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Phase field simulations of grain growth in materials containing second-phase particles

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Contents

- Introduction on Zener pinning
- Phase field model
- Grain boundary/particle interactions
- Large-scale 2D-simulations
- Conclusions

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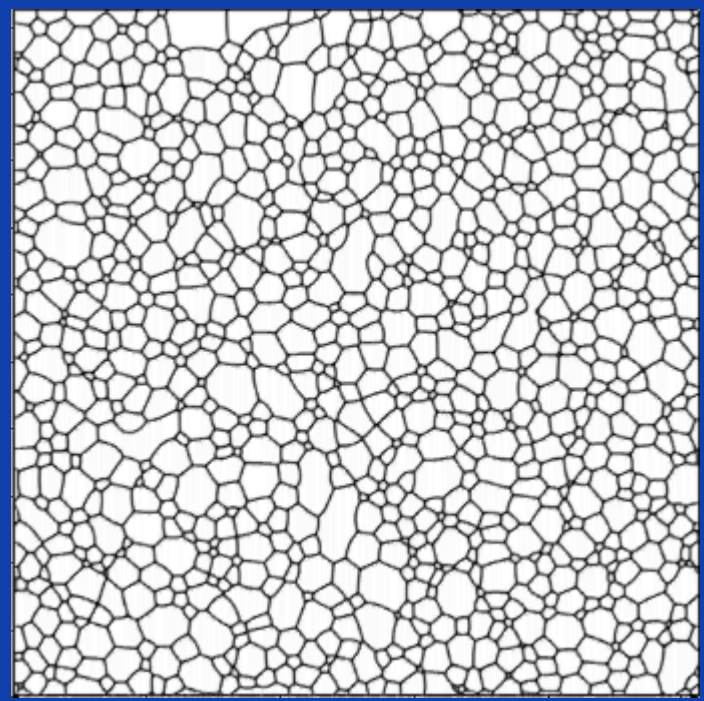
Grain growth

- Reduction of grain boundary energy
- Pure single phase materials
  - Parabolic growth law

$$\overline{R} = k * t^{1/2}$$

  - Grain size distribution time-invariant
- Real materials
  - Impurity drag
  - Zener pinning
  - Multiple phases



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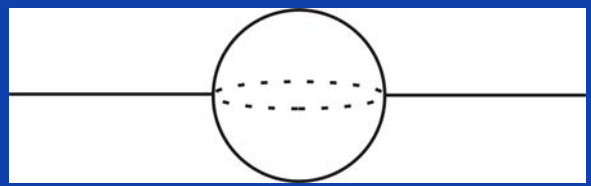
Zener pinning

- **Grain boundary-particle intersection**

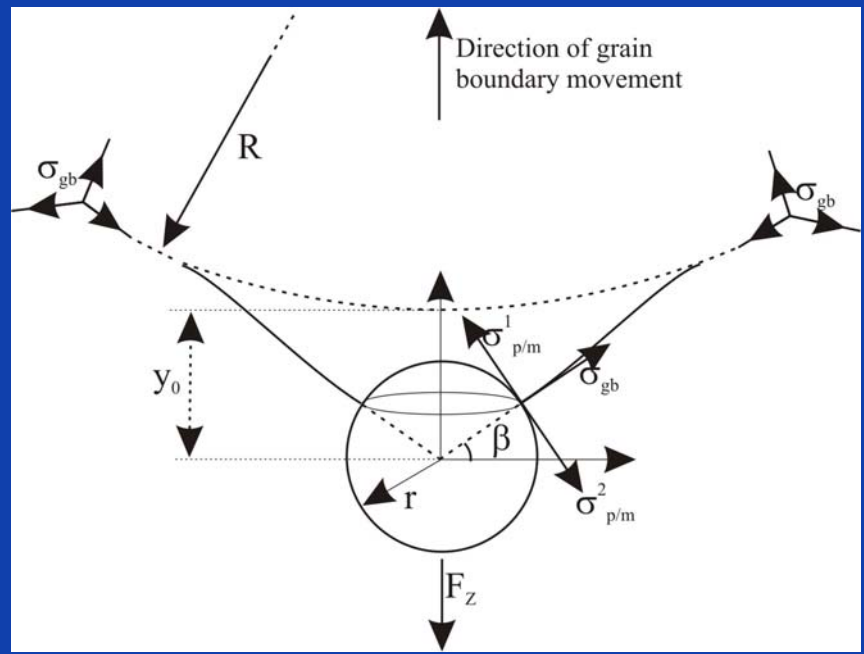


  - **=>Energy reduction**

$$2r\sigma_{gb}(2D)$$

$$\pi r^2\sigma_{gb}(3D)$$

  - **=> Interaction between grain boundaries and particles**
- **'Dimple shape'**
- **Limiting grain size:** $\dfrac{\overline{R_{\lim}}}{\bar{r}} = \dfrac{b}{f_V^{\beta}}$



