Interface Instabilities of Growing Hydrides

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Interface instabilities of growing hydrides

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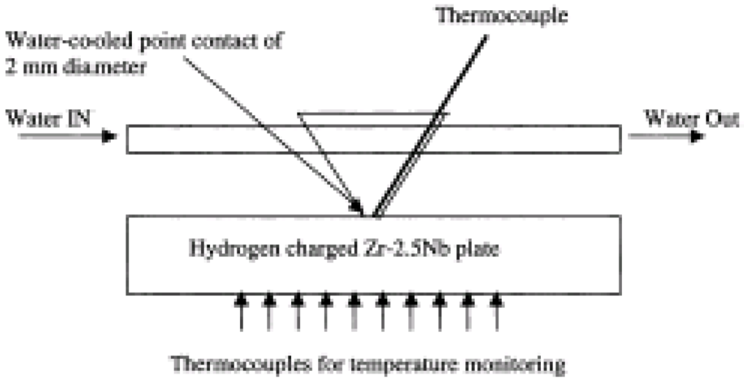
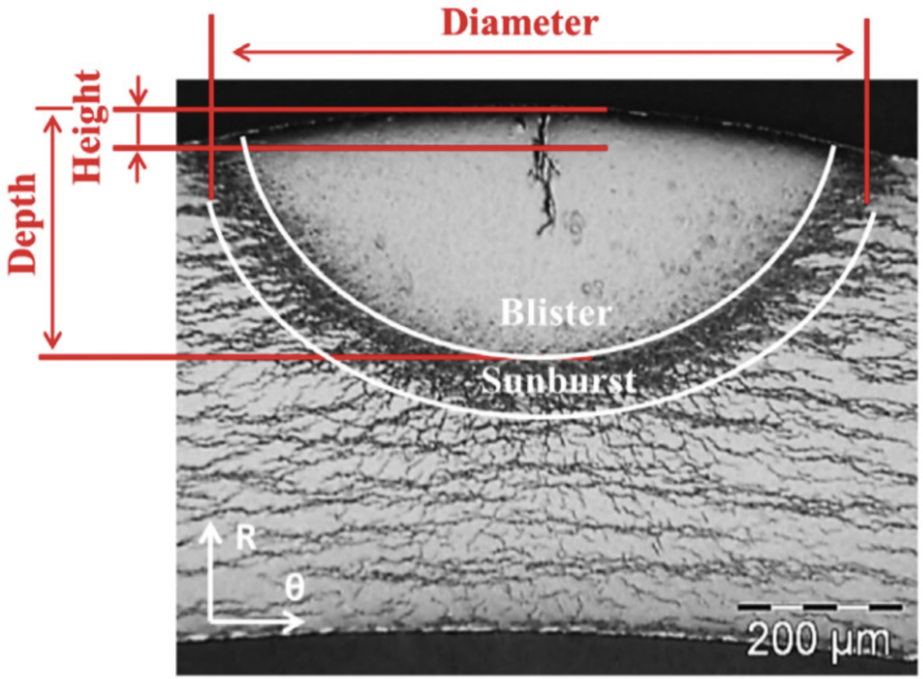
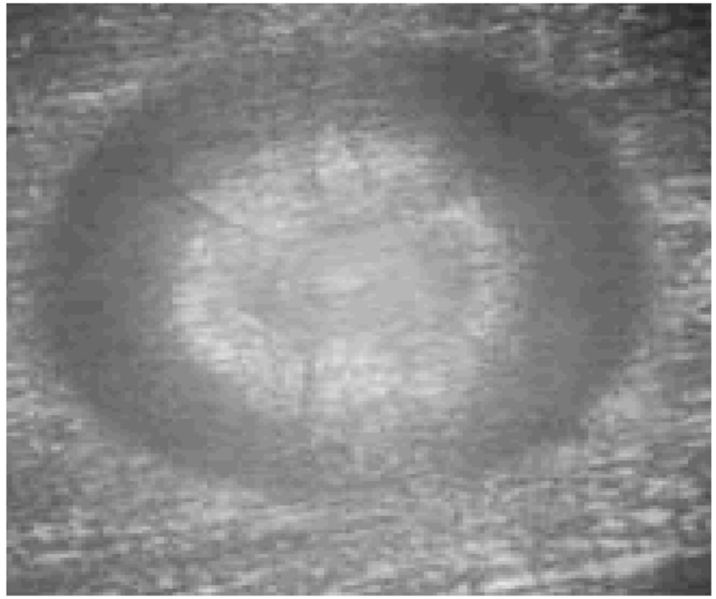


