Phase field simulations of the pinning effect of second-phase particles on grain boundaries:

Effect of particle shape and interfacial properties

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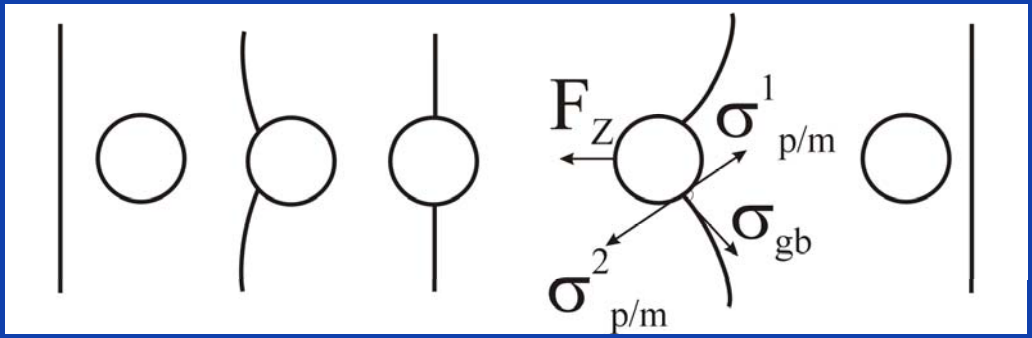
Content

- Zener pinning
- Model formulation + small scale simulations
- Model simplification and implementation for large grain structures + large scale simulations
- Conclusions + future research

Zener pinning

- **Local interaction between particles and grain boundaries**

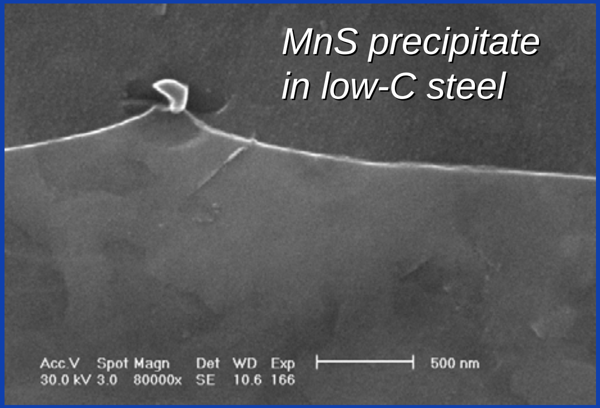


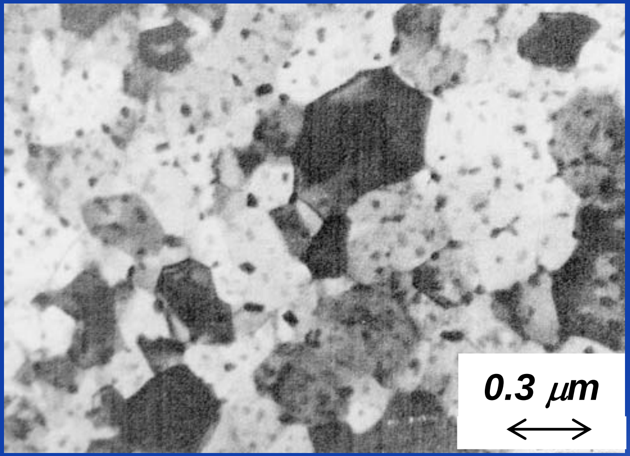
  - **Grain boundary reduction ⇒ pinning force**

- **Macroscopic effect:**
  - **Limiting mean grain size**

$$\frac{\overline{R}_{lim}}{\overline{r}} = K \frac{1}{f_V^b}$$

- **Effect of particle shape, interfacial energy, solubility ?**





Al film containing $CuAl_2$-particles
(H.P. Longworth and C.V. Thompson, 1991)

Model formulation

- **Based on model formulation of L.Q. Chen and Kazaryan et al.**
- **Grains + particles**

