Formation and growth of hydrides, 5th Broberg Symposium 2015.

Orationem Meam.

Ståhle, P.

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Formation and growth of hydrides

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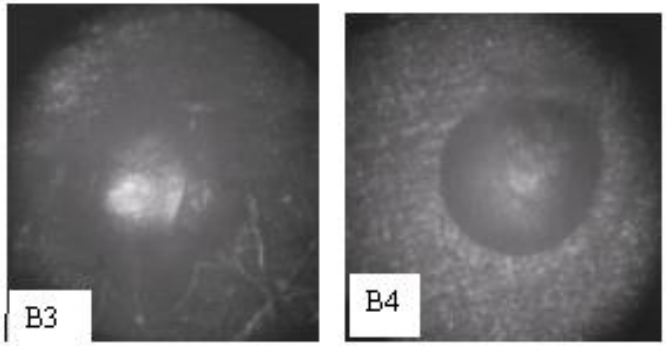
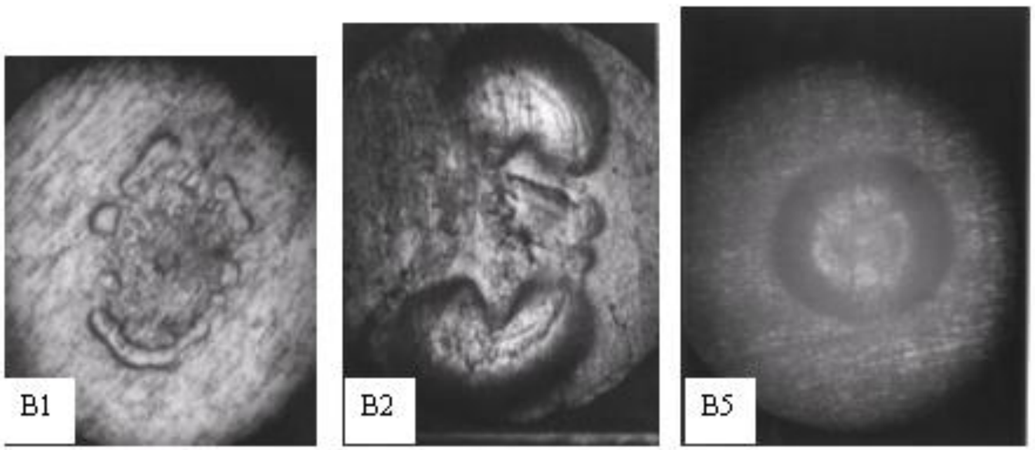
Hydride Blister

