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Phase Field Modeling of Gas Bubble Morphology in Solids

PRESENTED BY

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Overview

Developing a computational model to understand the interactions between mesoscale phenomena driving gas bubble morphology in materials

We will present

- Multiphysics of gas bubble morphology
- Analytical models of Eshelby Inclusions
- Numerical model - Phase Field
- Case studies of bubble morphology
- Summary and Future directions

Underlying Principals of Gas Bubble Morphology

Gas atoms are generated by various radiation processes

$$^{235}_{92}U \xrightarrow{Fission} {}^{135}_{52}Te \xrightarrow[19s]{\beta-} {}^{135}_{53}I \xrightarrow[6.6h]{\beta-} {}^{135}_{54}Xe \xrightarrow[9.2h]{\gamma} {}^{136}_{54}Xe$$

- Will diffuse and nucleate gas bubbles in host materials

These bubbles can be found in nuclear fuels, cladding materials, storage systems, and many other critical components

- Bubbles impact key material properties
- Result in reduced component lifetimes and component failure

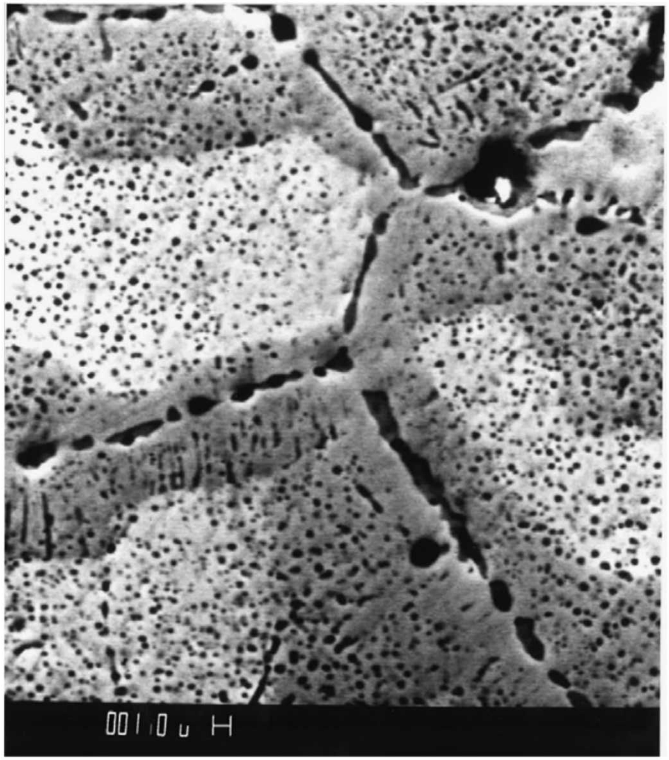


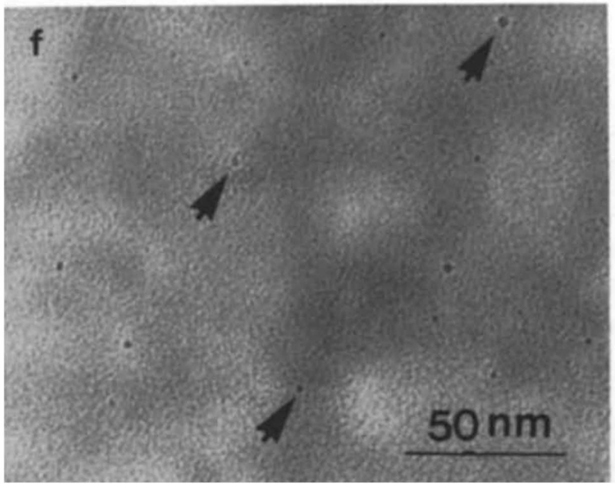
Fig. 5. SEM micrograph of the intermediate phasal zone of irradiated U–Pu–Zr fuel (3 at.% HM burnup, length of the scale bar in the bottom of the figure indicates the length of 1 μm).

