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On Phase-Field Modelling

Invited Talk given at Kunming University, Orationem Meam

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On Phase-Field Modelling

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Modelling of Whatever in Nature

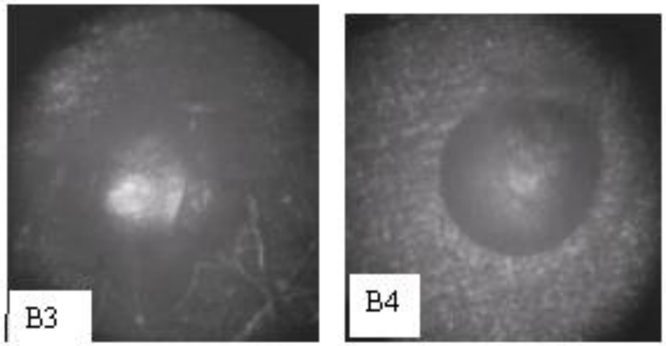
Free energy goes towards its minimum. Always.

Collect all relevant free energies like

gradient energy, electric energy, elastic energy, gravitational energy ... and chemical phase energy.

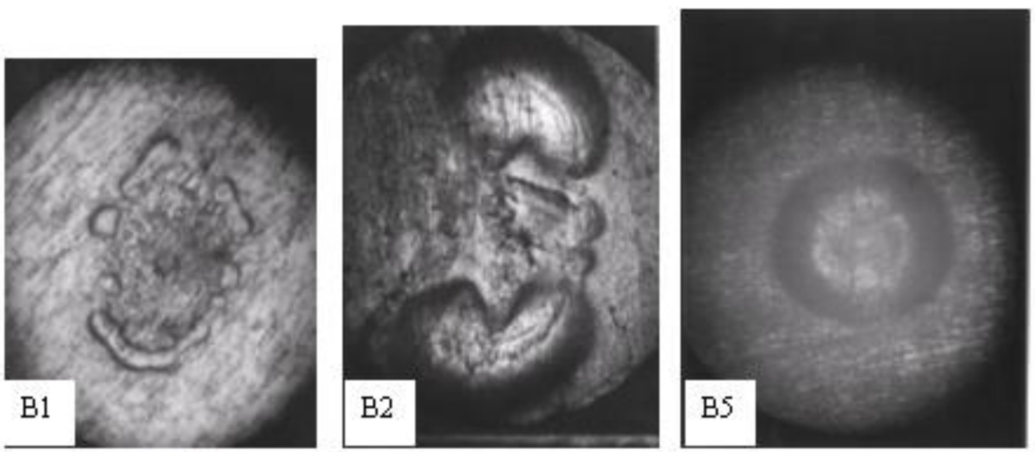
Hydride Blister

Prior solution annealing



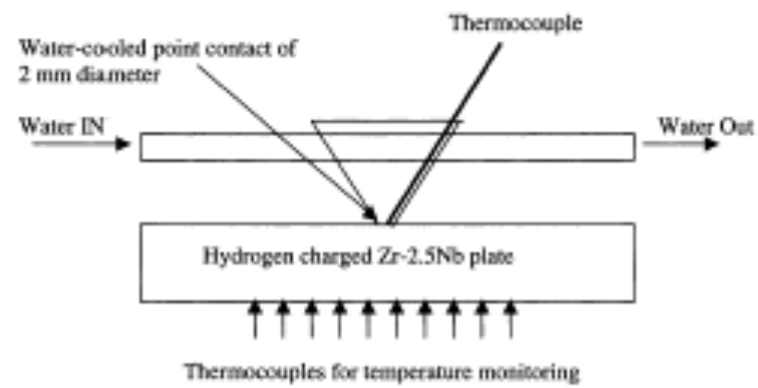
(a) Type I

Before cold finger is struck all the hydrogen is solid solution.
As cold finger makes contact hydride precipitation occurs at cold spot which grows with the arrival of thermally migrated hydrogen resulting in single blister



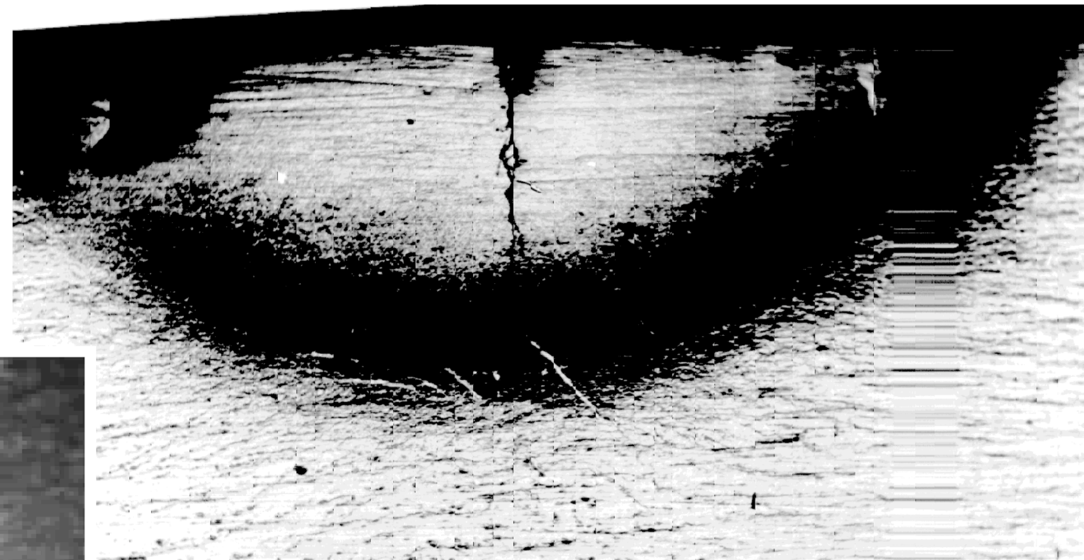
(b) Type II

Without solution annealing

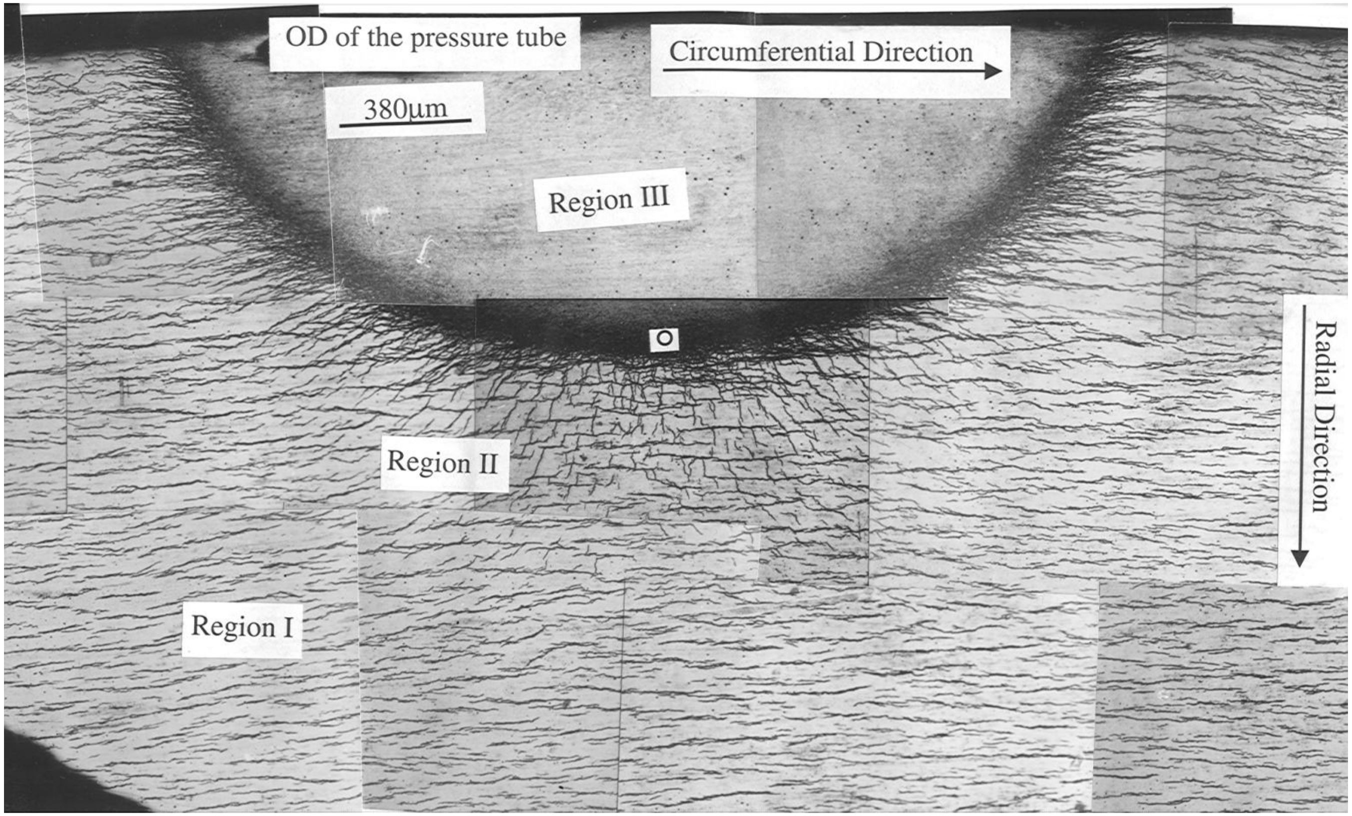


Cold finger is in contact all the time
Hydride precipitation occurs around the cold spot resulting in ring of blisterets

a hydride blister grown in Zr–2.5wt%Nb pressure tube alloy (Singh *et al.*, 2001)



