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## Formation and Fracture of Expanding Precipitates

Talk given at the annual meeting of the Italian Group of Fracture, Urbino, Italy. Orationem Meam.

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IGFXXIV, Urbino, Italy, March 2017

# Phase Field Modelling of Formation and Fracture of Expanding Precipitates

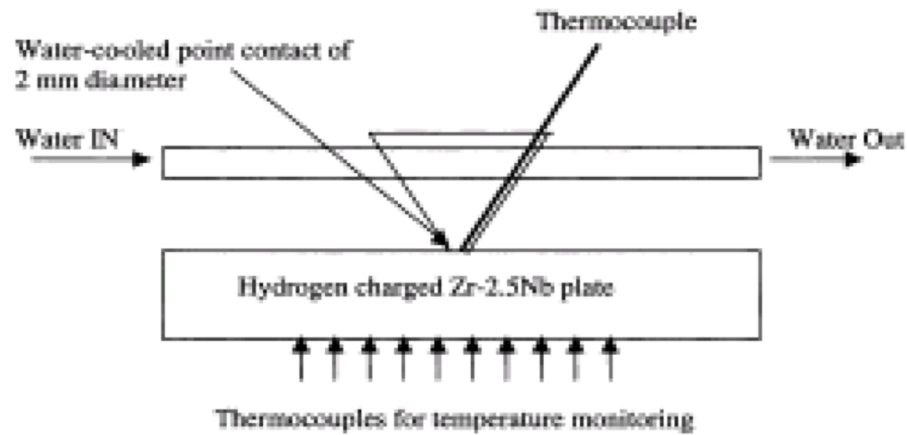
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Solid Mechanics,  
Lund University, Sweden

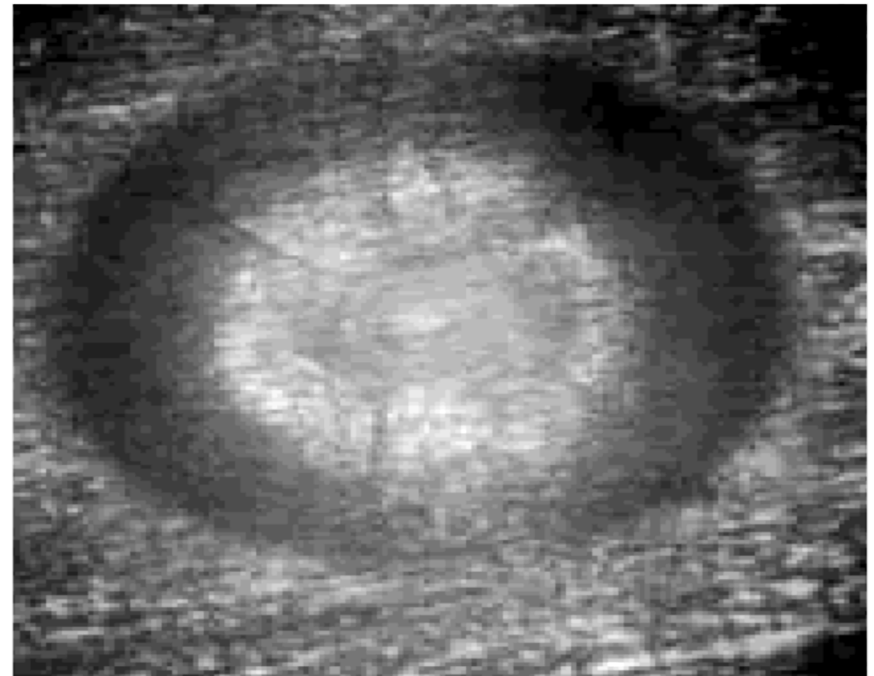
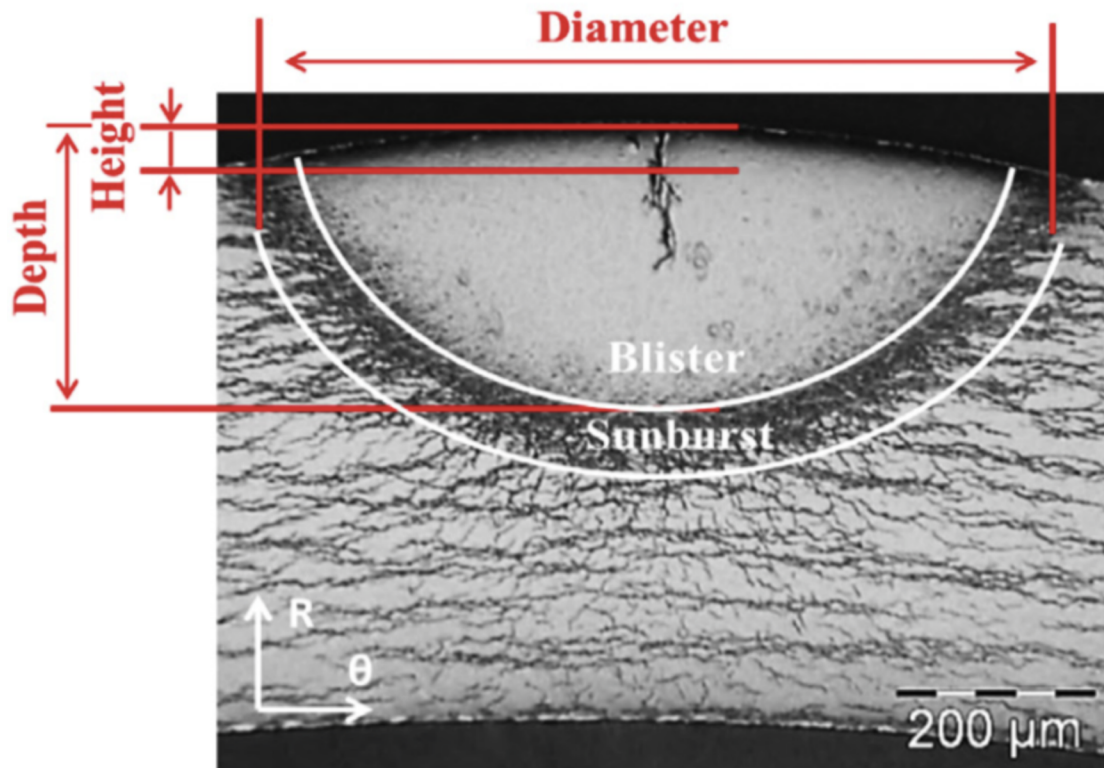