D. Yun, *et al.*, *J Nuclear Mater*, vol. 453, pp. 153-163, 2013.

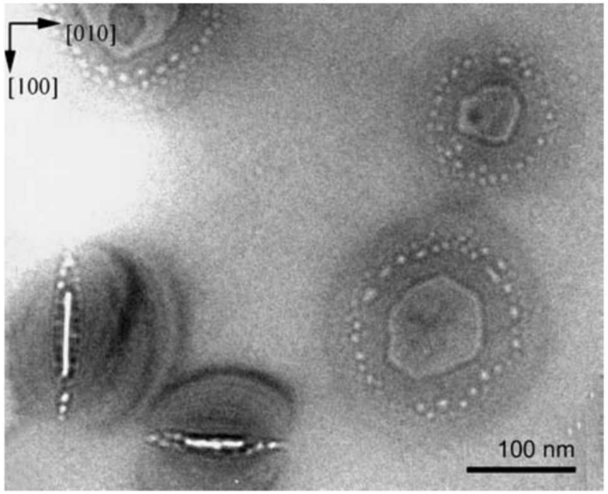
Gas Bubble Growth Physics

Complex multiphysics in to gas bubble evolution

- Evolving two phase system
- Microstructure is complex
- Length scales span from nanometers to microns
- Timescales can be on the order of seconds to decades
- Develop high internal pressures
- Surface and interfacial energies are significant
- Anisotropic material properties can impact growth and morphology



M. Shaw, *et al.*, *J Nuclear Mater*, vol. 115, pp. 1-10, 1983.



N. Hueging,*et al.*, *J Mater Sci*, vol. 41, pp. 4454-4465, 2006.

Eshelby Inclusions

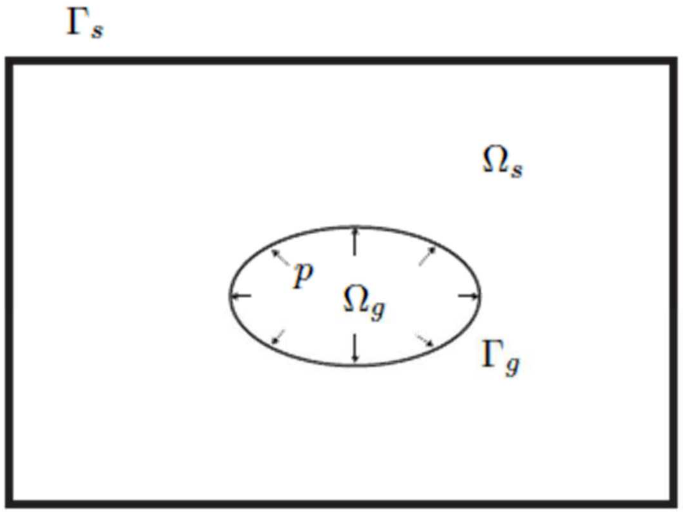
Significant work has focused on misfit strains from solid inclusions

- Driven by solutions to Eshelby equations
- Identifies bifurcation of particle shapes based on strain energy versus surface energy
  - Depends on material properties

Gas bubble evolution should be similar to pure dilatational strain cases

- However, the misfit strain from a gas bubble should be zero

Phase Field: Cahn-Hilliard Model



Problem domain (volume $\Omega = \Omega_s \cup \Omega_g$ and surface $\Gamma = \Gamma_s \cup \Gamma_g$).

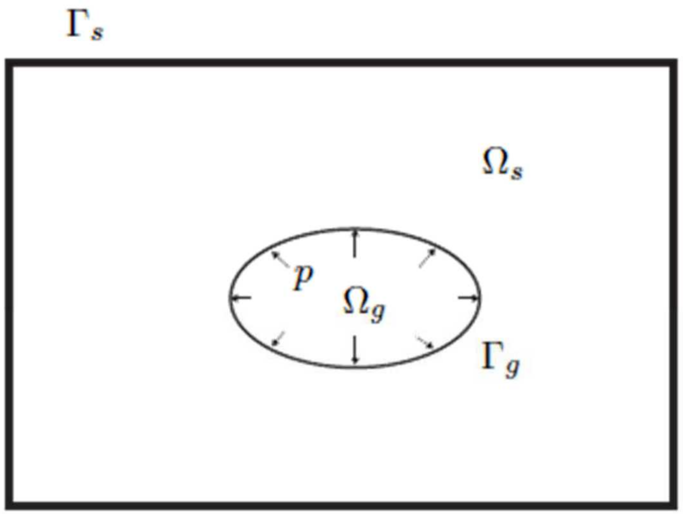
- Phase Energy Density

$$\Pi(\eta) = f(\eta) + \frac{1}{2}\nabla\eta \cdot \ \boldsymbol{\kappa}(\mathbf{n})\ \nabla\eta$$

- Phase Kinetics

$$\frac{\partial\eta}{\partial t} = \nabla \cdot (M\nabla\mu) + q$$

Phase Field: Cahn-Hilliard Model



Problem domain (volume $\Omega = \Omega_s \cup \Omega_g$ and surface $\Gamma = \Gamma_s \cup \Gamma_g$).