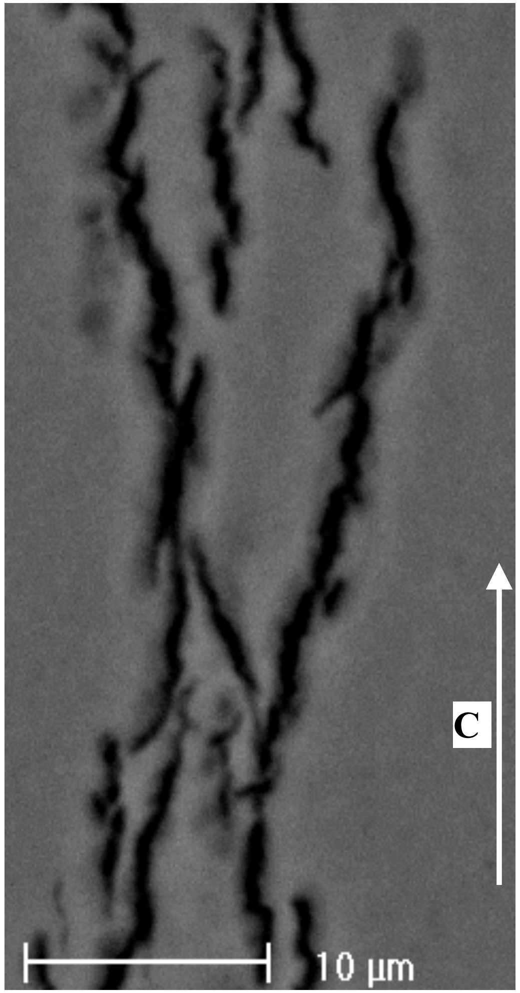
Hydride Blister section



Optical micrograph of hydride blister section, grown in Zr-2.5wt.% Nb pressure tube material. Three regions - Region I - matrix & circumferential hydrides, region II - matrix containing both radial and circumferential hydrides and region III - mainly of δ-hydride.

The basis of radial hydride formation is the stress field of blister in the matrix surrounding it.

Hydride – level of organization



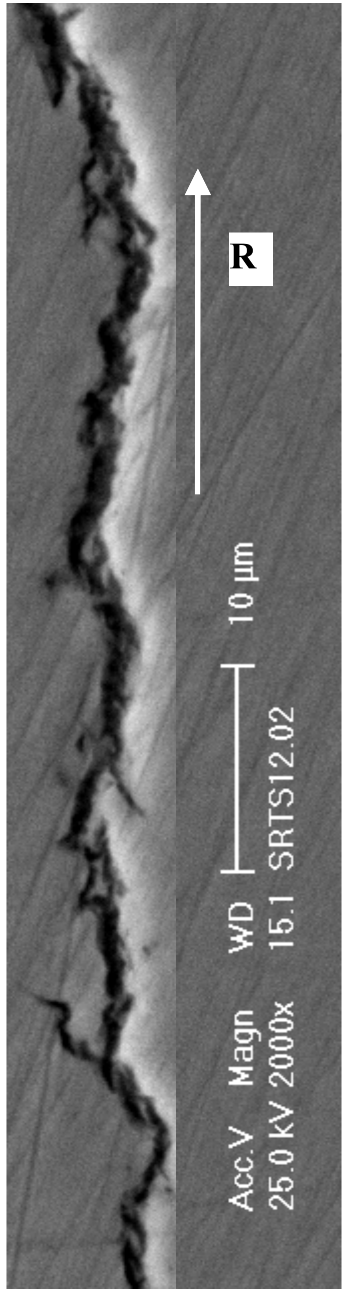
Hydride plate comprising of platelets stacked side by side

Each platelet comprising of sub-platelets stacked end to end

Circumferential hydride shows both level of organization

Radial hydride shows only sub-platelet level of organization

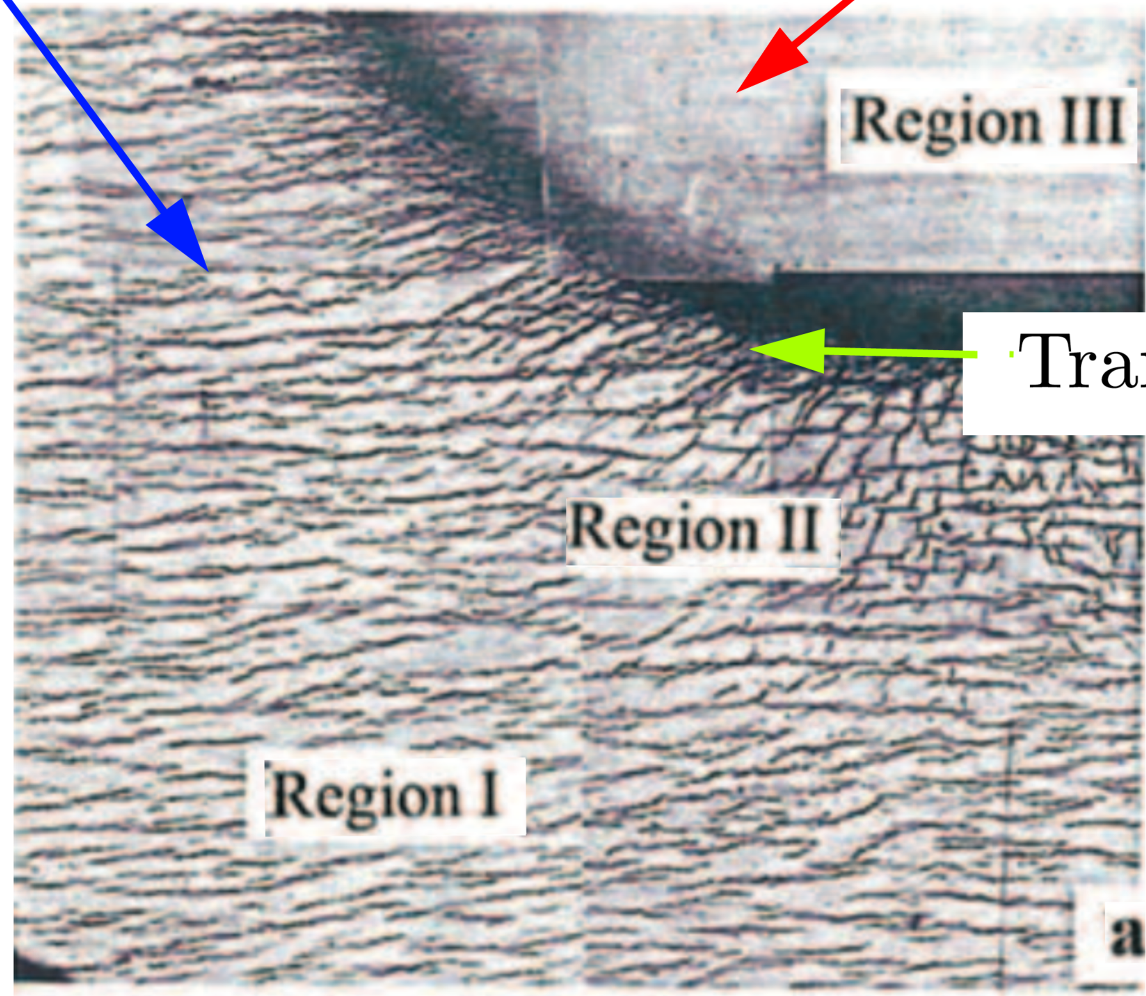
R. N. Singh et al. J. of Nucl. Mater. 2006



The Phase Field

$\psi = 0 \rightarrow$ Zr

$\psi = 1 \rightarrow Zr_n H$



Transient region

$0 < \psi < 1$

Hydride growth by:

0. Thermal diffusion
1. Concentration-driven diffusion
2. Uphill diffusion
3. Stress-driven diffusion

$$F = \int \mathcal{F} \mathrm{d}V = \int \left(\mathcal{F}_{gr} + \mathcal{F}_{ch} + \mathcal{F}_{el} \right) \mathrm{d}V$$

Contributions to the free energy

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

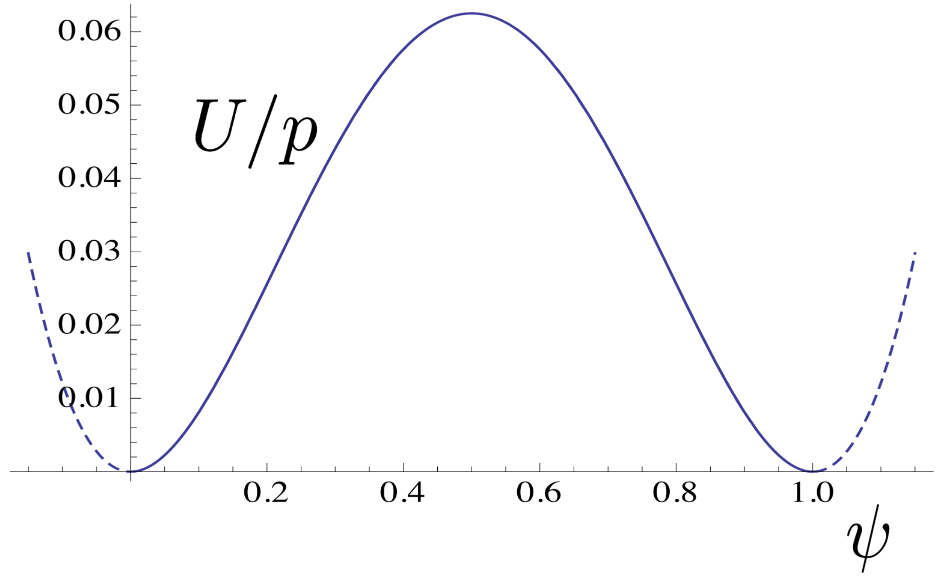
Elastic energy $$\mathcal{F}_{el} = \int \sigma_{ij} \mathrm{d}\epsilon_{ij}$$