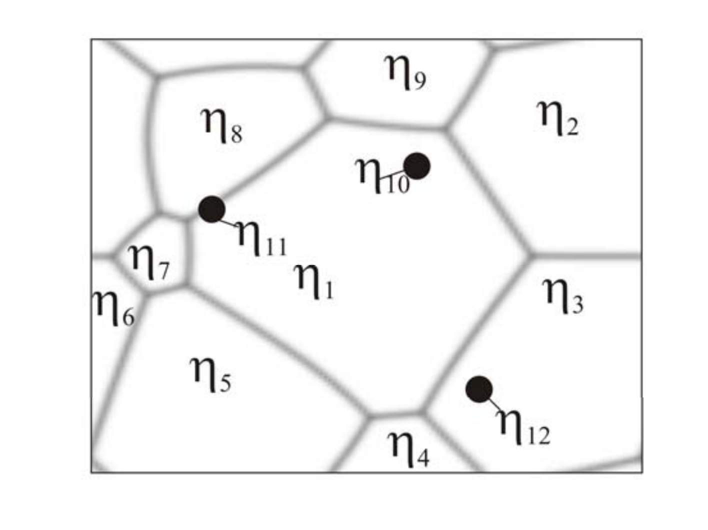
$$\eta_1, \eta_2, \ldots, \eta_i(\vec{r}, t), \ldots, \eta_{p'}, \eta_{p'+1}, \ldots, \eta_p$$

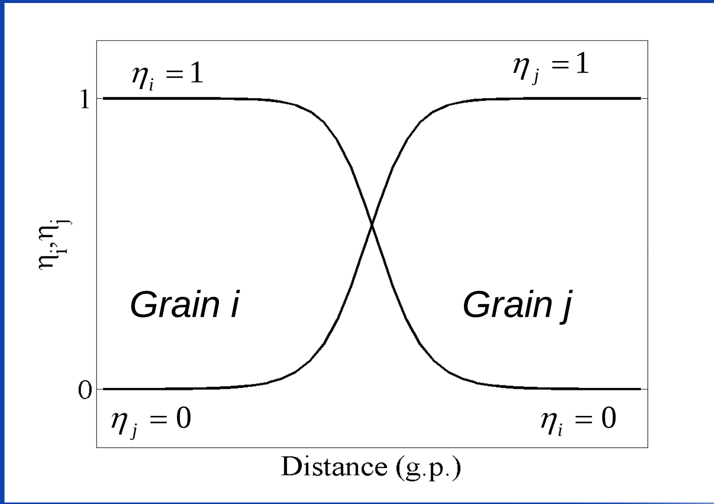
- **Within grains/particles:**

$$(\eta_1, \eta_2, \ldots, \eta_i, \ldots, \eta_p) = (0, 0, \ldots, 1, \ldots, 0)$$

- **Interfaces**

$$\eta_i^2 \eta_j^2 \neq 0$$





Model formulation

- **Temporal evolution**

$$\frac{\partial \eta_i(\vec{r},t)}{\partial t} = -L\frac{\partial F(\eta_1,\ldots,\eta_p)}{\partial \eta_i(\vec{r},t)}$$

- **Free energy**

$$F = \int_V [\, f_0 + \frac{\kappa}{2}\sum_{i=1}^{p}(\nabla \eta_i)^2]dV$$

$$f_0 = m\left(\sum_{i=1}^{p}\left(\frac{\eta_i^4}{4}-\frac{\eta_i^2}{2}\right)+\sum_{i=1}^{p}\sum_{j\neq i}^{p}\gamma_{i,j}\eta_i^2\eta_j^2\right)+\phi_\alpha f_\alpha(c_\alpha)+\phi_\beta f_\beta(c_\beta)+\mu(c-\sum_{\alpha,\beta}\phi_\alpha c_\alpha)$$

$$\kappa = \frac{\sum_{i=1}^{p}\sum_{j<i}^{p}\kappa_{i,j}\eta_i^2\eta_j^2}{\sum_{i=1}^{p}\sum_{j<i}^{p}\eta_i^2\eta_j^2} \Rightarrow \kappa = \kappa_{i,j}$$