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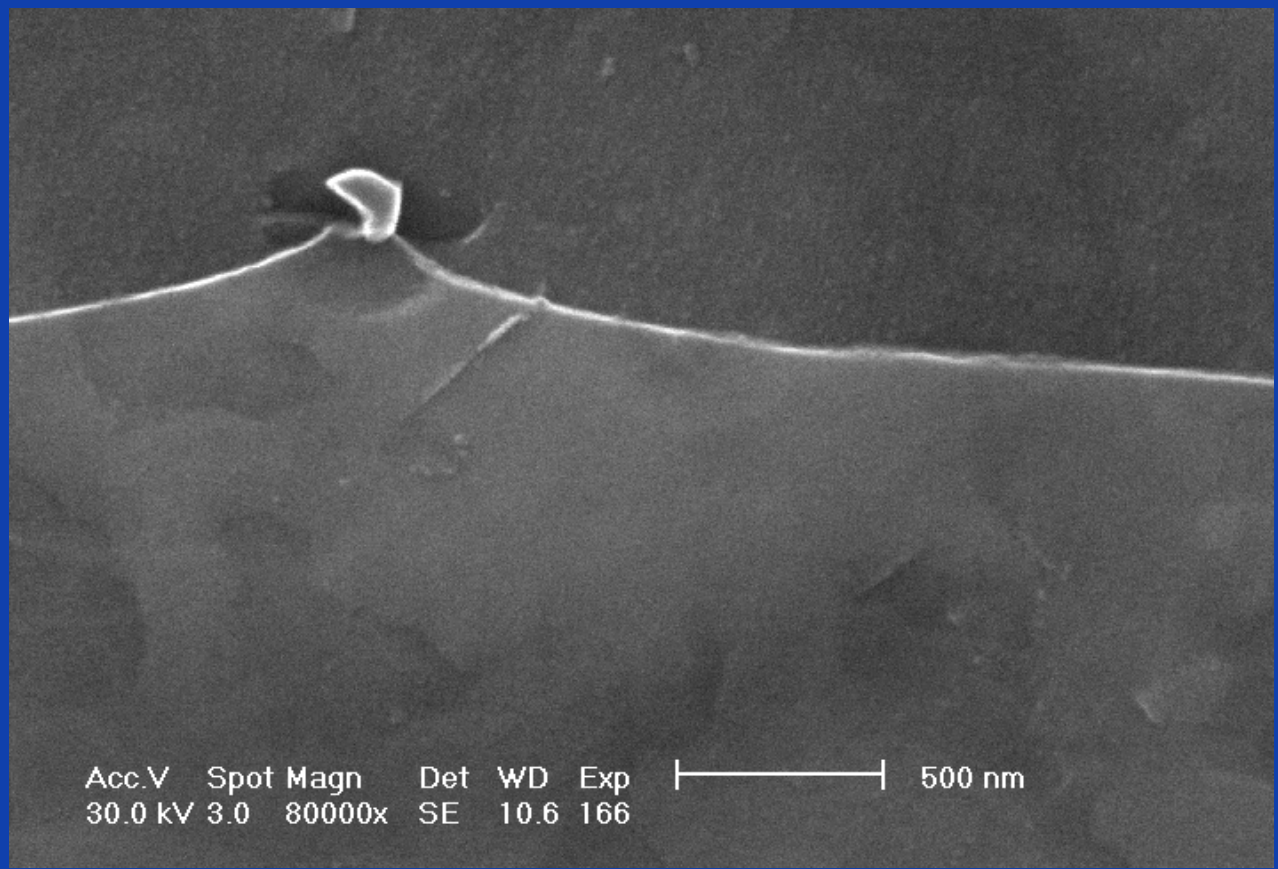
Experimental observation

- **MnS-particle in low-C steel**



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Phase field model

- **Extension of model of D. Fan and L.-Q. Chen for normal grain growth**
- **Phase field variables:**

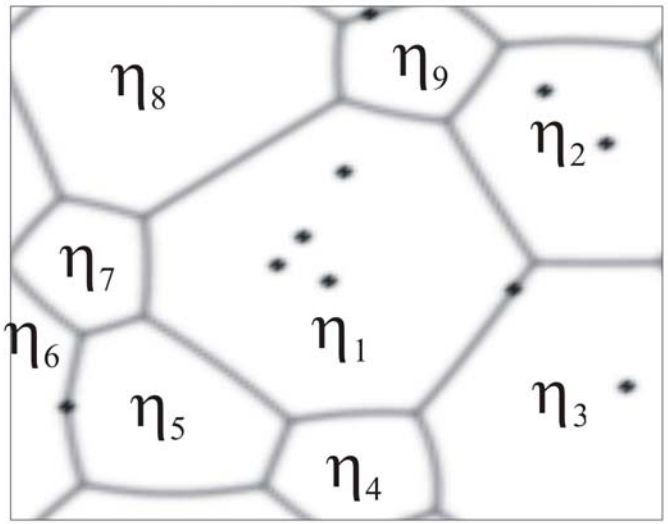
$$\eta_1, \eta_2, \ldots, \eta_i, \ldots, \eta_p$$

- **Particles : Φ=1**

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

- **Grain i of matrix-phase : Φ=0**

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



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Phase field model

- **Free energy**

$$F = \int_V \left[m\left(\sum_{i=1}^{p} \left(\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2}\right) + \sum_{i=1}^{p}\sum_{j\neq i}^{p} \eta_i^2 \eta_j^2 \right) + \varepsilon\Phi \sum_{i=1}^{p} \eta_i^2 + \sum_{i=1}^{p} \frac{\kappa}{2} (\nabla \eta_i)^2 \right] dV$$

- **Equilibrium**
  - **Φ=0 :** $(\eta_1, \eta_2, ..., \eta_p) = (1,0,...,0),(0,1,...,0),...(0,0,...,1),(-1,0,...,0),...$
  - **Φ=1 :** $(\eta_1, \eta_2, ..., \eta_p) = (0,0,...,0)$

