Formation and Fracture of Expanding Precipitates

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Phase Field Modelling of Formation and Fracture of Expanding Precipitates

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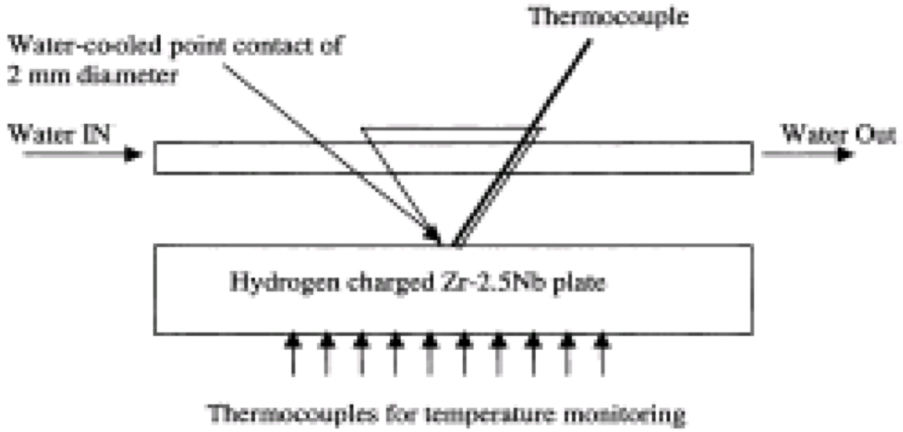
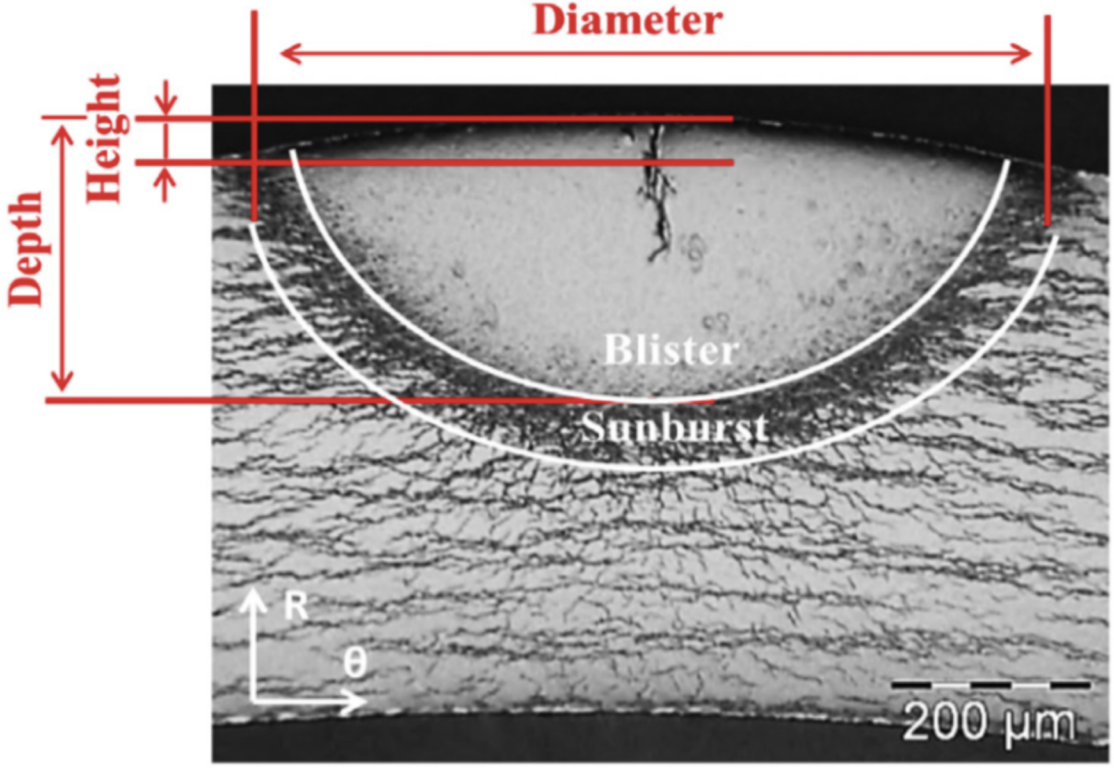
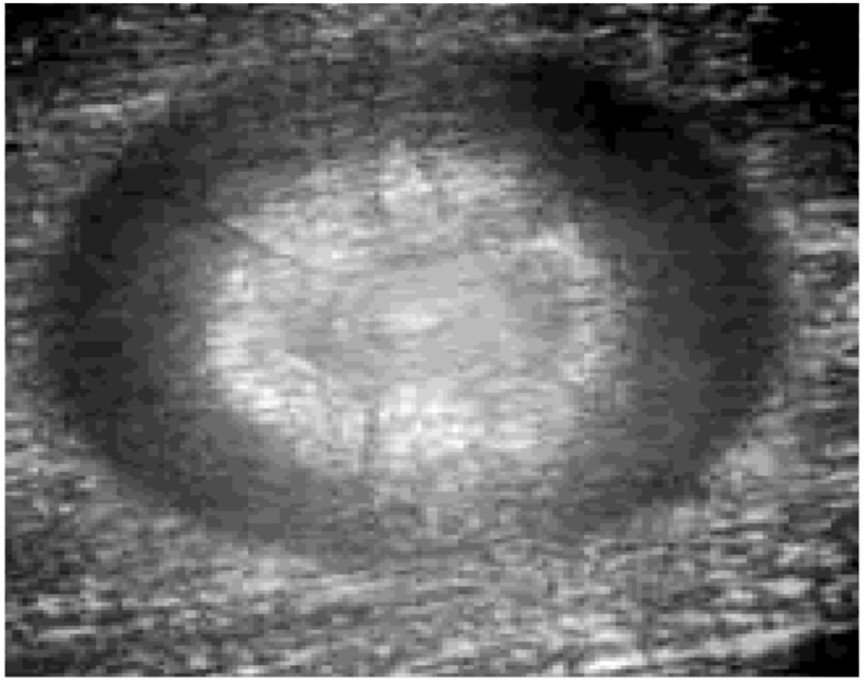
The experiment