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# The experiment



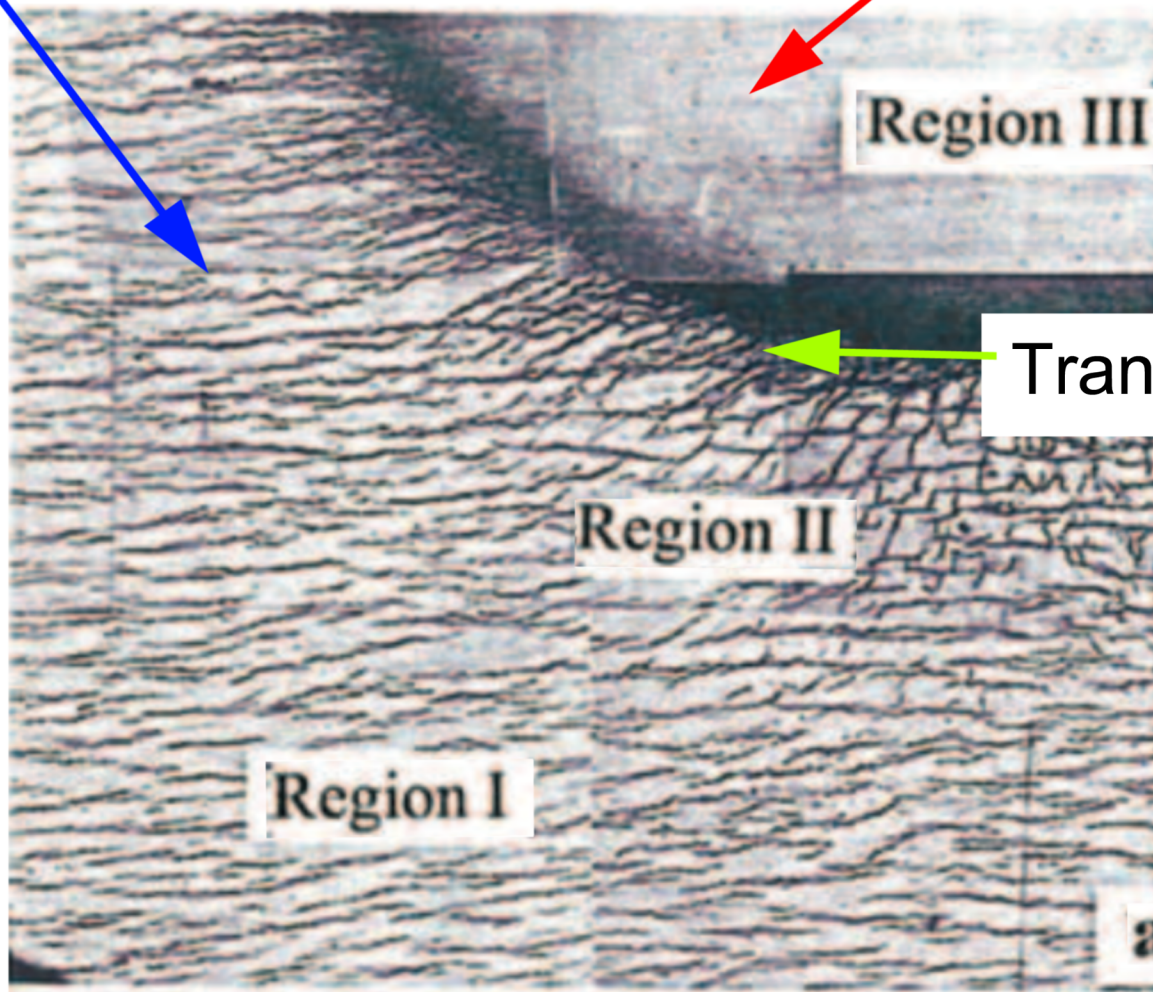
Initially hydrogen is in solid solution. As the cold finger makes contact hydride precipitation occurs. The hydride grows with the arrival of thermally migrated hydrogen