Initially hydrogen is in solid solution.
As the cold finger makes contact
hydride precipitation occurs.
The hydride grows with the arrival
of thermally migrated hydrogen

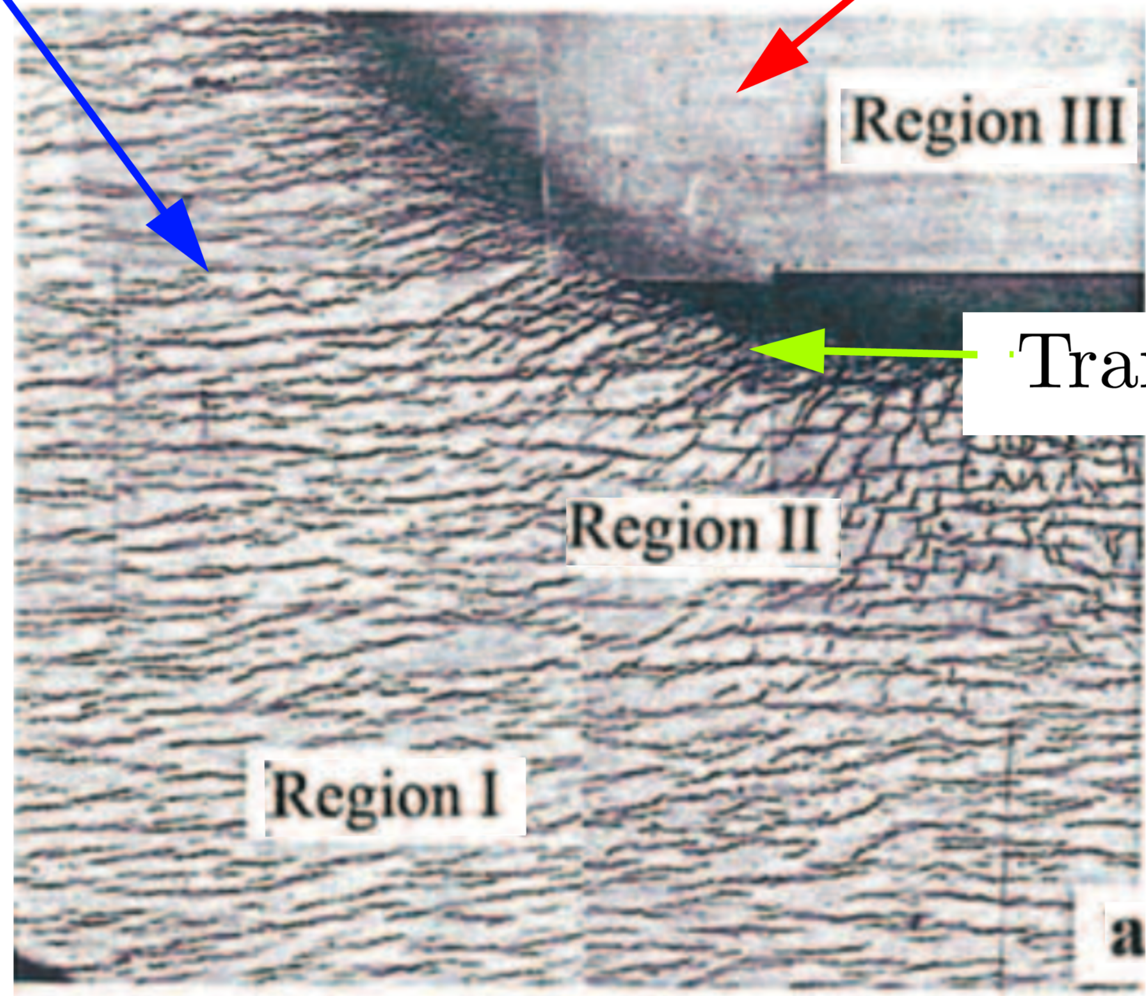




The Phase Field

$\psi = 0 \rightarrow$ Zr

$\psi = 1 \rightarrow$ Zr_nH



Transient region

$0 < \psi < 1$

Contributions to the free energy

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

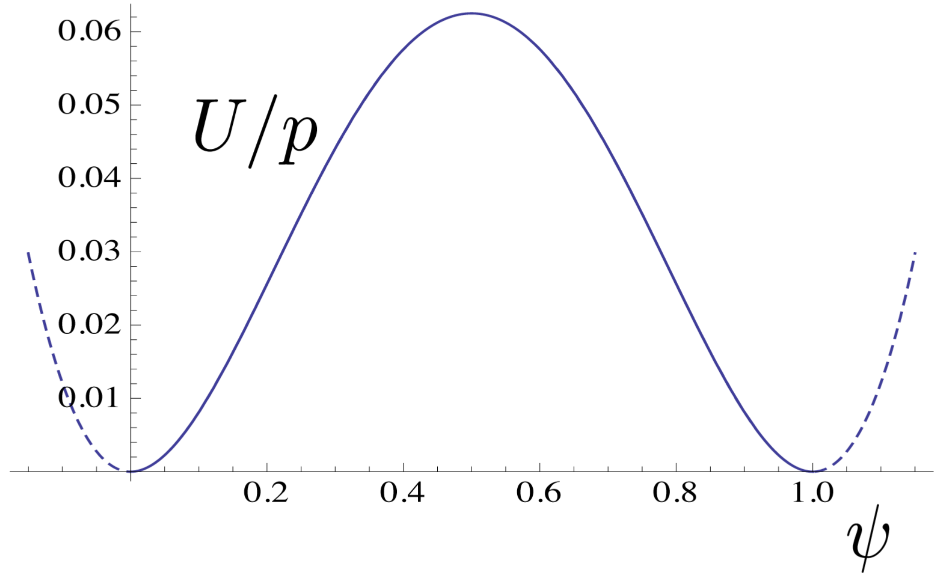
Elastic energy $$\mathcal{F}_{el} = \int \sigma_{ij} \mathrm{d}\epsilon_{ij}$$