- Anisotropic surface energies

$$\gamma(\hat{n}) = \gamma_0 \left[1 - \Sigma_i^N \epsilon_i (\hat{n} \cdot \hat{m}_i)^{w_i} H(\hat{n} \cdot \hat{m}_i)\right]$$

M. Salvalaglio, *et al.*, *Cryst Growth Des*, vol. 15, pp. 2787-2794, 2015.

$$\gamma \approx 2\sqrt{\kappa \Delta f}$$

Coupled Phase Field and Mechanics

- Total Free Energy

$$\Psi(\mathbf{u}, \eta) = \int_\Omega (\Pi(\eta) + g(\eta) W(\mathbf{u}))\ dV + \int_{\Gamma_g} \mathbf{u} \cdot p\mathbf{n}\ dS$$

$$\Psi(\mathbf{u}, \eta) = \int_\Omega \Pi(\eta) + g(W + p\nabla \cdot \mathbf{u})\ dV$$

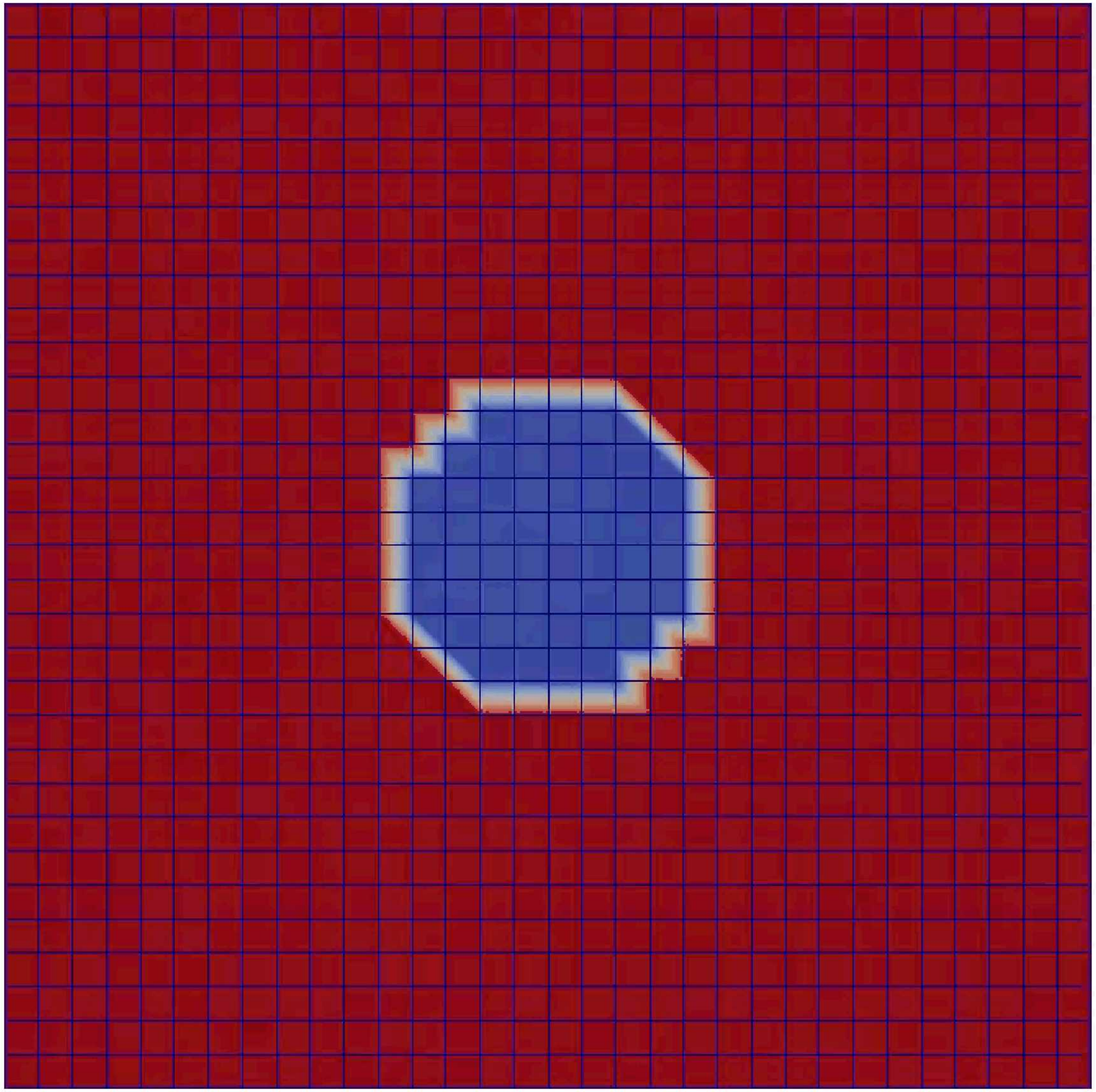
- Weak form of governing equations

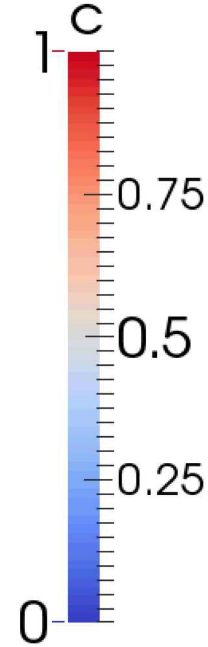
$$\int_\Omega w \left(\frac{\partial \eta}{\partial t} - q \right)\ dV + \int_\Omega w \nabla \cdot (M \nabla \mu)\ dV = 0$$

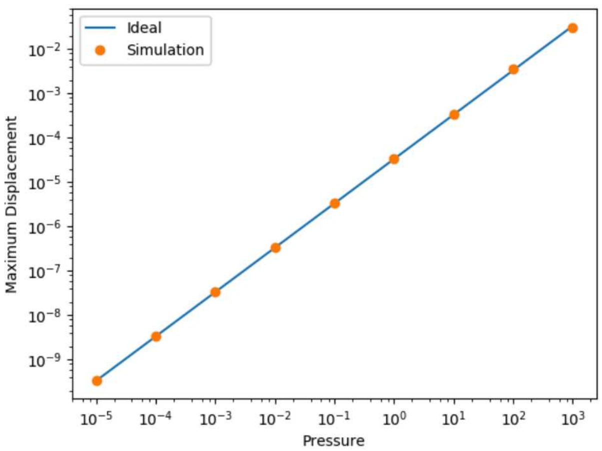
$$\int_\Omega \boldsymbol{\omega} \nabla \cdot (-g\boldsymbol{\sigma} - p\nabla g)\ dV + \int_{\Gamma_s} \boldsymbol{\omega}\ (g\boldsymbol{\sigma}) \cdot \mathbf{n}\ dS + \int_{\Gamma_s} (g\ p)\boldsymbol{\omega} \cdot \mathbf{n}\ dS = 0$$