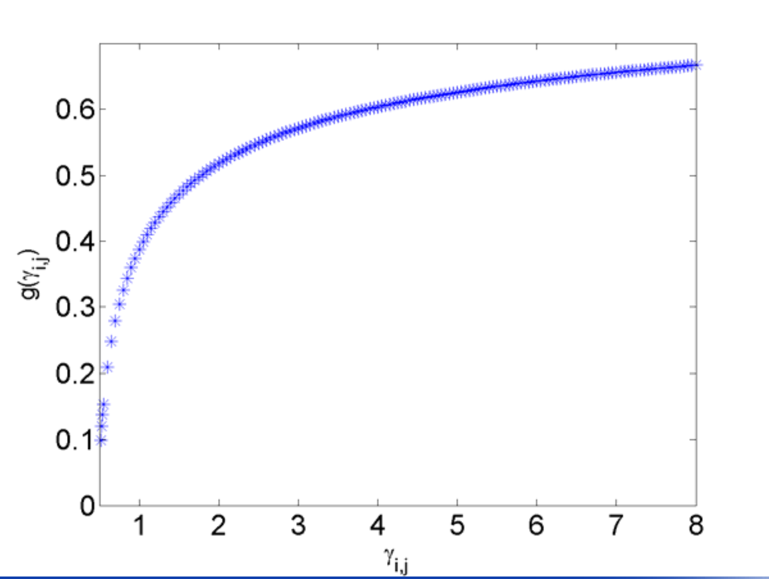
At the interface between grain i and j

Model formulation

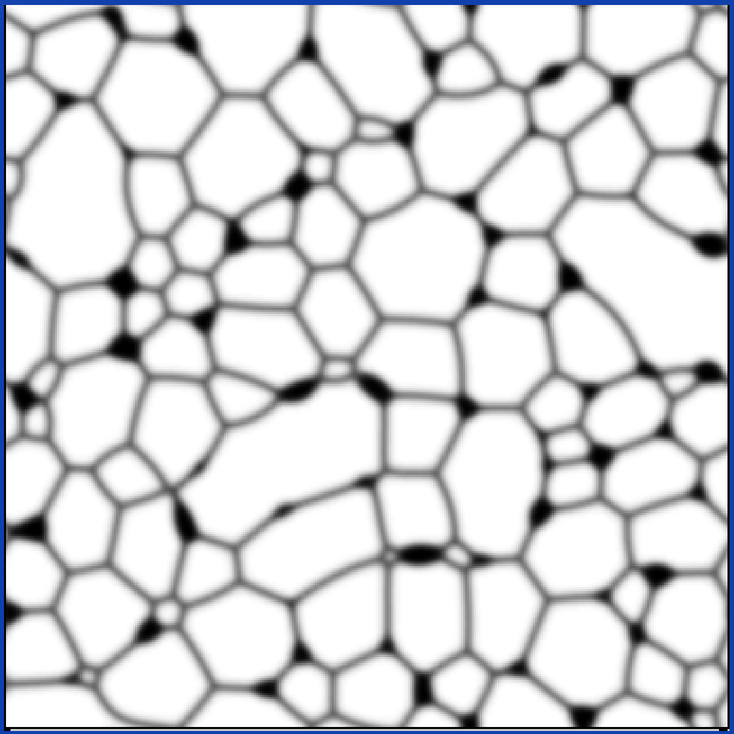
- **Bulk free energy**
  - **Based on multi-phase field approach**
  - **Phase fractions**

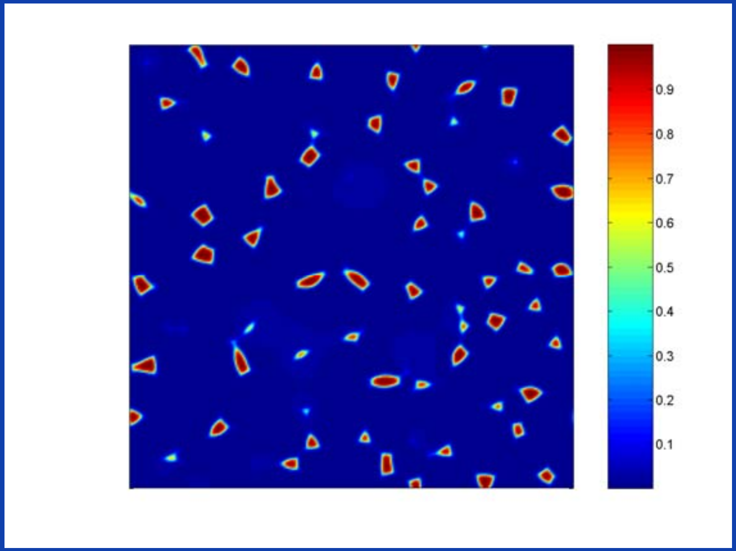
$$\phi_\alpha = \frac{\sum_{i,\alpha} \eta_i^2}{\sum_{i,\alpha} \eta_i^2 + \sum_{i,\beta} \eta_i^2}, \qquad \phi_\beta = \frac{\sum_{i,\beta} \eta_i^2}{\sum_{i,\alpha} \eta_i^2 + \sum_{i,\beta} \eta_i^2}$$