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

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

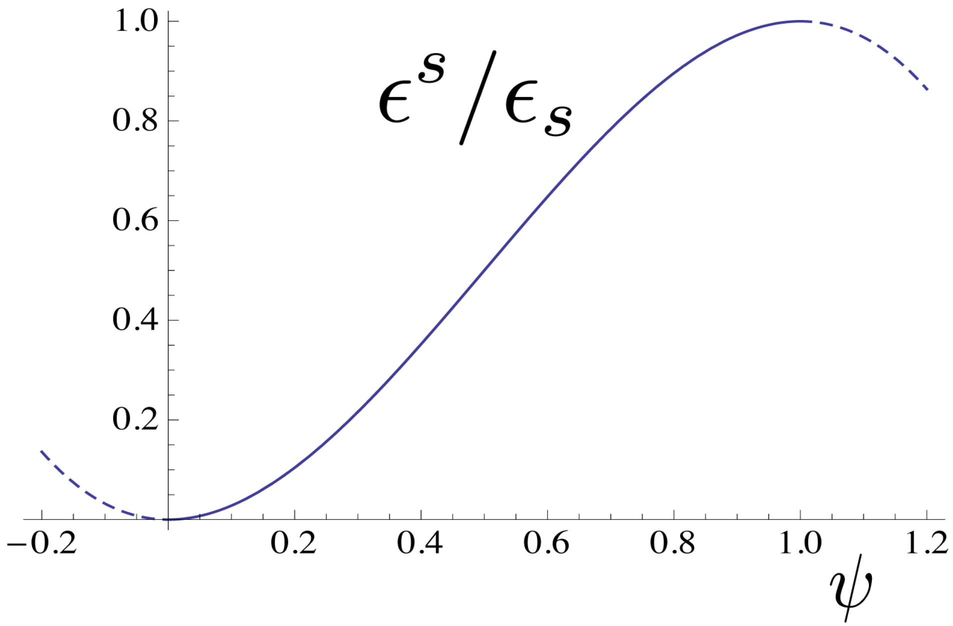
Double-well
chemical potential

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



Expansion

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



Unknown: ψ, u_1, u_2, u_3