- Implemented in deal.II FE framework

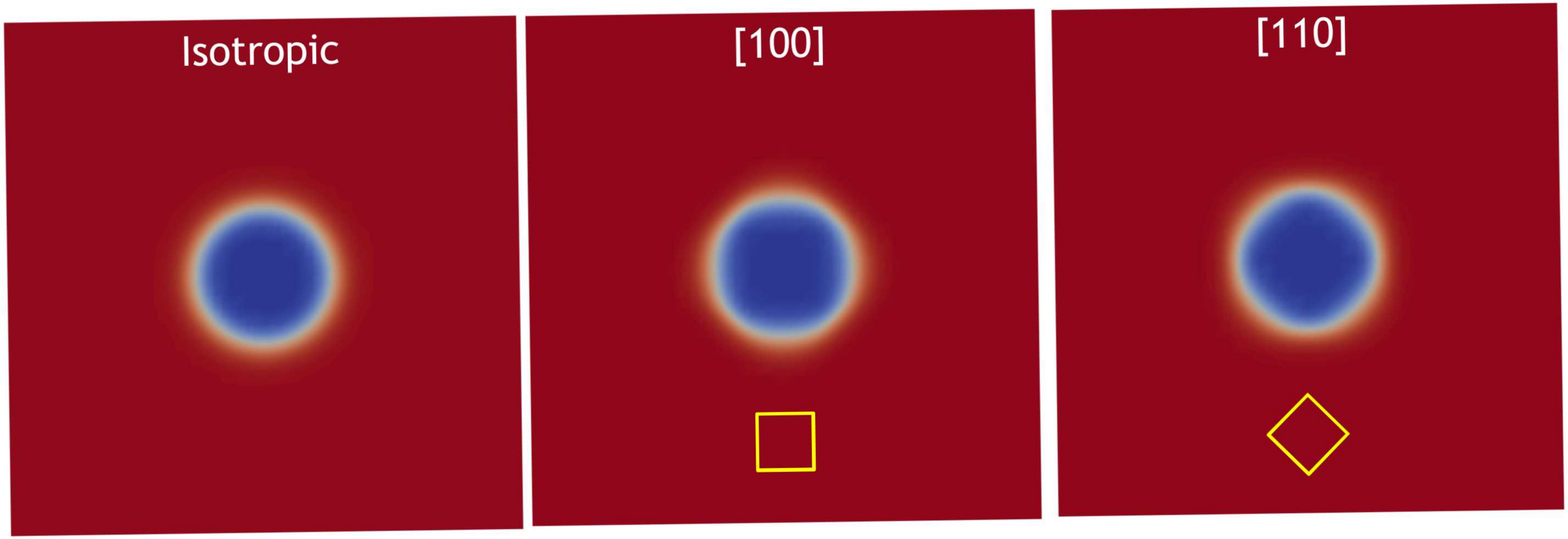
Results




c
1
0.75
0.5
0.25
0


Ideal
Simulation
Maximum Displacement
Pressure
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-5} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3}

Results - Anisotropy

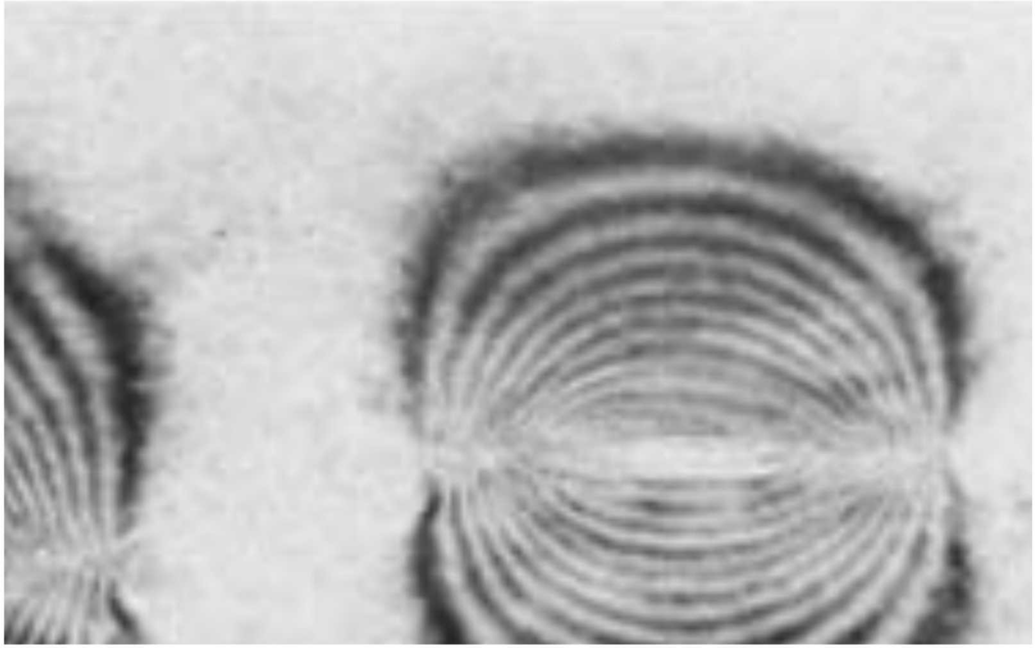


Results Favor Spherical Shapes

For mechanical and surface energy properties of relevant gas bubble material systems, we find that both surface energy and elastic energy favor spherical shapes

- Bifurcation seen in in Eshelby studies of solid inclusions is not seen for gas bubbles
- Need to do a more exhaustive search for what materials properties are needed to result in platelet geometries

