Microstructural Evolution Modeling

SAND2014-17075PE

Efraín Hernández–Rivera[1,2]

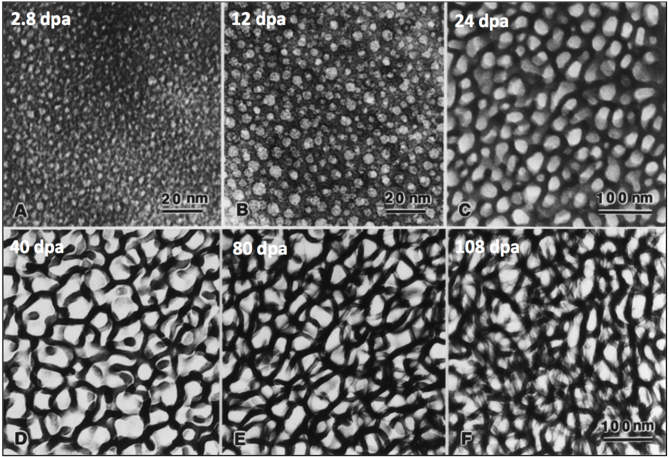
[1]University of Michigan, Ann Arbor MI
[2]Sandia National Laboratories, Albuquerque NM

August 12, 2014

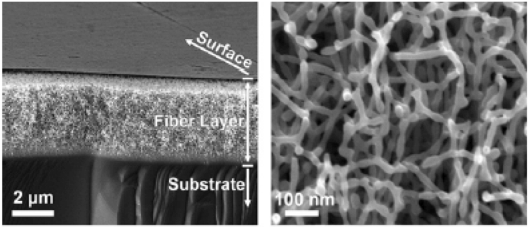
Sandia National Laboratories is a multi–program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE–AC04–94AL85000.

Outline

Ion Irradiation

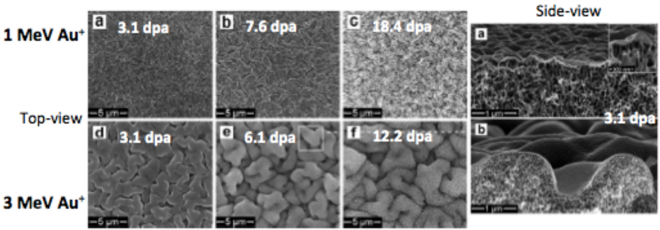


On Several Semiconductors

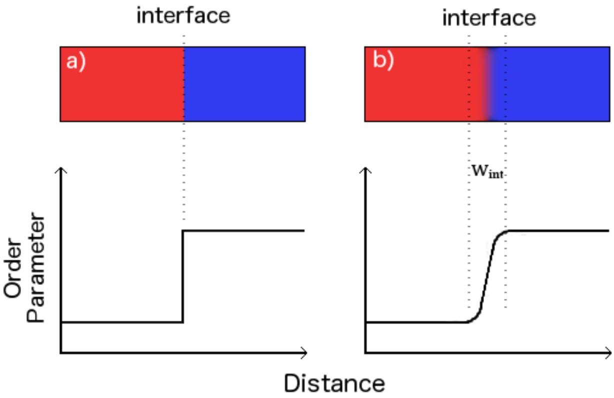


GaSb

InSb

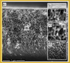


hPPF

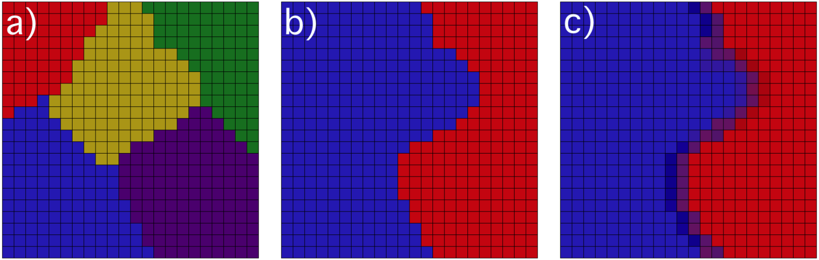


$$E_{Potts} = J \sum_{j=1}^{n} (1 - \delta_{s(i)s(j)}) \qquad E_{pf} = \int_{\mathcal{V}} (\frac{\gamma}{2} |\nabla C|^2) dV$$

