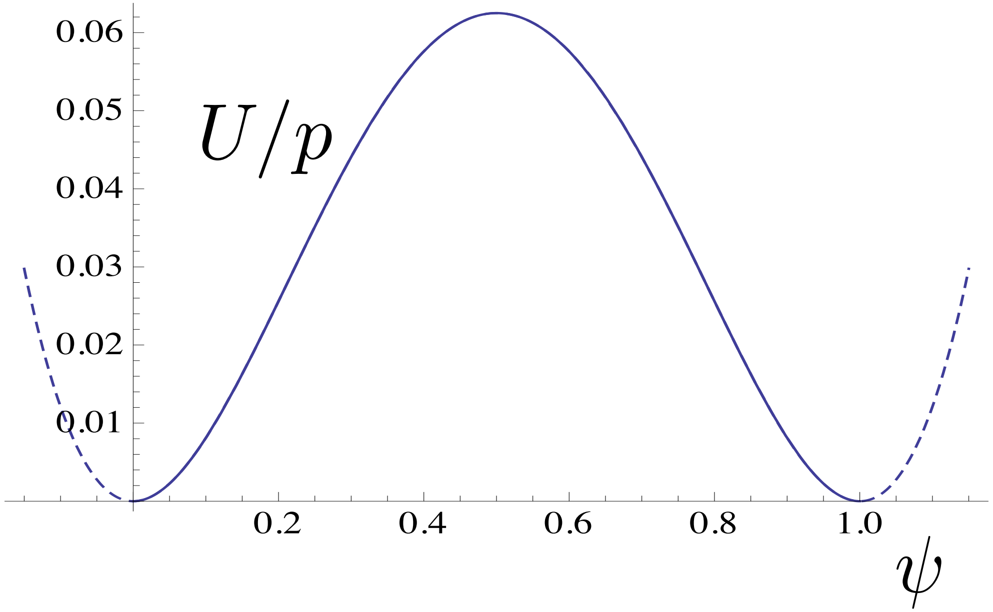
$$\mathcal{F}_e = \int \frac{G(\psi)}{2} (\nabla w)^2 \mathrm{d}V$$

$$\mathcal{F}_c = \int U(\psi) \, \mathrm{d}V$$

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

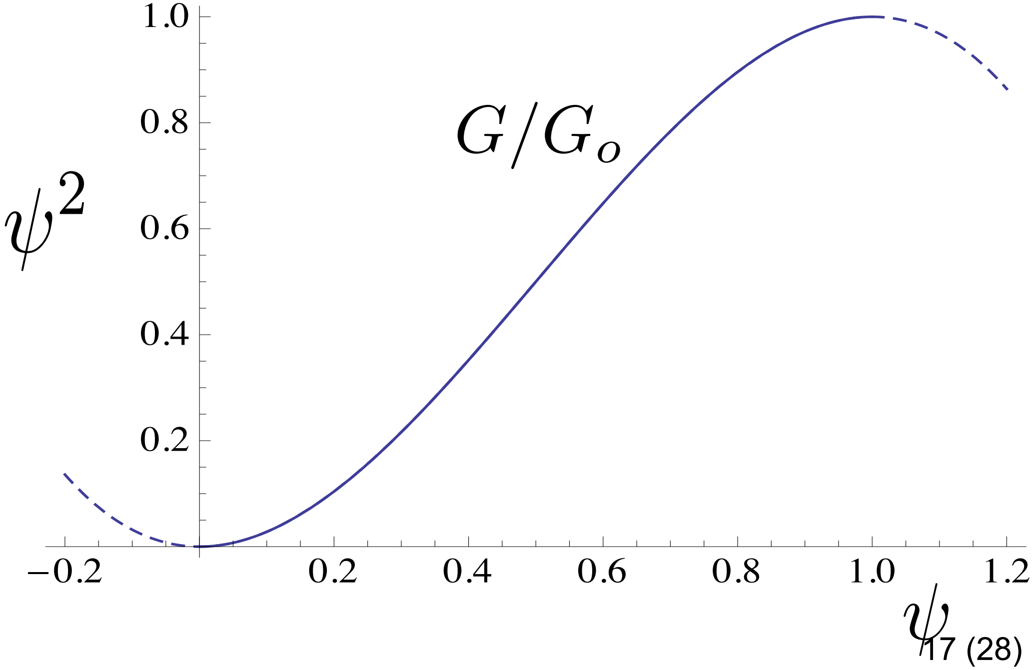
Double-well chemical potential

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



Shear modulus

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



Antiplane deformation $=>$ Two free variables

Displacements w and phase (density) ψ

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

Ginzburg, Landau (50)