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

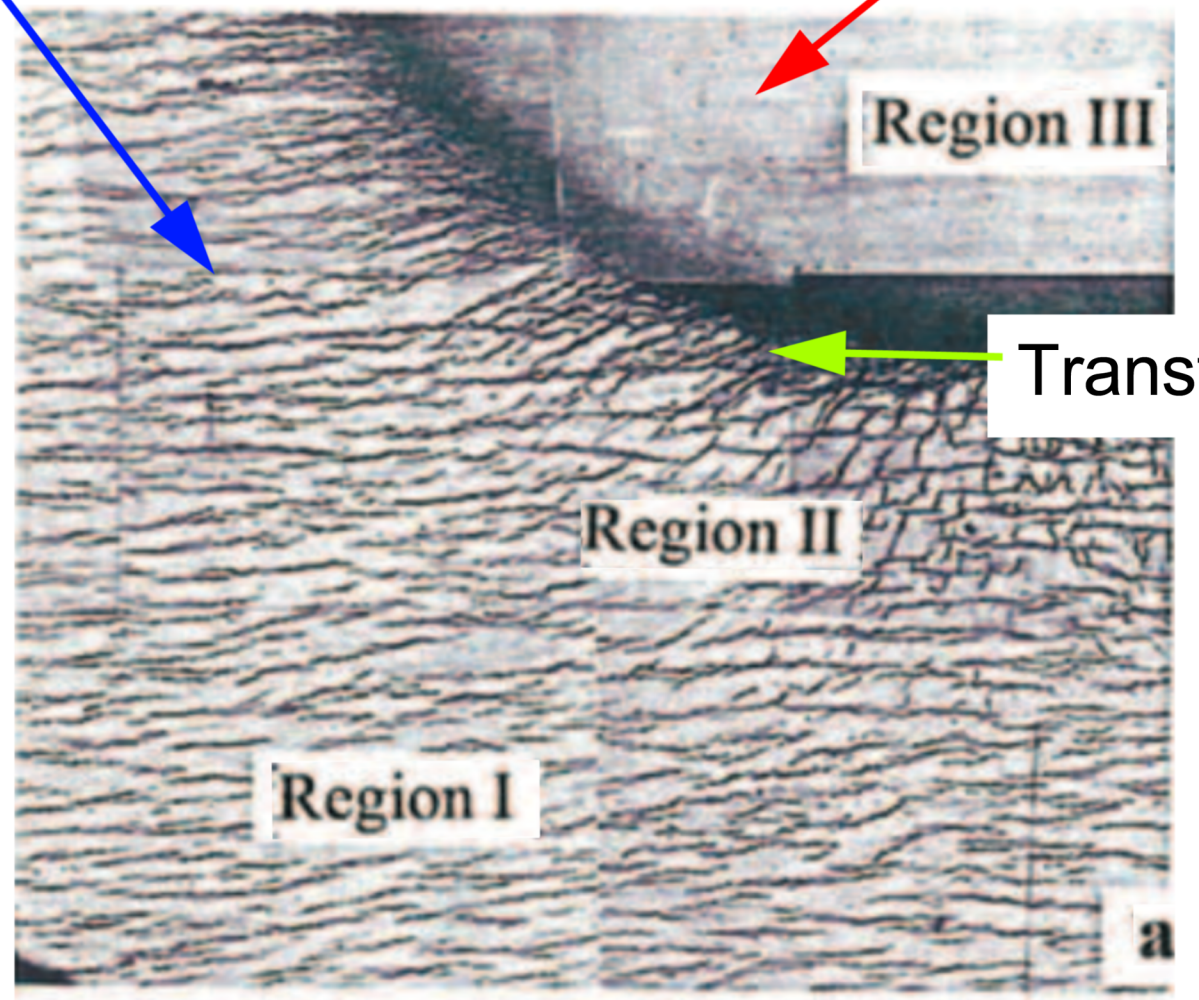




The Phase Field keeps track of the hydride

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

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

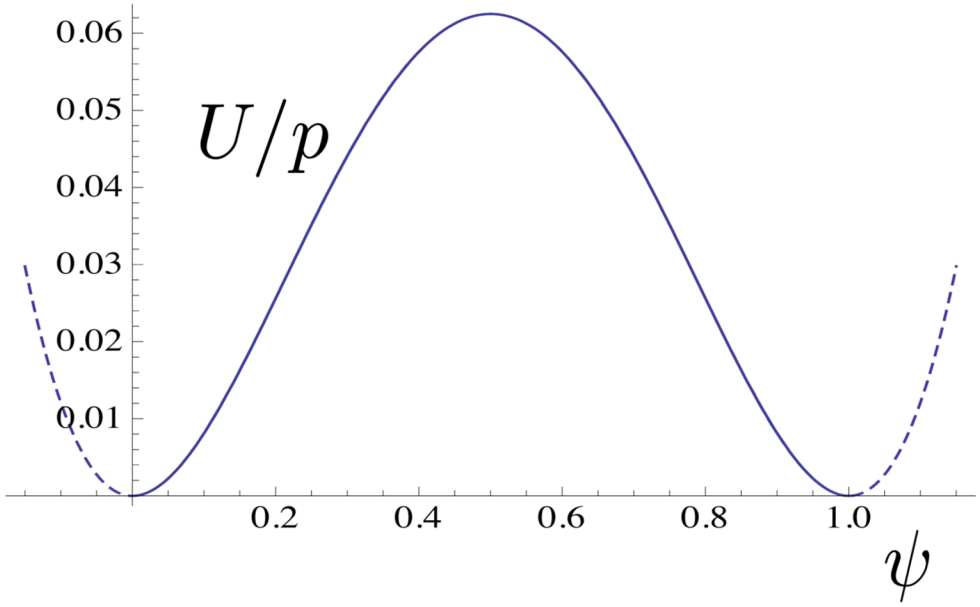