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

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

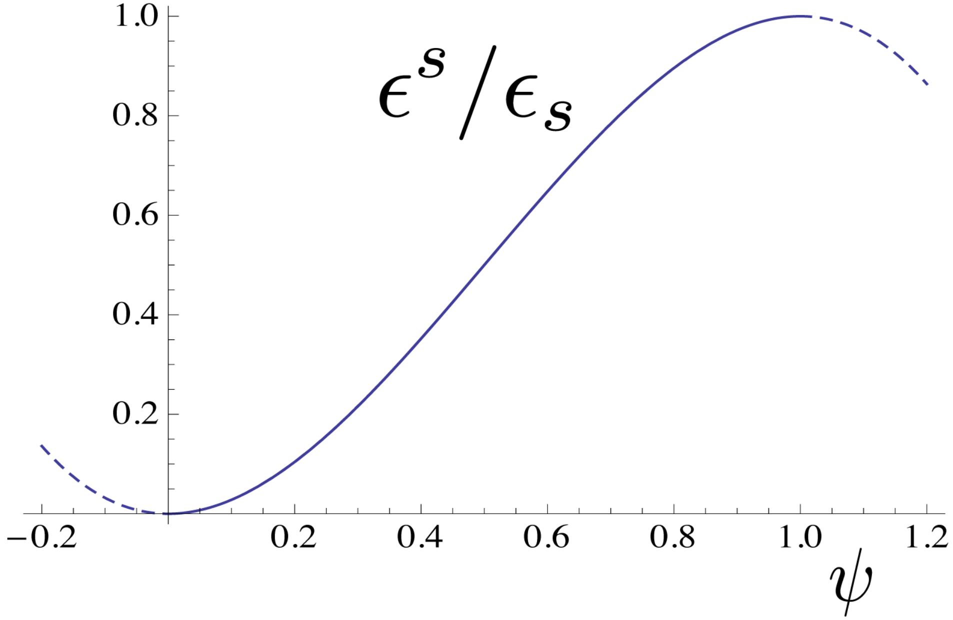
Double-well chemical potential

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



Expansion

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



Plane cases. Unknown: ψ, u_1, u_2

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

$$\frac{\partial \psi}{\partial t} = -L_{\psi}\left(\left\{3\sigma_{ii}\epsilon_s + 2p(1-2\psi)\right\}(1-\psi)\psi - g_b\psi_{,ii}\right)$$

Evolution of the displacements

$$\frac{\partial u_i}{\partial t} = \text{-}L_u(\mu u_{i,jj} + (\mu+\lambda)u_{j,ij} - (2\mu+3\lambda)\epsilon^s_{,i})$$

At equilibrium

$$\mu u_{i,jj} + (\mu+\lambda)u_{j,ij} - (2\mu+3\lambda)\epsilon^s_{,i} = 0$$

$$\frac{\partial \psi}{\partial t} = -L_{\psi} \left(\left\{ 3\sigma_{ii}\epsilon_s + 2p(1-2\psi) \right\} (1-\psi)\psi - g_b \psi_{,ii} \right)$$

$$\frac{g_b}{p} \psi_{,ii} - \frac{1}{pL_{\psi}} \frac{\partial \psi}{\partial t} = \left\{ 3\sigma_{ii}\epsilon_s/p + 2(1-2\psi) \right\} (1-\psi)\psi$$

$$\tilde{x}_i = \sqrt{p/g_b} x_i, \ \tilde{t} = pL_{\psi} t \qquad \tilde{u}_i = u_i/\sqrt{g_b p}$$

Heat transfer with heat generation

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

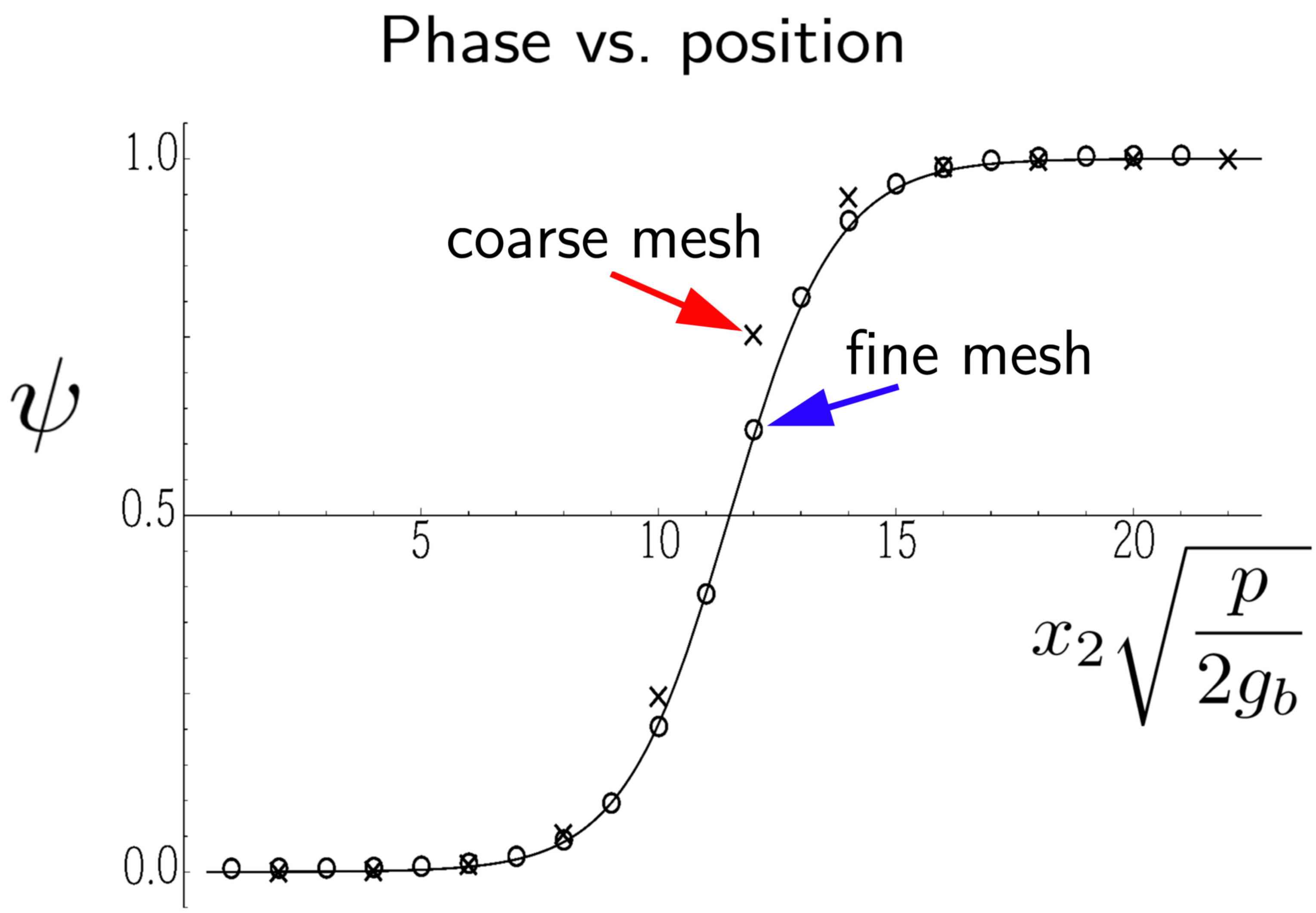
Mechanical equilibrium with thermal expansion

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

In analogy with a fully coupled thermal-stress

One dimension static (Ginzburg, Landau 1950)

$$g_b \psi_o'' - p\psi_o(\psi_o^2 - 1) = 0 \quad \text{solved by} \quad \psi_o = \tanh(x/\sqrt{2g_b})$$



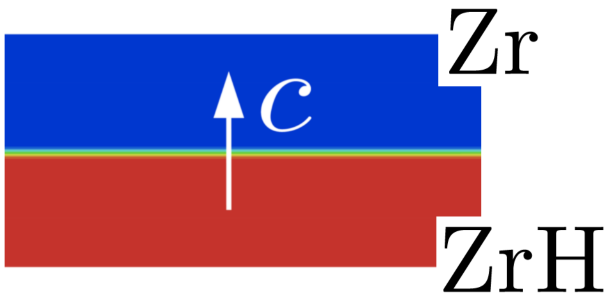
Dynamic with mechanical loading

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

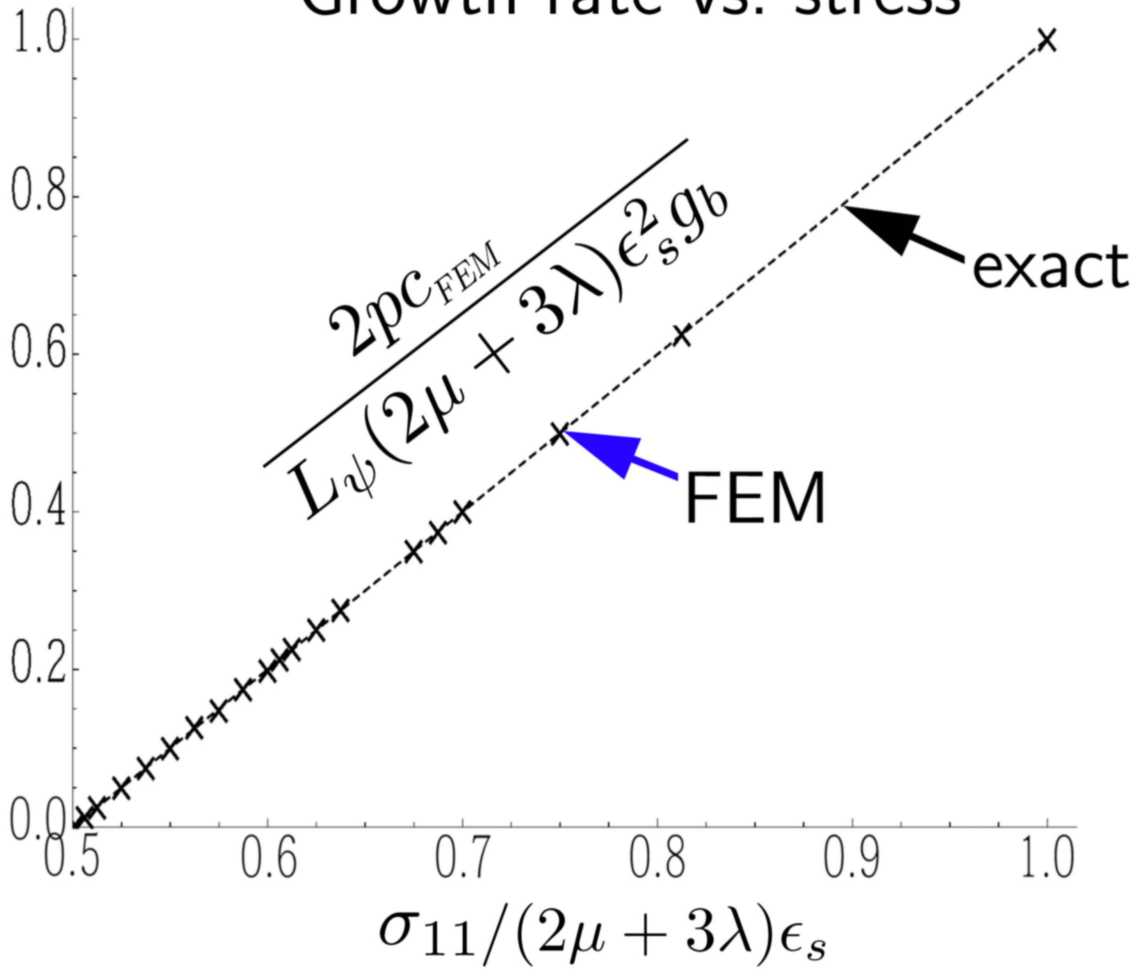
solved by $$\psi = 1 - \frac{1}{2}\tanh\left(\sqrt{\frac{p}{2g_b}}x_2 + \frac{1}{4}L_\psi \sigma_{11}\epsilon_s\sqrt{\frac{2g_b}{p}}t\right)$$