- **Kinetic equations (Ginzburg-Landau)**

$$\frac{\partial \eta_i(\vec{r},t)}{\partial t} = -L\frac{\partial F}{\partial \eta_i(\vec{r},t)} = -L\left(\frac{\partial f_0(\eta_1,\eta_2,...)}{\partial \eta_i(\vec{r},t)} - \kappa\nabla^2 \eta_i(\vec{r},t) \right)$$

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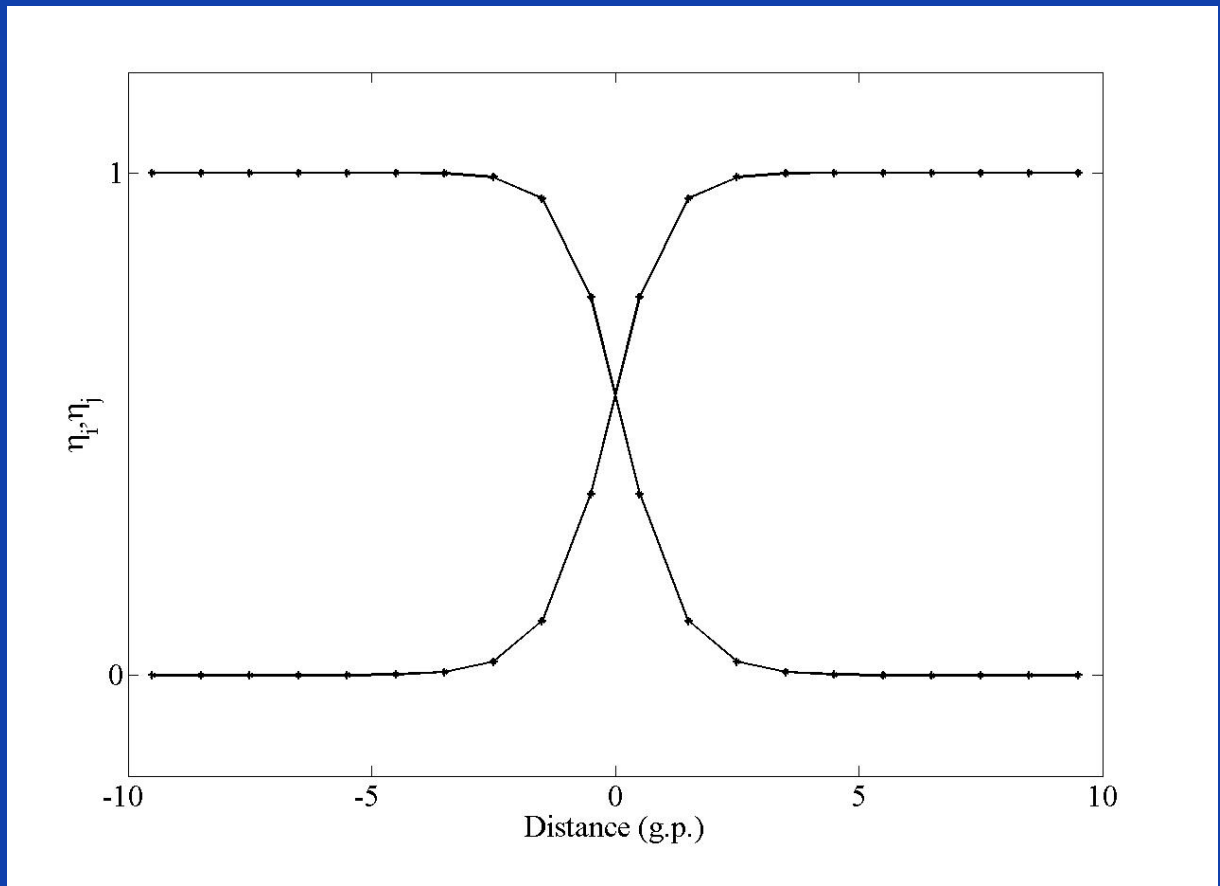
Diffuse grain boundaries