New Hypothesis: Crack/Defect Propagation



N. Hueging, *et al.*, *J Mater Sci*, vol. 41, pp. 4454–4465, 2006.

- At these size scales, physically unable to reproduce shapes with elasticity and chemical energy alone
- Experimental results show plate-like geometries at length scales dominated by surface energy
- First order attempt to capture physics through brittle crack growth

Phase Field Fracture Model

$$\Pi(\eta) = G_c \left(\frac{(1-\eta)^2}{4 * |\boldsymbol{\kappa}|} + \nabla\eta \cdot \; \boldsymbol{\kappa}(\mathbf{n}) \; \nabla\eta \right)$$

C. Miehe, *et al*., *Int. J. Numer. Eng.*, vol. 83, pp. 1273-1311, 2010.

- Switched to Allen-Cahn kinetics

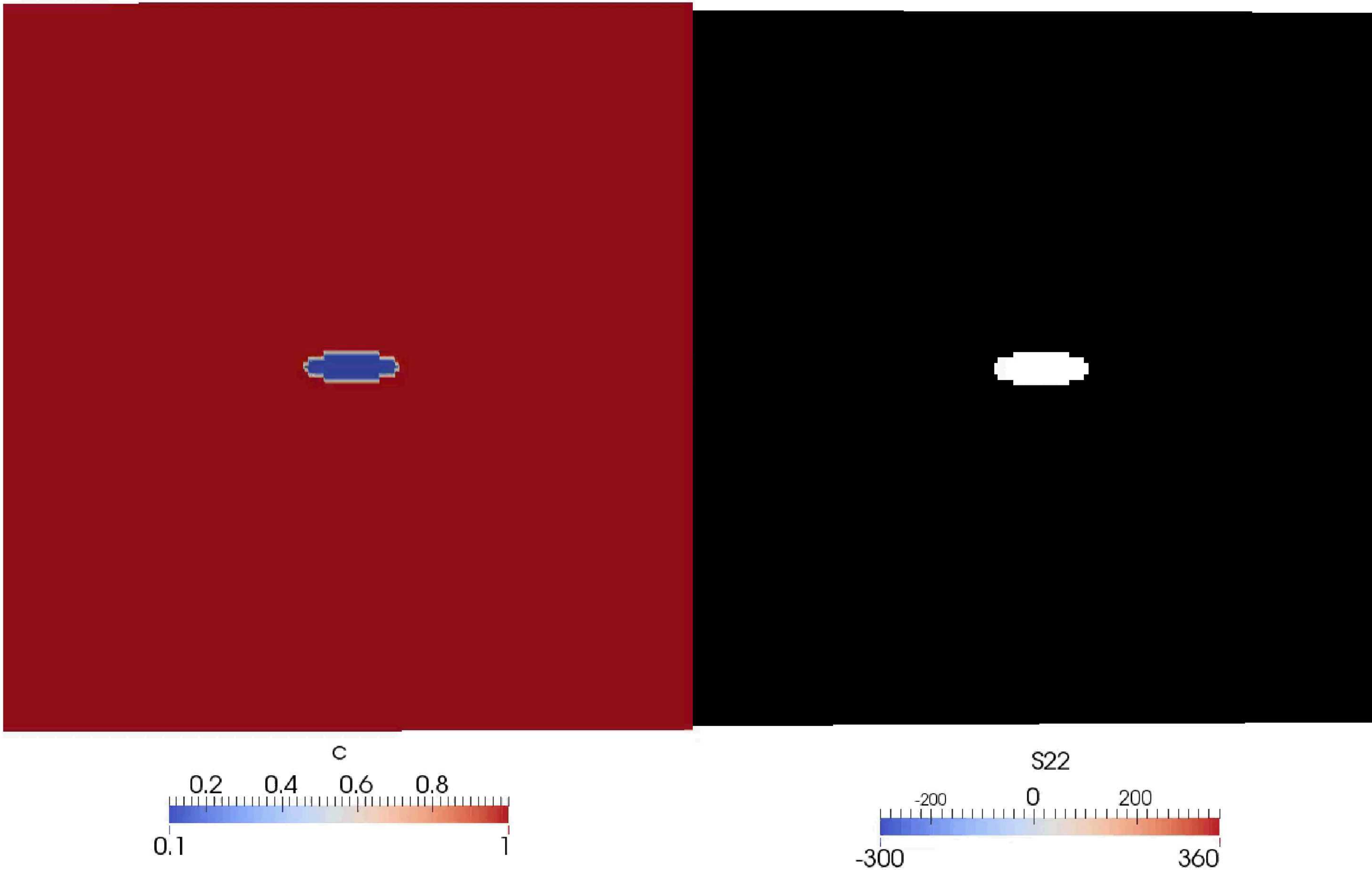
$$\frac{\partial\eta}{\partial t} = -M\mu + q$$

$$\int_\Omega w \left(\frac{\partial\eta}{\partial t} - q \right) \; dV + \int_\Omega wM\mu \; dV = 0$$