Evolution of the phase

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

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:

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

The result

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

gives

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

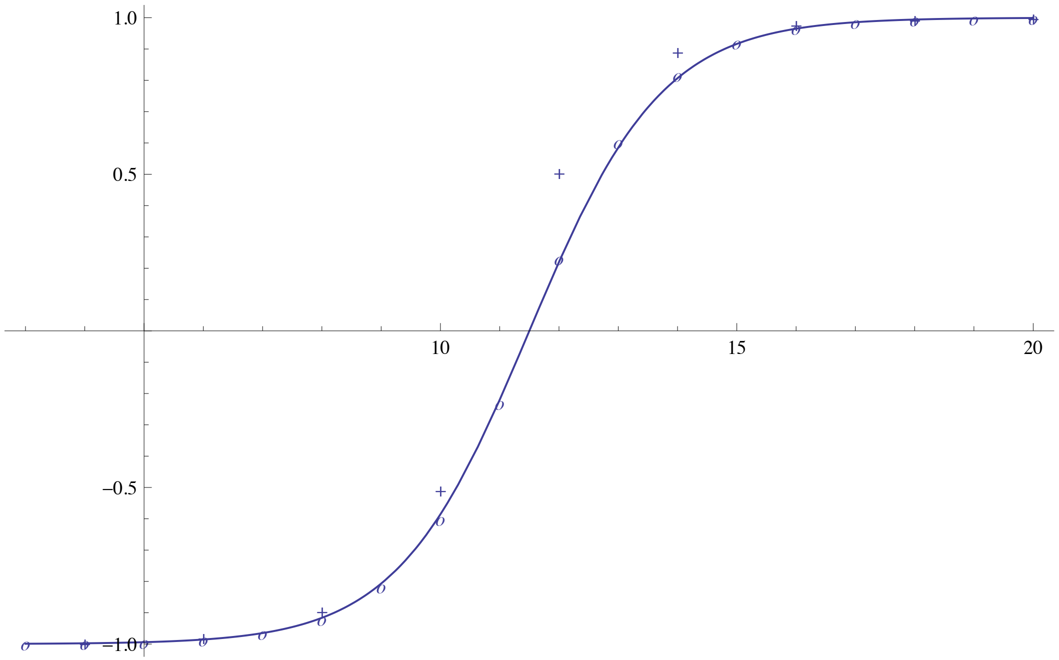
i.e. the speed of the corroding edge

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

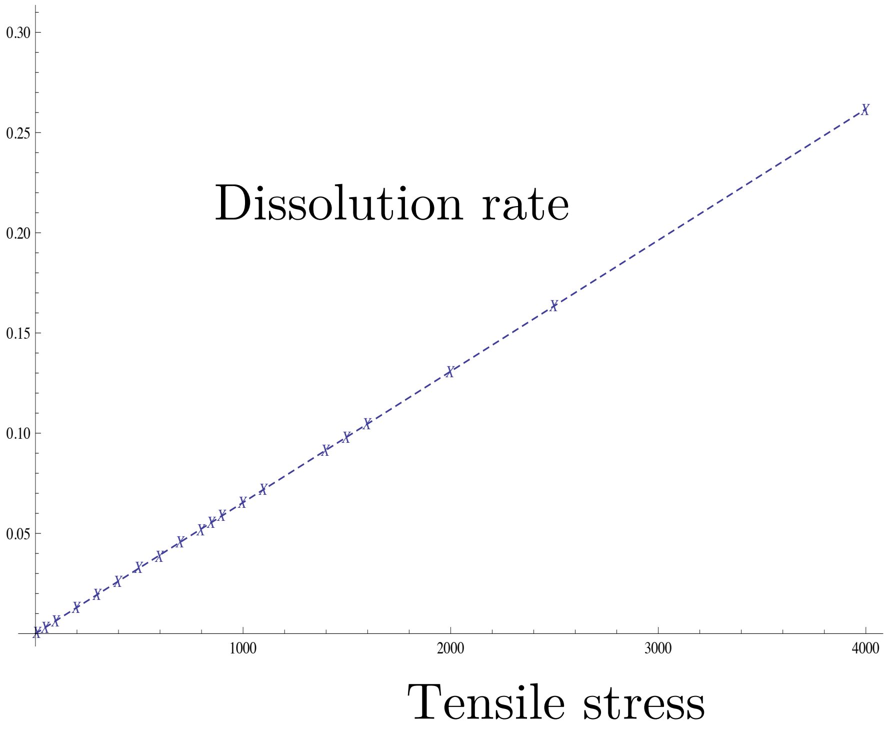
Steady state solution

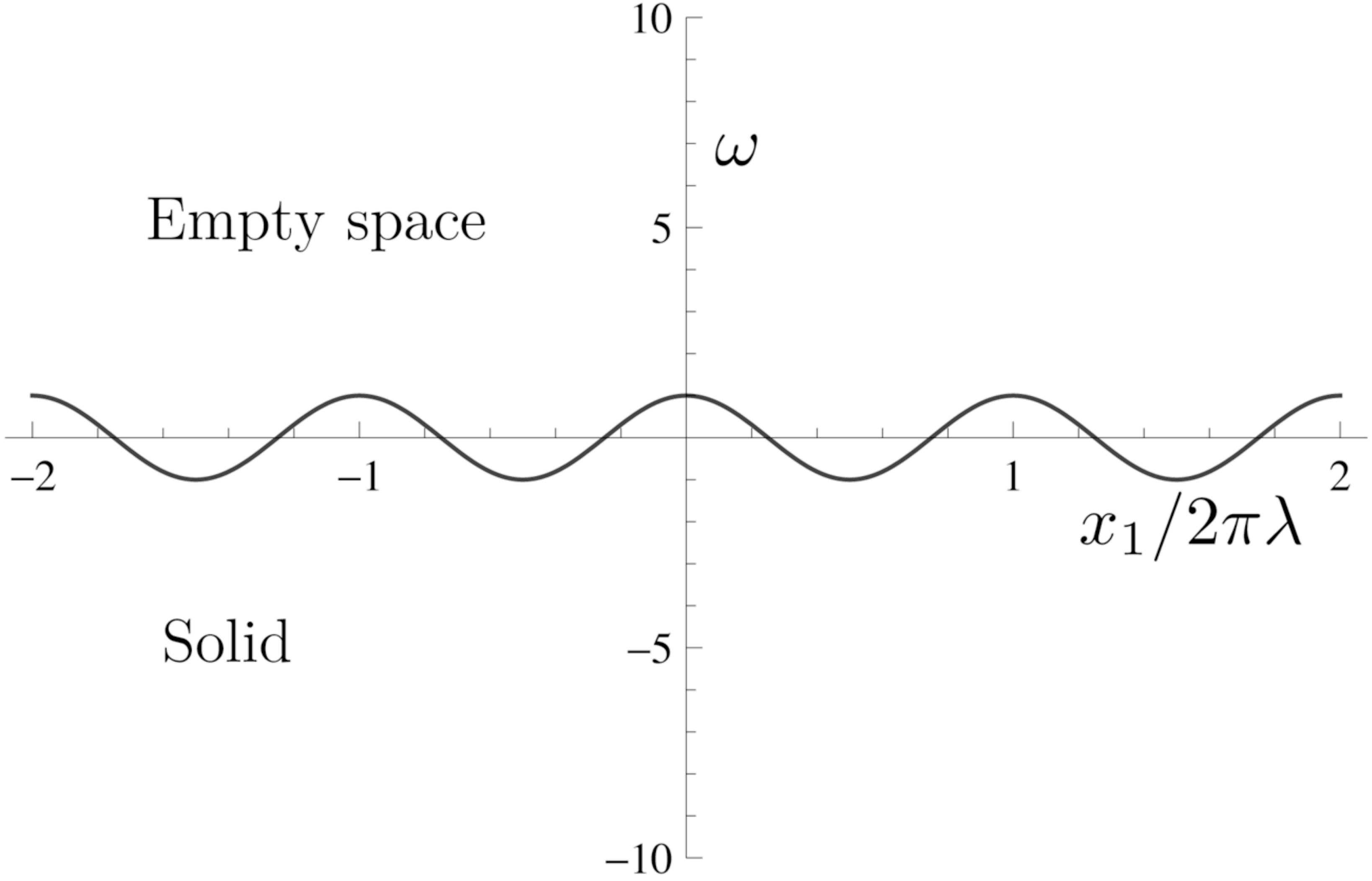
$$\psi = -\tanh(\sqrt{\frac{p}{2g_b}}x_2 + \frac{3}{4}L_\psi G_o(\nabla w)^2\sqrt{\frac{2g_b}{p}}t)$$