Outline



Microstructural Representation



Thermodynamics

The EoS is,

$$F = \int_{\mathcal{V}} f_0 dV + \int_{\mathcal{S}} \gamma dS = \int_{\mathcal{V}} f_0 dV + \frac{\gamma_{CH}}{2} \int_{\mathcal{V}} |\nabla C|^2 dV + \gamma_{Potts} \int_{\mathcal{S}} dS,$$

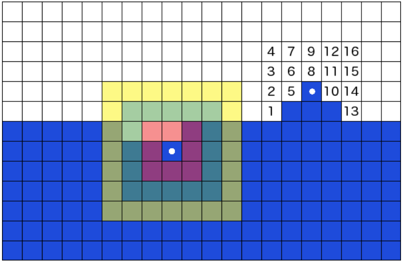
which can be discretized

$$F_{CH,i} = \sum_{i=1}^{N} \left(f_0(q_i, C_i) + \frac{\gamma_{CH}}{2} |\nabla C_i|^2 + J \sum_{j=1}^{n} (1 - \delta_{s(i)s(j)}) \right)$$

$$F_{Potts,i} = \sum_{i=1}^{N} \left(f_0(q_i, C_i) + J \sum_{j=1}^{n} (1 - \delta_{s(i)s(j)}) \right)$$

$$\frac{\delta F}{\delta C} = \gamma \frac{\delta S}{\delta C} = \gamma \frac{\delta V}{\delta C} \frac{\delta S}{\delta V} = \gamma \Omega \frac{8\pi R \delta r}{4\pi R^2 \delta r} = \frac{2\gamma\Omega}{R} \equiv \gamma \Omega \kappa$$

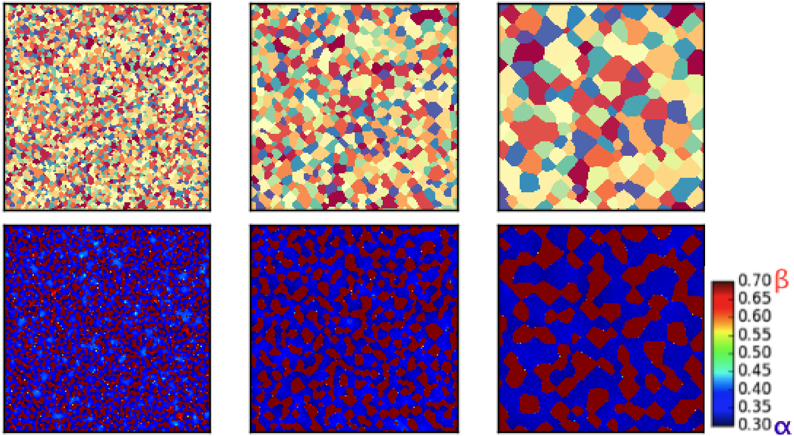
Curvature and Phenomenological Eqns



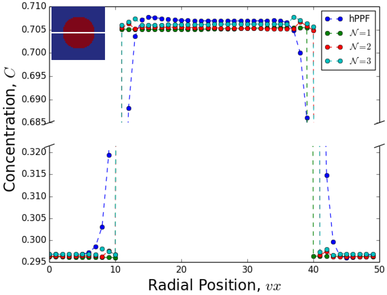
$$\kappa_i = \frac{\sum_{j=1}^{n_s}\left(1 - \delta_{q(i)q(j)}\right) - n_{base}}{n_s}$$