Prior solution annealing



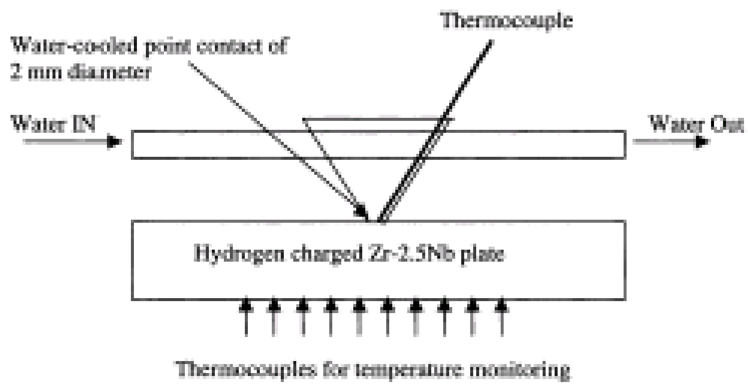
(a) Type I

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



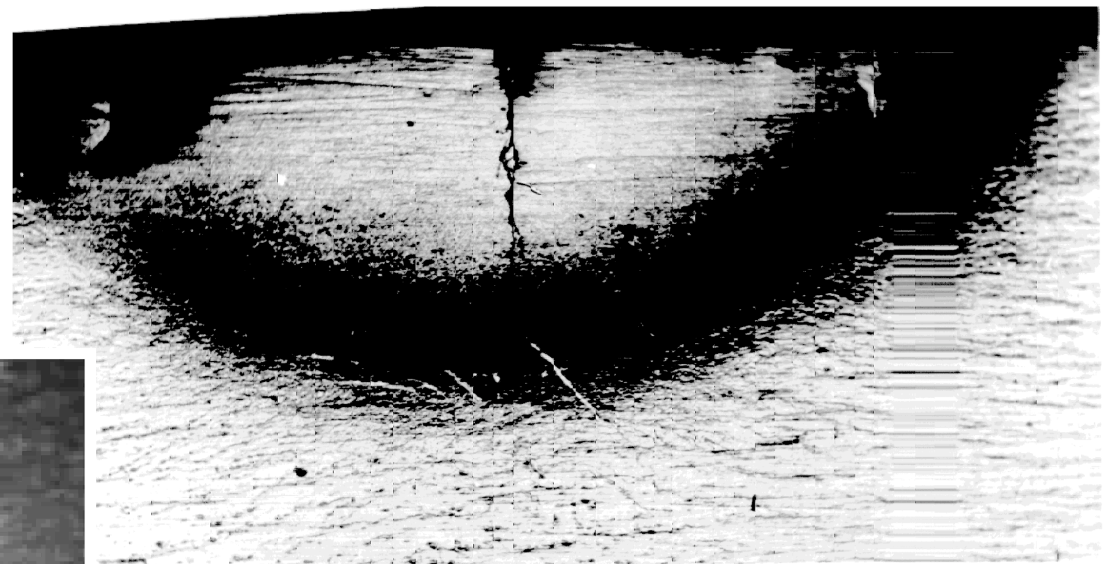
(b) Type II

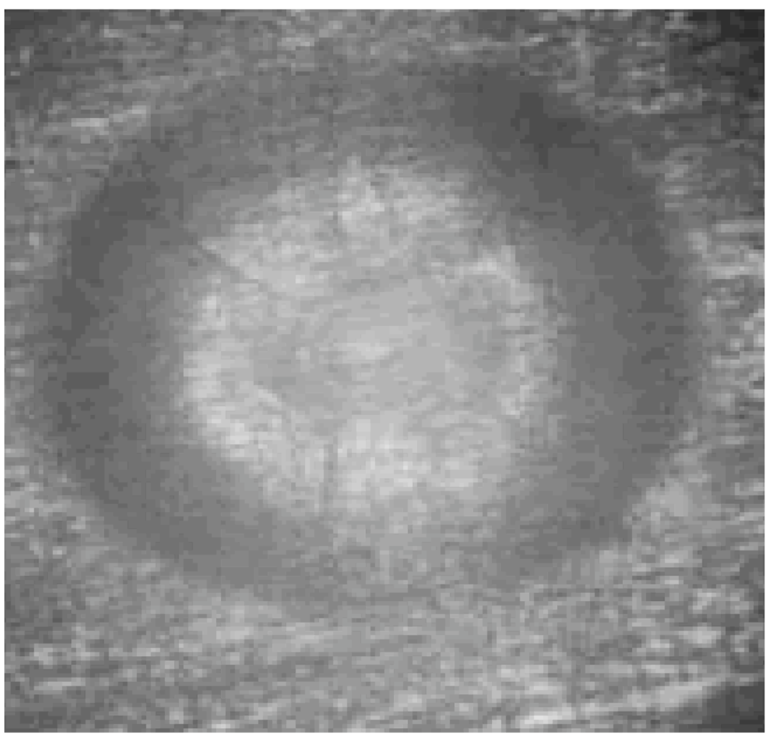
Without solution annealing



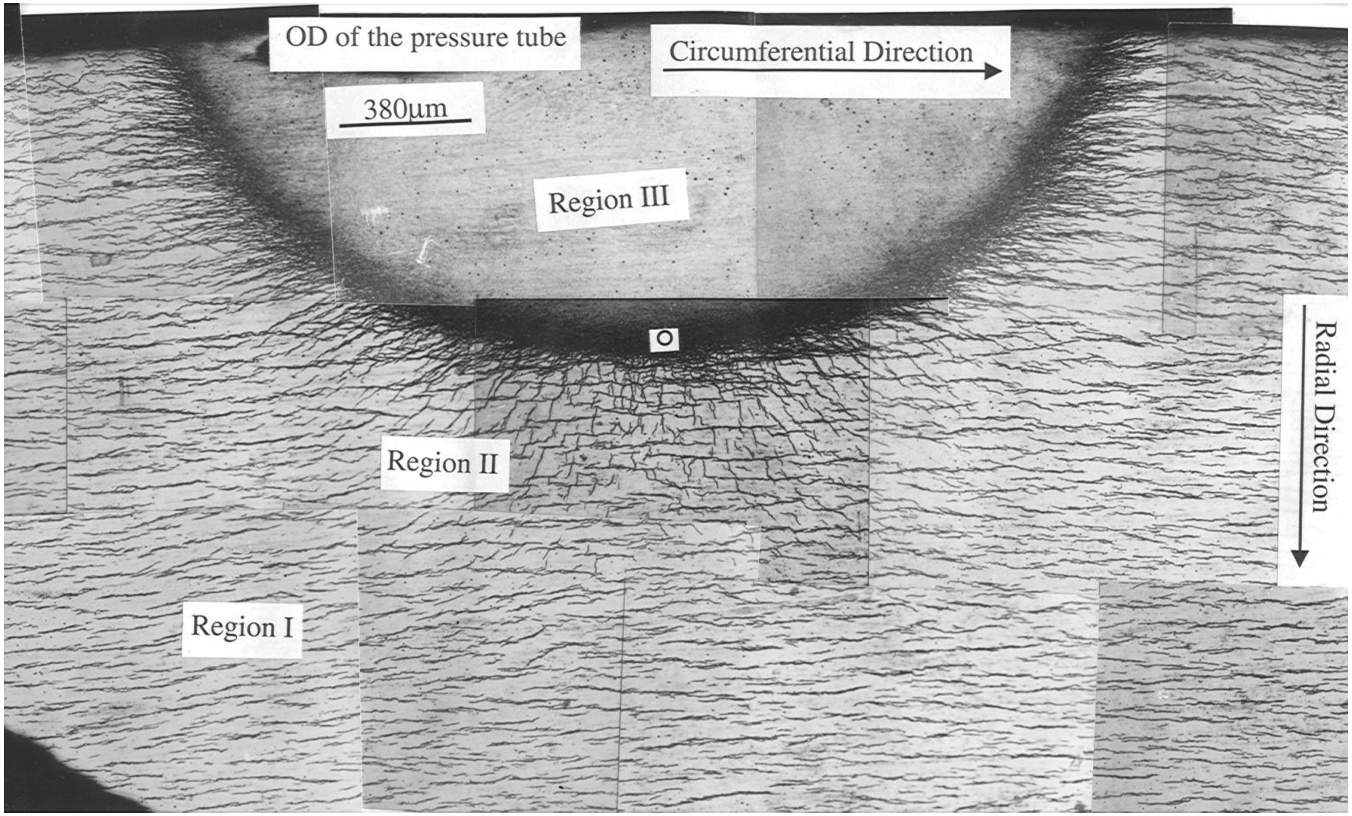
Cold finger is in contact all the time
Hydride precipitation occurs around the cold spot resulting in ring of blisterets