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

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

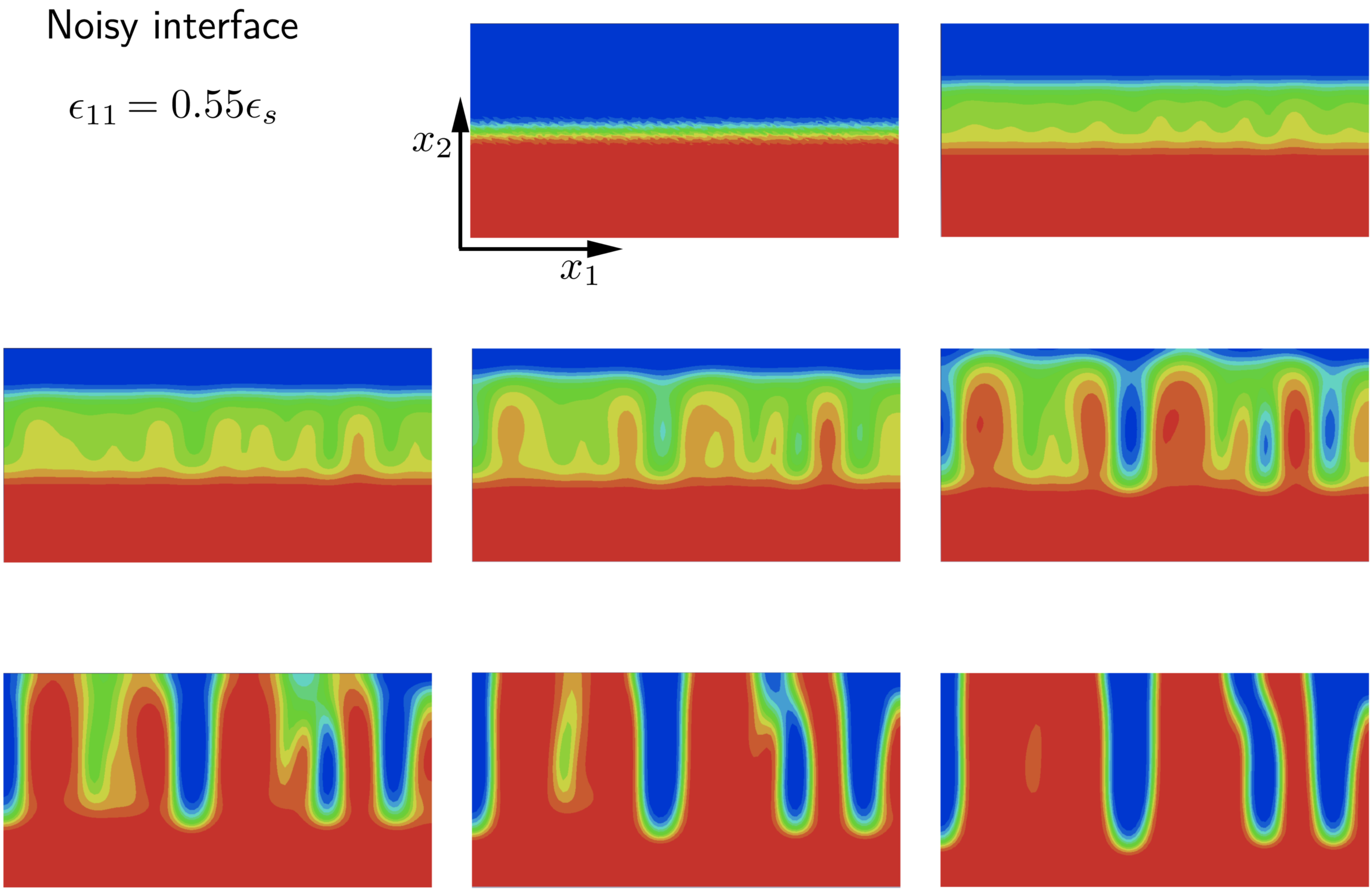
Evolution of the phase.

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

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
$\epsilon_{11} = 0.55\epsilon_s$
x_2
x_1