- **Grain boundary thickness** $\propto \sqrt{\frac{\kappa}{m}}$

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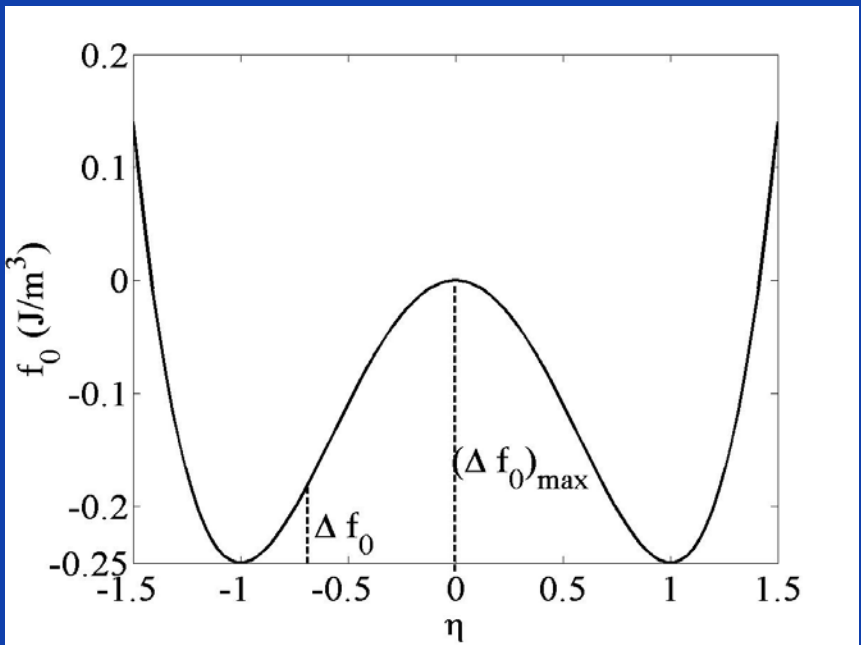
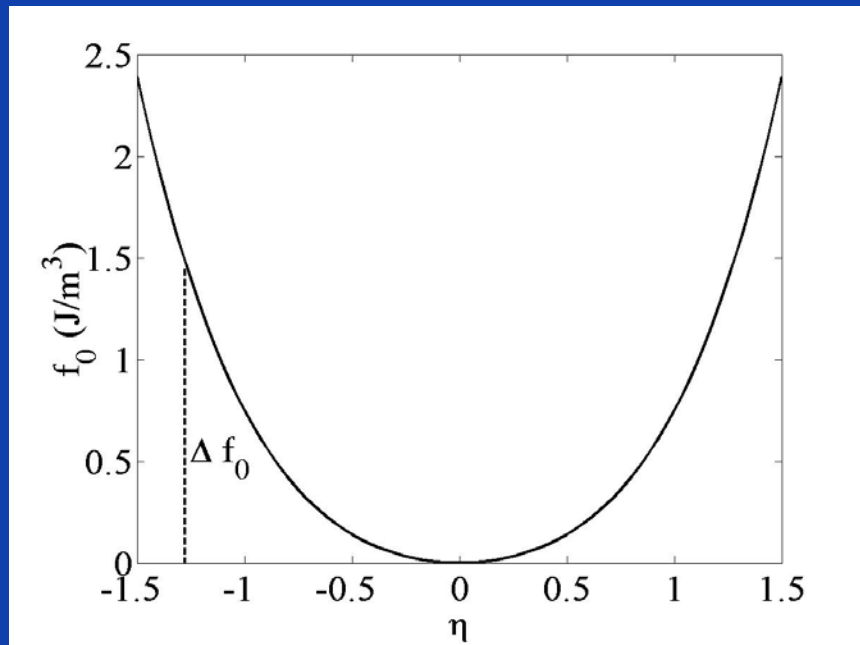
Local free energy

- **Matrix phase**



- **Second-phase particle**



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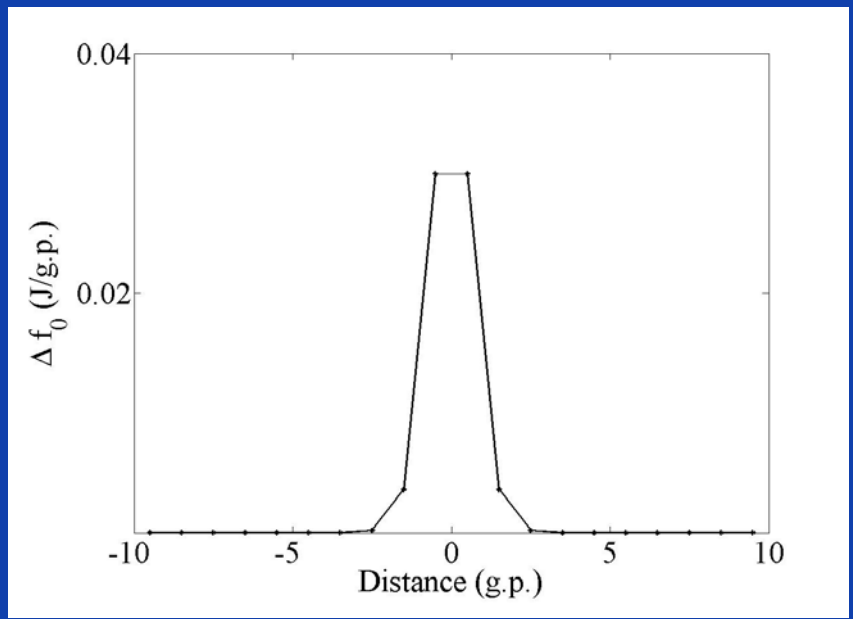
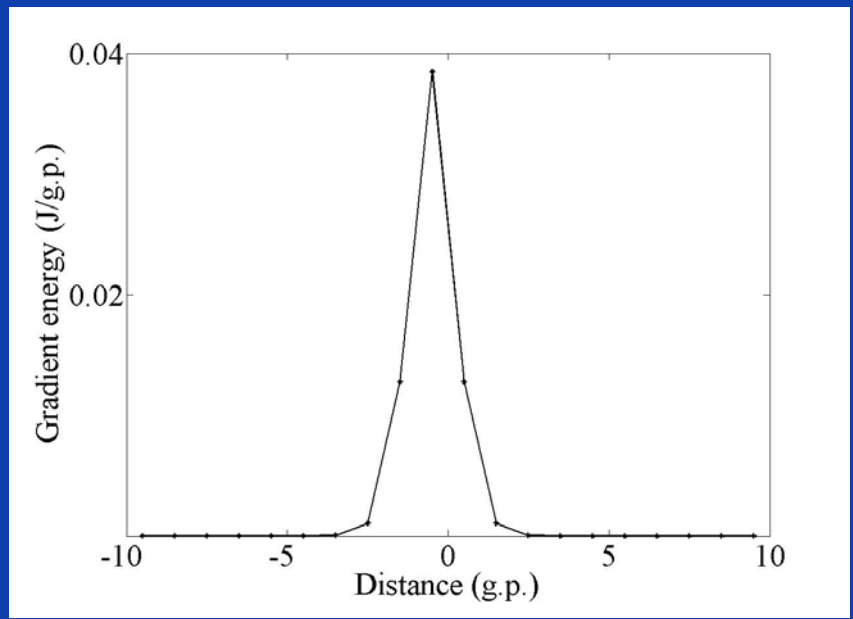
Grain boundary energy