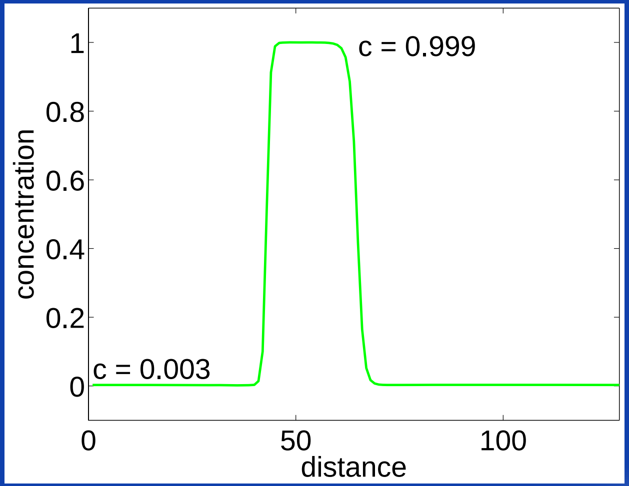
- **Interfacial/grain boundary properties**
  - **Energy** $\sigma_{i,j} = g(\gamma_{i,j})\sqrt{m\kappa_{i,j}}$
  - **Mobility** $\mu_{i,j} = L_{i,j}\sqrt{\frac{\kappa_{i,j}}{m(g(\gamma_{i,j}))^2}}$
  - **Thickness** $l \propto \sqrt{\frac{\kappa_{i,j}}{m(g(\gamma_{i,j}))^2}}$