# The Phase Field keeps track of the hydride

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

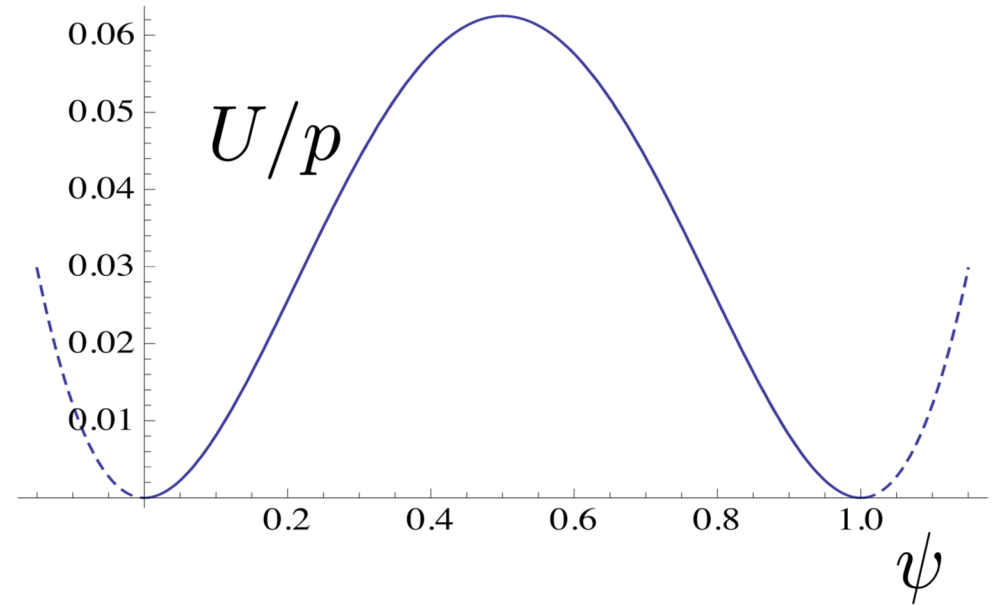
$\psi = 1 \rightarrow \text{Zr}_n\text{H}$