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



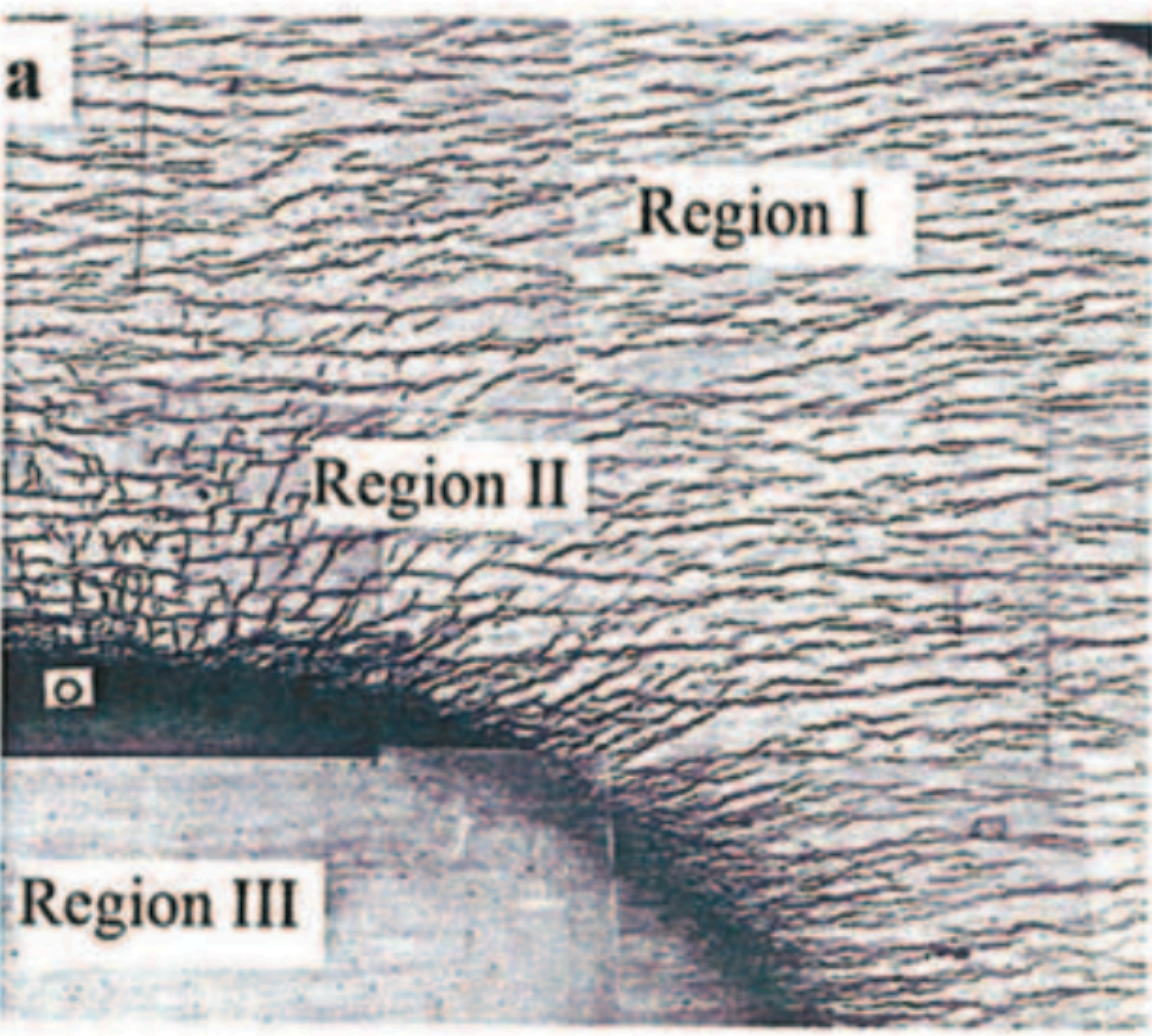


Hydride Blister section

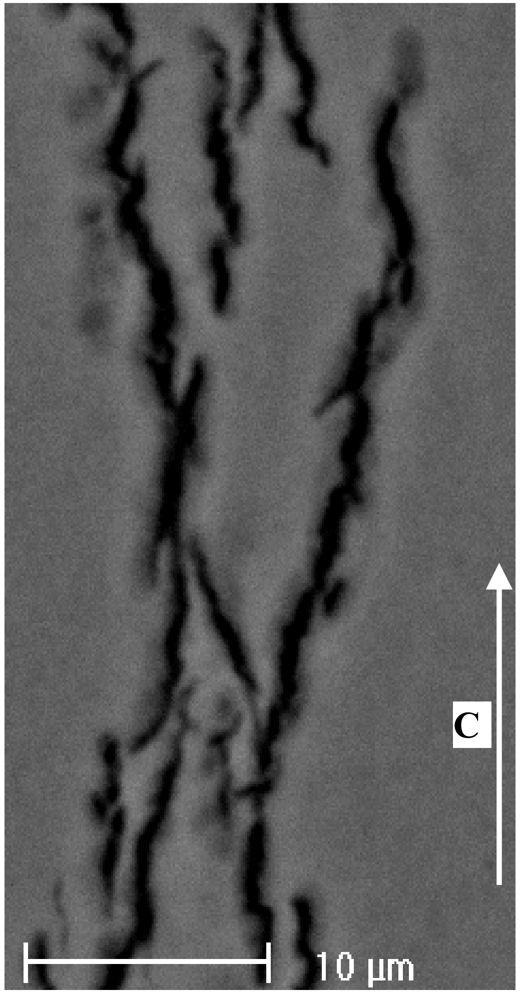


Optical micrograph of hydride blister section, grown in Zr-2.5wt.% Nb pressure tube material. Three regions - Region I - matrix & circumferential hydrides, region II - matrix containing both radial and circumferential hydrides and region III - mainly of δ-hydride.

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


a
Region I
Region II
o
Region III

Hydride – level of organization



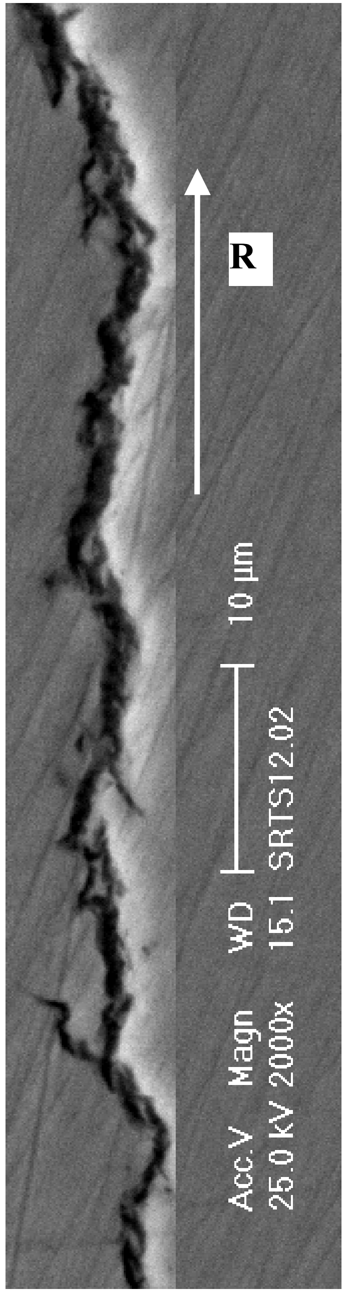
Hydride plate comprising of platelets stacked side by side