Transformation region

$0 < \psi < 1$

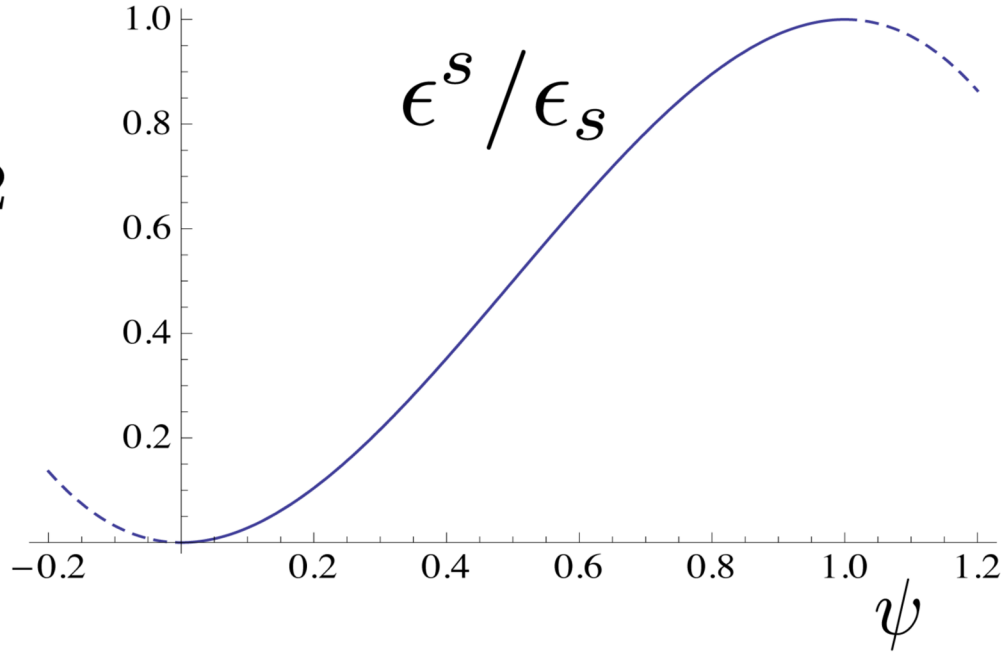
Double-well
chemical potential

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



Expansion

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