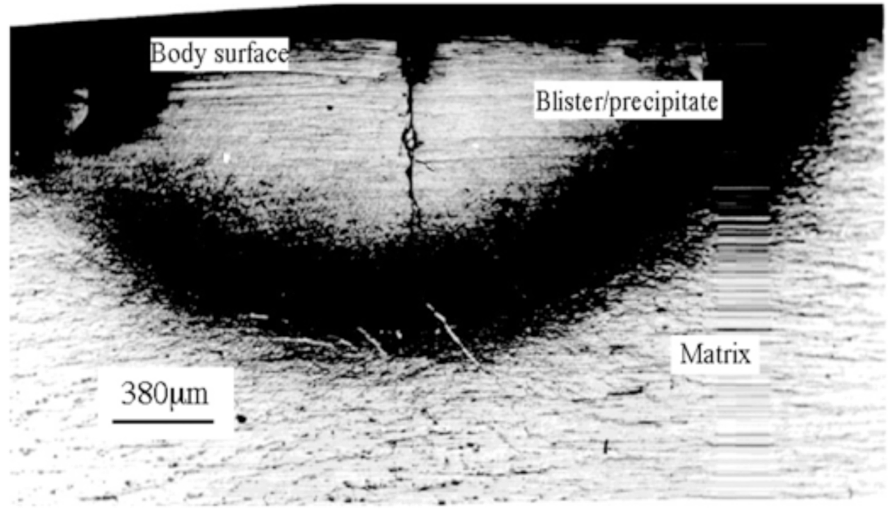
Surface energy $\gamma = \sqrt{2pg_b}$ [F/L]

Strain energy density $W = \sigma_{ii}\epsilon_s$ [F/ L^2]

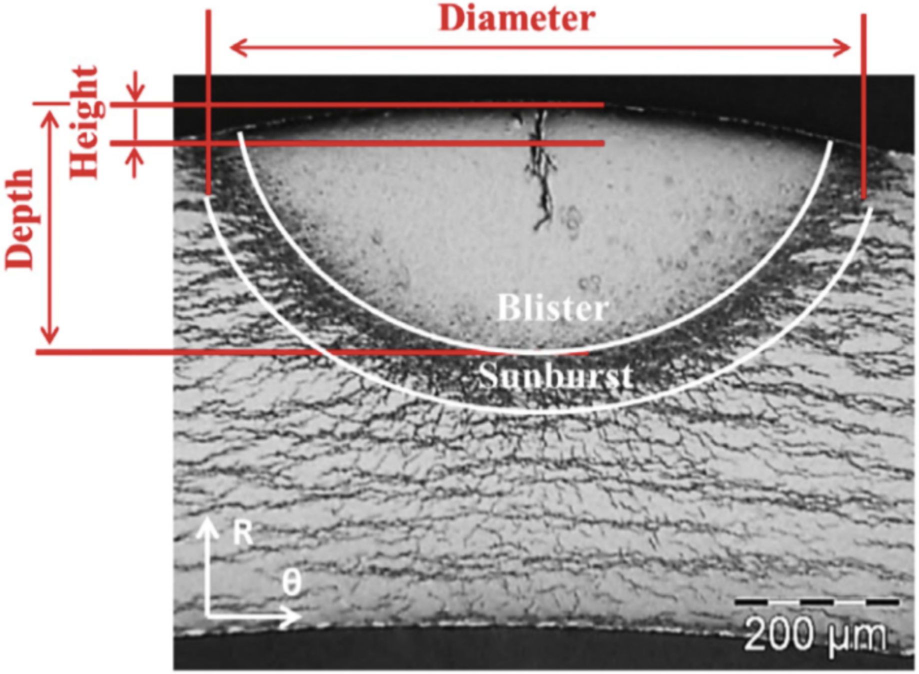
Length parameter γ/W [L]

Cracks appear in the expanded hydride

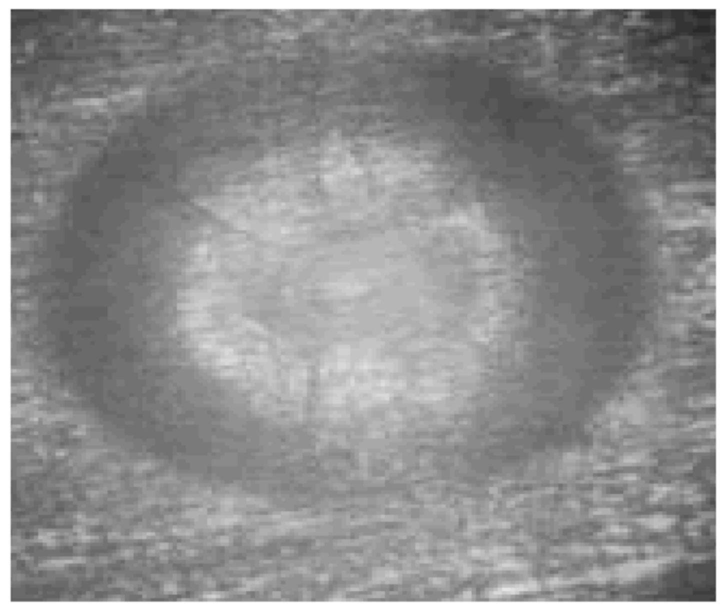
Precipitate is commonly believed to be comresssed