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



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

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

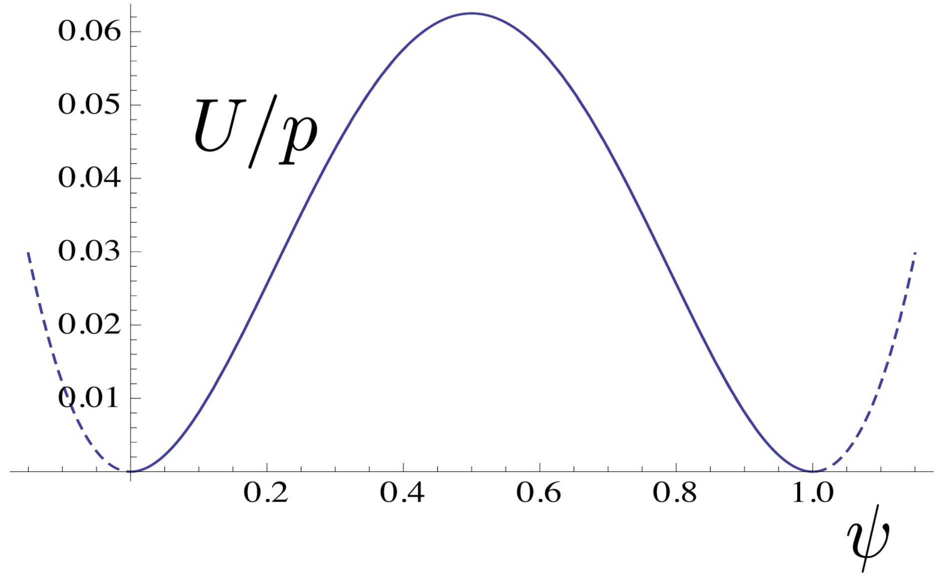
Elastic energy $$\mathcal{F}_{el} = \int \sigma_{ij} \mathrm{d}\epsilon_{ij}$$

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

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

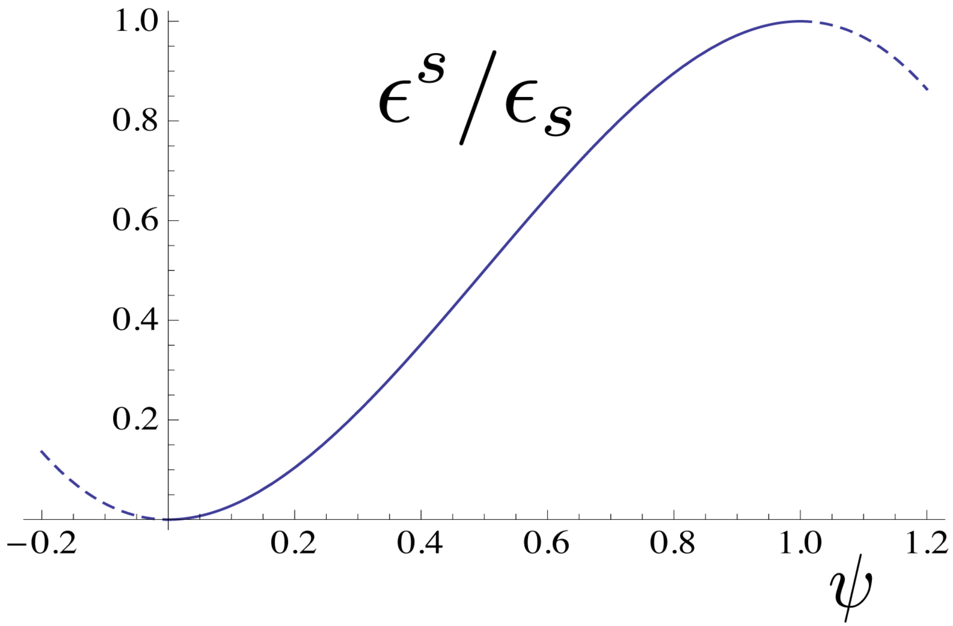
Double-well chemical potential

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



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

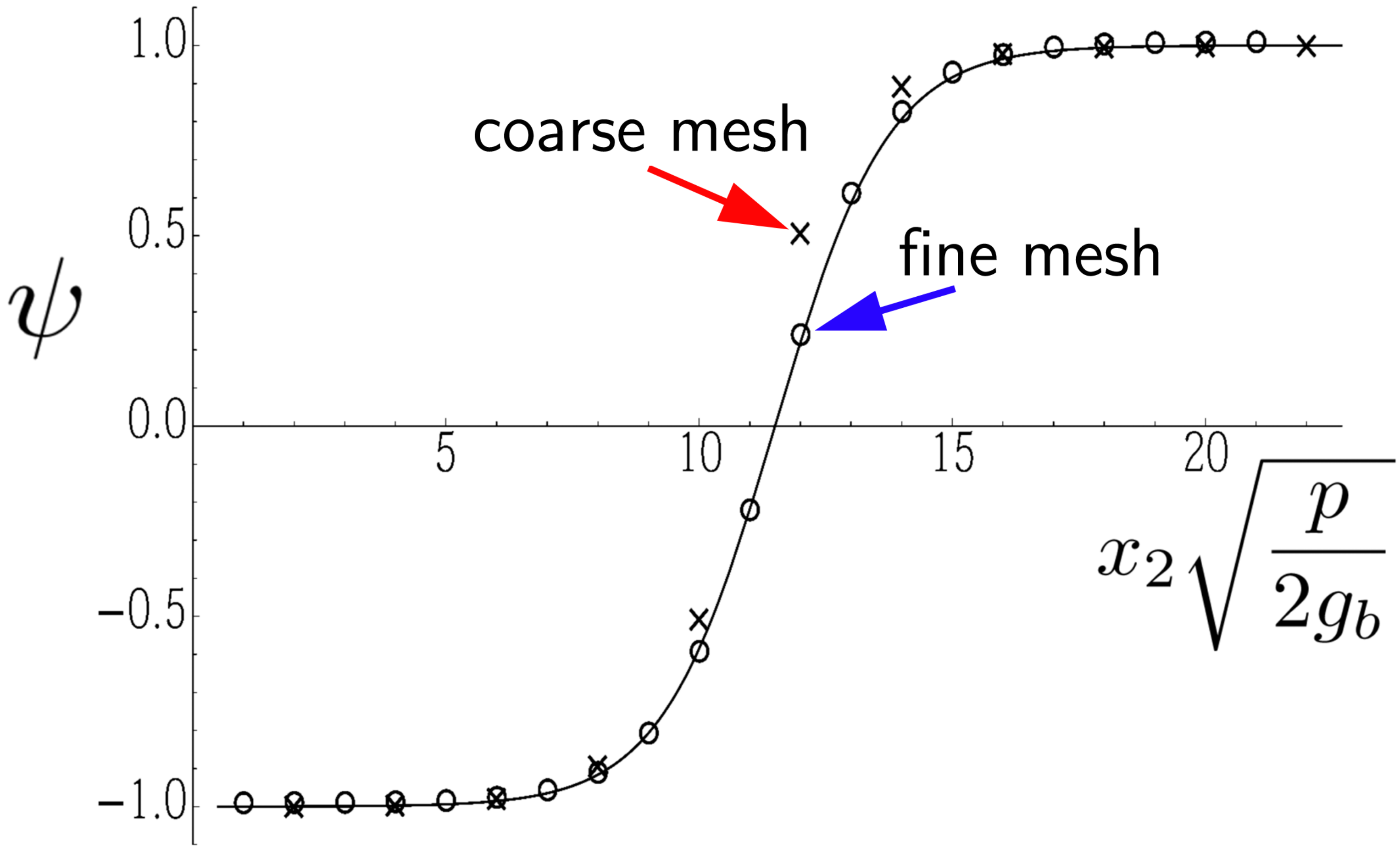
$$\tilde{u}_{i,jj} + \frac{1}{1-2\nu} \tilde{u}_{j,ij} - (\tilde{\epsilon}_s)_{,j} = 0$$