Transformation region  
 $0 < \psi < 1$

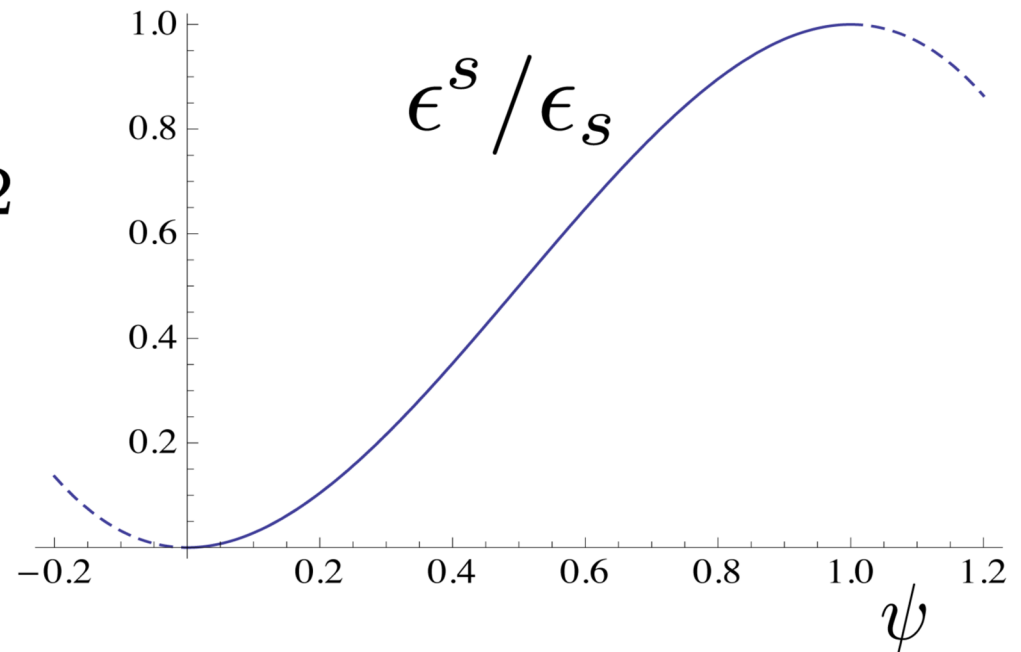
Double-well  
chemical potential

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



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

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

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

Unknown:  $\psi, u_1, u_2, u_3$

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

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

Evolution of the phase.