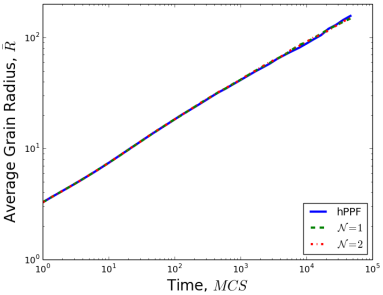
$$\frac{\partial C}{\partial \tilde{t}} = \tilde{\nabla} \cdot \left[\tilde{\nabla} \left(\frac{\partial \tilde{f}_0}{\partial C} - \tilde{\nabla}^2 C \right) \right] \qquad \frac{\partial C}{\partial \tilde{t}} = \tilde{\nabla} \cdot \left[\tilde{\nabla} \left(\frac{\partial \tilde{f}_0}{\partial C} + \tilde{\kappa} \right) \right]$$

Microstructural Evolution



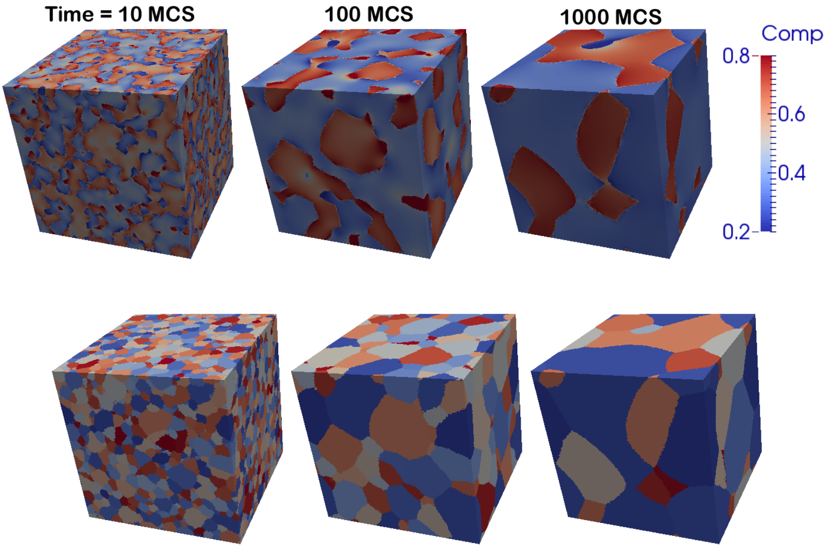
Grain Growth Results





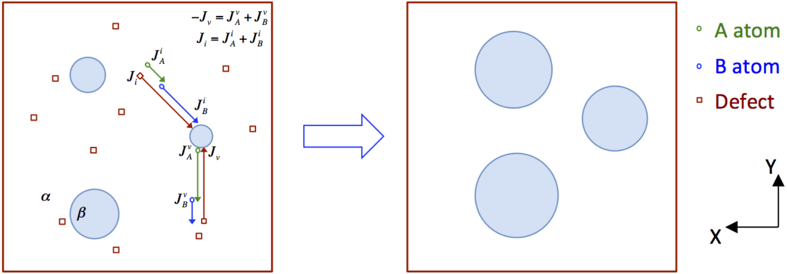
hPPF	$\mathcal{N}$		$\mathcal{N}_{3D}=1$
	1	2	
0.350	0.337	0.345	0.353

3D Microstructural Evolution

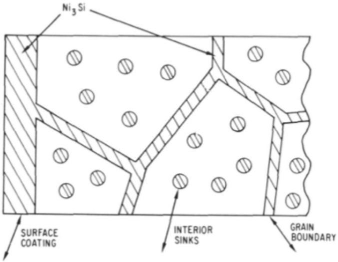


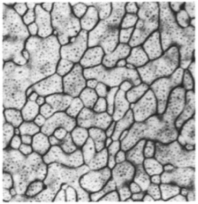
RIS: General Description

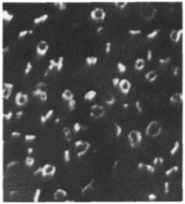
$$J_i^a + J_i^b = J_i$$
$$J_v^a + J_v^b = -J_v$$
$$J_a + J_b = J_i - J_v$$

