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Interface Instabilities of Growing Hydrides

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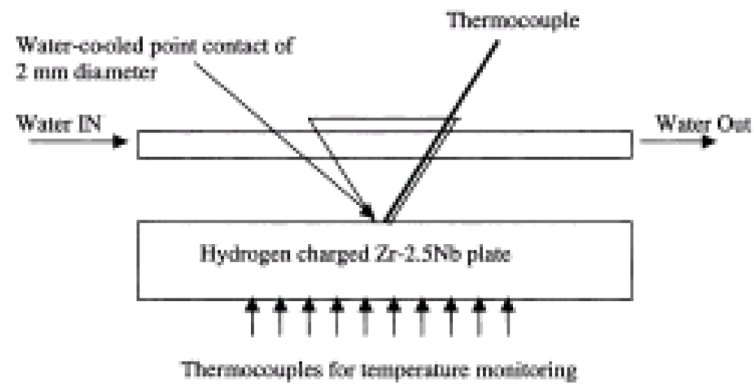
21st European Conference of Fracture, Catania 2016

Interface instabilities of growing hydrides

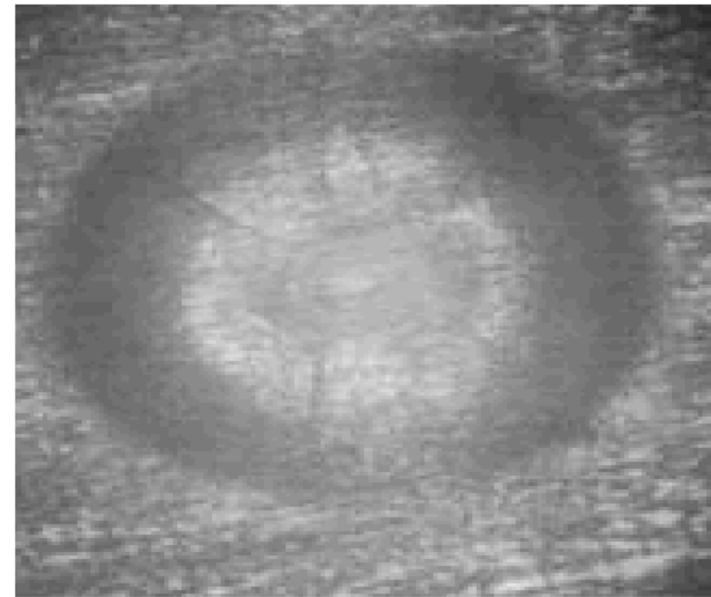
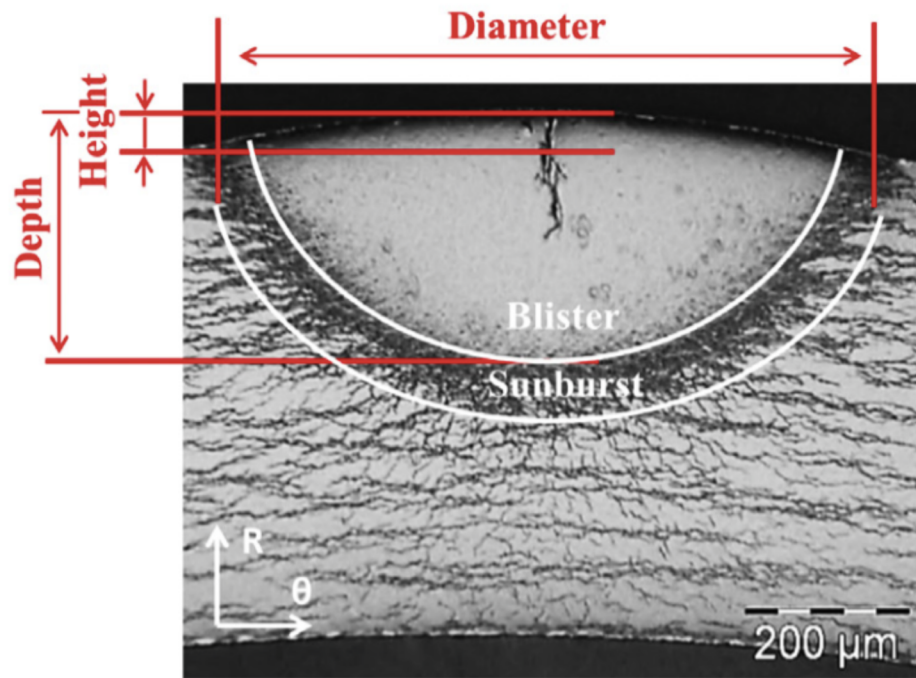
Per Ståhle and Wurigul Reheman

