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

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Zener pinning

- **Grain growth:**

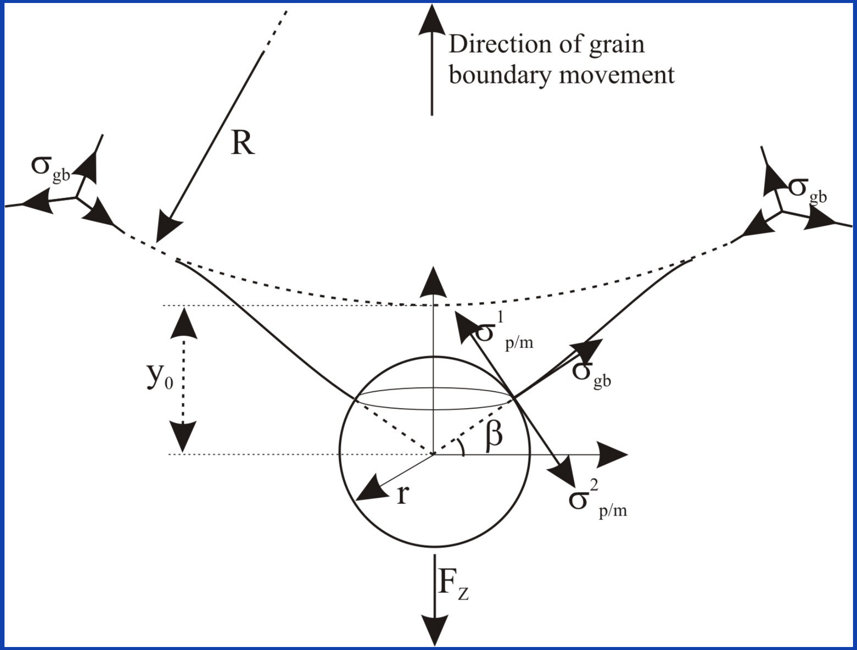
$$P = \sigma_{gb}\left(\frac{1}{R_1} + \frac{1}{R_2}\right)$$

- **Zener pinning:**

$$F_Z^{\max} = \pi r \sigma_{gb} (3D)$$

- **'Dimple shape'**
- **Limiting grain size:**

$$\frac{\overline{R_{\lim}}}{\bar{r}} = \frac{b}{f_V^{\beta}}$$



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Phase field model

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

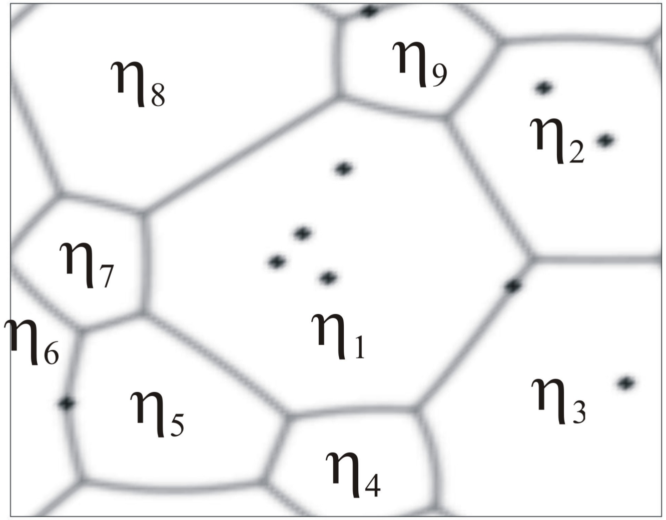
$$\eta_1, \eta_2, \ldots, \eta_i, \ldots, \eta_p$$

- 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**

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

- **Equilibrium**
  - **Φ=0 :** $(\eta_1, \eta_2, \ldots, \eta_p) = (1,0,\ldots,0), (0,1,\ldots,0), \ldots (0,0,\ldots,1), (-1,0,\ldots,0), \ldots$
  - **Φ=1 :** $(\eta_1, \eta_2, \ldots, \eta_p) = (0,0,\ldots,0)$
- **Kinetic equations (Ginzburg-Landau)**

$$\frac{\partial \eta_i(\vec{r},t)}{\partial t} = -L_i \frac{\partial F}{\partial \eta_i(\vec{r},t)} = -L_i \left(\frac{\partial f(\eta_1, \eta_2, \ldots)}{\partial \eta_i(\vec{r},t)} - \kappa_i \nabla^2 \eta_i(\vec{r},t) \right)$$