Evolving particles



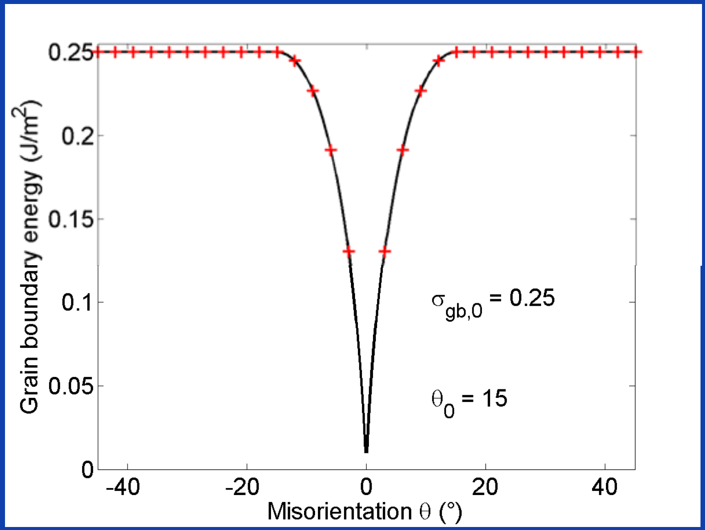


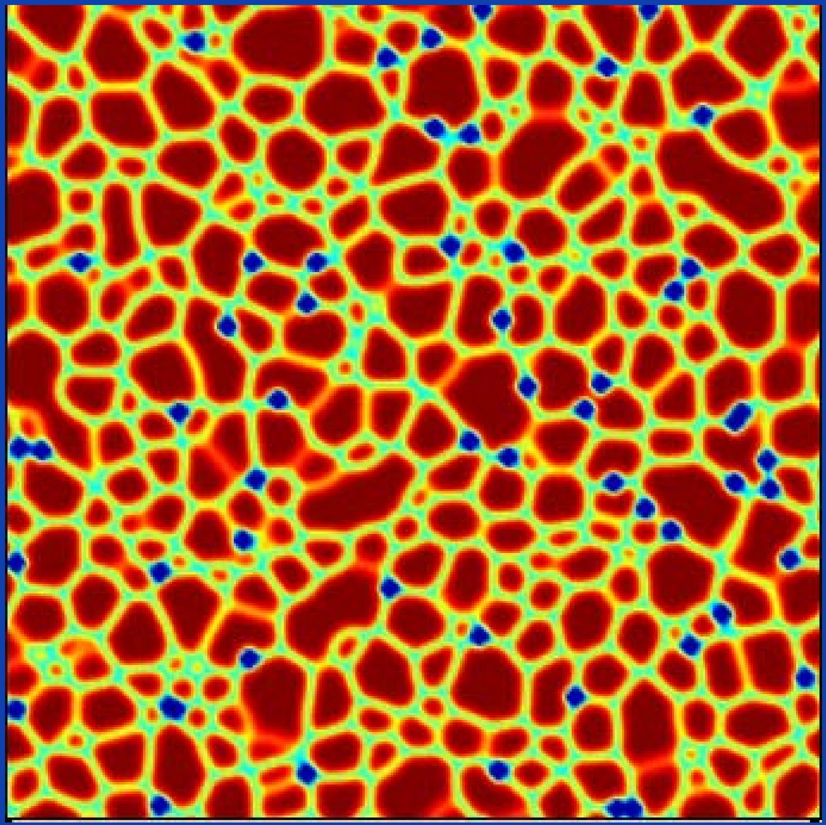


$c_{eq,part}$ =0.001, $c_{eq,matrix}$ = 0.999
D_{part} = 0.01, D_{matrix} = 0.1
σ_{gb} = 0.25, σ_{int} = 0.2
c_{total} = 0.05
30 + 1 order parameters

Misorientation dependent grain boundary energy

$c_{eq,part}$ =0.000001, $c_{eq,matrix}$ = 0.999999
D_{part} = 0, D_{matrix} = 0
c_{total} = 0.05
σ_{int} = 0.2
σ_{gb} = 0.25 (high angle)
30 +1 order parameters

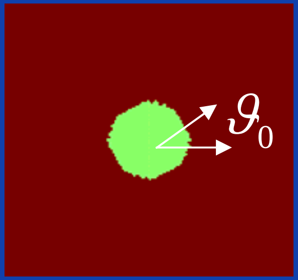


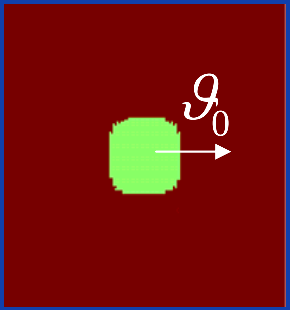


Read-Shockly: $\sigma_{gb} = \sigma_{gb,0} \frac{|\theta|}{\theta_0}\left(1 - \ln\left(\frac{|\theta|}{\theta_0}\right)\right), \quad 0 < |\theta| < \theta_0$

Particle shape

- **Strong anisotropy**
  - **Plates (2D):** $\sigma_{\text{int}} = \bar{\sigma}(1+\delta_\sigma \,|\sin(\vartheta_0+\vartheta)|)$
  - **Cubes (2D):** $\sigma_{\text{int}} = \bar{\sigma}(1+\delta_\sigma \,|\sin(\vartheta_0+2\vartheta)|)$





- **Introduced via κ and γ**

$$\kappa_{i,j} = \bar{\kappa}_{i,j}(1+\delta_\sigma \,|\sin(\vartheta_0+\vartheta)|)$$

$$g(\gamma_{i,j}) = g(\gamma_{i,j})\sqrt{(1+\delta_\sigma \,|\sin(\vartheta_0+\vartheta)|)}$$