Solid Mechanics,
Lund University, Sweden





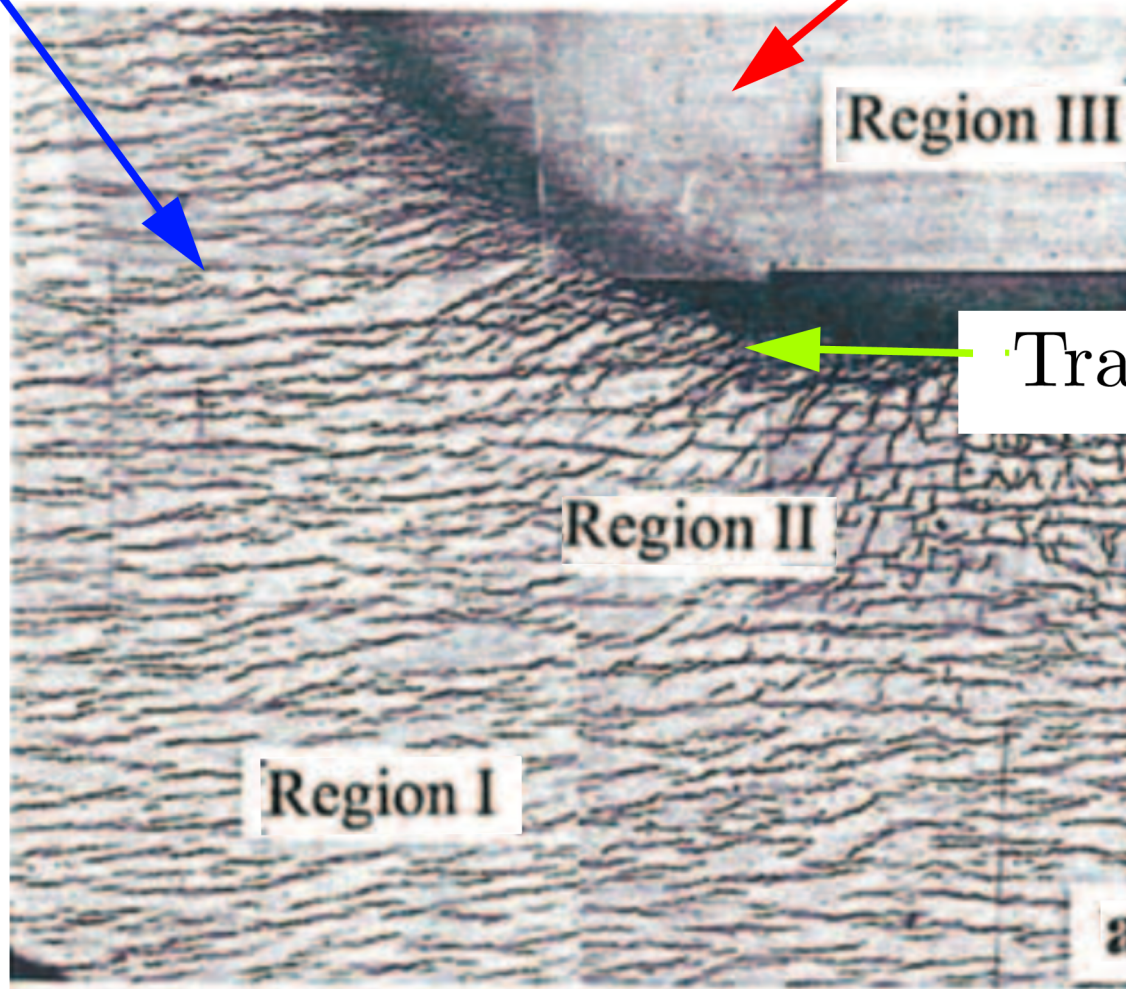
Initially hydrogen is in solid solution.
 As the cold finger makes contact
 hydride precipitation occurs.
 The hydride grows with the arrival
 of thermally migrated hydrogen