Growth rate

$$c = L_\psi \sigma_{11}\epsilon_s \frac{g_b}{2p}$$



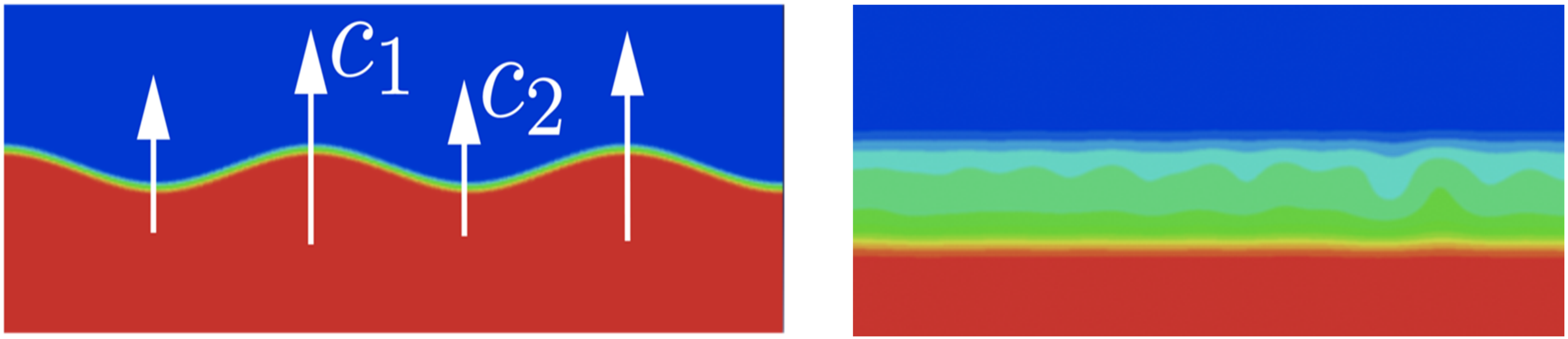
Growth rate vs. stress

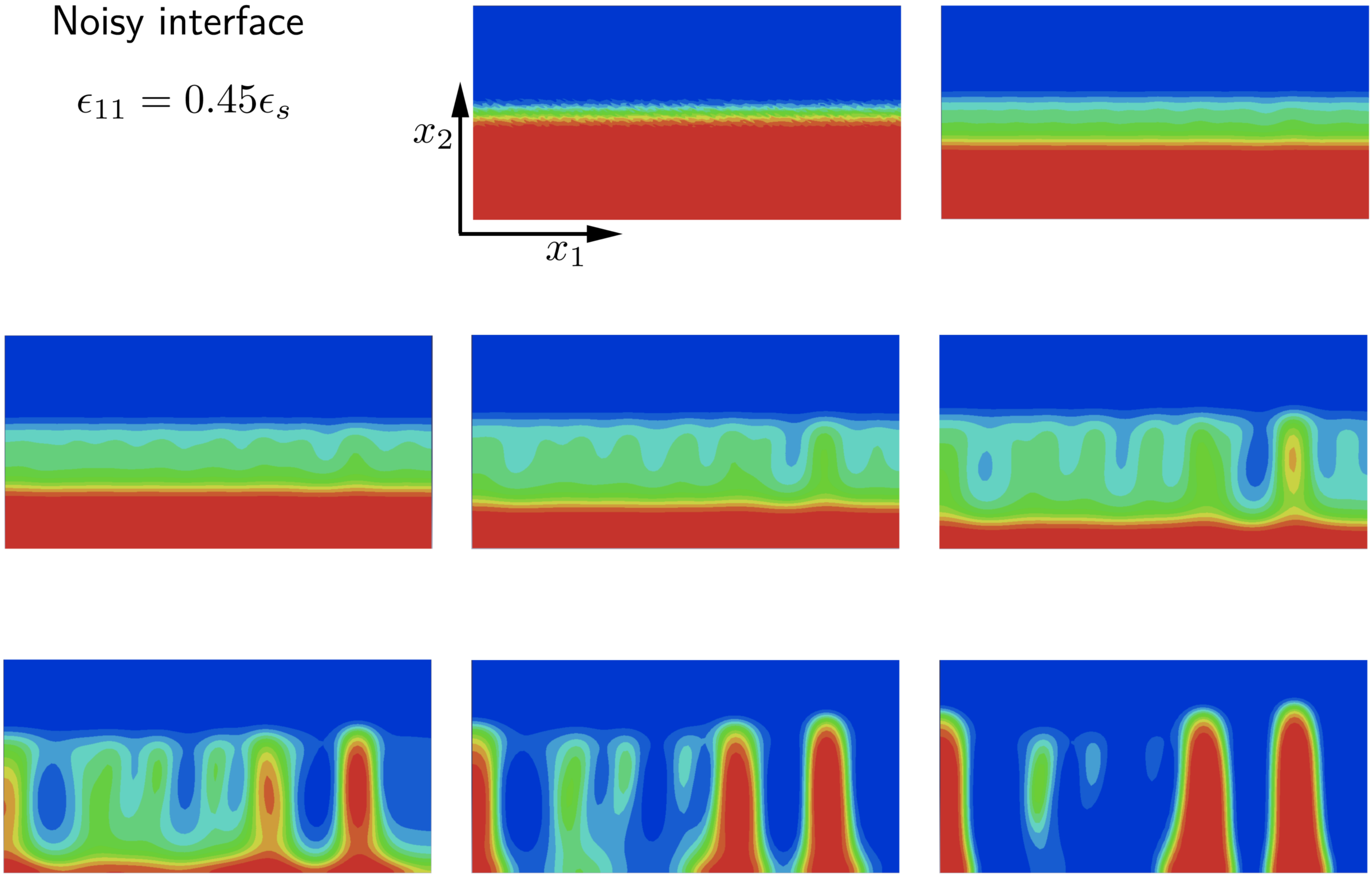


Surface energy $\gamma = \sqrt{2pg_b}$ [F/L]

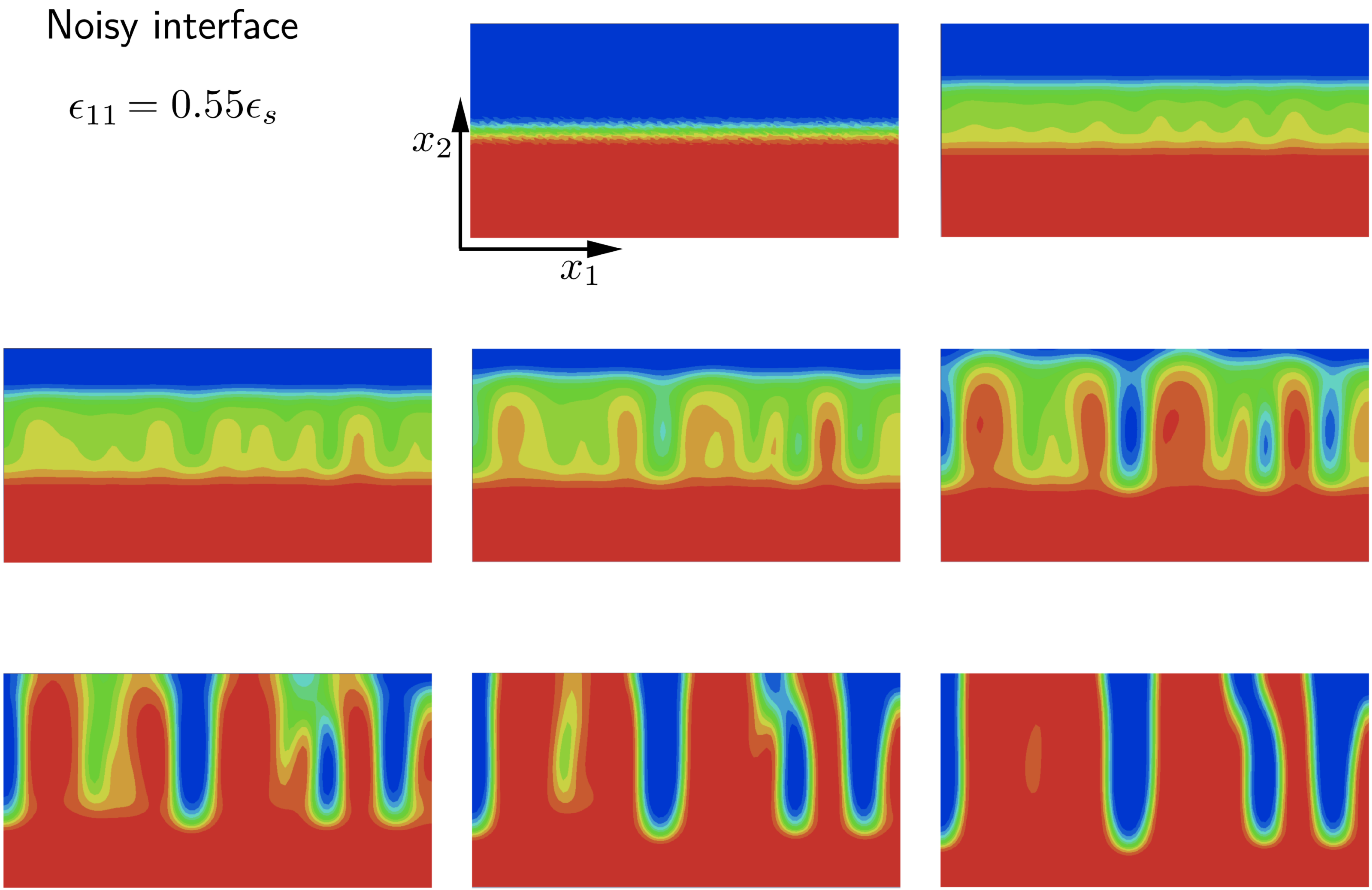
Strain energy density $W = \sigma_{ii}\epsilon_s$ [F/ L^2]