Transition Rate vs. Distance

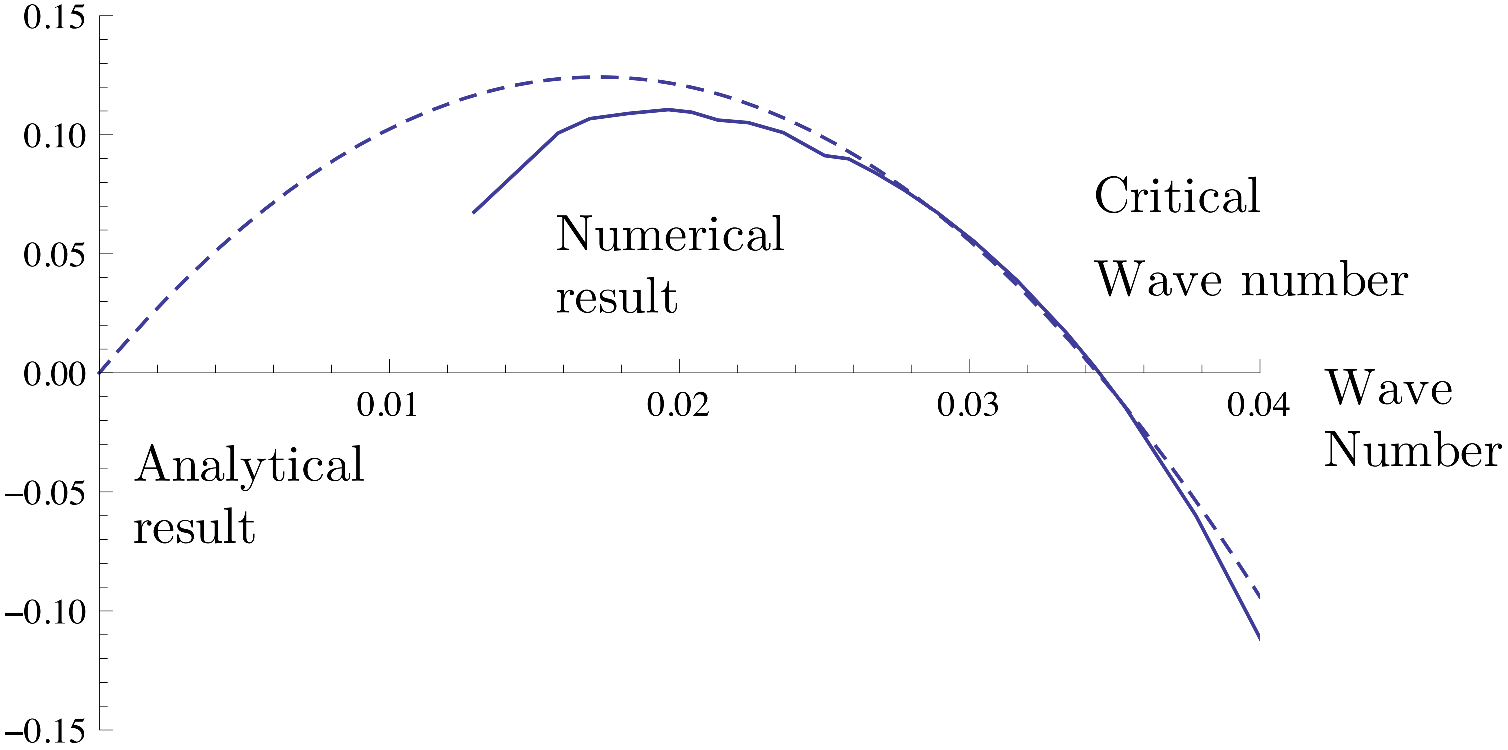


Dissolution Rate vs. Tensile Stress



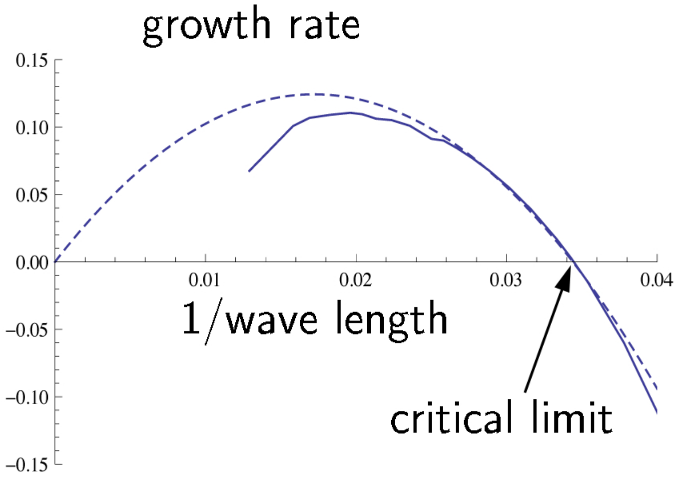

10
ω