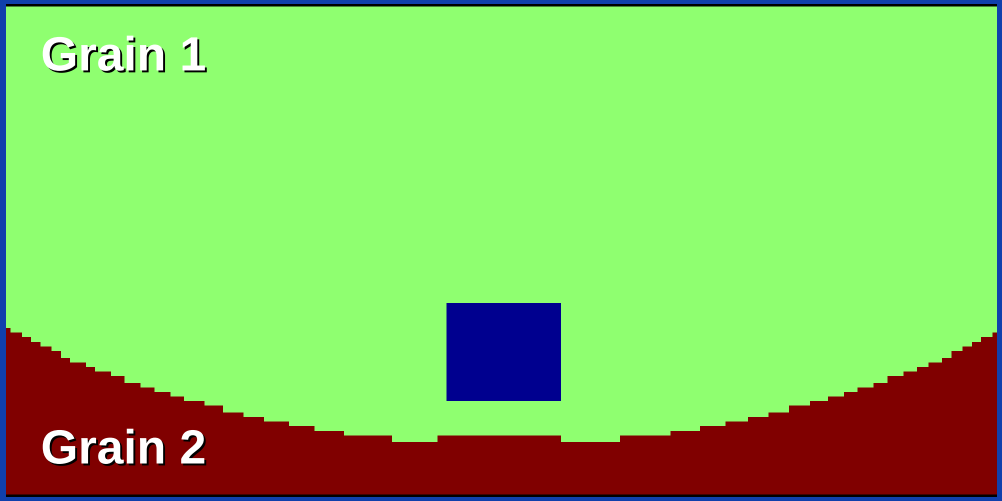
- $\Rightarrow$

$$\sigma_{i,j} = g(\gamma_{i,j})\sqrt{m\kappa_{i,j}}$$

$$l \propto \sqrt{\frac{\kappa_{i,j}}{m(g(\gamma_{i,j}))^2}} = cte$$

Coherent->incoherent

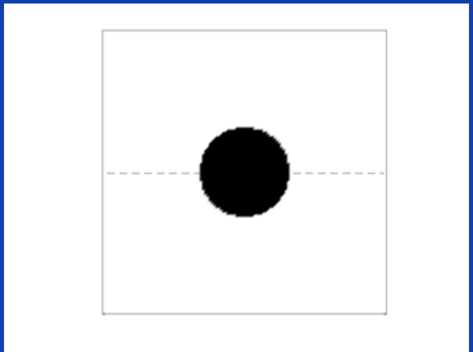
- **Coherent interface:** $\sigma_1 = 0.3(1+1.6\,|\sin(2\vartheta)|)$
- **Incoherent interface:** $\sigma_2 = 0.78$



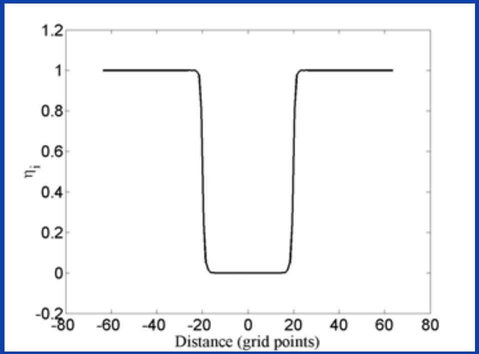
$c_{eq,part} = 0.001$, $c_{eq,matrix} = 0.999$
$D_{part} = 0.01$, $D_{matrix} = 0.1$

Model simplifications and implementation for large grain structures

- **Fixed sharp-interface representation for the particles**
  - **Less grid points required per particle**
  - **Less equations to solve**