Length parameter γ / W [L]

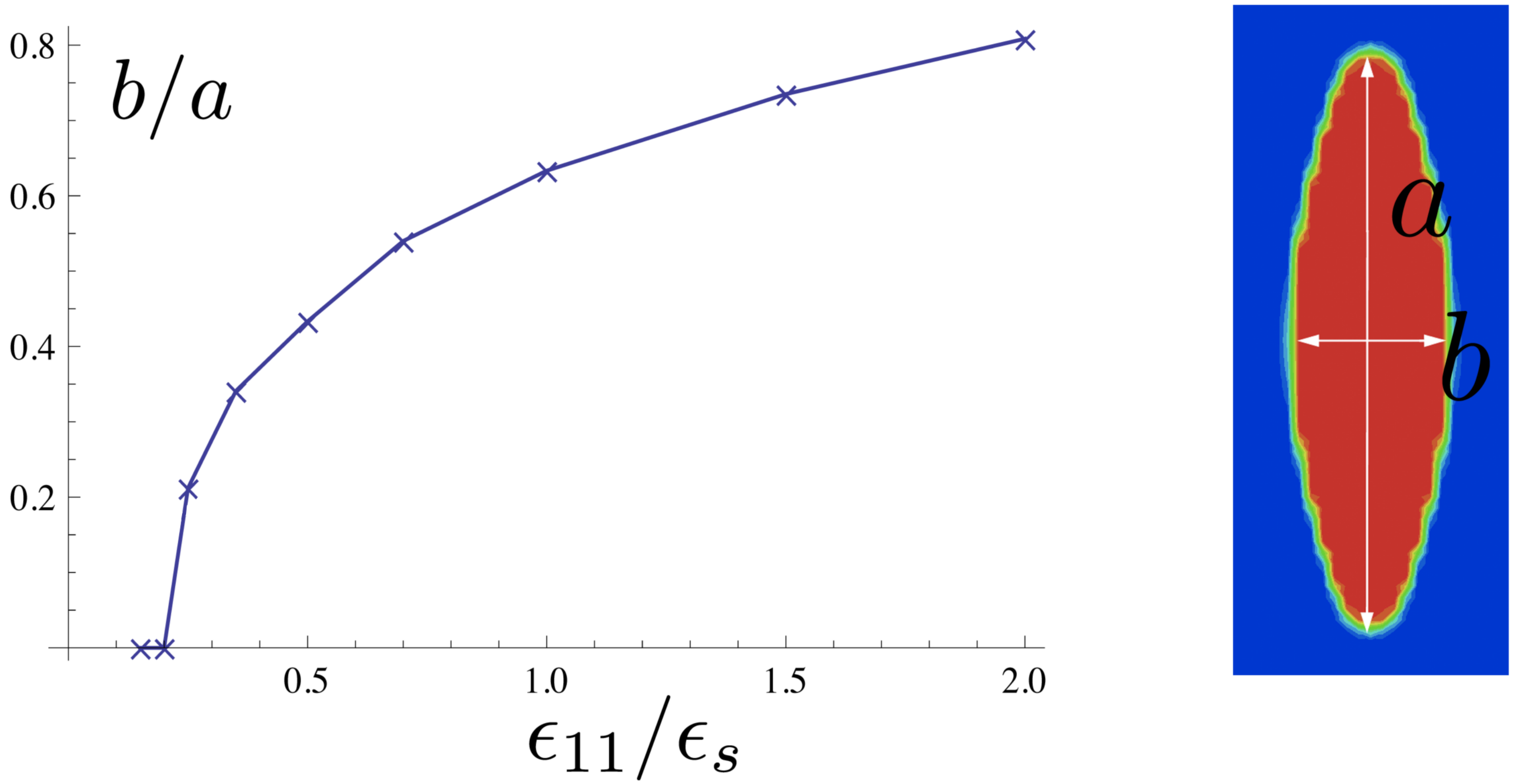


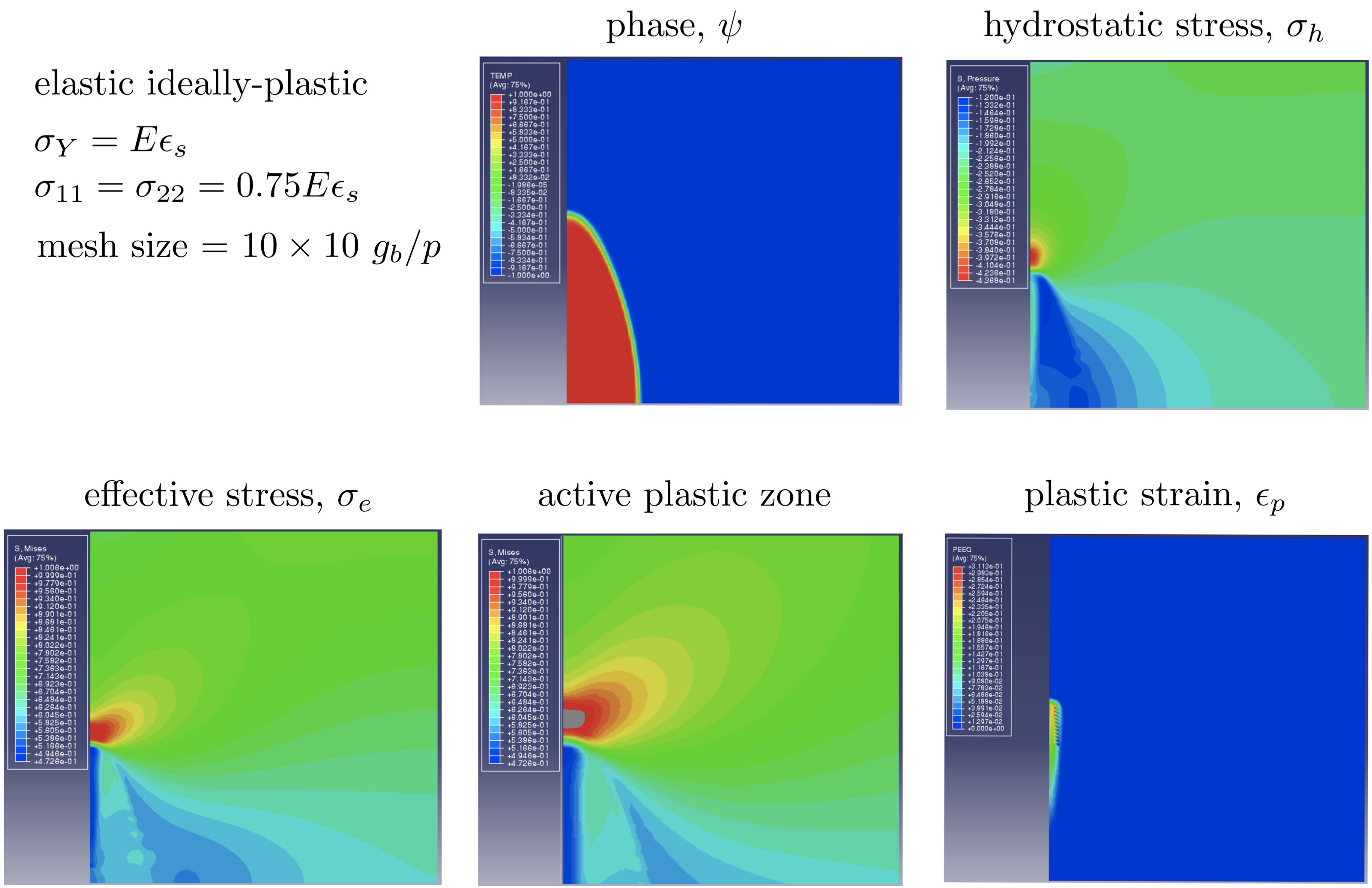


Noisy interface
$\epsilon_{11} = 0.45\epsilon_s$
x_2
x_1


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

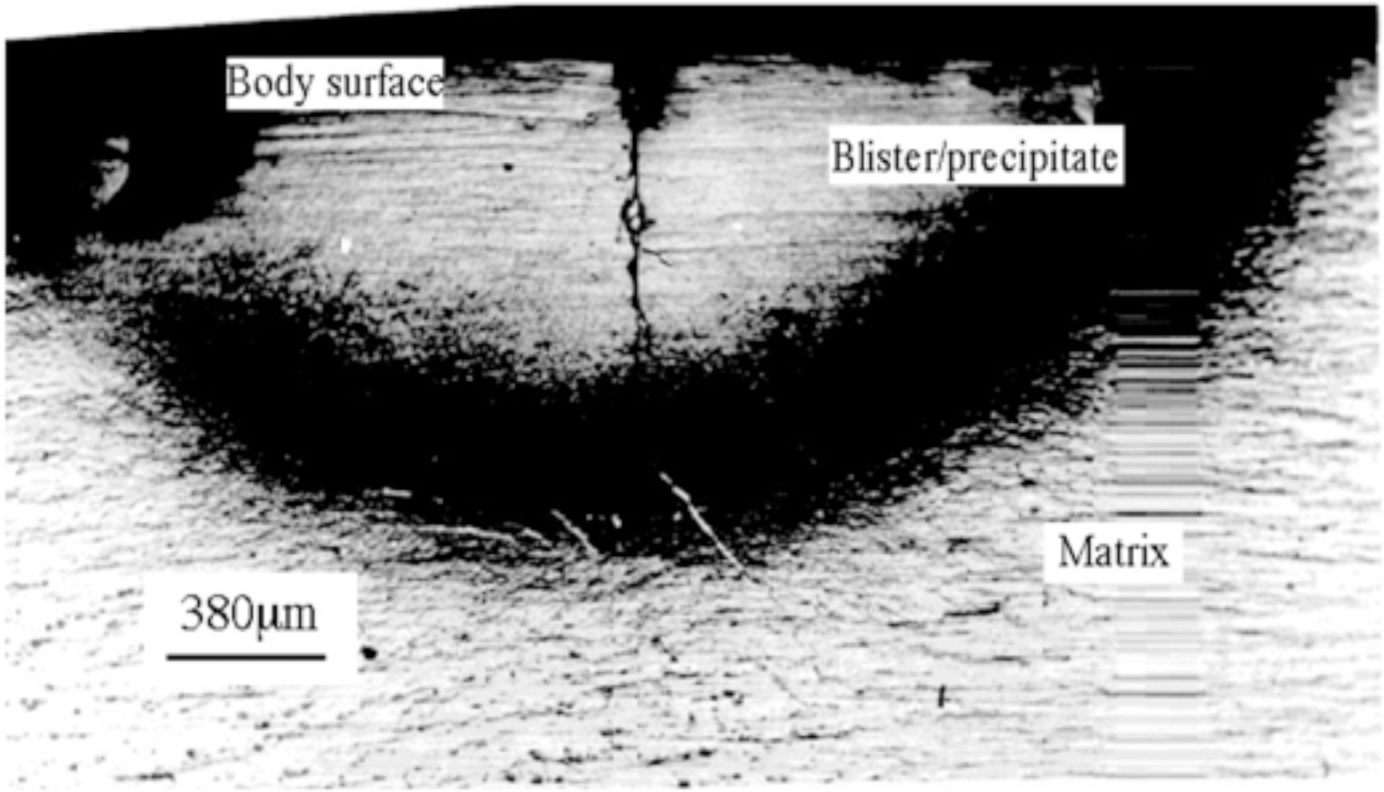
Aspect ratio of platelet axes