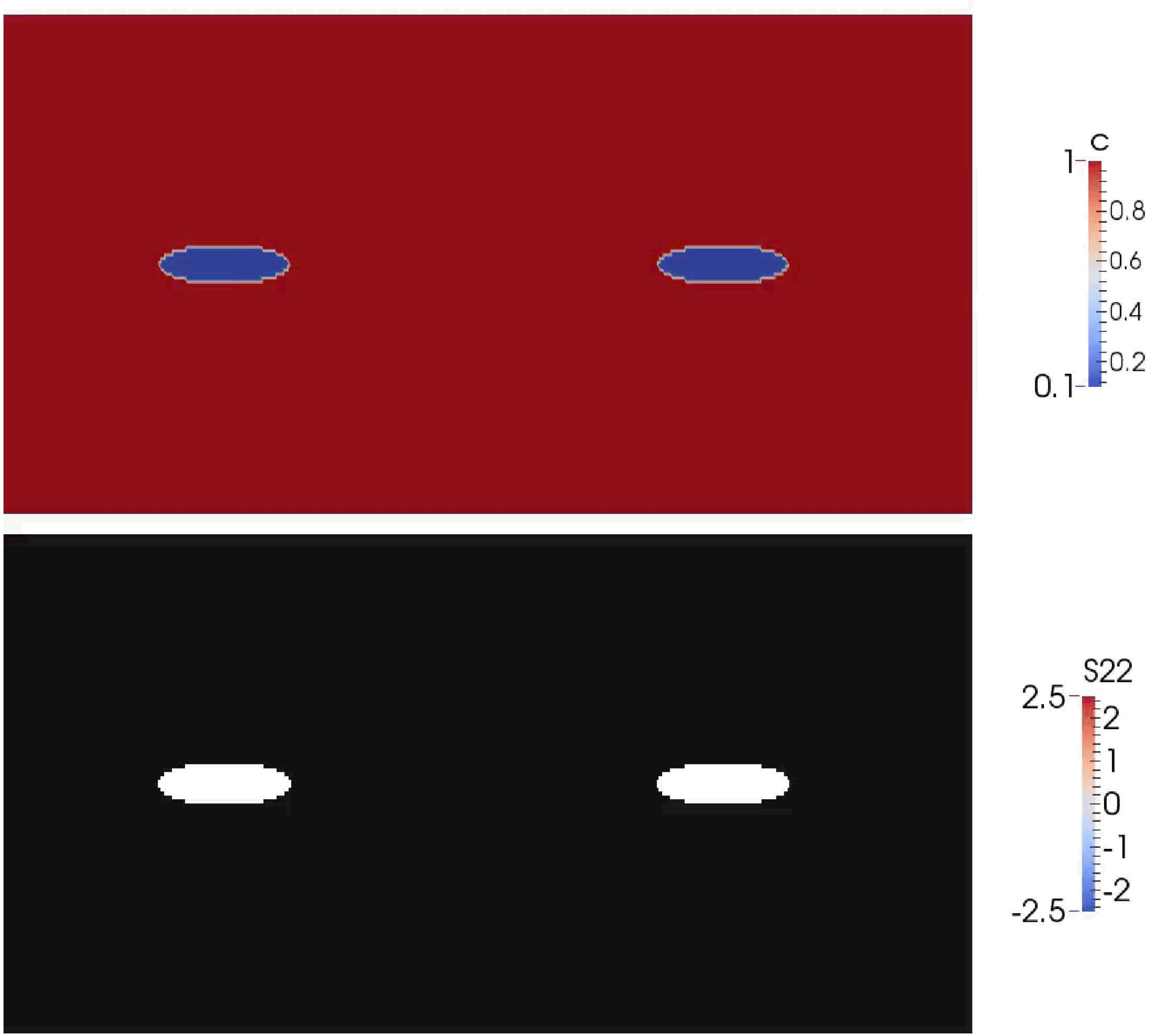
$$\Psi(\mathbf{u}, \eta) = \int_\Omega (\Pi(\eta) + g(\eta)W(\mathbf{u})) \; dV + \int_{\Gamma_g} \mathbf{u} \cdot p\mathbf{n} \; dS$$