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

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.

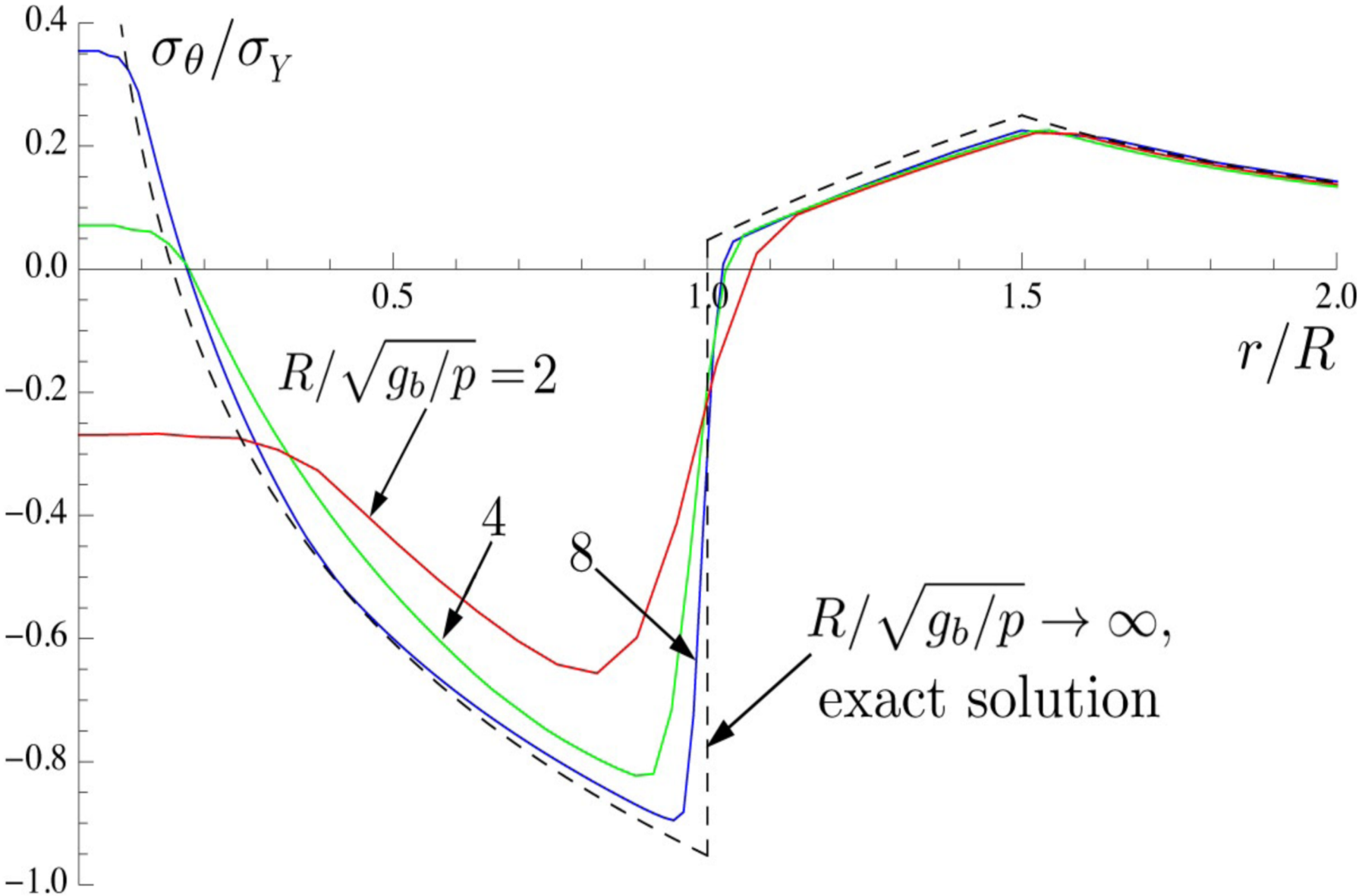
$$\psi_{,ii} - \frac{\partial \psi}{\partial \tilde{t}} = \left\{ 3\epsilon_{ii}^{el} \tilde{\epsilon}_s + 2(1-2\psi) \right\} (1-\psi)\psi$$