Empty space
5
−2
−1
1
2
$x_1/2\pi\lambda$
Solid
−5
−10

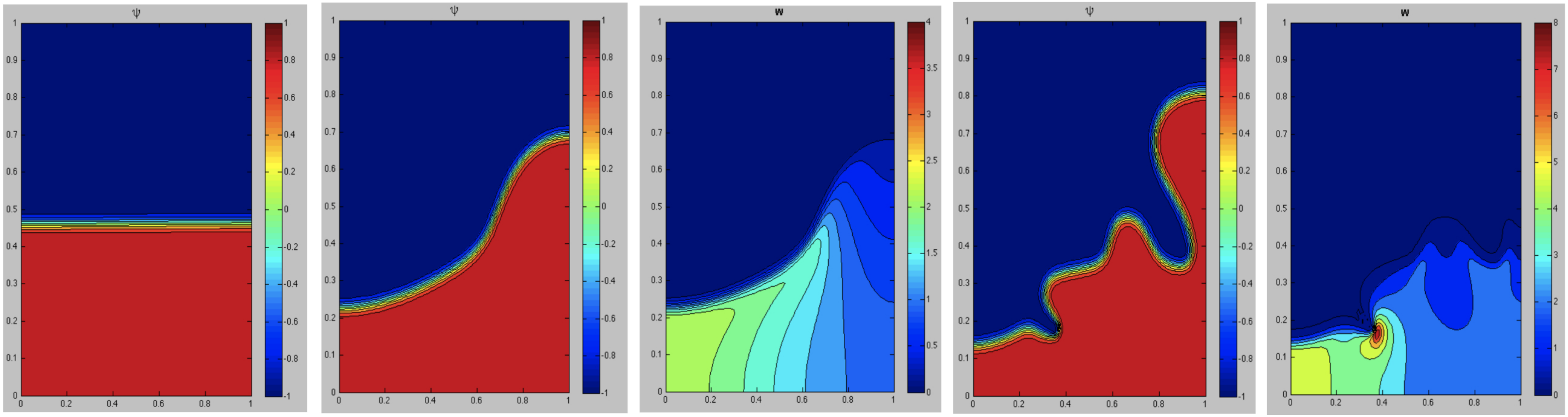
Relative Growth Rate



$$(\frac{\mathrm{d}}{\mathrm{d}x_2} - 2\beta)(f' + f^2 - 1) = 0$$