The Phase Field

$\psi = 0 \rightarrow \text{Zr}$

$\psi = 1 \rightarrow \text{Zr}_n\text{H}$



Transient region
 $0 < \psi < 1$

Contributions to the free energy

$$\mathcal{F} = \mathcal{F}_{el} + \mathcal{F}_{ch} + \mathcal{F}_{gr}$$

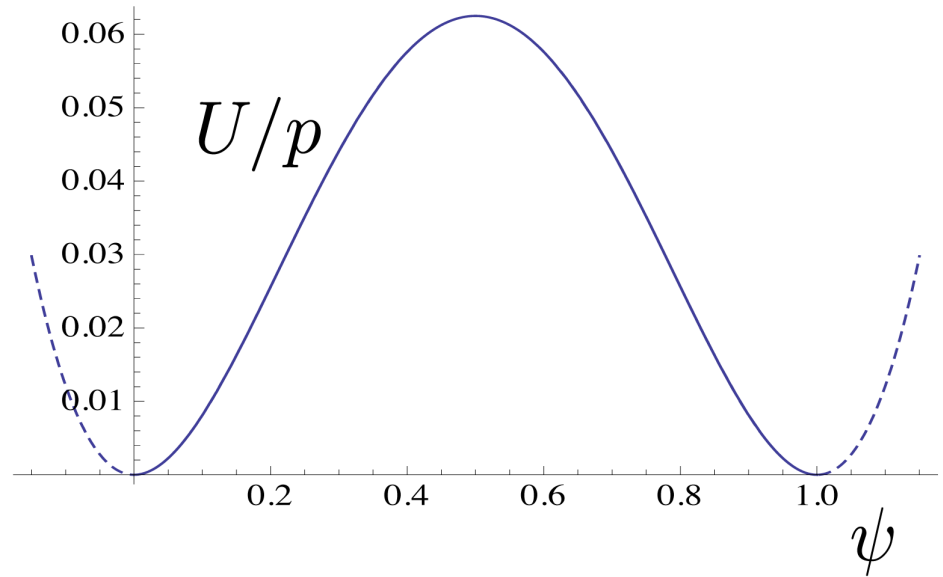
Elastic energy $\mathcal{F}_{el} = \int \sigma_{ij} d\epsilon_{ij}$

Chemical energy $\mathcal{F}_{ch} = U(\psi)$

Gradient energy $\mathcal{F}_{gr} = \frac{g_r}{2} (\psi_{,i})^2$

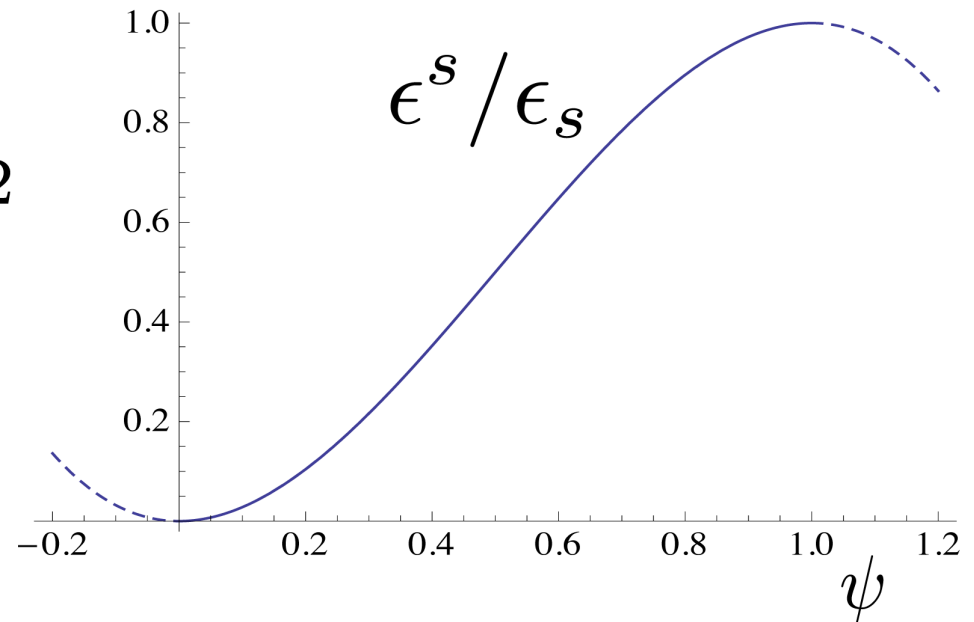
Double-well
chemical potential

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



Expansion

$$\epsilon^s(\psi) = \epsilon_s(3 - 2\psi)\psi^2$$



Unknown: ψ, u_1, u_2, u_3

$$\text{Phase: } \frac{\partial \psi}{\partial t} = -L_{\psi} \left(\frac{\partial \mathcal{F}}{\partial \psi} - \nabla \frac{\partial \mathcal{F}}{\partial (\nabla \psi)} \right)$$

$$\text{Displ.: } \frac{\partial u_i}{\partial t} = -L_{u_i} \left(\frac{\partial \mathcal{F}}{\partial u_i} - \nabla \frac{\partial \mathcal{F}}{\partial (\nabla u_i)} \right)$$

Evolution of the phase.

$$\psi_{,ii} - \frac{\partial \psi}{\partial \tilde{t}} = \{3\epsilon_{ii}^{el} \tilde{\epsilon}_s + 2(1 - 2\psi)\} (1 - \psi)\psi$$