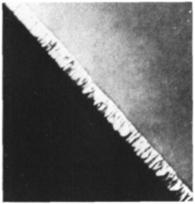


Experimentally Observed









Phenomenological Equations

$$\frac{\partial C_i}{\partial \tilde{t}} = \frac{\eta_s(\vec{x})}{\Delta \tilde{t}} + \tilde{\Theta}_b \tilde{\nabla} \cdot \left(\frac{D_i}{D_b} \tilde{\nabla} C_i + C_i \tilde{\nabla} C_b \right) - \tilde{k}_{iv} C_i C_v - \tilde{S}_{fs} - \tilde{S}_{\alpha\beta}$$

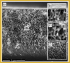
$$\frac{\partial C_v}{\partial \tilde{t}} = \frac{\eta_s(\vec{x})}{\Delta \tilde{t}} + \tilde{\Theta}_b \tilde{\nabla} \cdot \left(\frac{D_v}{D_b} \tilde{\nabla} C_v - C_v \tilde{\nabla} C_b \right) - \tilde{k}_{iv} C_i C_v - \tilde{S}_{fs} - \tilde{S}_{\alpha\beta}$$

$$\frac{\partial C_b}{\partial \tilde{t}} = \tilde{\nabla} \cdot \left(\tilde{\nabla} \left[\frac{\partial \tilde{G}}{\partial C_b} - \tilde{\nabla}^2 C_b \right] + \tilde{\Theta}_b C_b \left[\frac{D_i}{D_b} \tilde{\nabla} C_i - \frac{D_v}{D_b} \tilde{\nabla} C_v \right] \right)$$