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

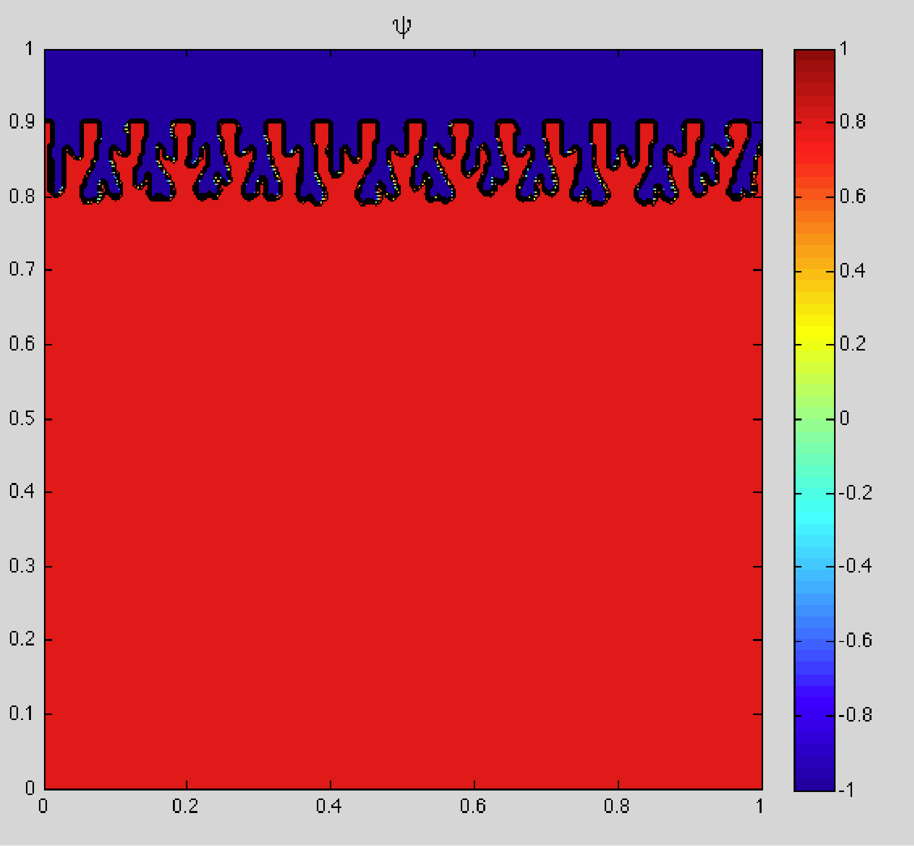




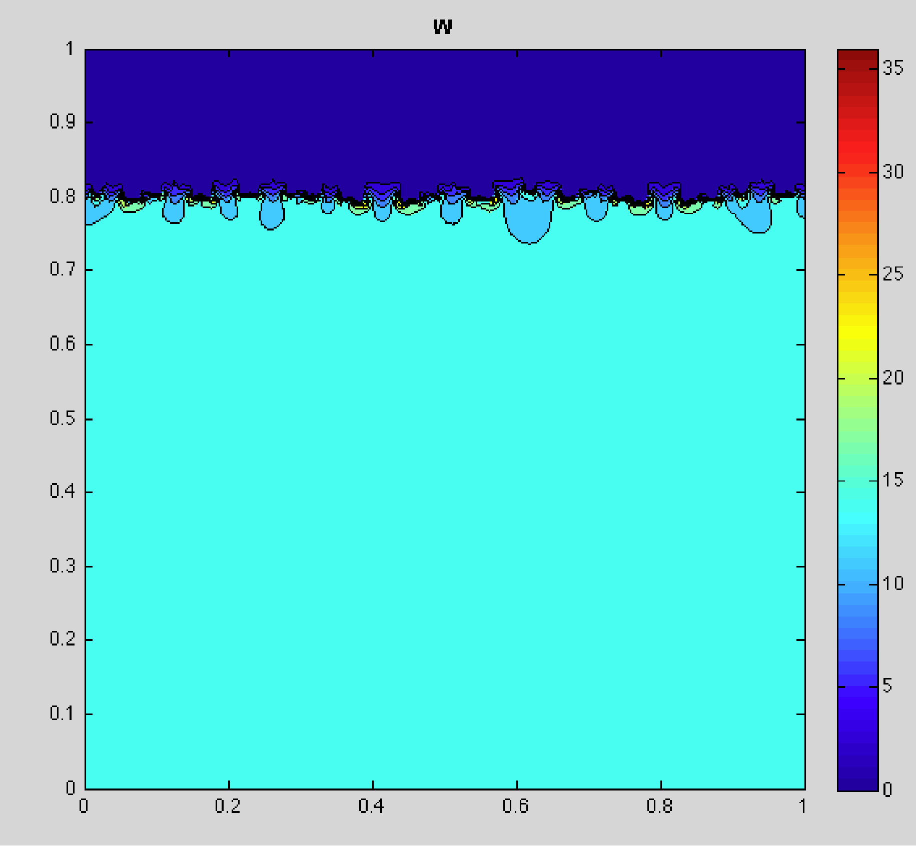