Model parameters

- **Equations** $$\frac{\partial \eta_i(\vec{r},t)}{\partial t} = -L_i \left(\frac{\partial f(\eta_1,\eta_2,\ldots)}{\partial \eta_i(\vec{r},t)} - \kappa_i \nabla^2 \eta_i(\vec{r},t) \right)$$
  - **with** $$f = m\left(\sum_{i=1}^{p} \left(\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2}\right) + \sum_{i=1}^{p} \sum_{j\neq i}^{p} \eta_i^2 \eta_j^2 \right) + \varepsilon \Phi \sum_{i=1}^{p} \eta_i^2$$
- **Grain boundary energy (expressed in J/g.p.)**

$$\kappa = 0.5, m = 1 \Rightarrow \sigma_{gb} = 0.40$$

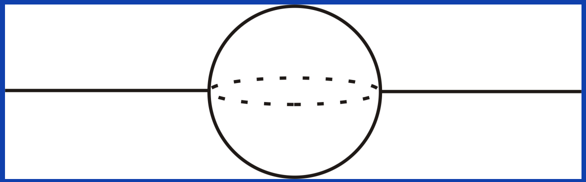
$$\kappa = 4, m = 1 \Rightarrow \sigma_{gb} = 1.16$$

$$\kappa = 1, m = 0.25 \Rightarrow \sigma_{gb} = 0.29$$

- **Interfacial energy particles:** $m/2 < \varepsilon < 2.5$
- **Interfacial thickness :** $\propto \sqrt{\frac{\kappa}{m}}$
- **Growth rate :** $\propto \kappa L\left(\frac{1}{R_1} + \frac{1}{R_2}\right)$

Grain boundary/particle interaction

- Energetic consideration:
  - Geometry:



  - 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
- Evolution spherical grain boundary pinned by single particle
  - 'dimple shape'