Mechanical equilibrium with expansion

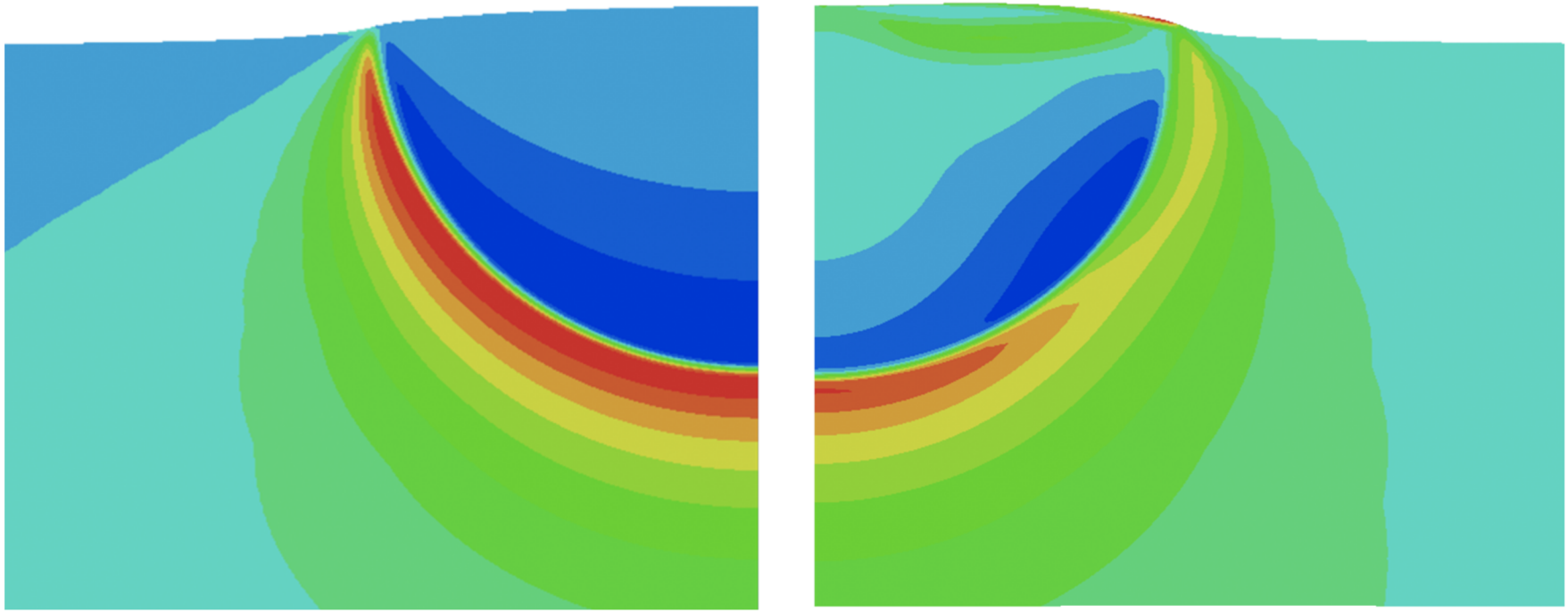
$$\tilde{u}_{i,jj} + \frac{1}{1-2\nu} \tilde{u}_{j,ij} = 2\tilde{\epsilon}^{p}_{ij,j} + \tilde{\epsilon}^{s}_{,i}$$