with boundary condition at the *free surface*

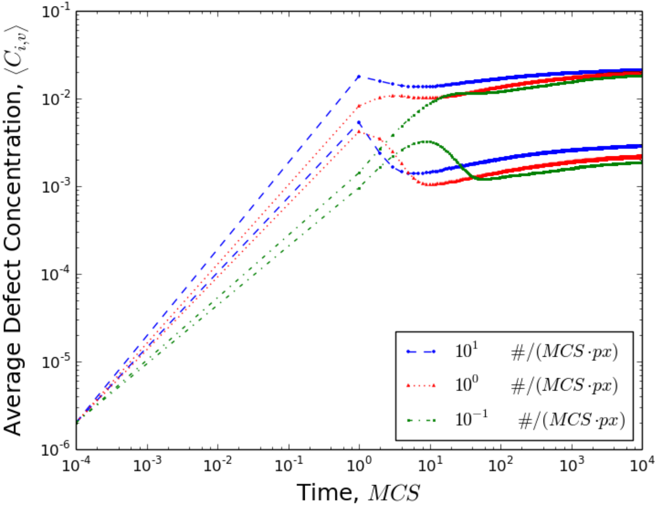
$$\mathbf{J} \cdot \mathbf{n} = 0$$

$$C_{i,v} = C_{i,v}^{eq}$$



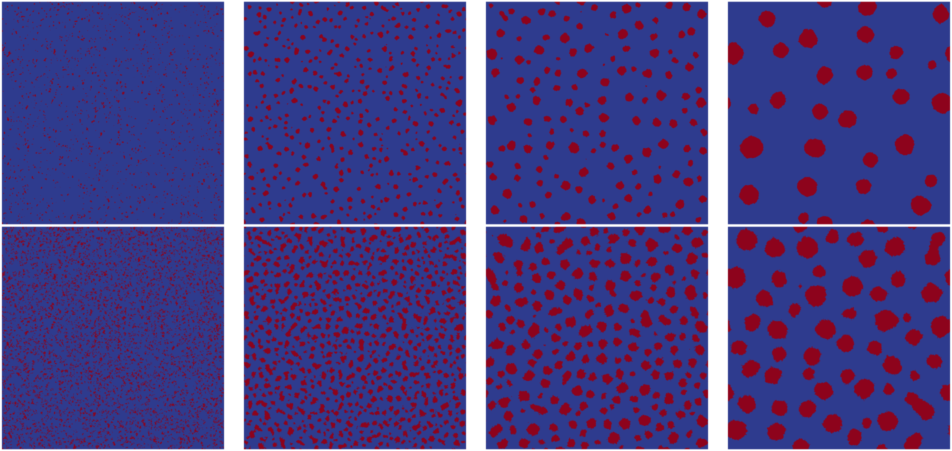
Radiation Characteristics

Low T/Intermediate ρ_s

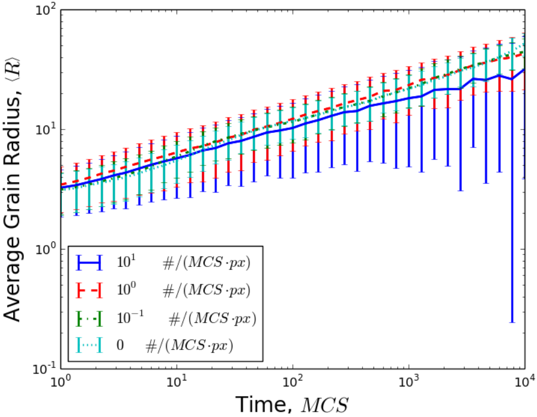


Phase Evolution

$\tau = 1\ MCS$ $\tau = 100\ MCS$ $\tau = 1000\ MCS$ $\tau = 10000\ MCS$



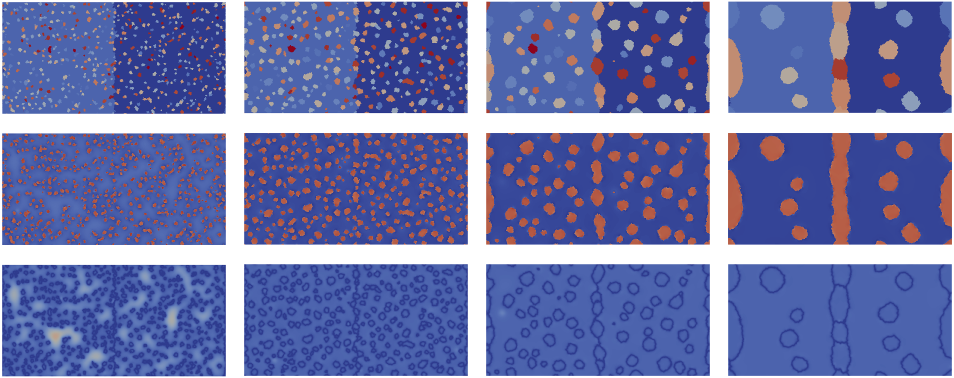
Grain Growth Kinetics



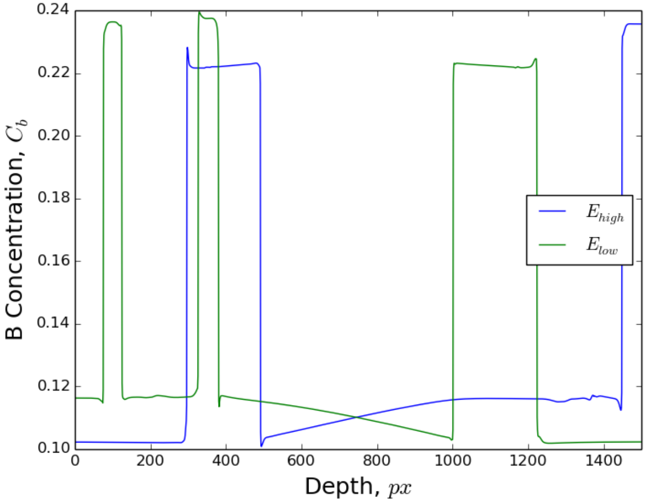
Dose $[\#/(MCS \cdot px)]$	$\sim 10^{1}$	$\sim 10^{0}$	$\sim 10^{-1}$	0
n	4.21	3.62	3.35	3.04