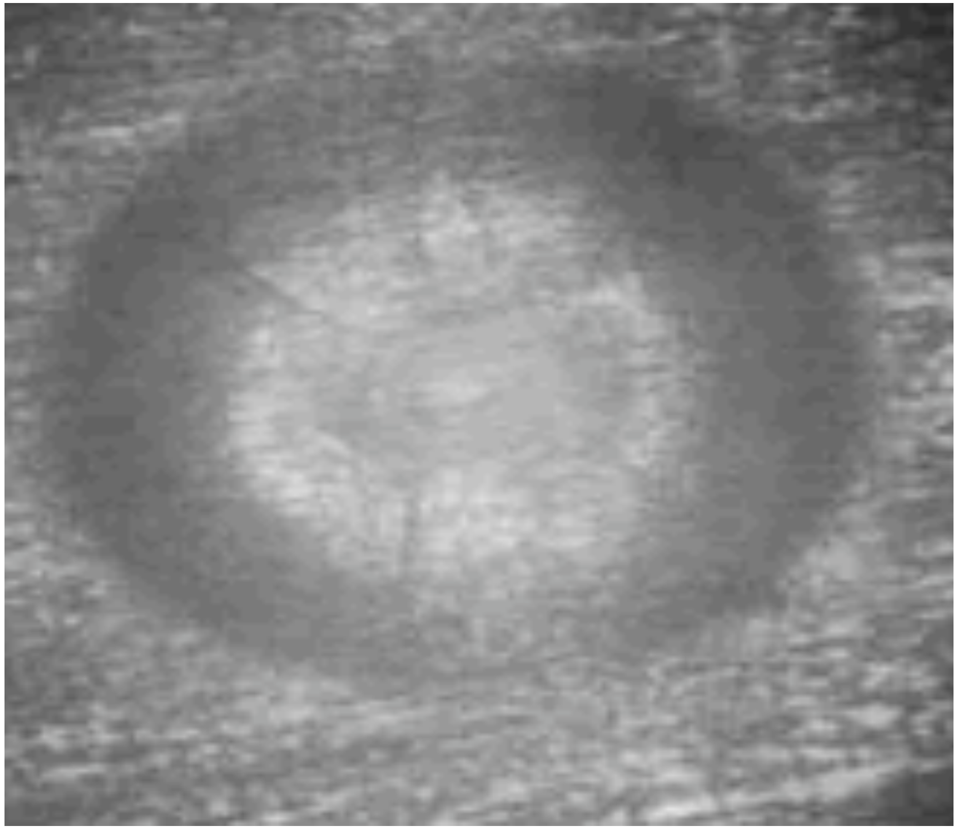


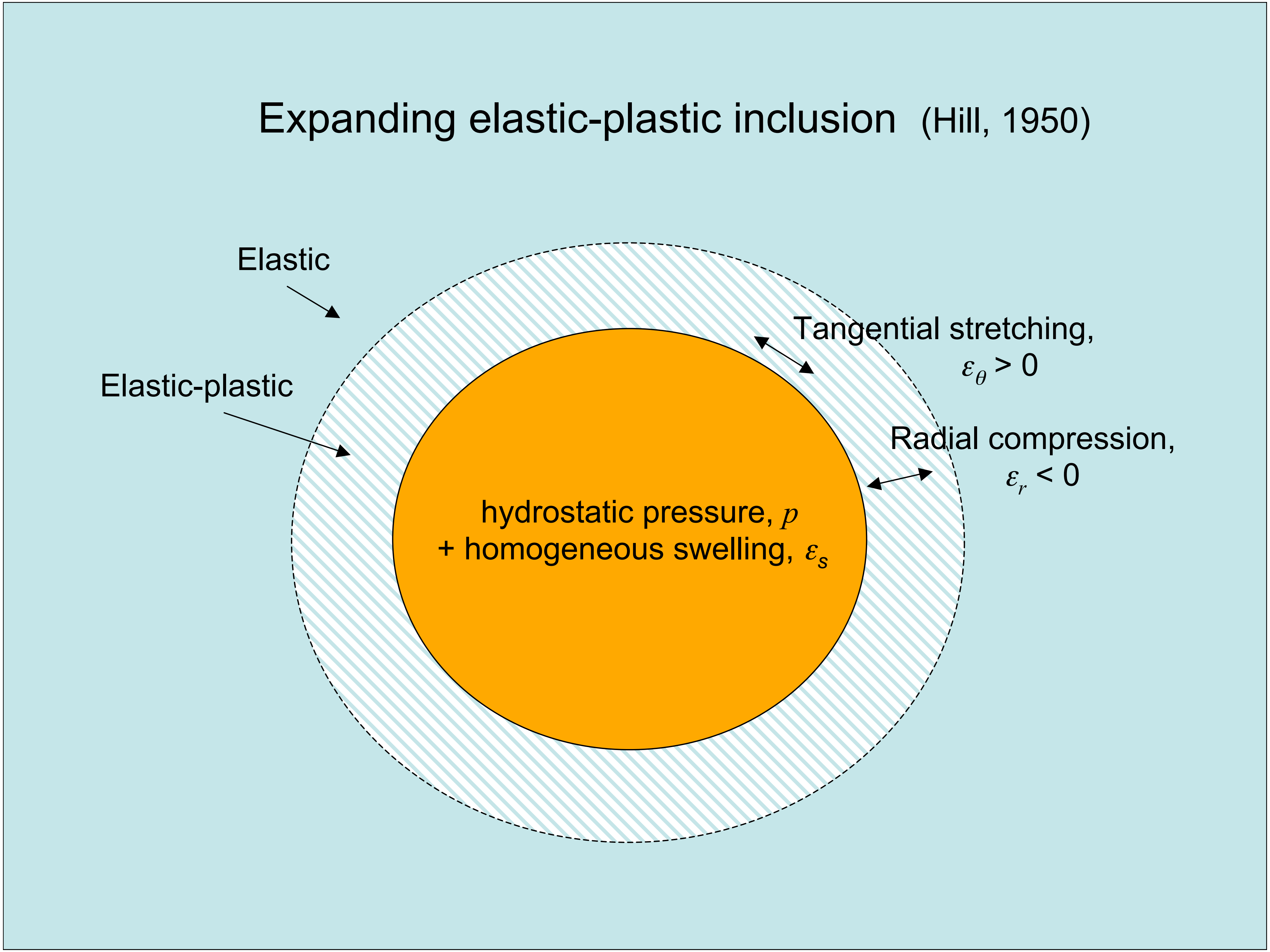
elastic ideally-plastic
$\sigma_Y = E\epsilon_s$
$\sigma_{11} = \sigma_{22} = 0.75E\epsilon_s$
mesh size $= 10 \times 10 \ g_b/p$
phase, ψ
hydrostatic stress, σ_h
effective stress, σ_e
active plastic zone
plastic strain, ϵ_p