In analogy with a fully coupled thermal-stress

One dimension static (Ginzburg, Landau 1950)

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

Phase vs. position



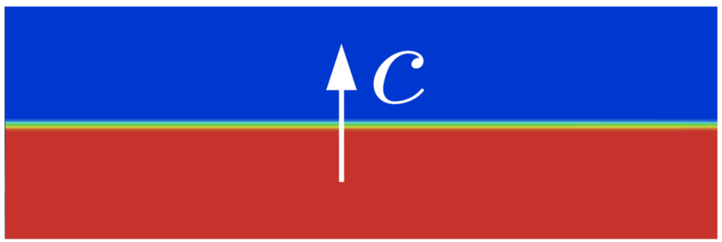
Dynamic with mechanical loading

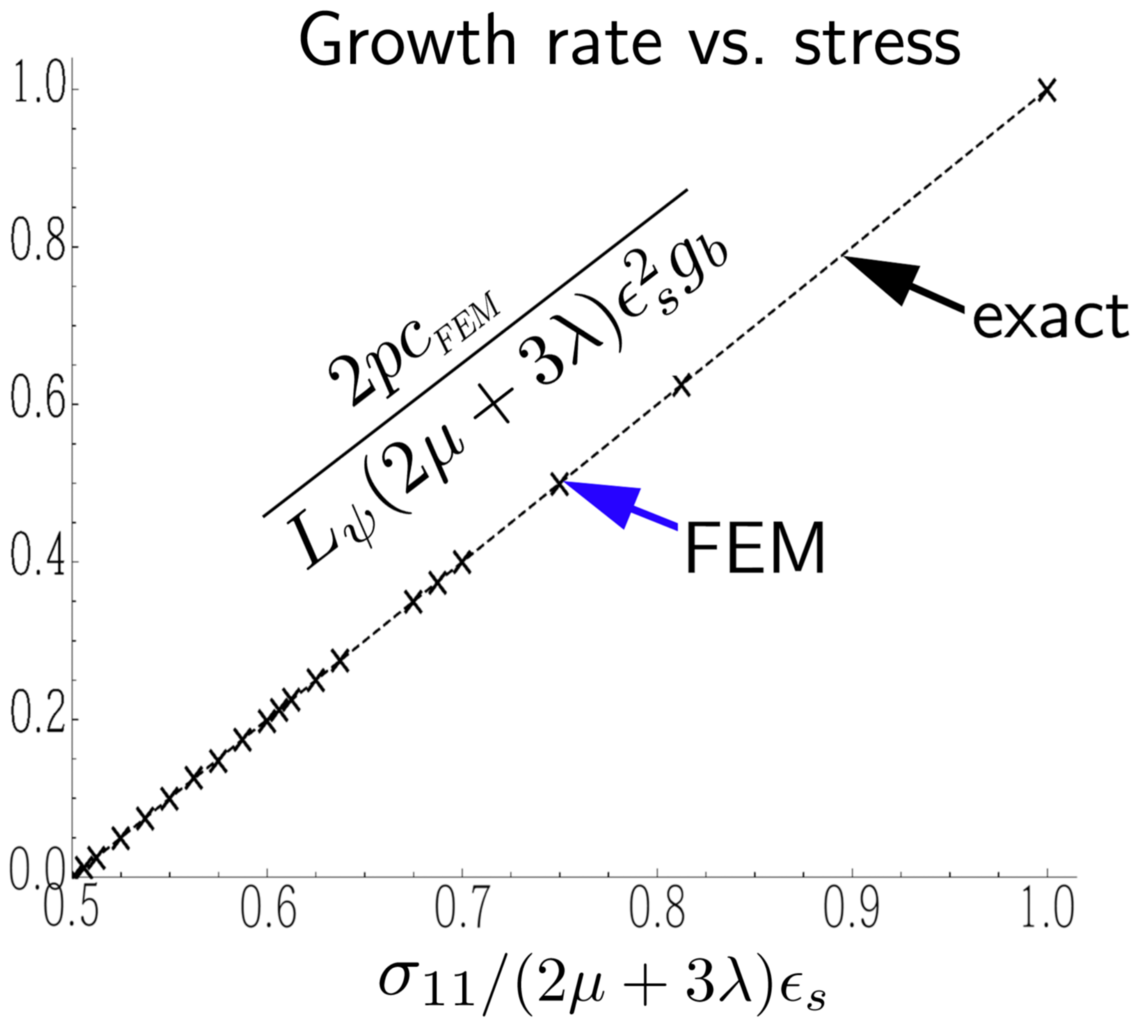
$$g_b\psi'' - p\psi(\psi^2-1) + \kappa p(\psi^2-1) - \frac{c}{L_\psi}\psi' = 0$$