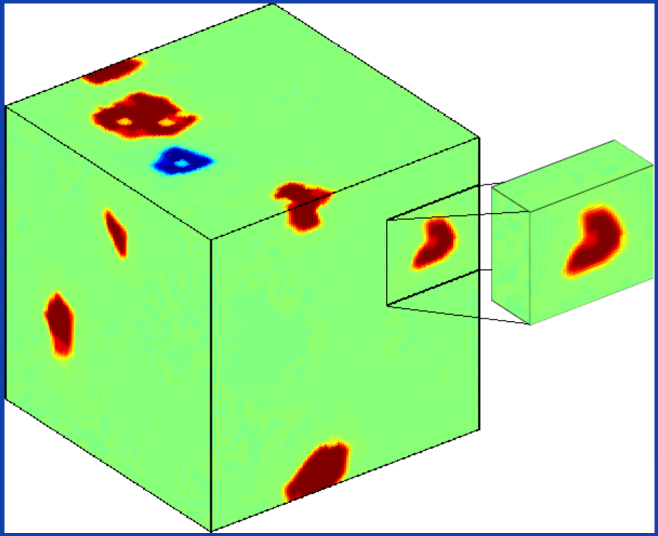


η_{part}



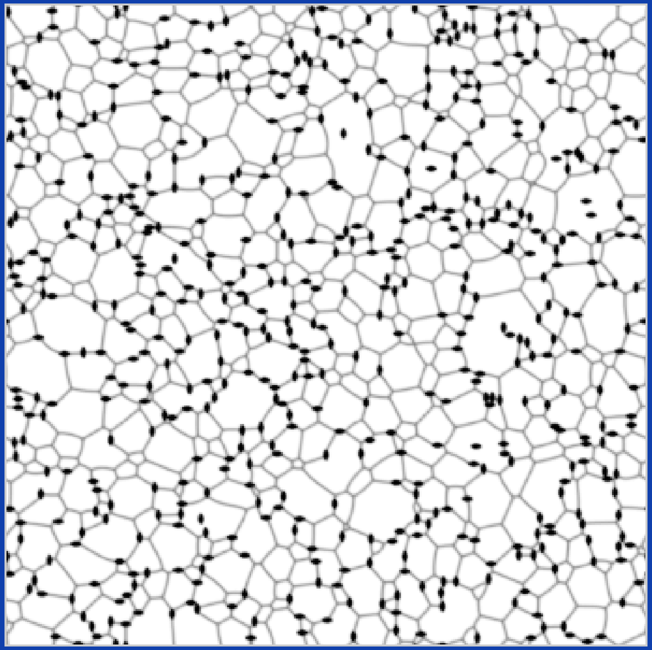
η_{grain}

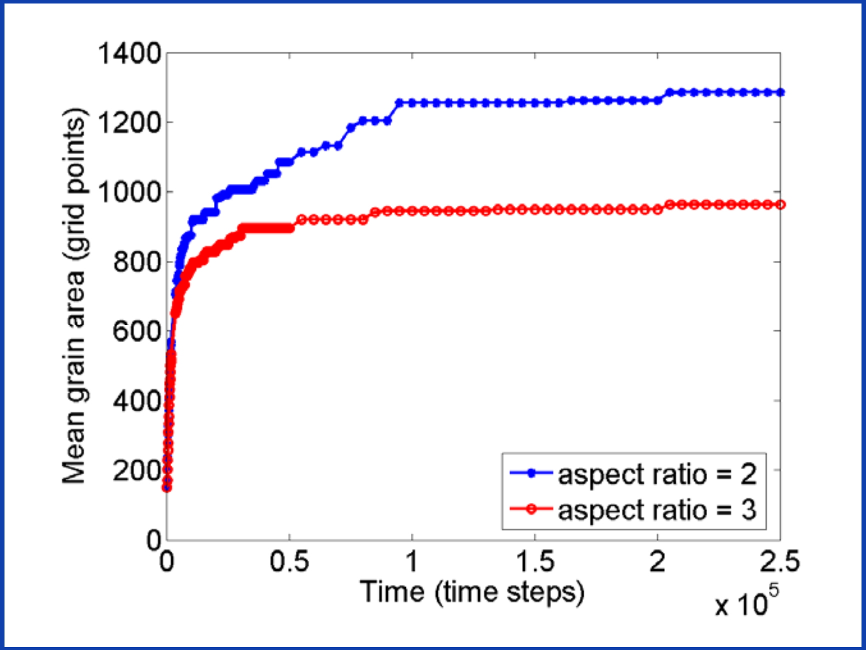
- **Bounding box algorithm**
  - **Equations are only solved locally**
  - **Boxes allow a semi-implicit time stepping**
  - **Prevents grain coalescence**