Red is remaining material

Effective Stress

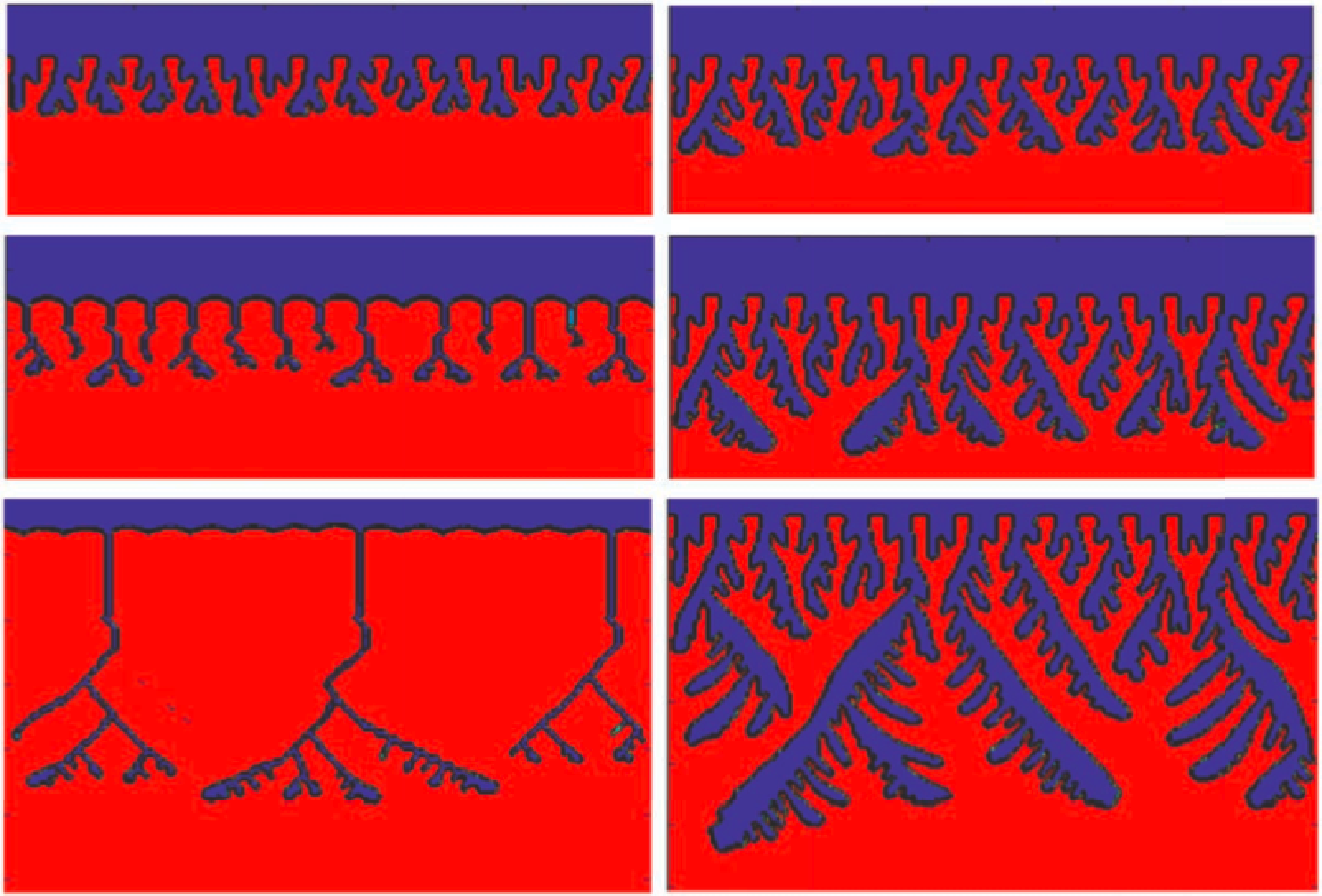
Effective Stress



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