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

Growth rate

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

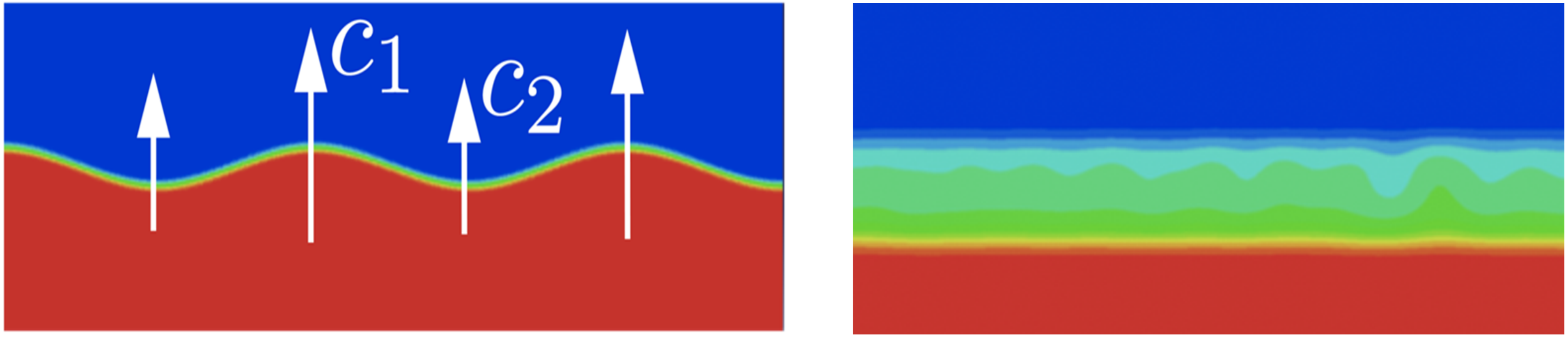


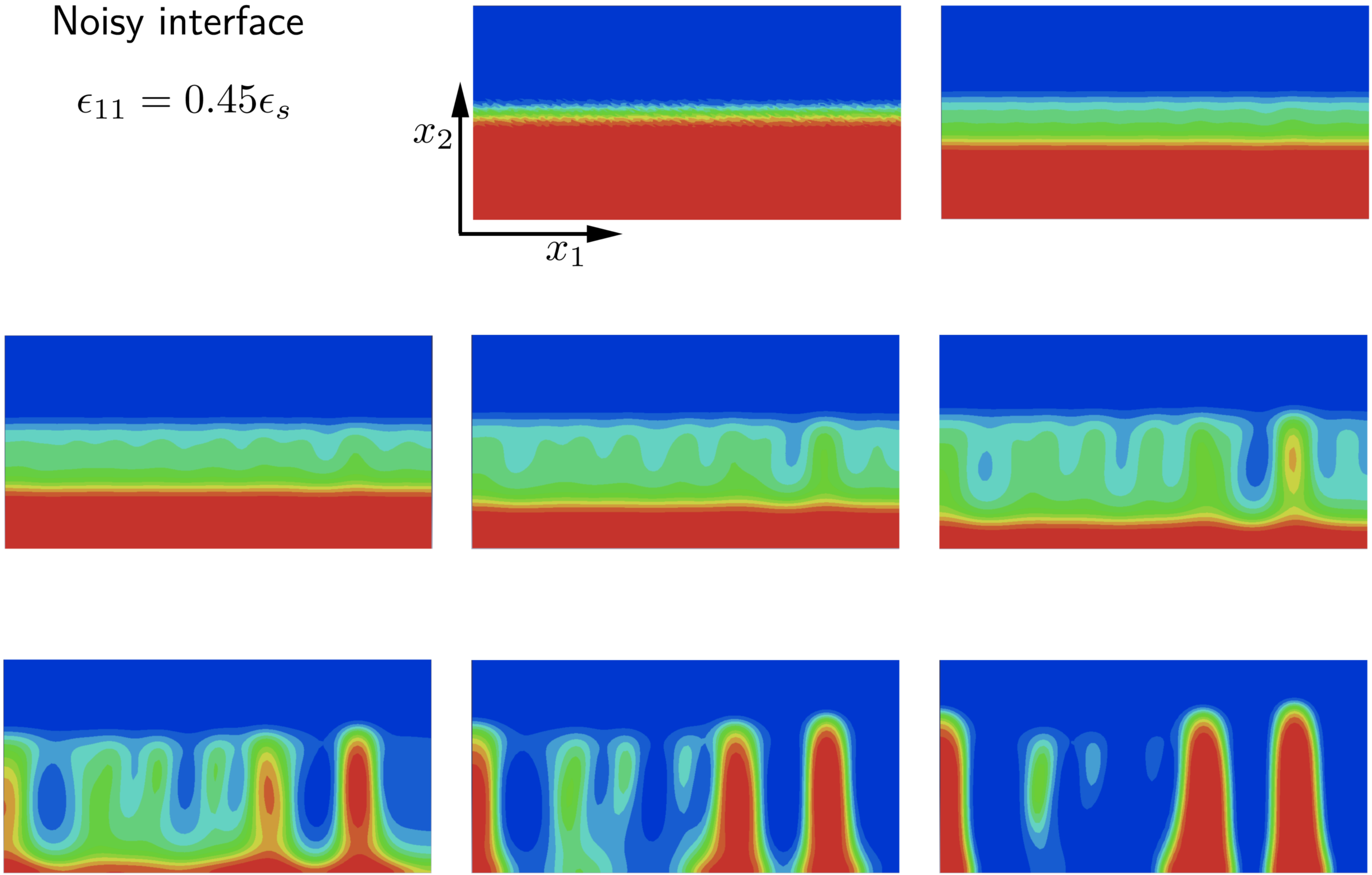


Surface energy $\gamma = \sqrt{2pg_b}$ [F/L]