Nucleation at Grain Boundaries

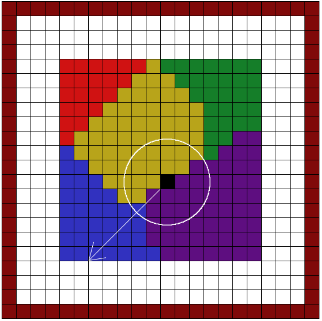
$\tau = 10\ MCS$ | $\tau = 100$ | $\tau = 1000$ | $\tau = 10000$

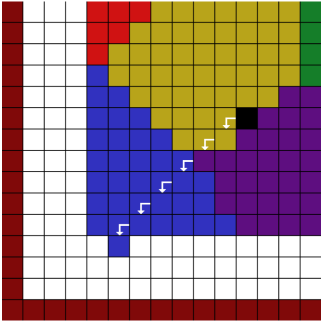


Concentration Profile



Bulk Volumetric Swelling





Swelling simulated by a site exchange mechanism

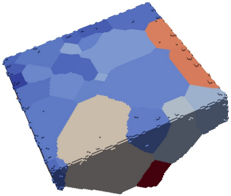
Choosing a random direction

$$p_x = \cos(\phi)\sin(\theta) \qquad p_y = \sin(\phi)\sin(\theta) \qquad p_z = \cos(\theta)$$

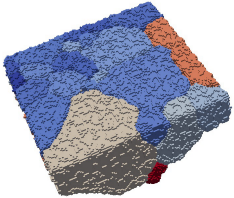
Essentially, "reverse" sintering [*García-Cardona, Tikare* (2011)]

Stages of Percolation

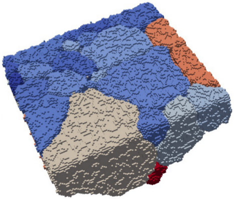
Initial Microstructure (time = 0 MCS)



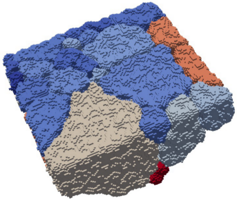
Early Stage (4503 MCS)



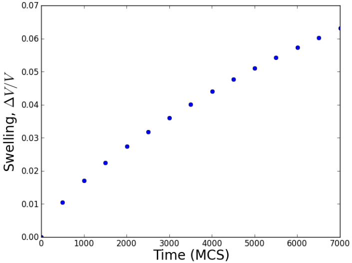
Moderate Stage (8000 MCS)

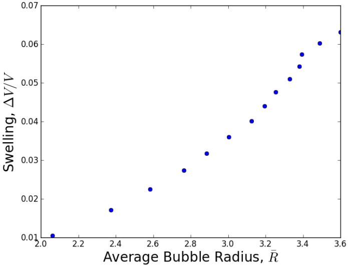


Advanced Stage (23006 MCS)



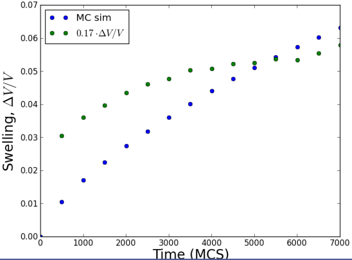
Gas Bubble Swelling



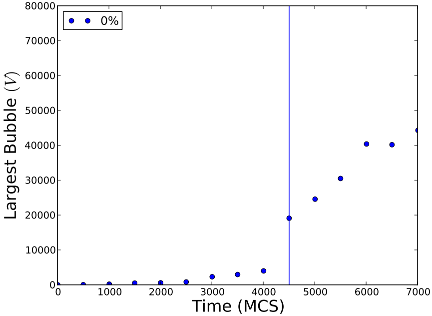


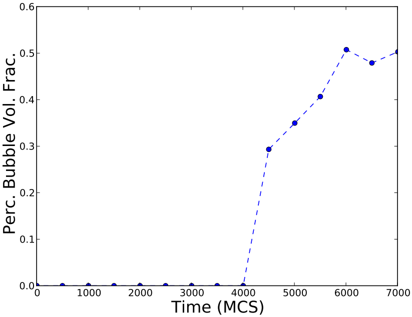
$$\frac{\Delta V}{V} = \frac{2(R_{gb}/a)(R_{gb}/\mathcal{R})^2}{1 - 2(R_{gb}/a)(R_{gb}/\mathcal{R})^2}$$