Ellipsoidal particles: 2D simulations

- **Effect of aspect ratio**

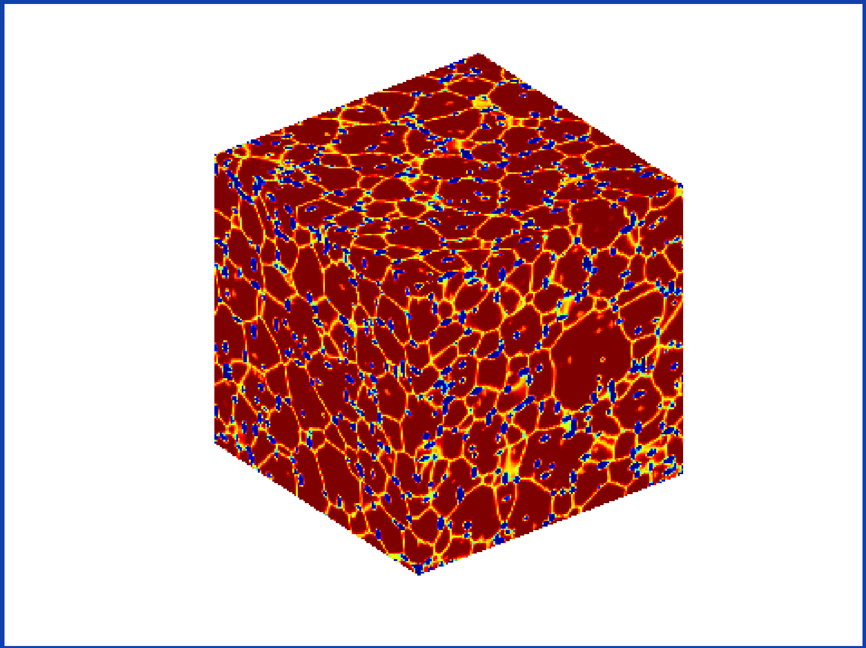


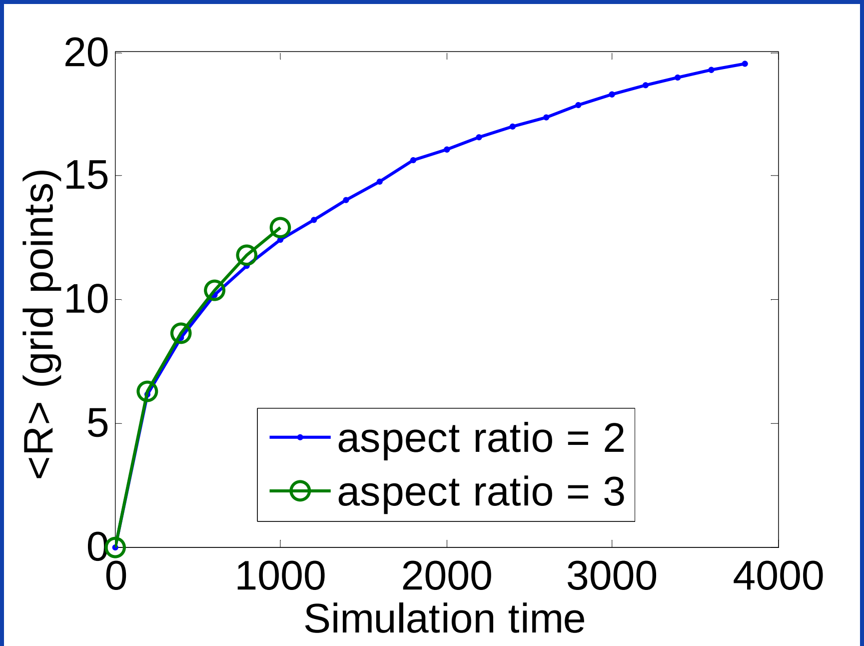


f_V = 0.05, aspect ratio = 2

100 + 1 order parameters

Ellipsoidal particles: 3D simulations





f_V = 0.05, aspect ratio 2

1 order parameter / grain

Conclusions

- We presented a phase field model and simulations for grain growth in the presence of second-phase particles
  - The model can account for the interfacial properties and stability of the second phase
- We proposed an approach to treat large grain structures
- Further research
  - Add more features to the bounding box implementation
  - Initialization grain structure
  - Data storage / post processing
  - Validation of the simulations