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

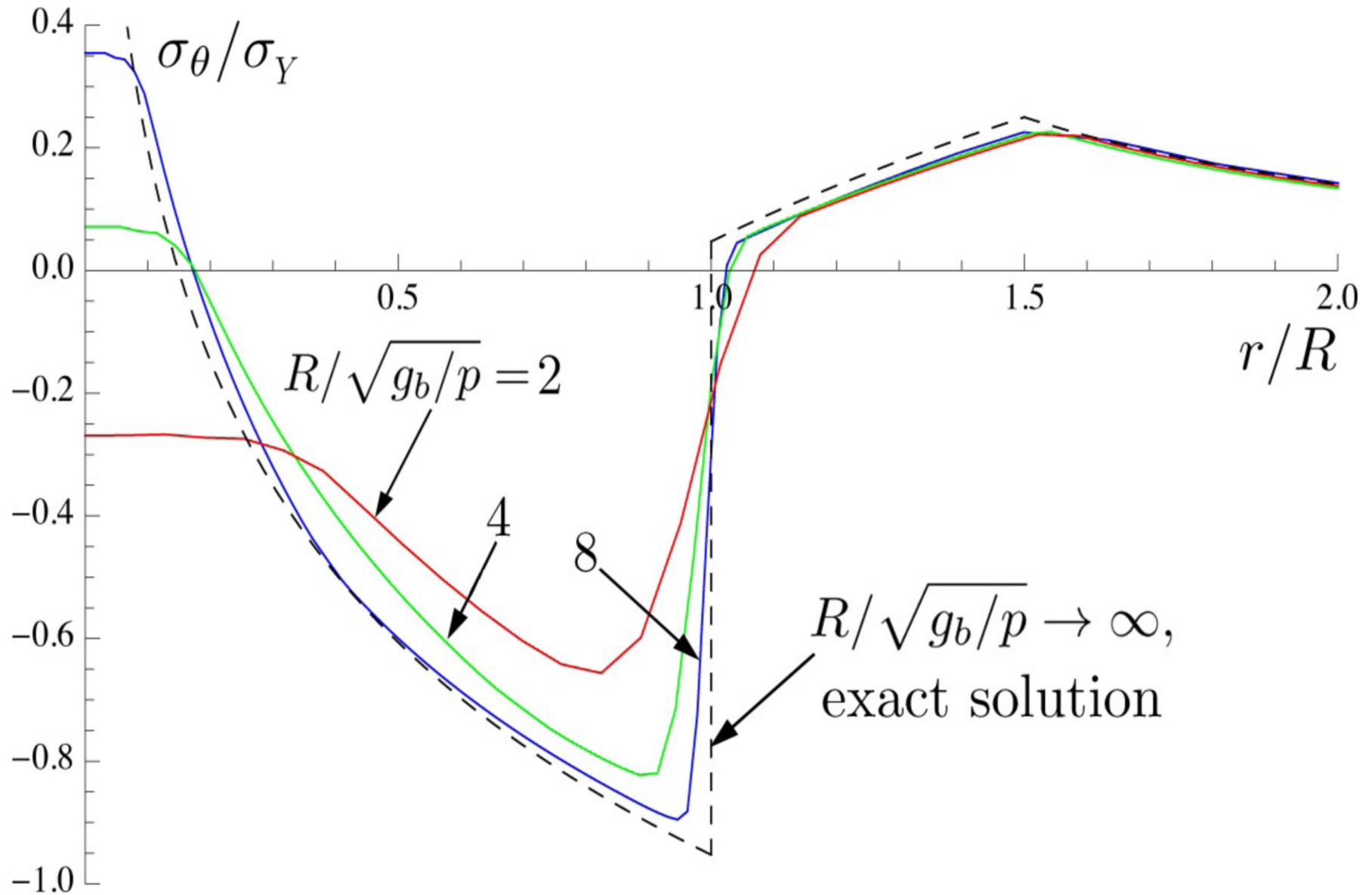
Mechanical equilibrium with expansion

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

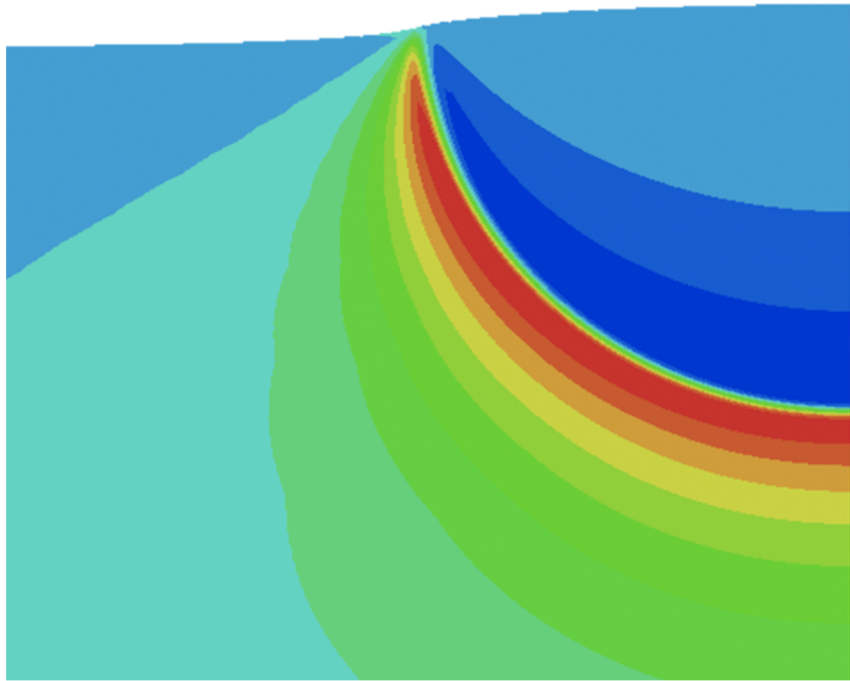
In analogy with a fully coupled thermal-stress