Large-scale 2D-simulations

- **Isotropic grain boundary properties:**

$$\kappa_i = 0.5, L_i = 1, m = 1, \varepsilon = 1$$

- **Round particles:** $r = 2.5$

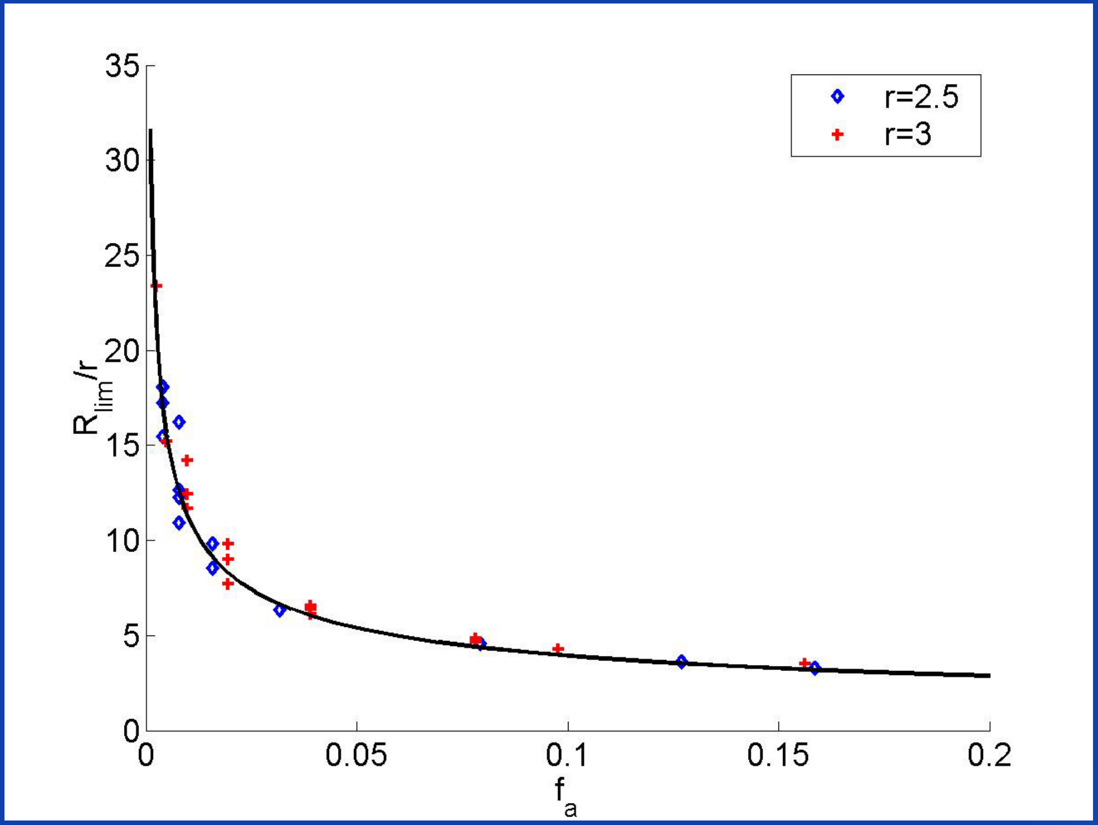
  $r = 3$
- **Area fraction:**

$$f_a = 0.004 - 0.16$$

- **System size: 256x256 and 512x512**
- **Initial microstructure:**
  - **Grain nucleation in presence of particles (R_0=0)**
  - **Grain nucleation and initial grain growth without particles (R_0>0)**
- **Random particle distribution**

Comparison with theory

- **High scatter for low f_a**
- **Fitting:** $$\frac{\overline{R_{\lim}}}{\bar{r}} = \frac{b}{f_V^{\beta}}$$
  - **Theory:** $$\beta = 0.5$$
  - **Phase field (R_0=0):** $$\beta = 0.46, b = 1.38$$
  - **Monte Carlo:** $$\beta = 0.5, b = 1.7$$ $$\beta = 0.54, b = 1.2$$
  - **Front-tracking:** $$\beta = 0.46$$ $$\beta = 0.5$$



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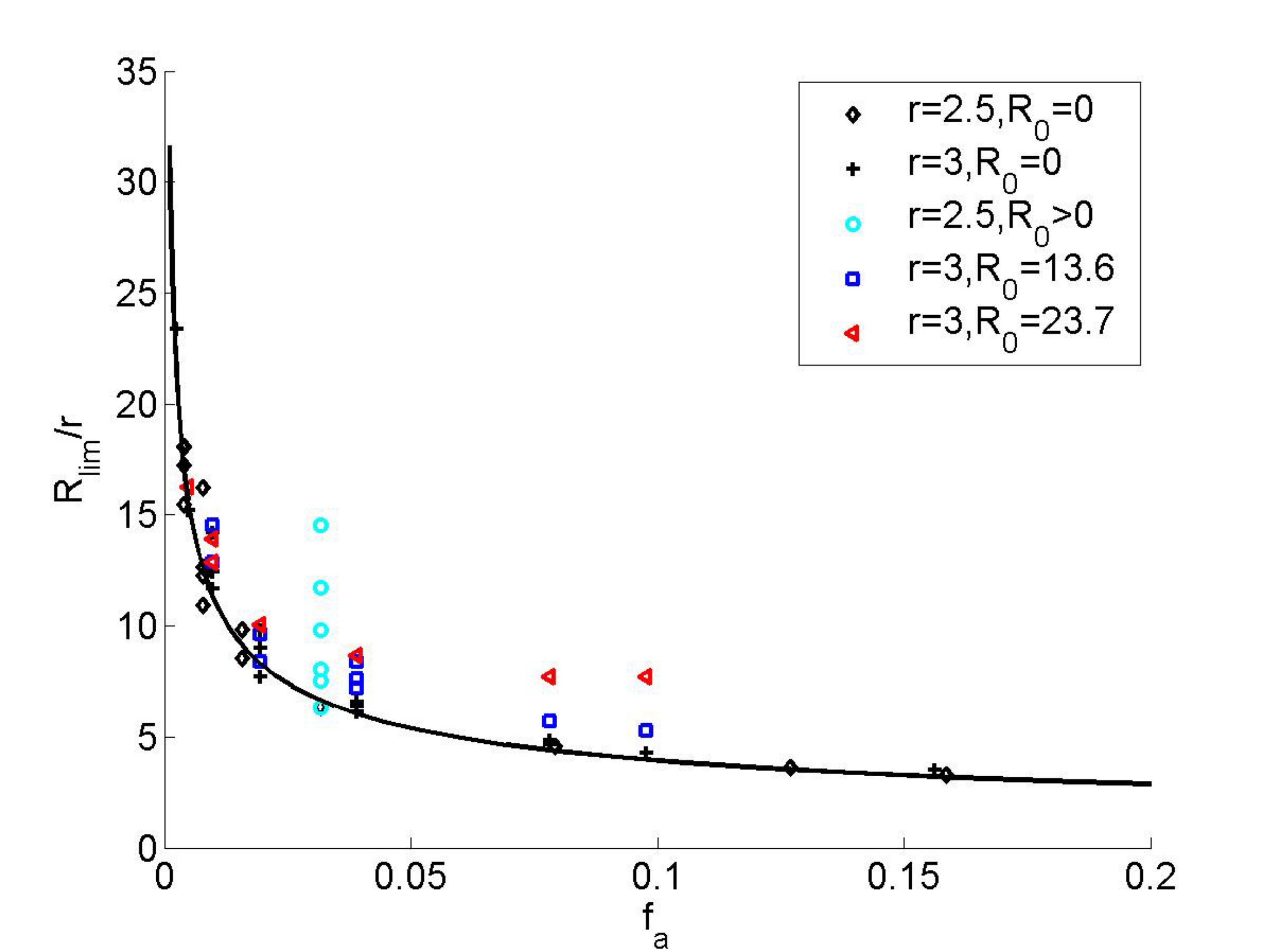
Role initial grain size