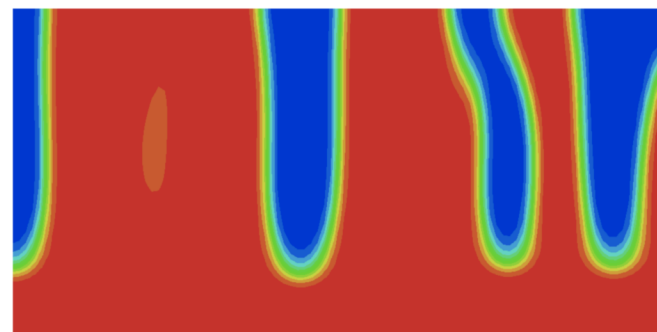
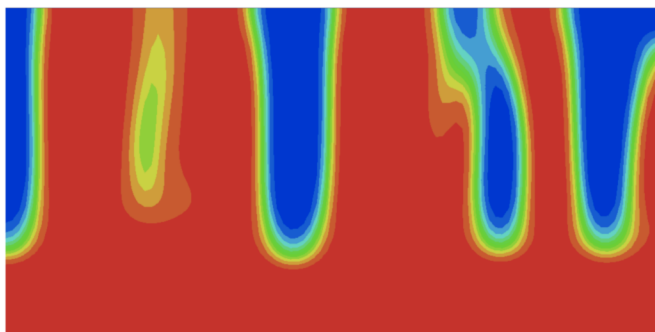
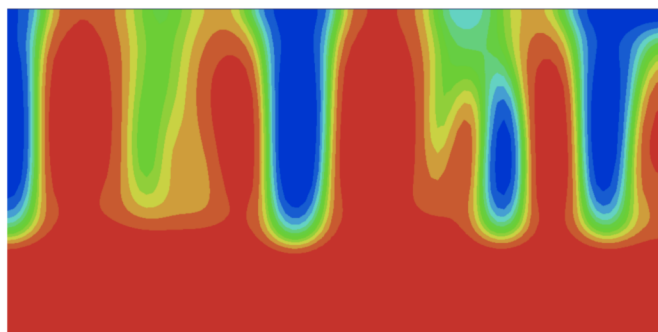
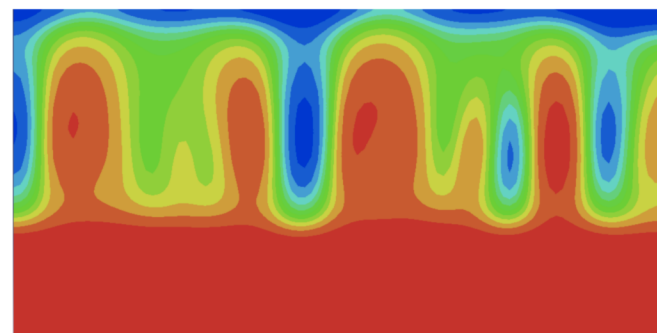
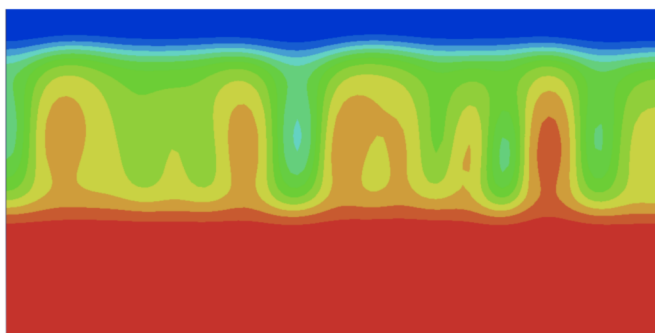
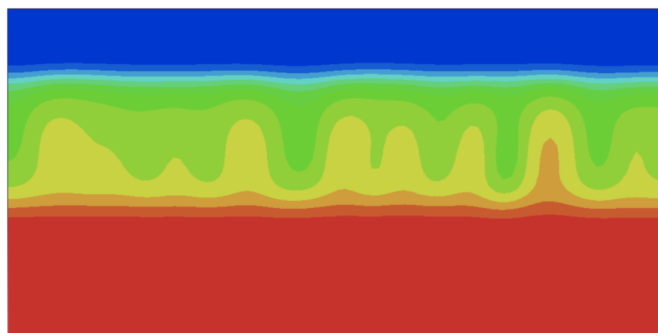
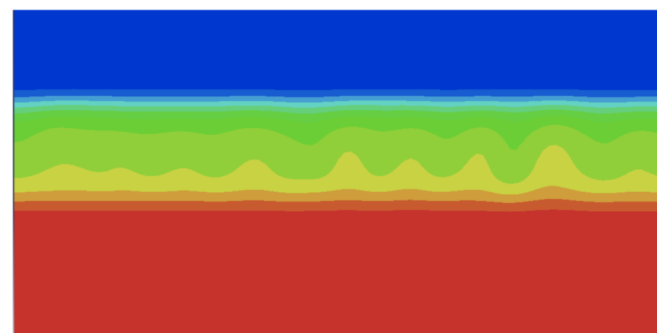
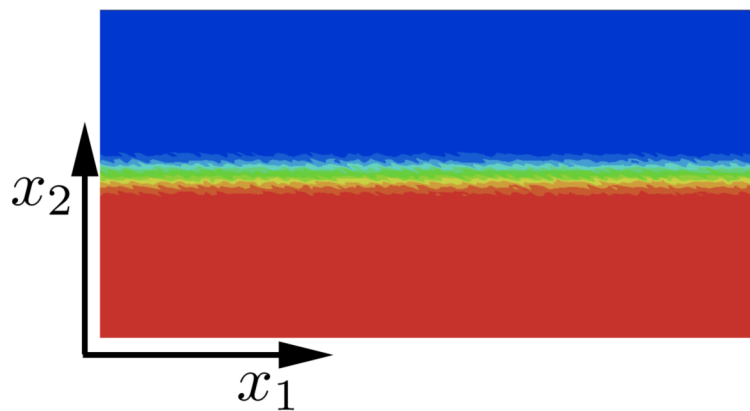
Mechanical equilibrium with expansion

$$\tilde{u}_{i,jj} + \frac{1}{1 - 2\nu} \tilde{u}_{j,ij} - (\tilde{\epsilon}_s)_{,i} = 0$$