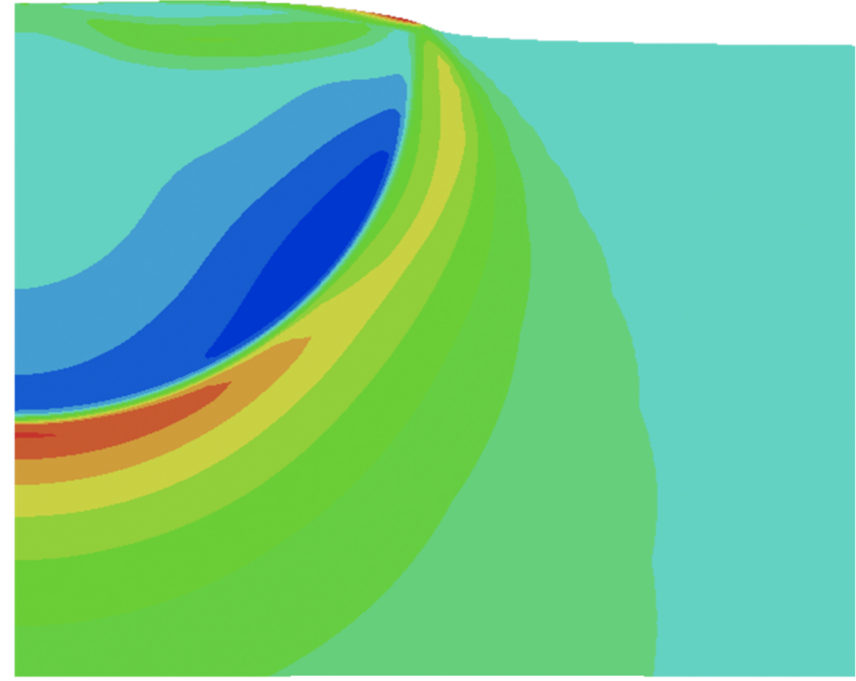
# Emedded Cylinder - Phase Field



# Largest Principal Stress