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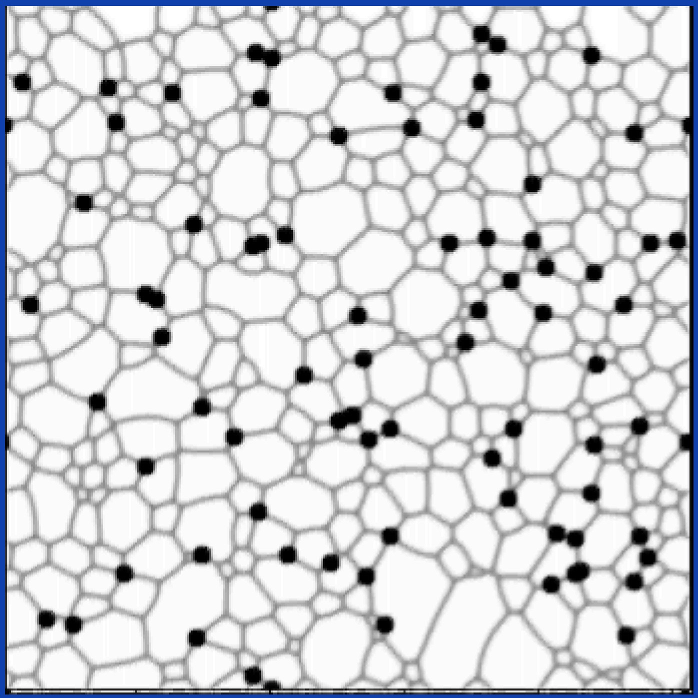
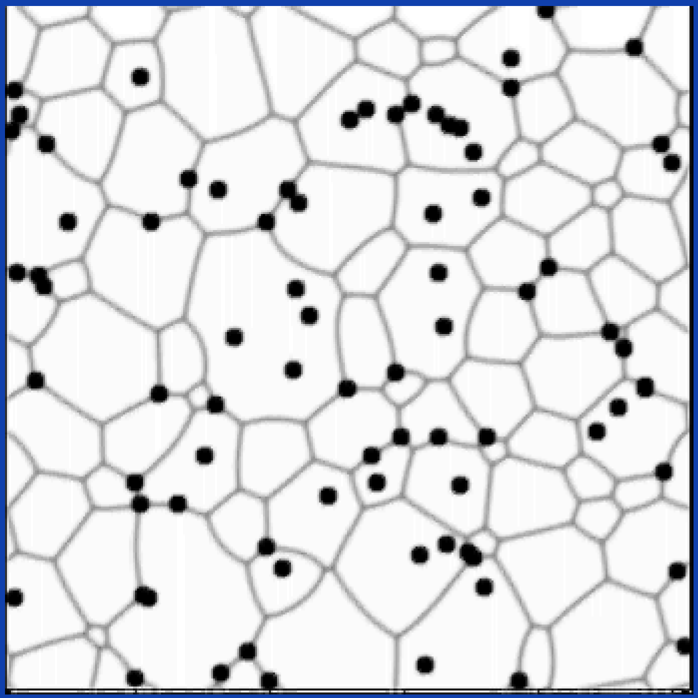
Role initial grain size