- Crack evolution only driven by tension and cannot heal

Single Bubble Evolution



Multi-bubble Evolution



Summary and Next Steps

- Summary
  - Developed a phase field based formulation for pressure driven bubble growth
  - Investigated shapes and multi-bubble dynamics under various anisotropies (elastic, chemical)
  - Trying to link to observed experimental growth of bubbles over decades in irradiated materials
- Next steps
  - Studying the dynamics of bubble clusters and the potential failure patterns of the underlying material
  - Extension to include plasticity and stress driven growth mechanisms

COMPUTATIONAL MATERIALS GROUP

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* 25+ students involved in Informatics Skunkworks
https://skunkworks.engr.wisc.edu/

Informatics Skunkworks

Computational Materials Group

Thank you!

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Questions?

Surface Energy Anisotropy

More of a numerical approach
- Many fitting parameters to accommodate different surfaces
- Can be reduced to fit previous forms

Assumes there are N minima with directions (m) [±100], [0±10], [00±1], [±1±10], [±10±1], [0±1±1], [±1±1±1]
- ~8 for 2D and ~27 for 3D
- Each minima has a depth value given by ϵ_i
- Each minima has width value given by w_i
- Heaviside function ensures that negative direction values are not counted twice

$$\gamma(\hat{n}) = \gamma_0 \left[1 - \Sigma_i^N \epsilon_i (\hat{n} \cdot \hat{m}_i)^{w_i} H(\hat{n} \cdot \hat{m}_i)\right]$$

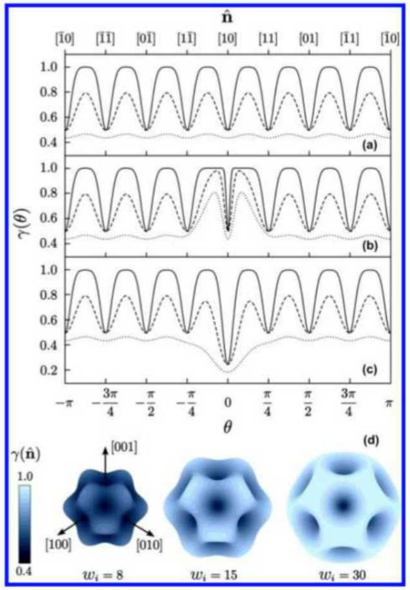
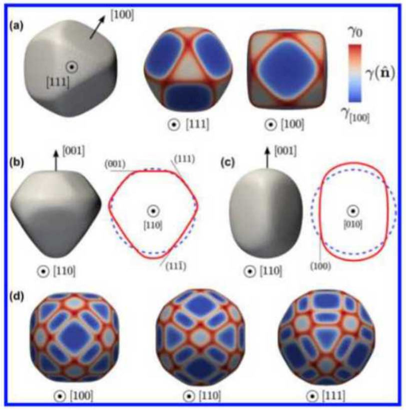


Figure 2. Examples of surface energy density from eq 7. (a−c) Plot of 2D $\gamma(\theta)$ function with minima at $\bar{\theta}_i = i\pi/4$ (⟨10⟩ and ⟨11⟩ directions) with $\alpha_i = 0.5$ and $\gamma_0 = 1$. (a) $w_i = 8$ (dotted line), $w_i = 20$ (dashed line), and $w_i = 100$ (solid line). (b) as in panel (a) with w_0 increased by a factor 10. (c) as in panel (a) with $\alpha = 0.75$ for the $\bar{\theta}_0$ minimum. (d) Three-dimensional $\gamma(\hat{\mathbf{n}})$-plot with minima along ⟨100⟩ and ⟨111⟩ directions, $\alpha_i = 0.5$ and $\gamma_0 = 1$, for three w_i values. $\gamma(\hat{\mathbf{n}})$ values are also plotted as surface color map.



Mesh Adaptivity

- Mesh refinement is based on the order parameter to focus the finest meshes in the area of most interest