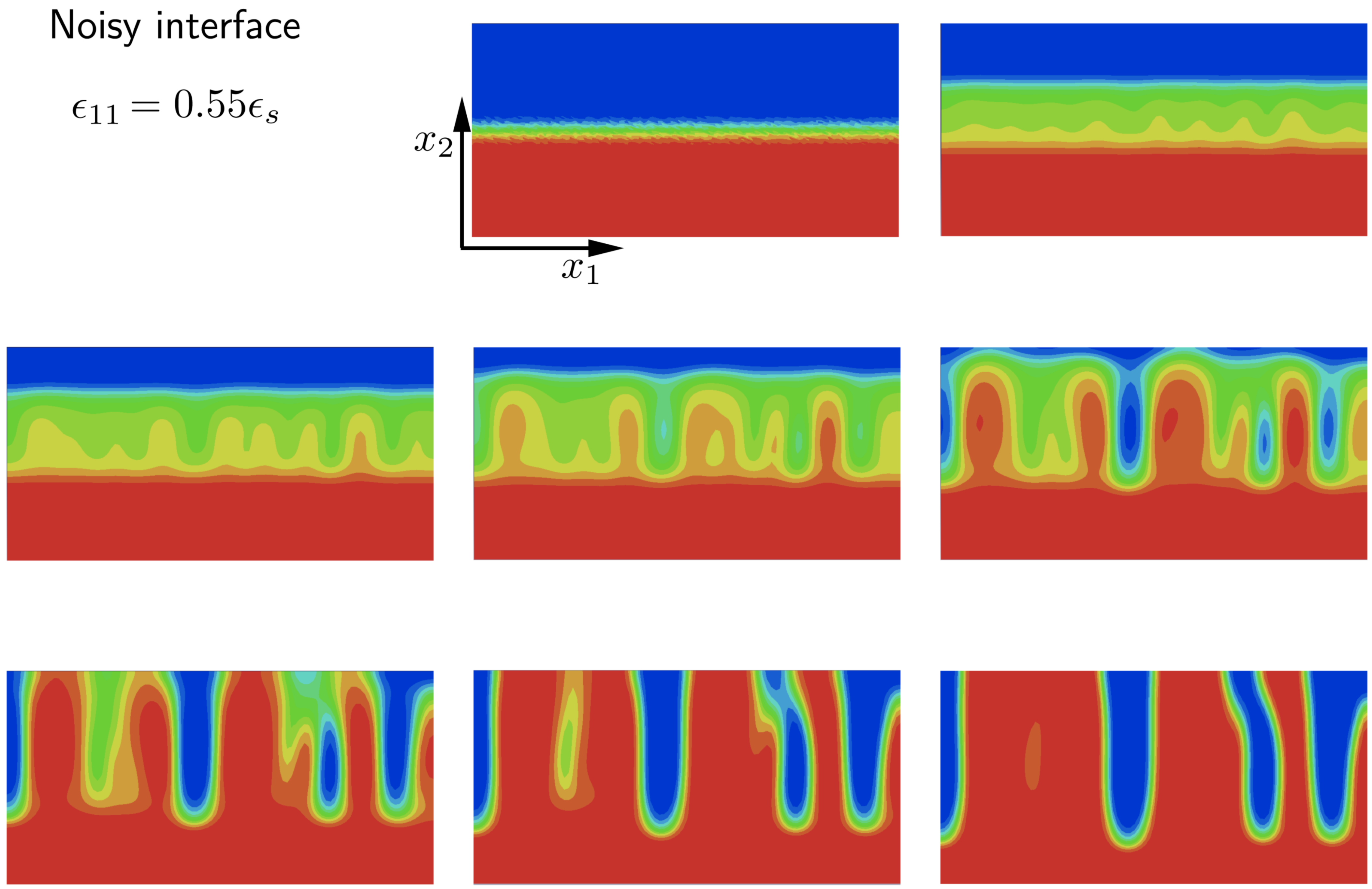
Strain energy density $W = \sigma_{ii}\epsilon_s$ [F/ L^2]