Stress and strain in the expanding hydride



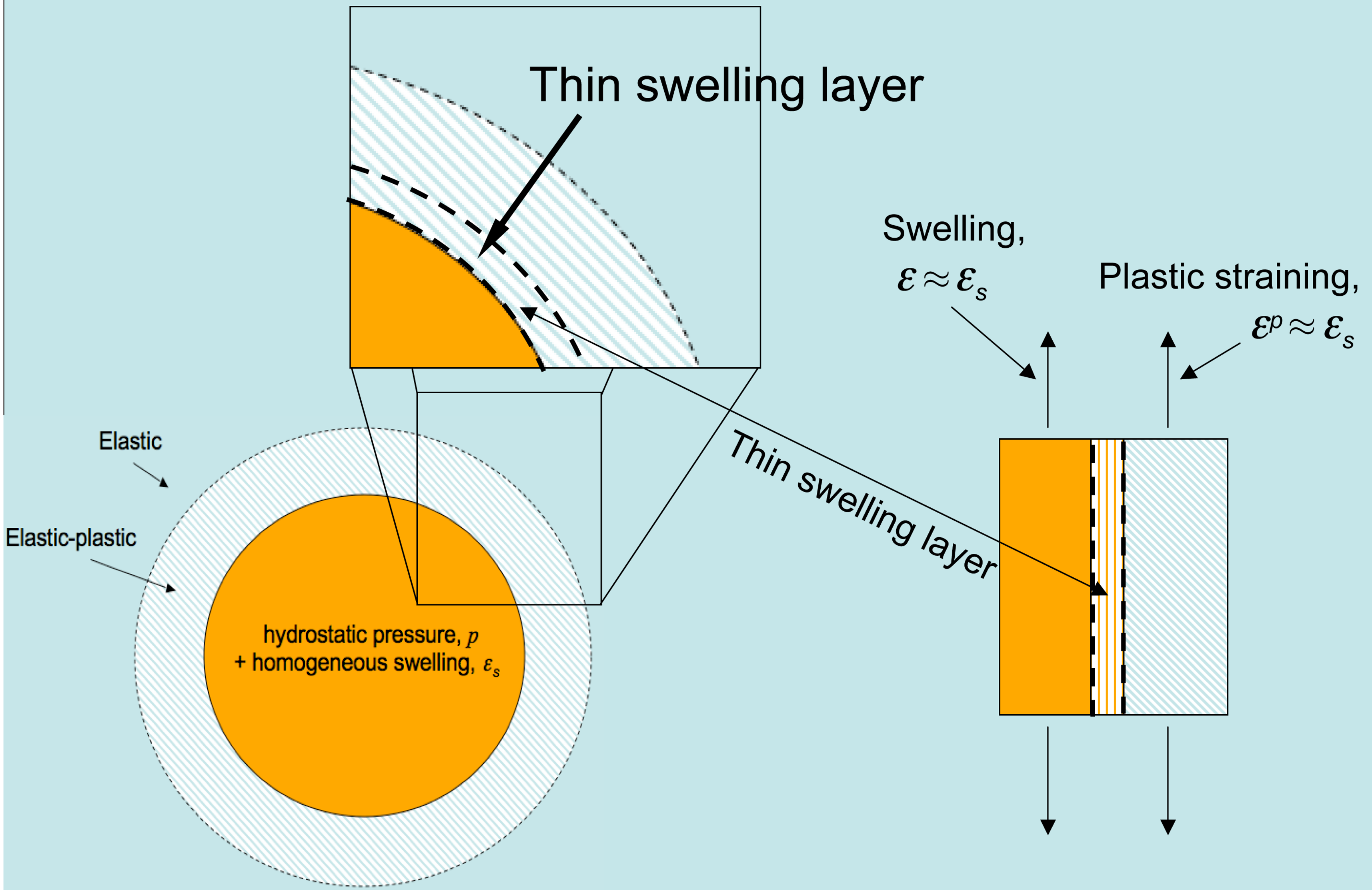
Top view of a hydride blister grown in
Zr–2.5wt%Nb pressure tube alloy (Singh *et al.*, 2001)



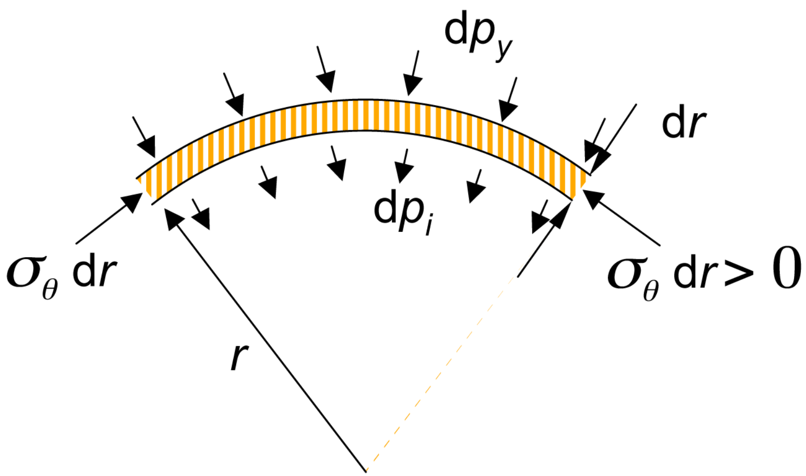


Expanding elastic-plastic inclusion (Hill, 1950)
Elastic
Elastic-plastic
Tangential stretching,
$\varepsilon_\theta > 0$
Radial compression,
$\varepsilon_r < 0$
hydrostatic pressure, p
+ homogeneous swelling, ε_s

Thin layer increasing inclusion volume (and mass)

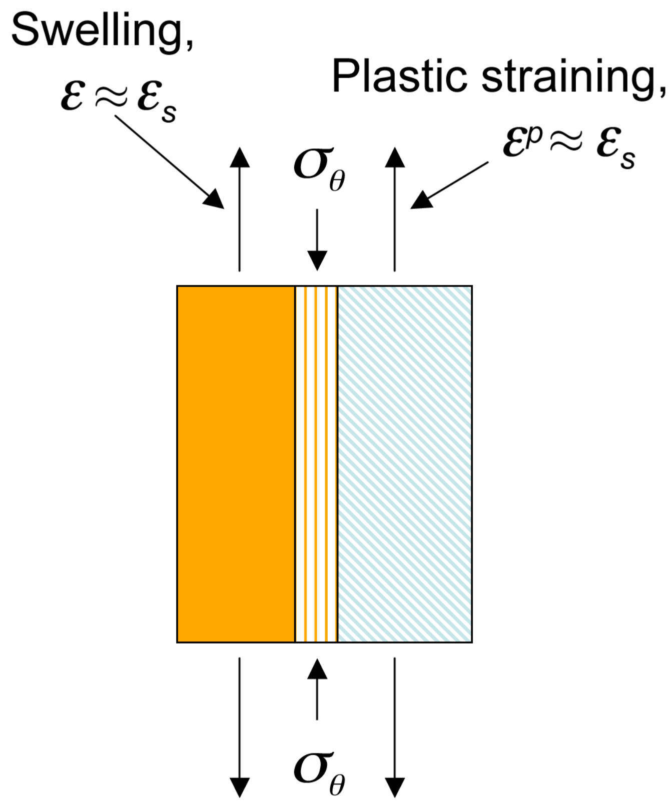


The swelling of a thin layer

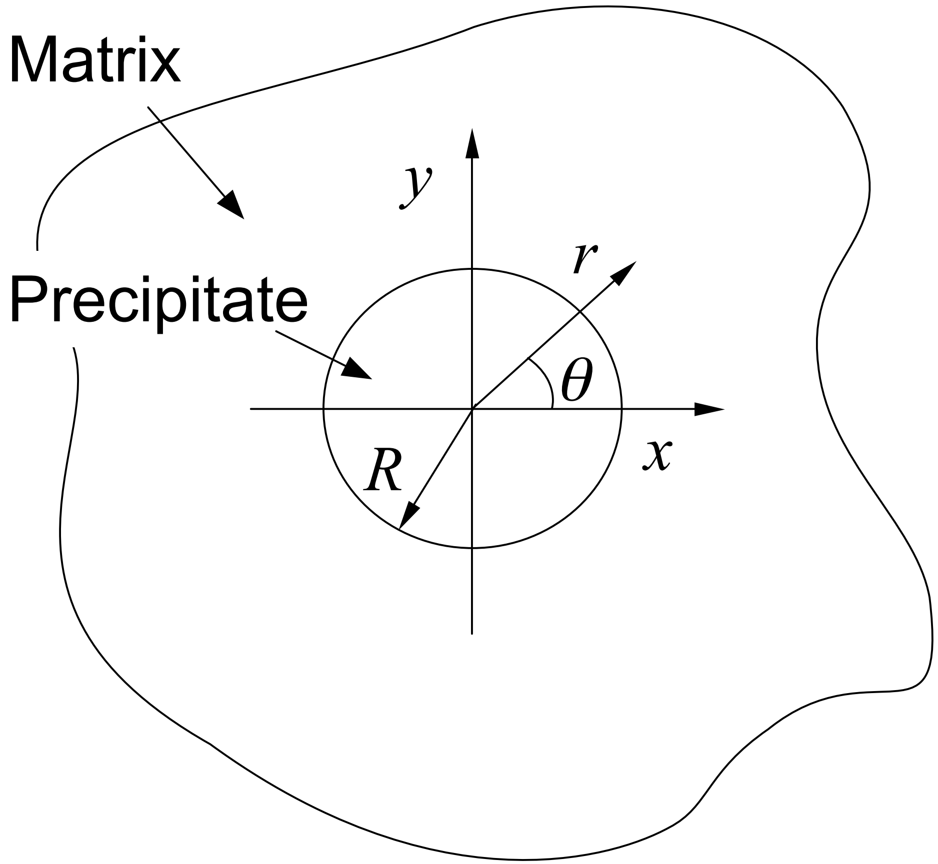


$$(\mathrm{d}p_i + \mathrm{d}p_y) r = \sigma_\theta \, \mathrm{d}r$$

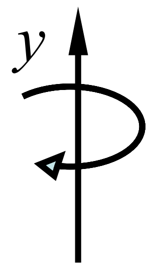
$$\Rightarrow \quad p_i + p_y = \sigma_\theta \ln(r)$$