In analogy with a fully coupled thermal-stress

Noisy interface

$$\epsilon_{11} = 0.55\epsilon_s$$



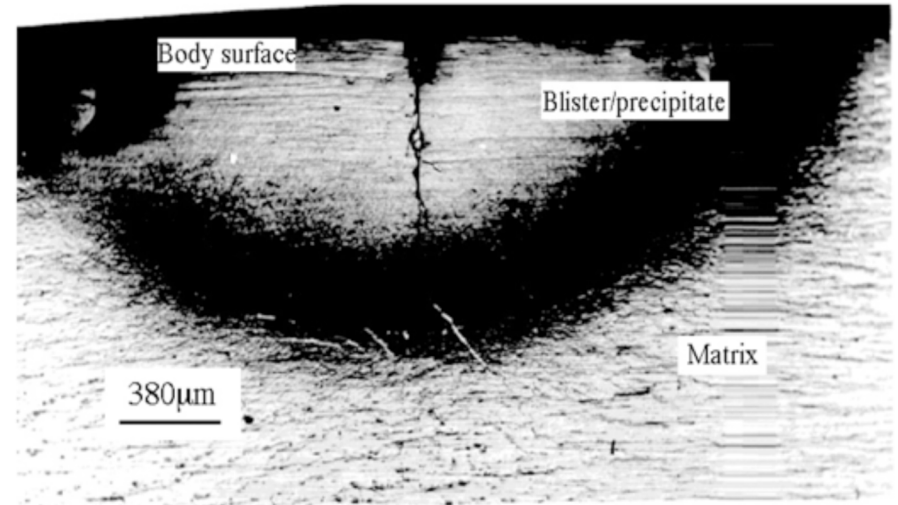
Surface energy $\gamma = \sqrt{2pg_b}$ [F/L]

Strain energy density $W = \sigma_{ii}\epsilon_s$ [F/L²]

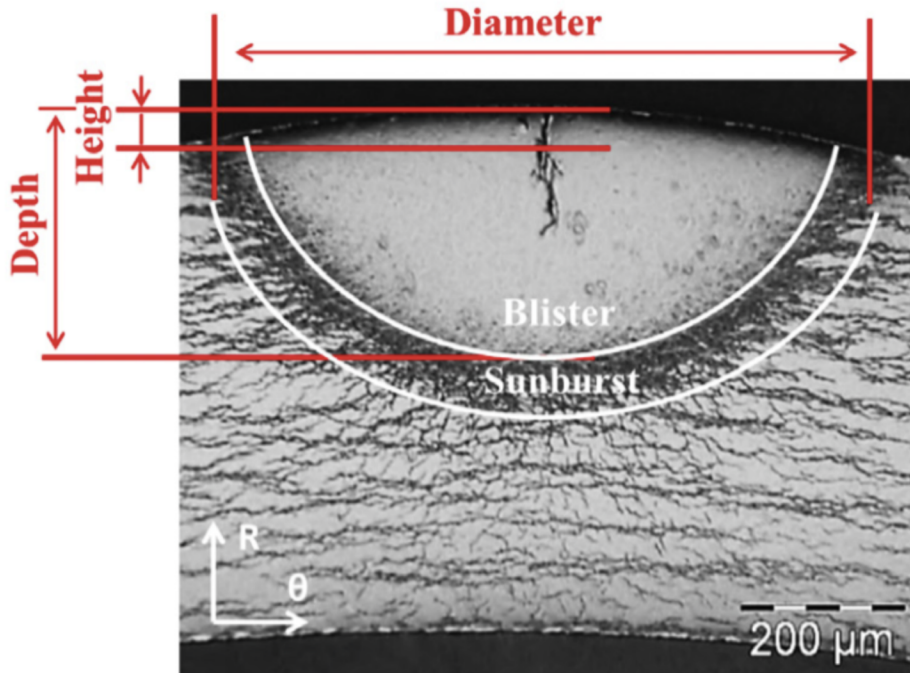
Length parameter γ/W [L]