In analogy with a fully coupled thermal-stress

Emedded Cylinder - Phase Field



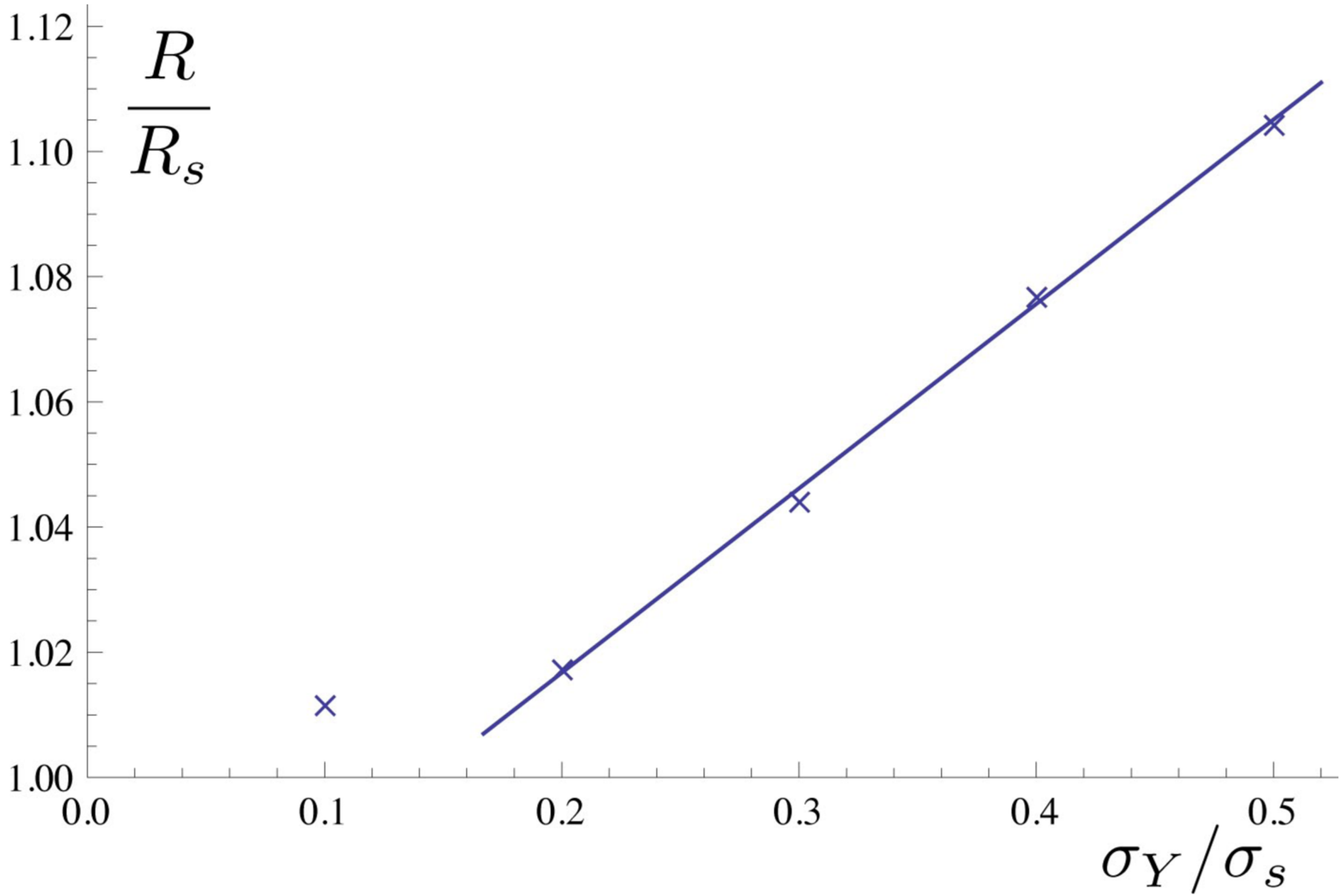
Largest Principal Stress

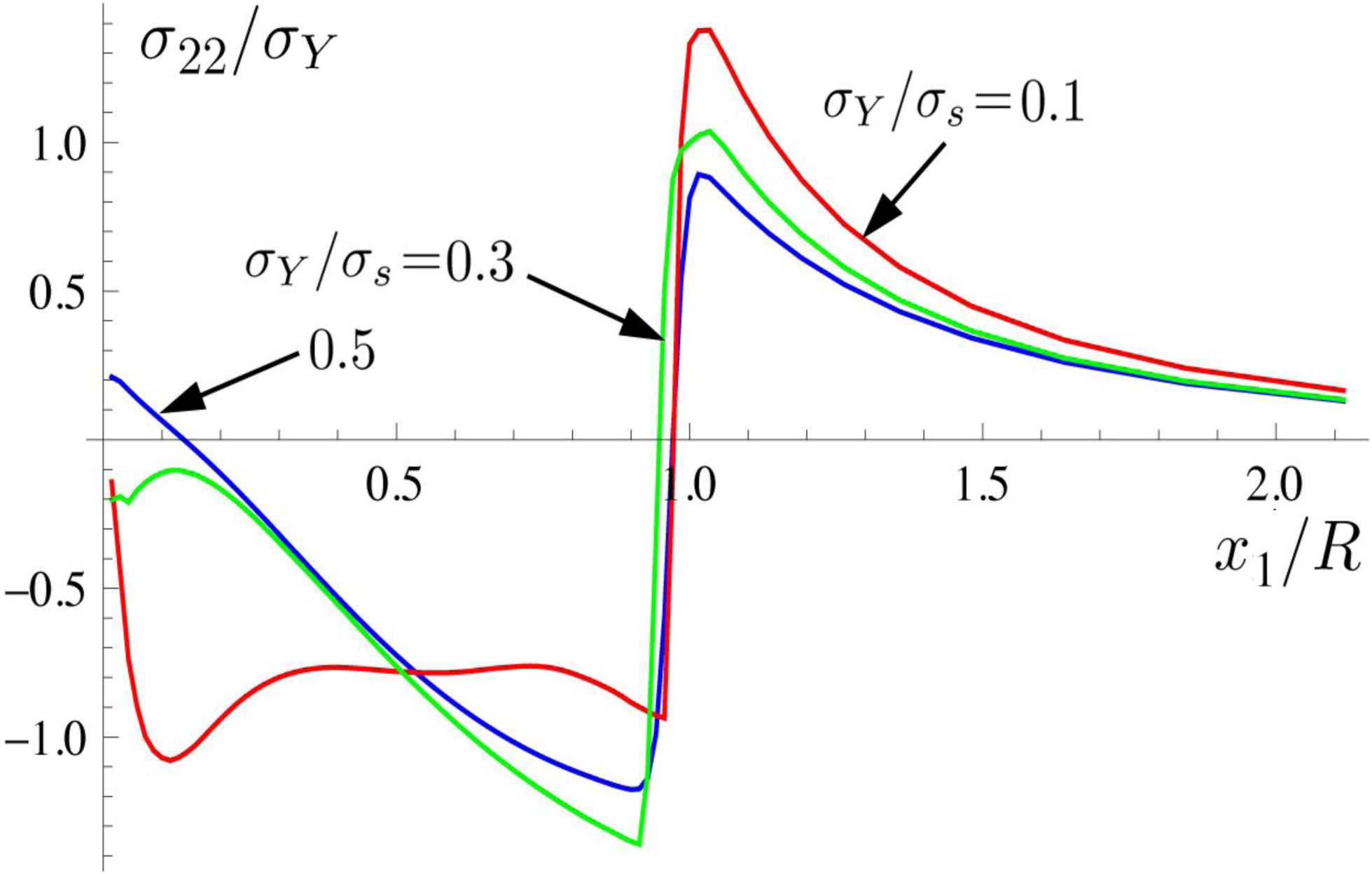


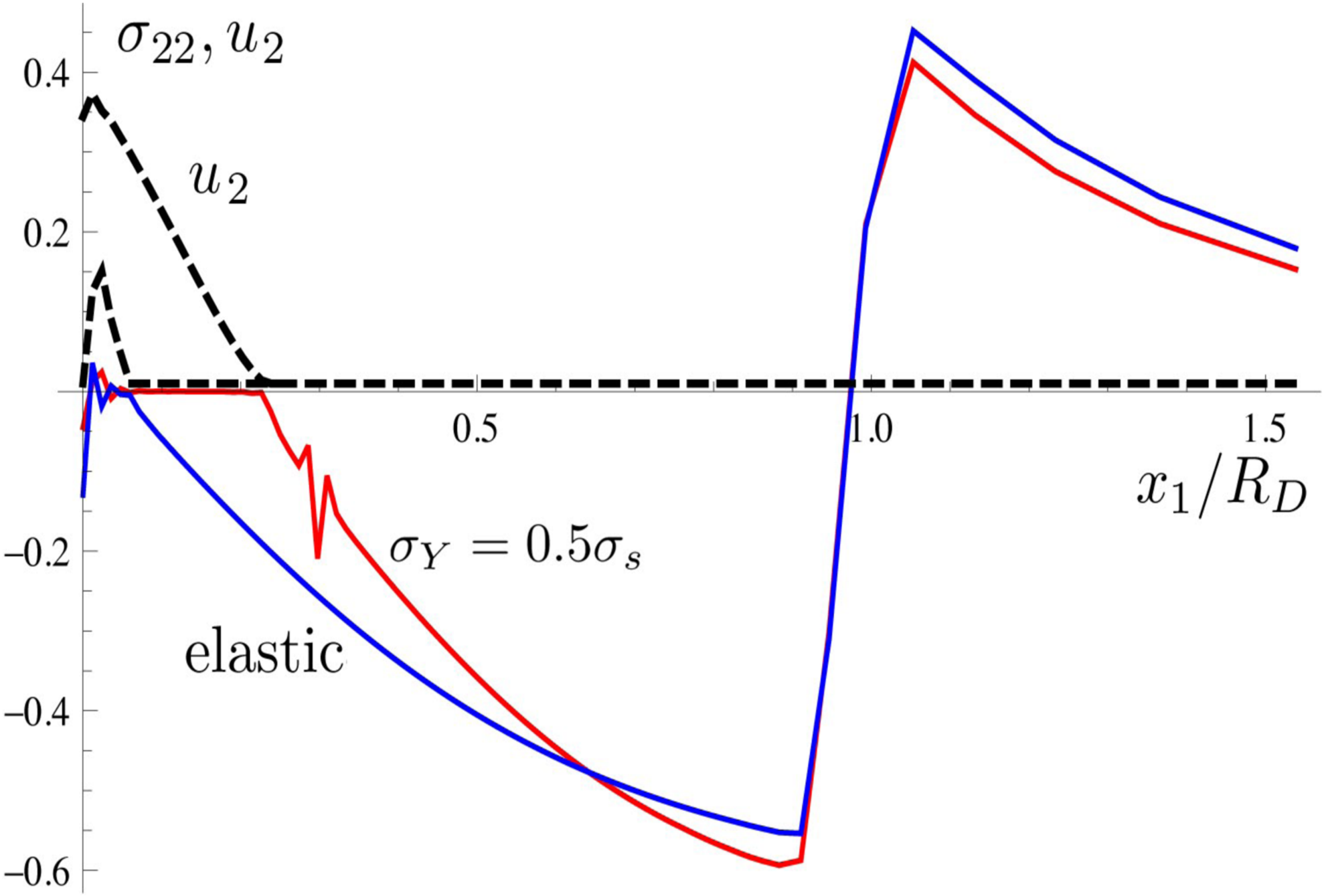
Stationary blister

Growing blister

Blister Depth vs Radius




σ_{22}/σ_Y
$\sigma_Y/\sigma_s=0.1$
$\sigma_Y/\sigma_s=0.3$
0.5
1.0
0.5
−0.5
−1.0
0.5
1.0
1.5
2.0
x_1/R


σ_{22}, u_2
0.4
0.2
u_2
0.5
1.0
1.5
x_1/R_D
$\sigma_Y = 0.5\sigma_s$
elastic
–0.2
–0.4
–0.6

Summary

Growing hydrides are studied using a phase field model

The expanding hydride develops internal tensile stress

The fracture of surface hydrides is possibly explained