Body described in a spherical coordinate system



Direction of revolution



$$r = (x^2 + y^2 + z^2)^{1/2}$$

$$\varphi = \arctan(y/(x^2 + z^2)^{1/2})$$

$$\theta = \arctan(z/x)$$

Shear stress components vanish everywhere:

$$\sigma_{r\theta} = \sigma_{r\psi} = \sigma_{\theta\varphi} = 0 \quad .$$

Symmetry also results in

$$\sigma_{\theta} = \sigma_{\psi} \quad .$$

The equations of equilibrium are reduced to

$$\frac{d\sigma_r}{dr} + 2\frac{\sigma_r - \sigma_\theta}{r} = 0 \quad ,$$

General solution for an elastic hollow sphere

$$u_r = c_o r + c_1 r^{-2} \quad .$$

$$\sigma_r = (2\mu + 3\lambda)c_o - 4\mu c_1 r^{-3}$$

$$\sigma_\theta = (2\mu + 3\lambda)c_o + 2\mu c_1 r^{-3} \quad .$$

Elastic-Plastic hollow sphere

The spherical symmetry give the same yield stress for both Tresca's and von Mises' effective stresses. The shear stress given by

$$\tau = \frac{\sigma_r - \sigma_\theta}{2} = \mu(\varepsilon_r - \varepsilon_\theta) \quad ,$$

If the yield shear stress, k, is meet *i.e.* if $|\tau| = k$ and $d\varepsilon_p / dt > 0$, where

$$d\epsilon^p = [\frac{3}{2}(d\epsilon_r^{p2} + d\epsilon_\theta^{p2} + d\epsilon_\psi^{p2})]^{1/2} = [\frac{3}{2}((d\frac{du}{dr})^2 + 2(\frac{du}{r})^2)]^{1/2} \quad ,$$

the equilibrium equation (3) at plastic deformation reads

$$\frac{d\sigma_r}{dr} \pm 4\frac{k}{r} = 0 \quad ,$$

The general solution is

$$\sigma_r = \mp 4k \ln r + q \text{ and } \sigma_\theta = \mp 4k \ln r + q \mp 2k \quad ,$$

where q is an arbitrary constant.

cf. (Hill, 1950).

Results for an expanding growing inclusion

$$\sigma_r = -4\mu c_1 r^{-3}$$

$$\sigma_\theta = 2\mu c_1 r^{-3} \quad .$$

If $c_1 > 0$ because of the supposed compressive stresses exerted by the expanding sphere. Yield stress is meet at

$$r = r_p = \sqrt[3]{\frac{3\mu c_1}{k}} \quad .$$

Because of the expansion of the sphere $\tau = -k$ in the region $R < r \leq r_p$.

$$\sigma_r = 2k[2\ln(\frac{r}{r_p}) - \frac{2}{3}]$$

$$\sigma_\theta = 2k[2\ln(\frac{r}{r_p}) + \frac{1}{3}] \quad .$$

In the region $r < R$ the stresses are obtained through (13) using $\tau = k$,

$$\sigma_r = 2k[2\ln(\frac{R^2}{rr_p}) - \frac{2}{3}]$$

$$\sigma_\theta = 2k[2\ln(\frac{R^2}{rr_p}) - \frac{5}{3}] \quad .$$

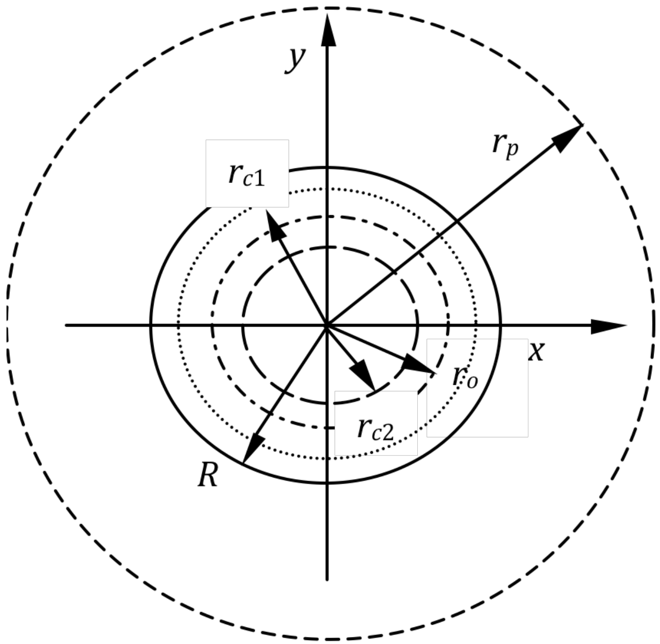
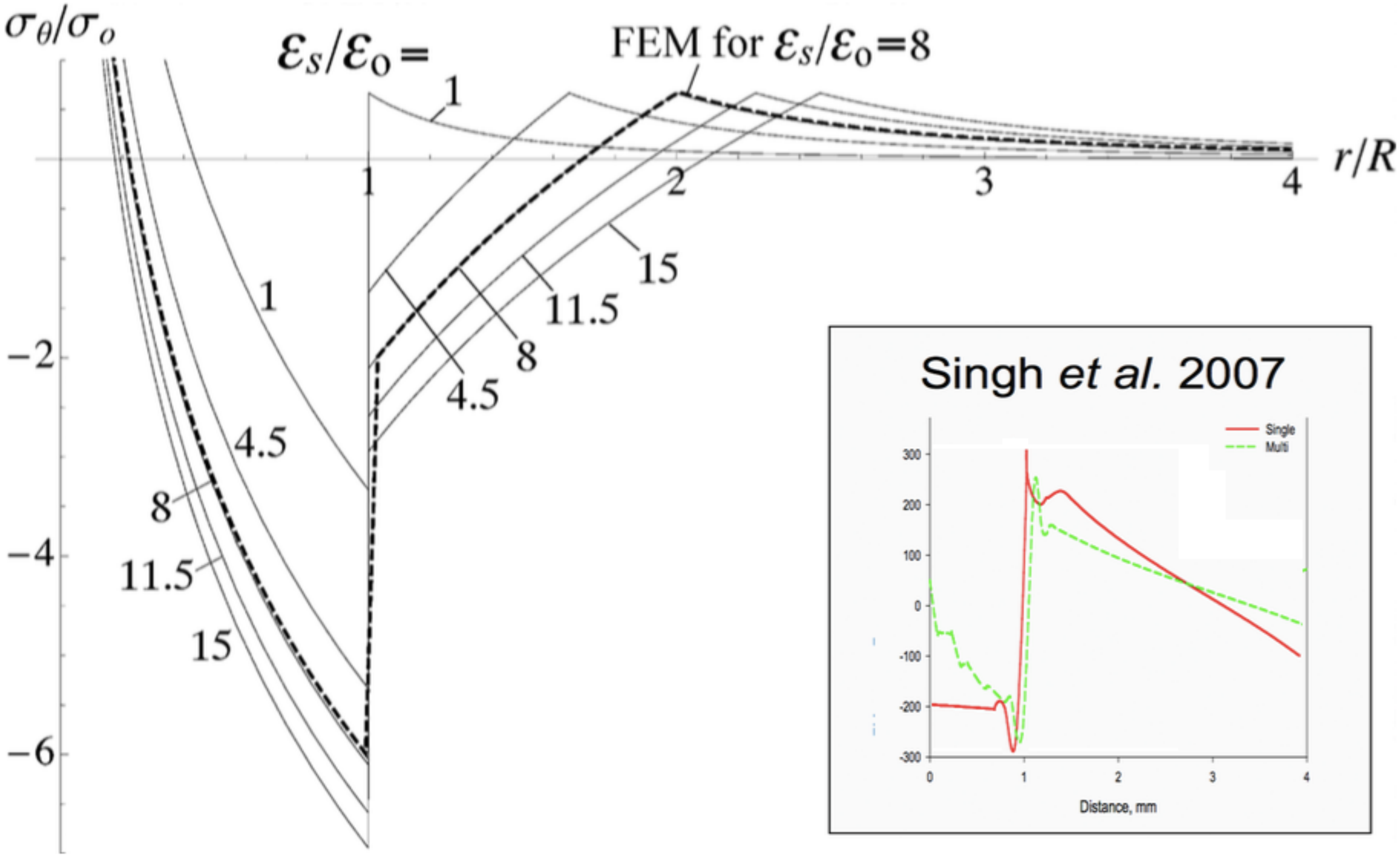


Fig. 2 Different characteristic regions of the solution. In $r > r_p$ the material is elastic; in $r \leq r_p$ the material is plastic; in $r_{c1} < r < R$ no tensile stress; in $r_o < r < r_{c1}$ tensile radial stress; in $r_{c2} < r < r_o$ tensile radial stress and hydrostatic stress; in $r < r_{c2}$ all stresses are tensile.

$$r < r_{c1} = \frac{R^2}{r_p e^{1/3}}, \quad r < r_o = \frac{R^2}{r_p e^{2/3}} \quad \text{and} \quad r < r_{c2} = \frac{R^2}{r_p e^{5/6}}$$



σ_θ/σ_o
$\varepsilon_s/\varepsilon_o =$
FEM for $\varepsilon_s/\varepsilon_o$=8
r/R
1
2
3
4
−2
−4
−6
1
4.5
8
11.5
15
Singh *et al.* 2007
Single
Multi
Distance, mm

Summary

Phase field modellig can be used in studies of phenomena occuring near the hydride surface

The hydride surface is unstable on a length scale given by the ratio of the surface energy and the strain energy density

Platelet shape is affected by the ratio of stress free expansion strain and the elastic strain

Inclusions that grow at its edges obtain reduced compression closer to its center

At self similar growth stress becomes tensile and logarithmically singular