- **Contribution local free energy**



- **Contribution due to gradient**



- **Total grain boundary energy** $\propto \sqrt{\kappa m}$

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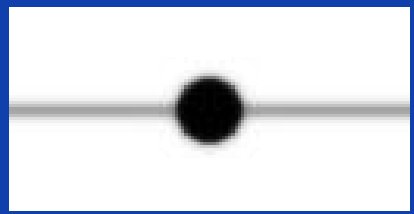
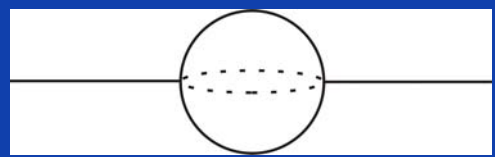
Grain boundary/particle interaction

- **Energetic consideration:**
  - **Geometry :**



  - **Theoretical interaction energy:**



$$2r\sigma_{gb}(2D)$$

$$\pi r^2\sigma_{gb}(3D)$$

- **Diffuse grain boundaries**
  - **Interaction energy slightly too negative**
  - **Lower limit on particle size**

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Local interactions: spherical grain

- **Grain boundary moving through particle: 3D-simulation**
  - $\kappa = 0.5, m = 1, L = 1$

    $r = 8, R_0 = 90, d_{c-p} = 76$

- **'dimple shape'**

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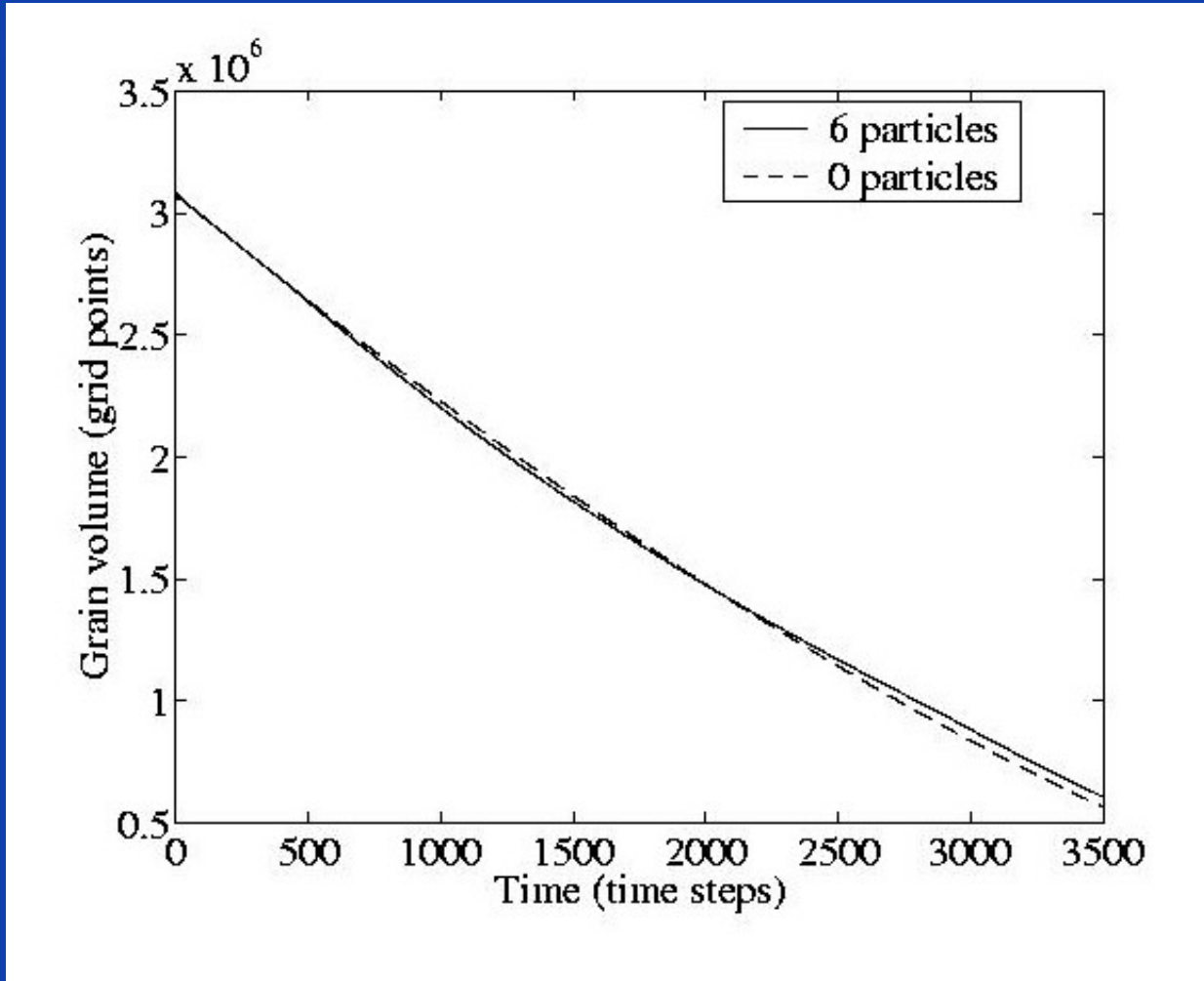
Temporal evolution spherical grain