Agrees with *Kagana*, $\sim 86.3 \pm 3.9\%$ ($\sim 83\%$ at percolation) lower swelling for interlinkage



Bubble Evolution





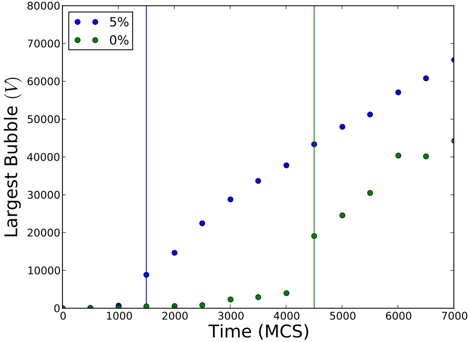
- Substantial increase in bubble volume
- Abrupt increase in volume at $t = t_{perc} \approx 4500$ MCS

Initial Porosity of 5%

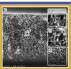
- Initial porosity has significant consequences
  - Percolation time significantly reduced

$$\frac{t_{perc}^{\rho=95\%}}{t_{perc}^{\rho=100\%}} \sim 33\%$$

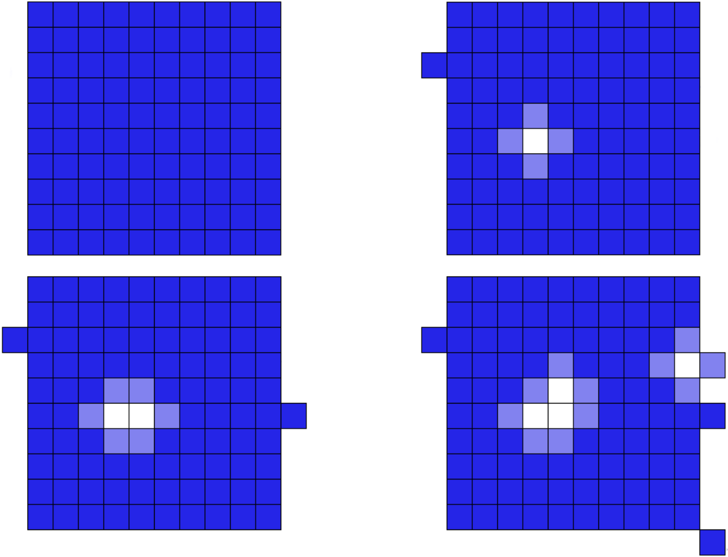
  - Percolation happens with smaller bubbles



Outline



Example of Swelling



Alternative Surface Treatment

Using the "true" definition of a curvature, we define it as

$$\kappa_{S_f} = \nabla \cdot \hat{\mathbf{n}} = \nabla \cdot \left(\frac{\nabla S_f}{\left| \nabla S_f \right|} \right)$$

and the solid fraction evolution is proportional to the Laplacian of the curvature ($\propto \nabla_s^2 \kappa_{S_f}$), where surface gradient is given by

$$\nabla_s = \nabla - \hat{\mathbf{n}}(\hat{\mathbf{n}} \cdot \nabla)$$

$$\begin{aligned}
\nabla_s \kappa_{S_f} &= \nabla \kappa_{s_f} - \hat{\mathbf{n}}\left(\hat{\mathbf{n}} \cdot \nabla \kappa_{S_f}\right) \\
&= \left(\nabla_x \hat{i} + \nabla_y \hat{j} + \nabla_z \hat{k}\right) \kappa_{S_f} \\
&\qquad - \left(n_x \hat{i} + n_y \hat{j} + n_z \hat{k}\right)\left(n_x \nabla_x + n_y \nabla_y + n_z \nabla_z\right) \kappa_{S_f} \\
&= A\hat{i} + B\hat{j} + C\hat{k}
\end{aligned}$$