Cracks appear in the expanded hydride

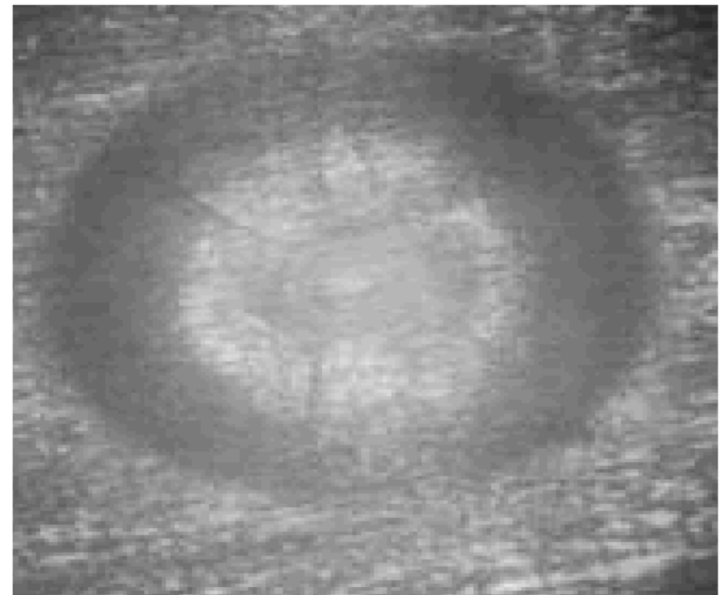
Precipitate is commonly believed to be compressed

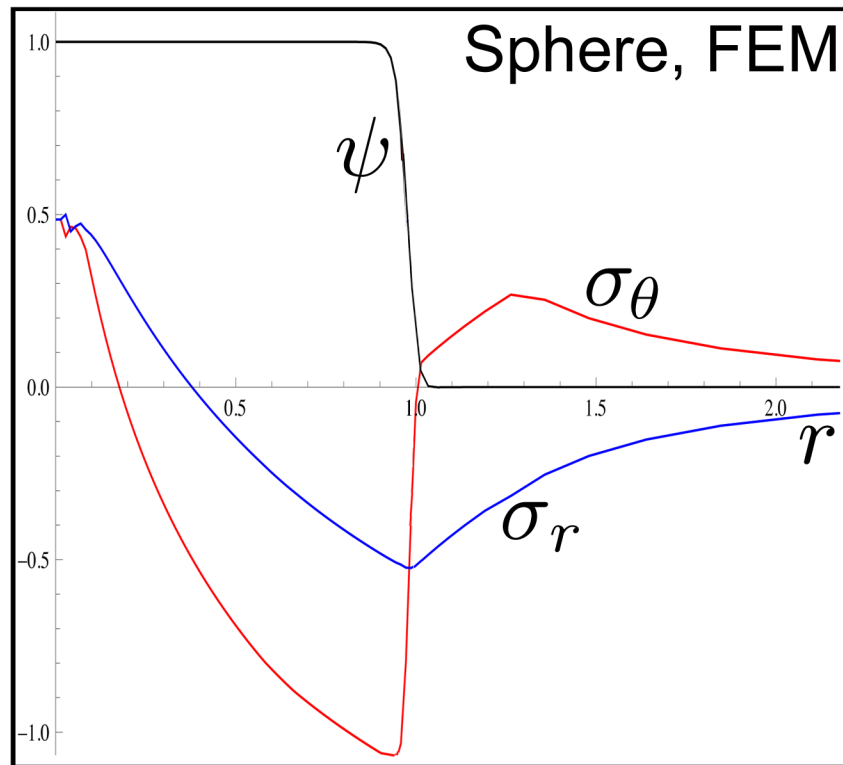
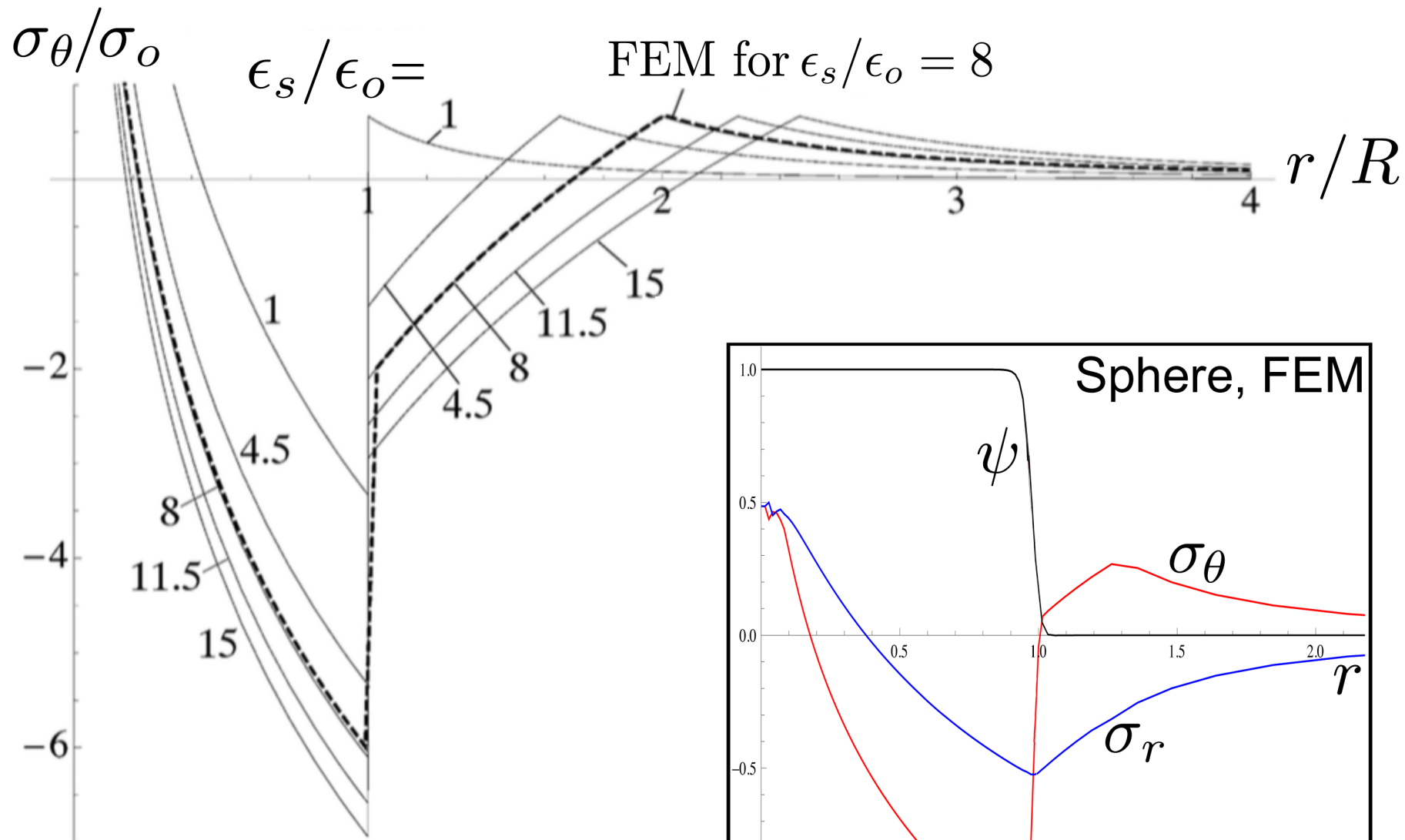