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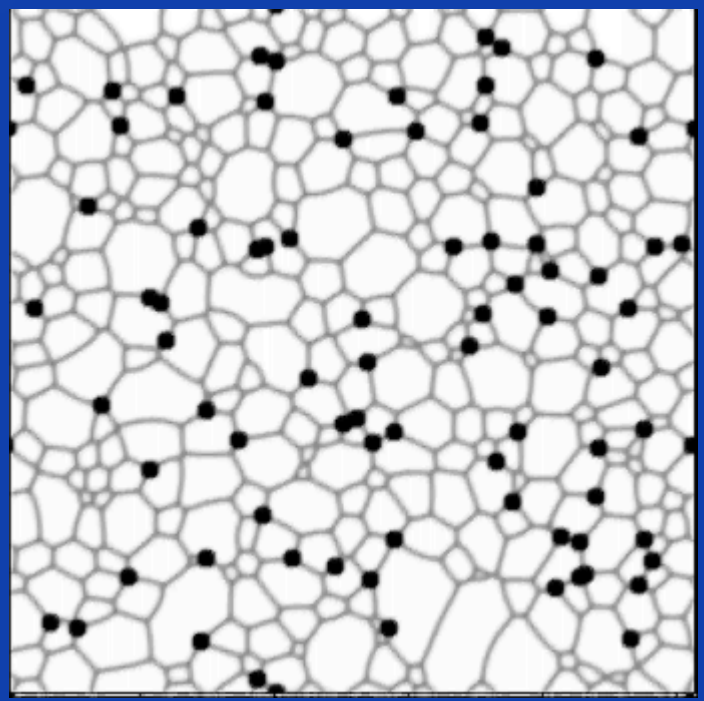
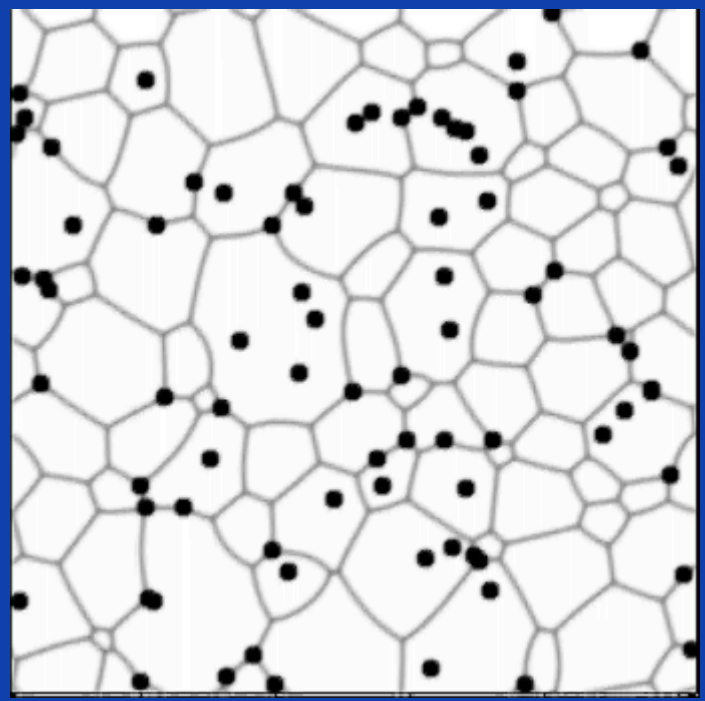
Large-scale 2D-simulations



$r = 3,\ f_a = 0.04,\ \overline{R}_0 = 0$



$r = 3,\ f_a = 0.04,\ \overline{R}_0 = 13.6$

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Final grain size

- $\frac{\overline{R_{\lim}}}{\overline{r}} = \frac{b}{f_a^{\beta}}$
- **Phase field ($R_0 = 0$):**