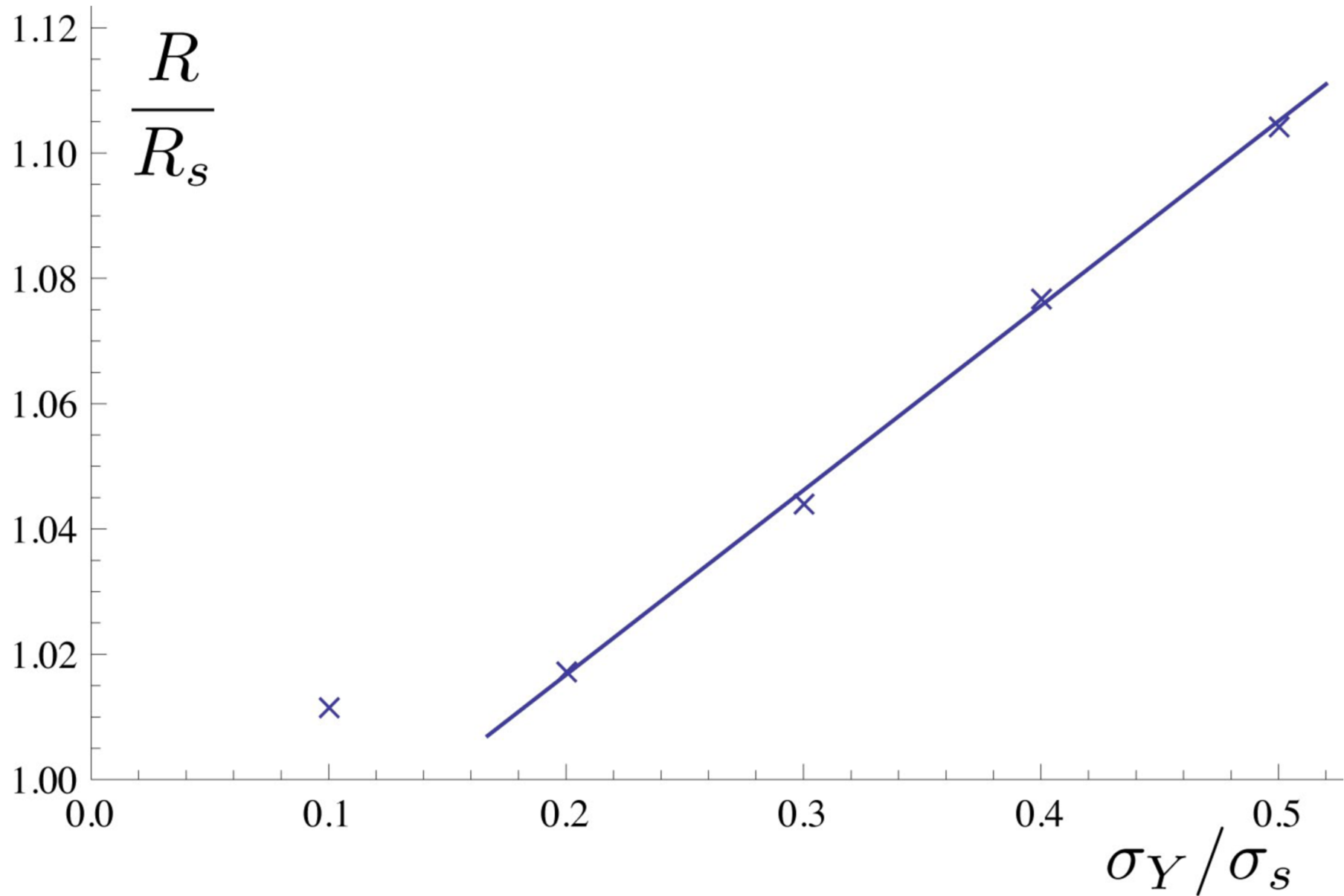


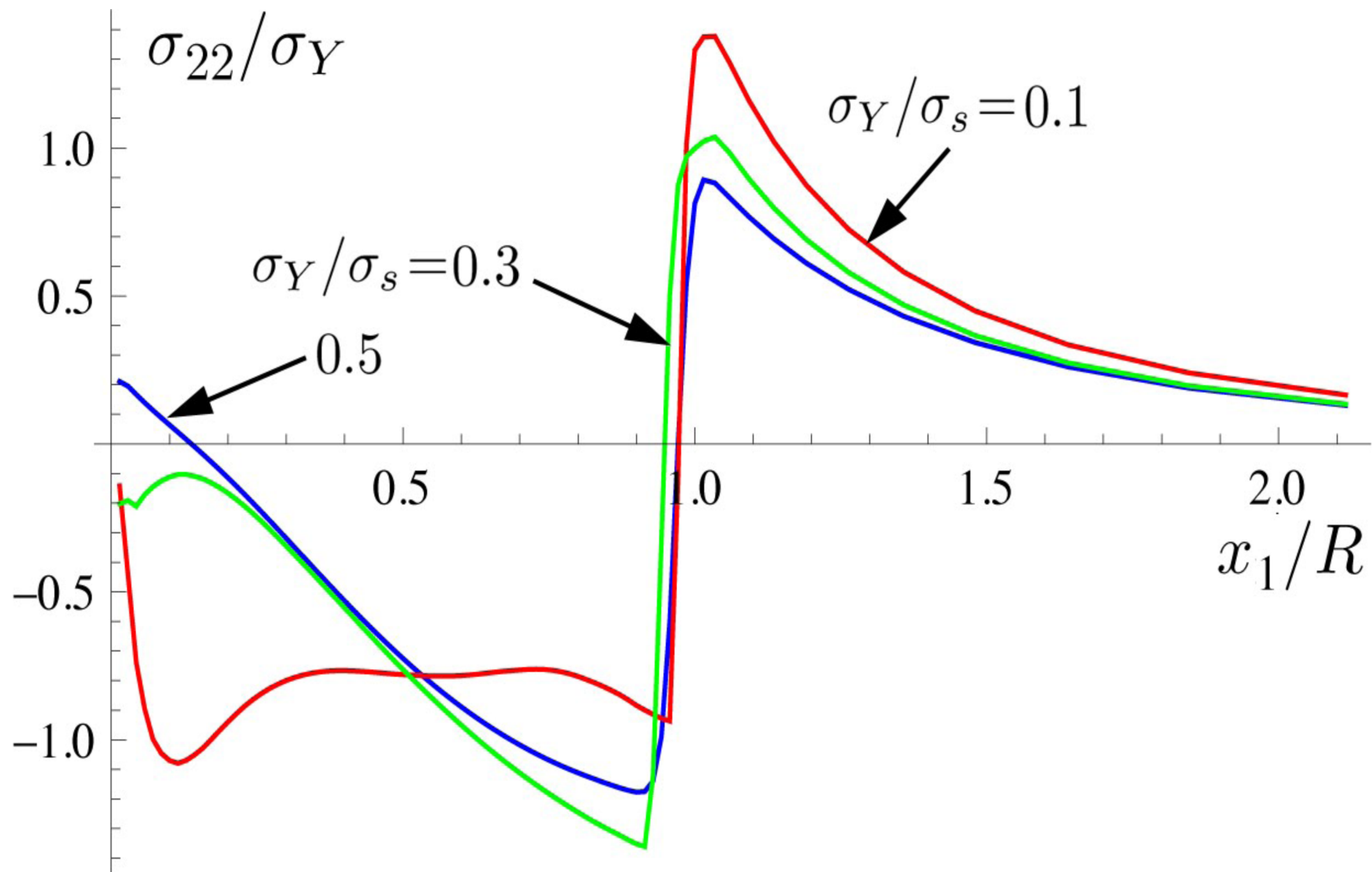
Stationary blister

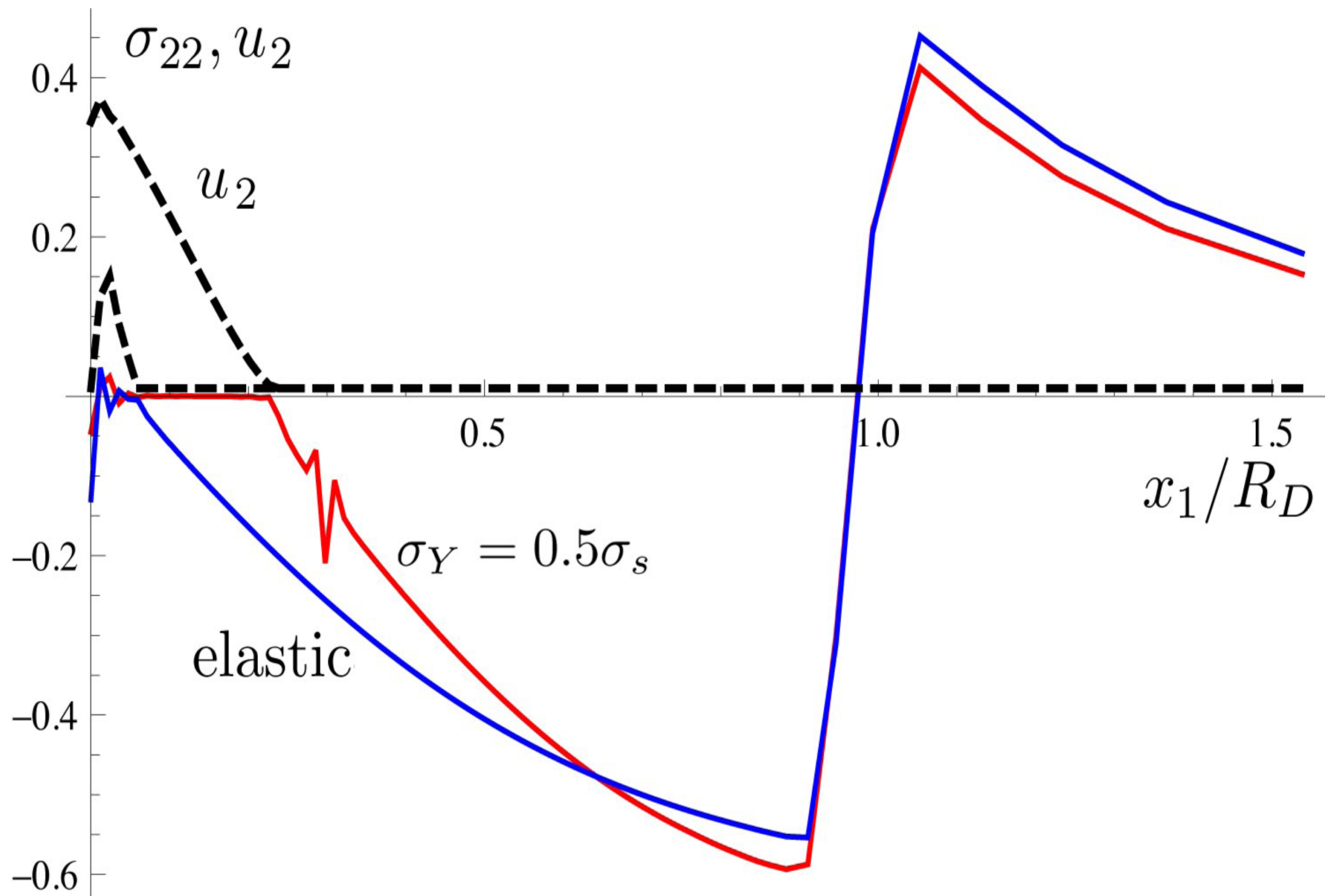


Growing blister

# Blister Depth vs Radius







## 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