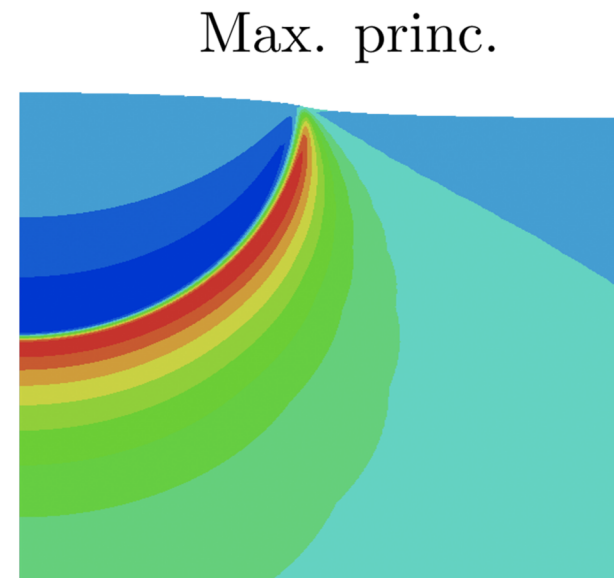
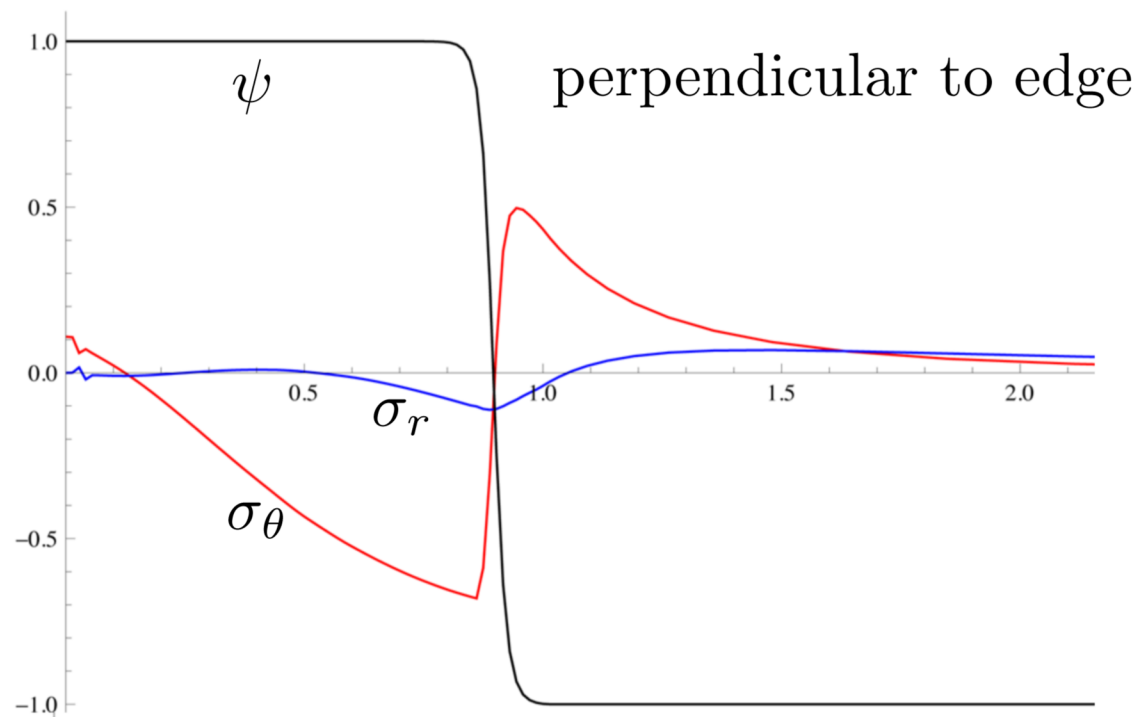
Ma et al. 2006