$\beta = 0.48 \pm 0.05$

$b = 1.24 \pm 0.30$

Theory

$\beta = 0.5, b = \sqrt{3}$

Monte Carlo

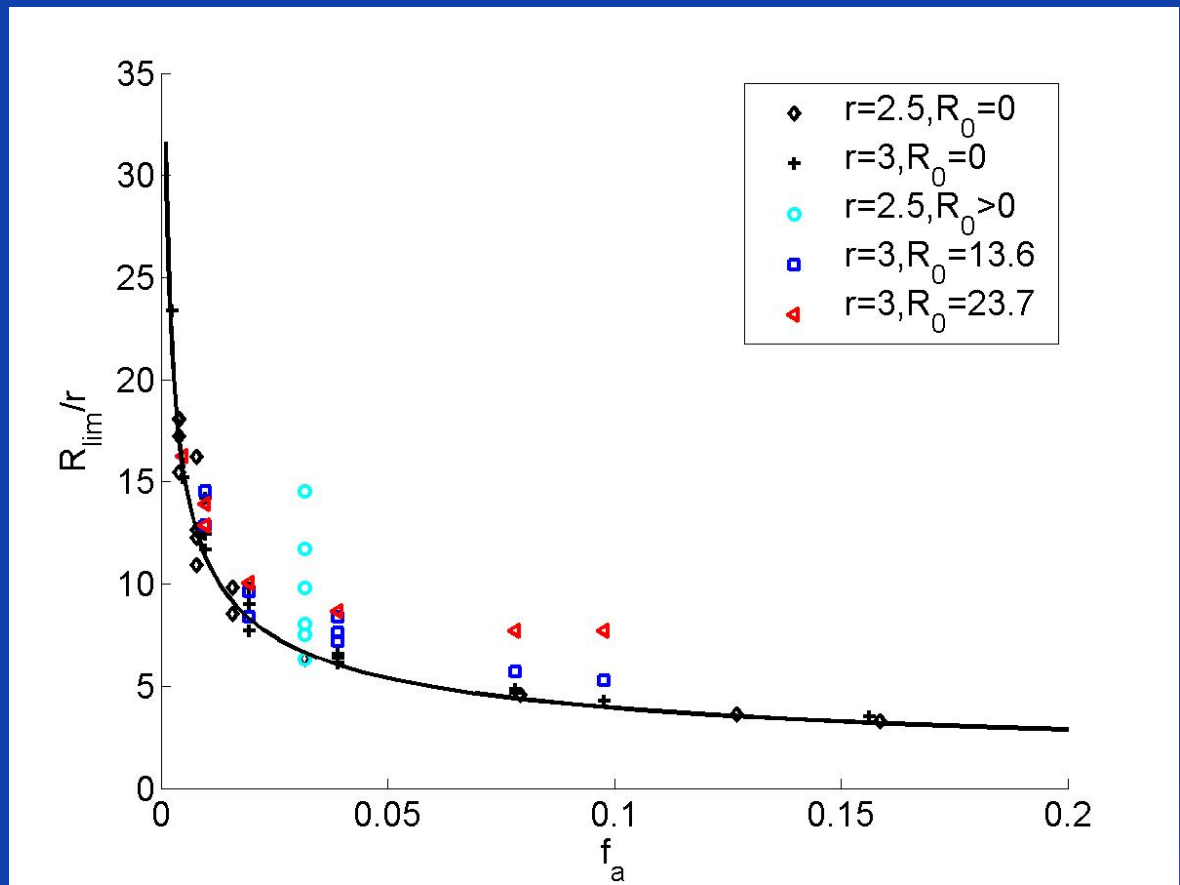
$\beta = 0.5, b = 1.7$

$\beta = 0.54, b = 1.2$

Vertex

$\beta = 0.46$

$\beta = 0.5$



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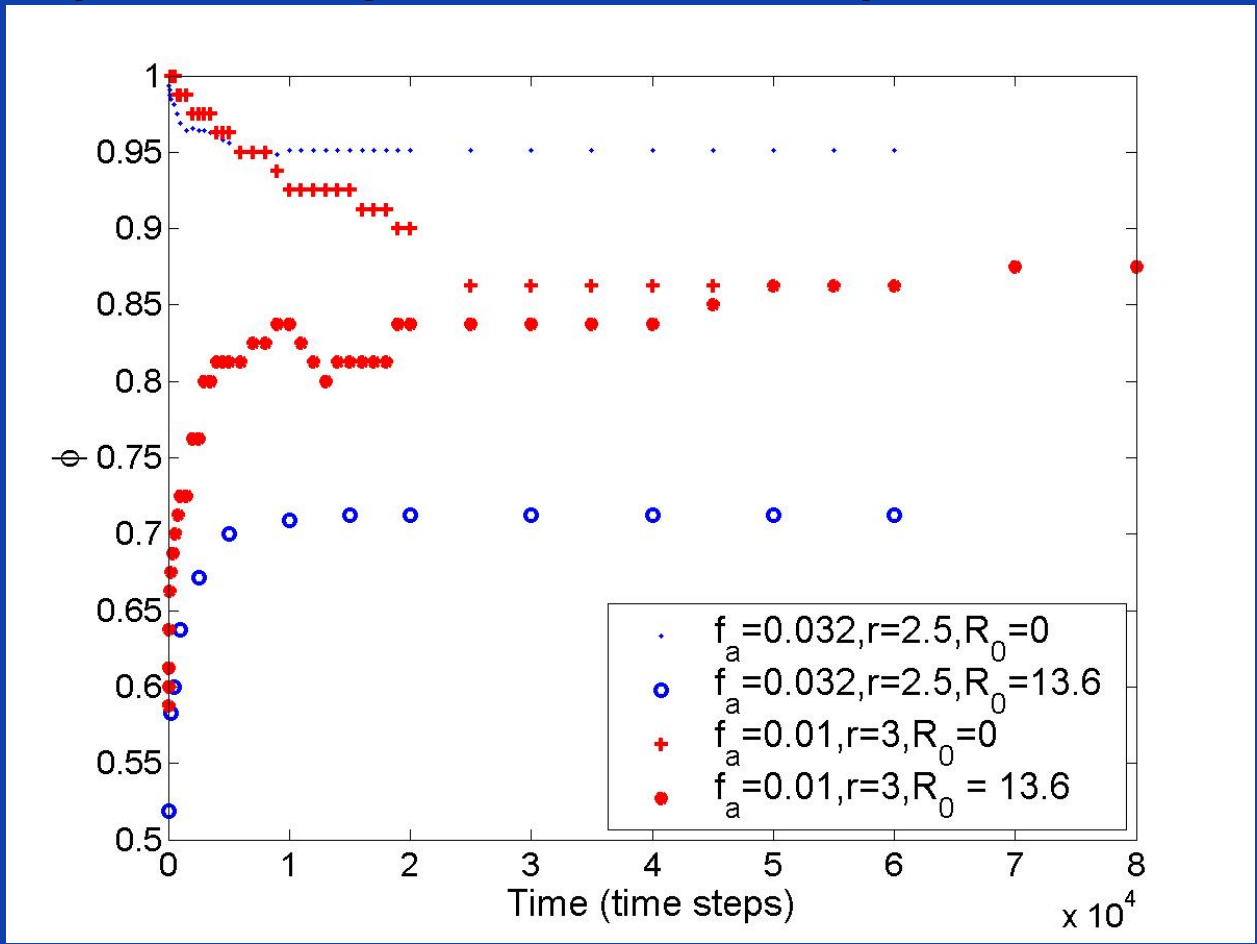
Role initial grain size