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

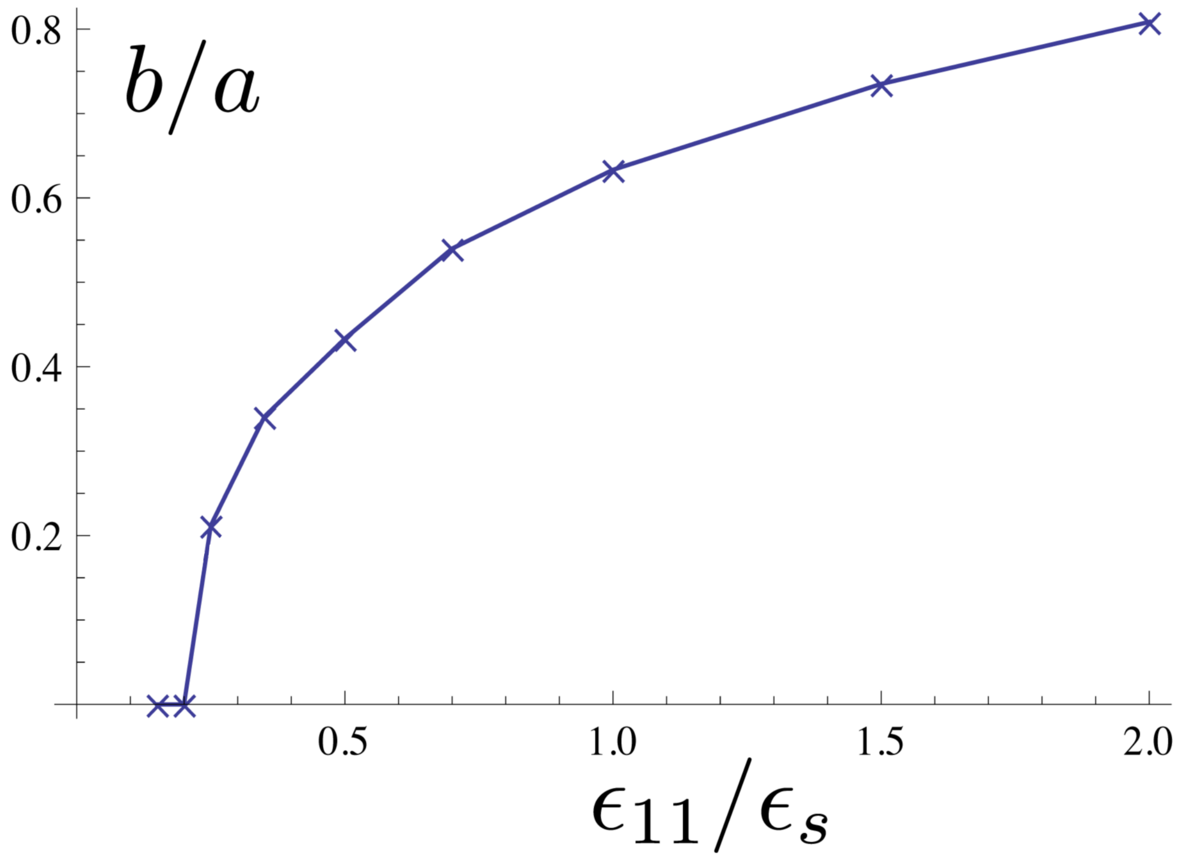
Summary

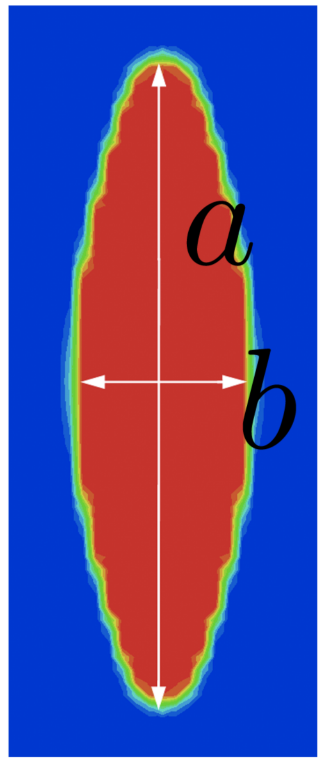
Phase field modellig can be used in studies of phenomena occuring near the hydride surface

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

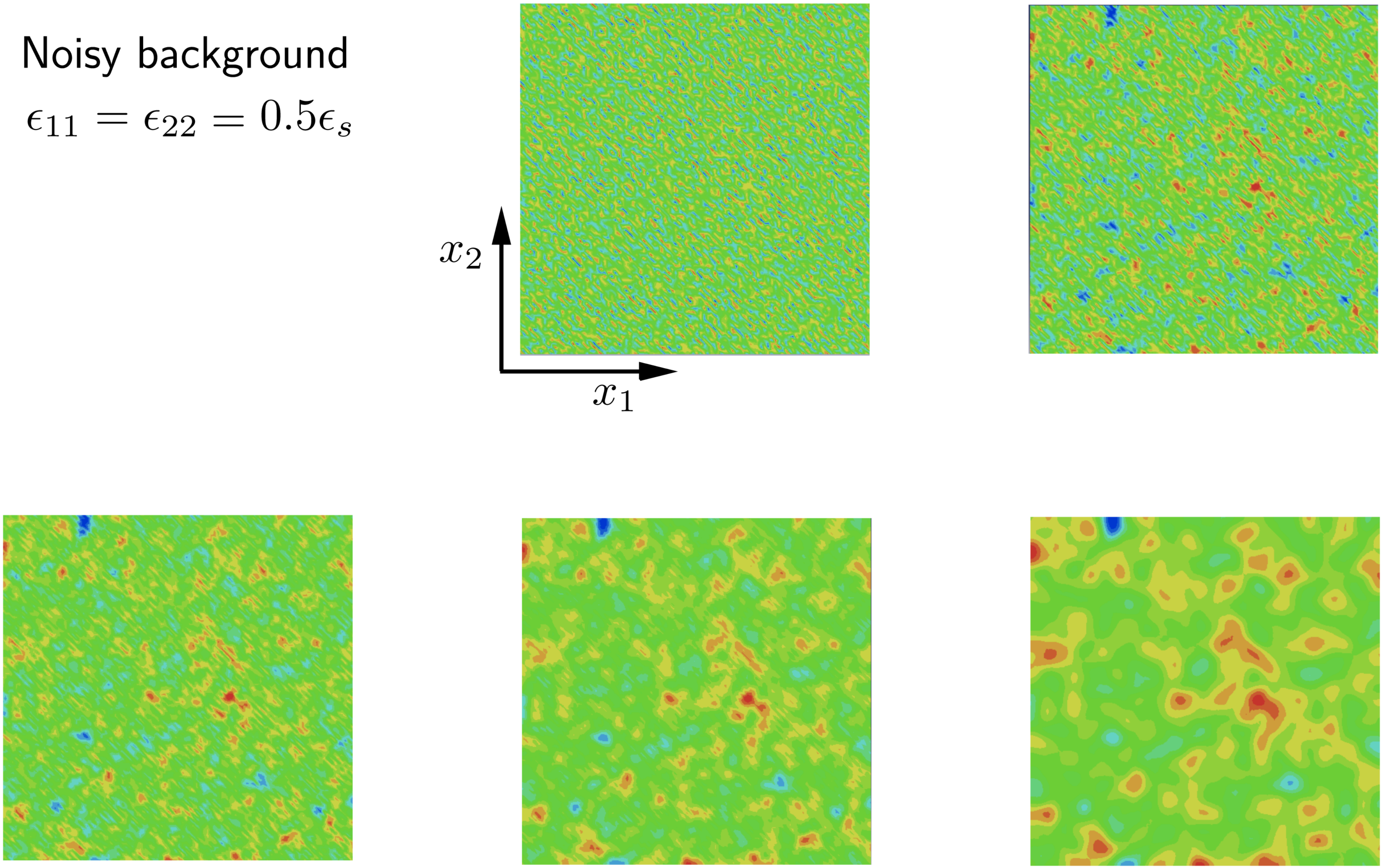
Aspect ratio of platelet axes





Noisy background

$\epsilon_{11} = \epsilon_{22} = 0.5\epsilon_s$



Noisy background

$$\epsilon_{11} = 0.5\epsilon_s$$