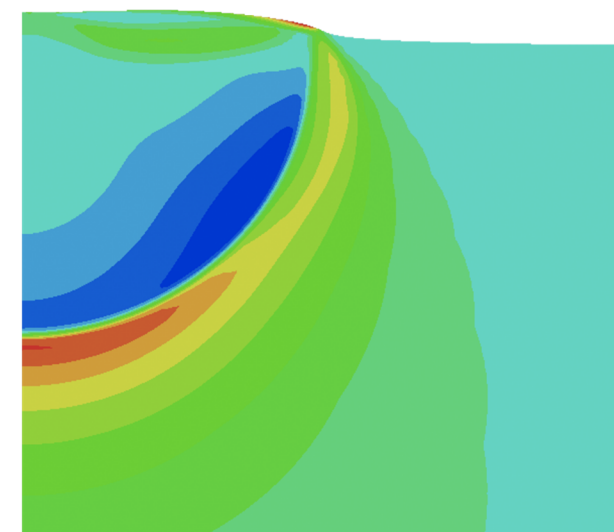
Singh et al. 2001



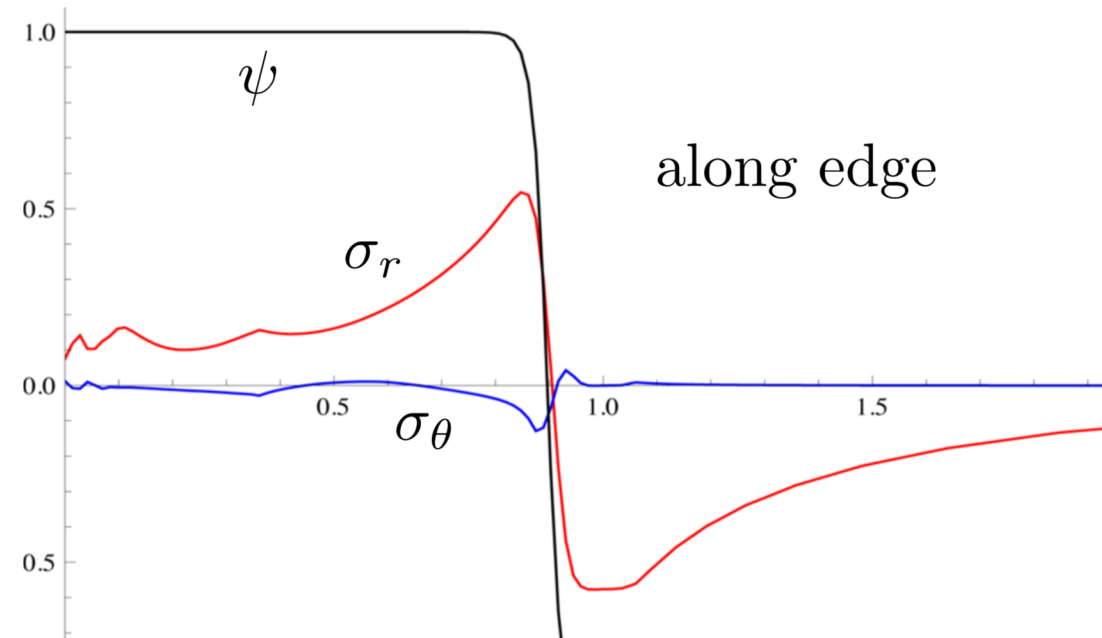




Stationary blister



Growing blister



Summary

- A stretched surface of an expanding precipitate is unstable
- The surface develops finger like morphology
- Surface energy vs. strain energy gives the length scale
- Spherical precipitates develop central stress singularities
- Surface blisters crack from tensile stress