- **Fraction of particles on grain boundaries: temporal evolution**



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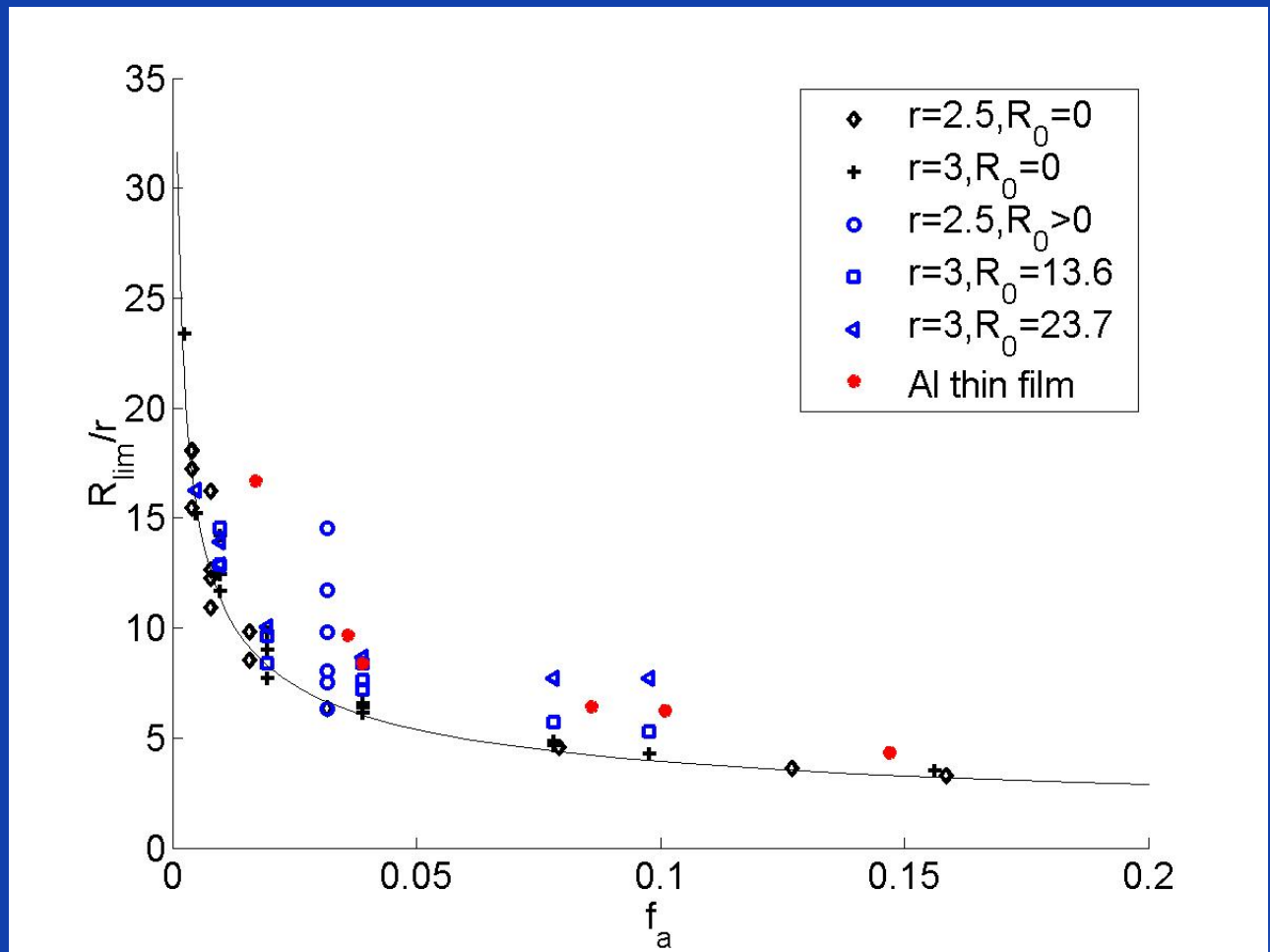
Comparison with experiment

- Thin Al-films
  - Columnar grains
  - 2D- structure
  - $CuAl_2$-particles



Data from H.P. Longworth and C.V. Thompson

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Conclusions

- Zener pinning was studied as a function of
  - Particle size
  - Area fraction of particles
  - Initial microstructure
- Good correspondence with models and previous simulations
- Experiments indicate that more parameters should be included
- Systematic experimental information on grain boundary energy and mobility is required

End

Thank you for your attention !

http://www.ulyssis.org/~nele/

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References

- N. Moelans, B. Blanpain, P. Wollants, "A phase field model for the simulation of grain growth in materials containing finely dispersed incoherent second-phase particles", Acta Mater., 53, pp 1771-1781, 2005.

- N. Moelans, B. Blanpain, P. Wollants, "Phase field simulations of grain growth in 2-dimensional systems containing finely dispersed second-phase particles", submitted to Acta Mater.

- Available on http://www.ulyssis.org/~nele/