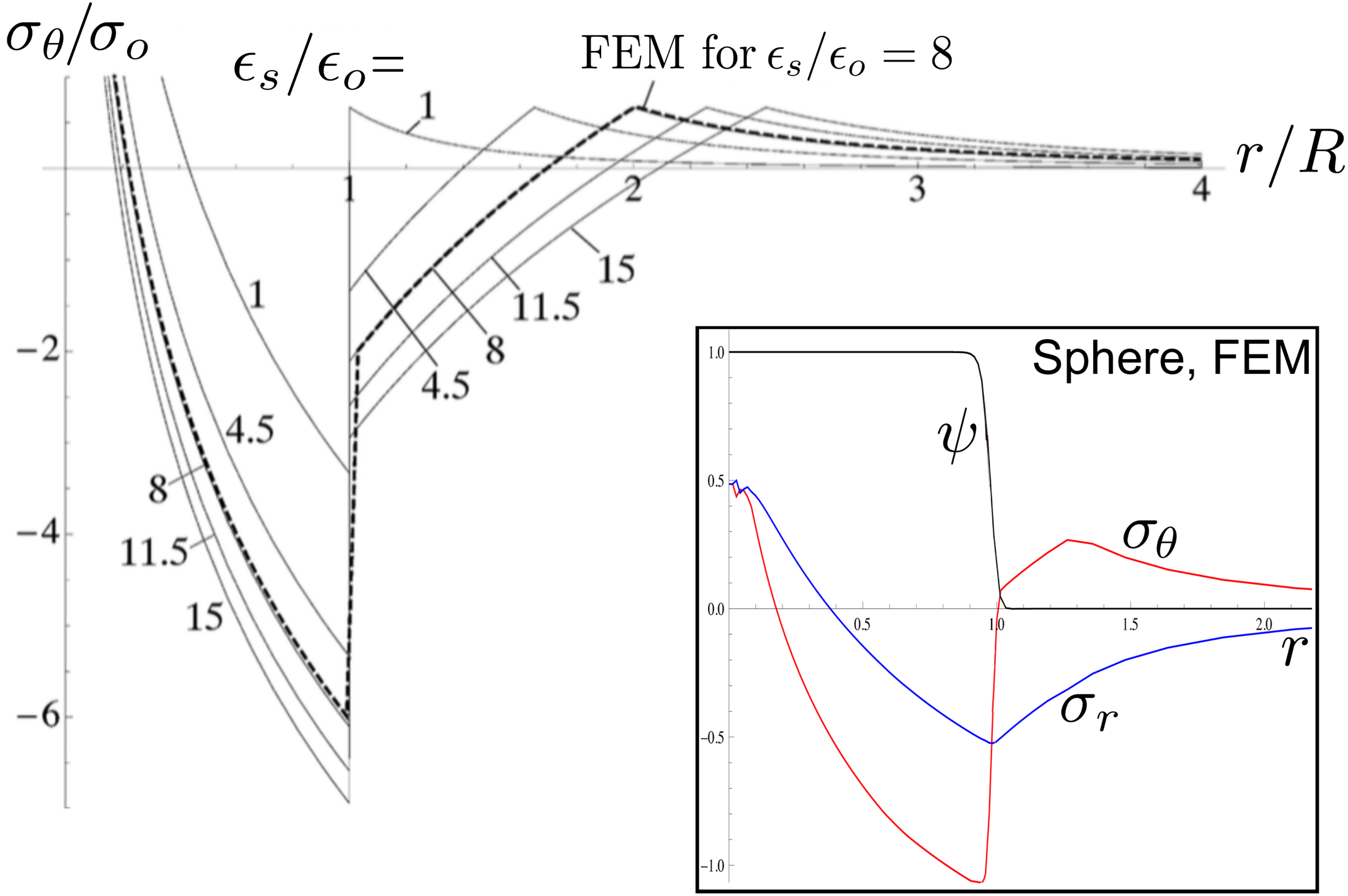


Ma et al. 2006

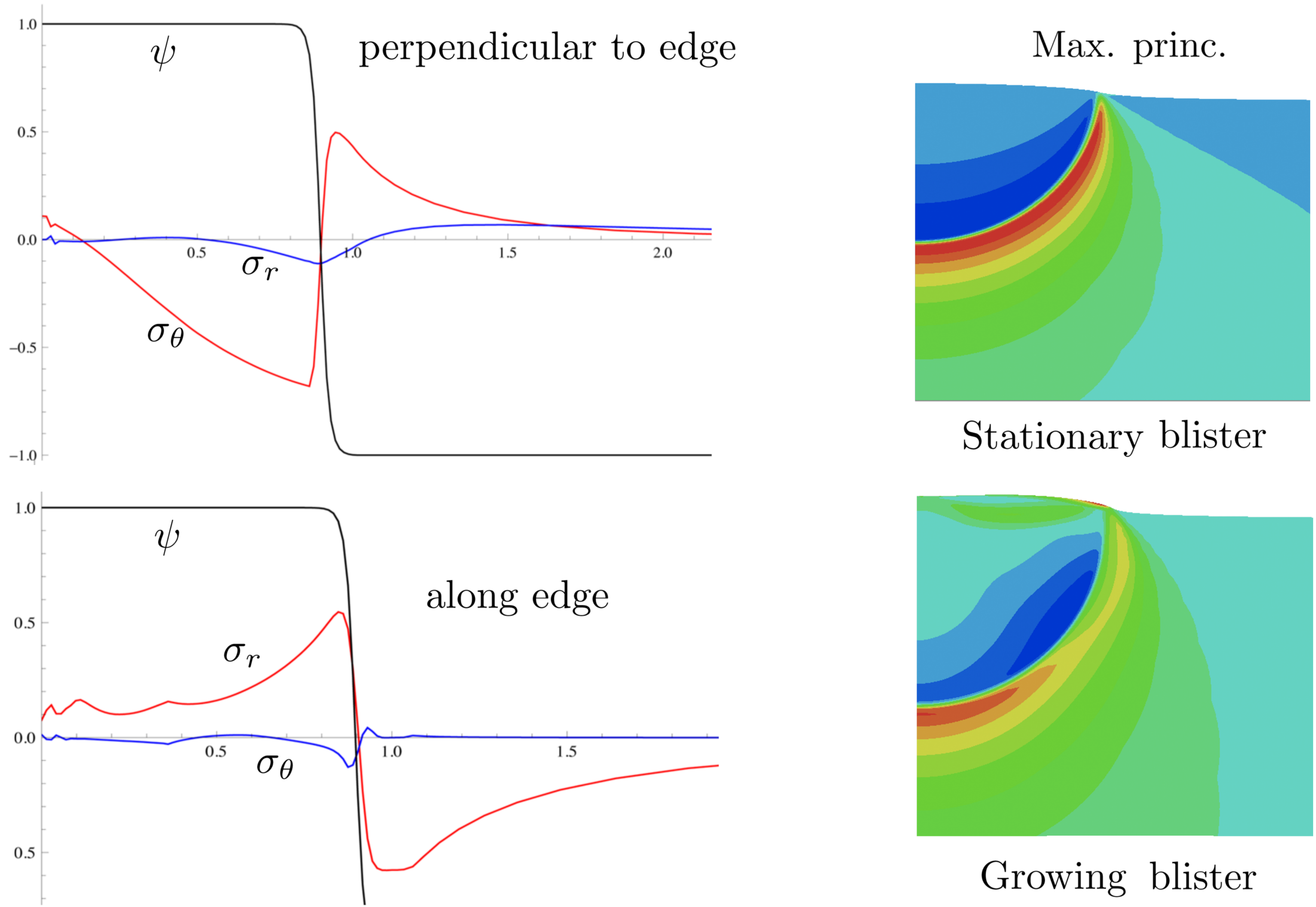


Singh at el. 2001





σ_θ/σ_o
$\epsilon_s/\epsilon_o=$
FEM for $\epsilon_s/\epsilon_o = 8$
r/R
1
1
4.5
8
11.5
15
1
2
3
4
−2
−4
−6
1
4.5
8
11.5
15
Sphere, FEM
ψ
σ_θ
σ_r
r
1.0
0.5
0.0
−0.5
−1.0
0.5
1.0
1.5
2.0



perpendicular to edge
ψ
σ_r
σ_θ
1.0
0.5
0.0
−0.5
−1.0
0.5
1.0
1.5
2.0
along edge
ψ
σ_r
σ_θ
1.0
0.5
0.0
0.5
0.5
1.0
1.5
Max. princ.
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