- $R_0 = 0$:



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

- $R_0 > 0$



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

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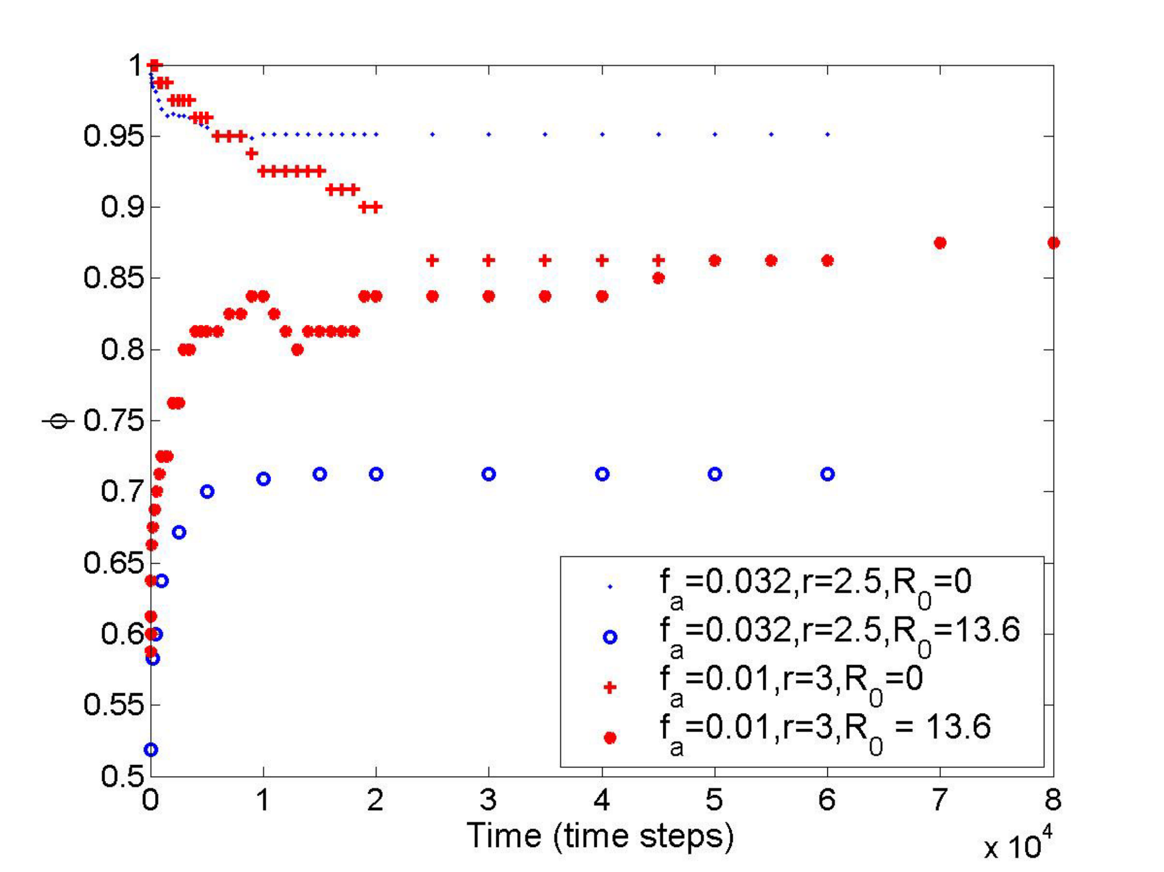
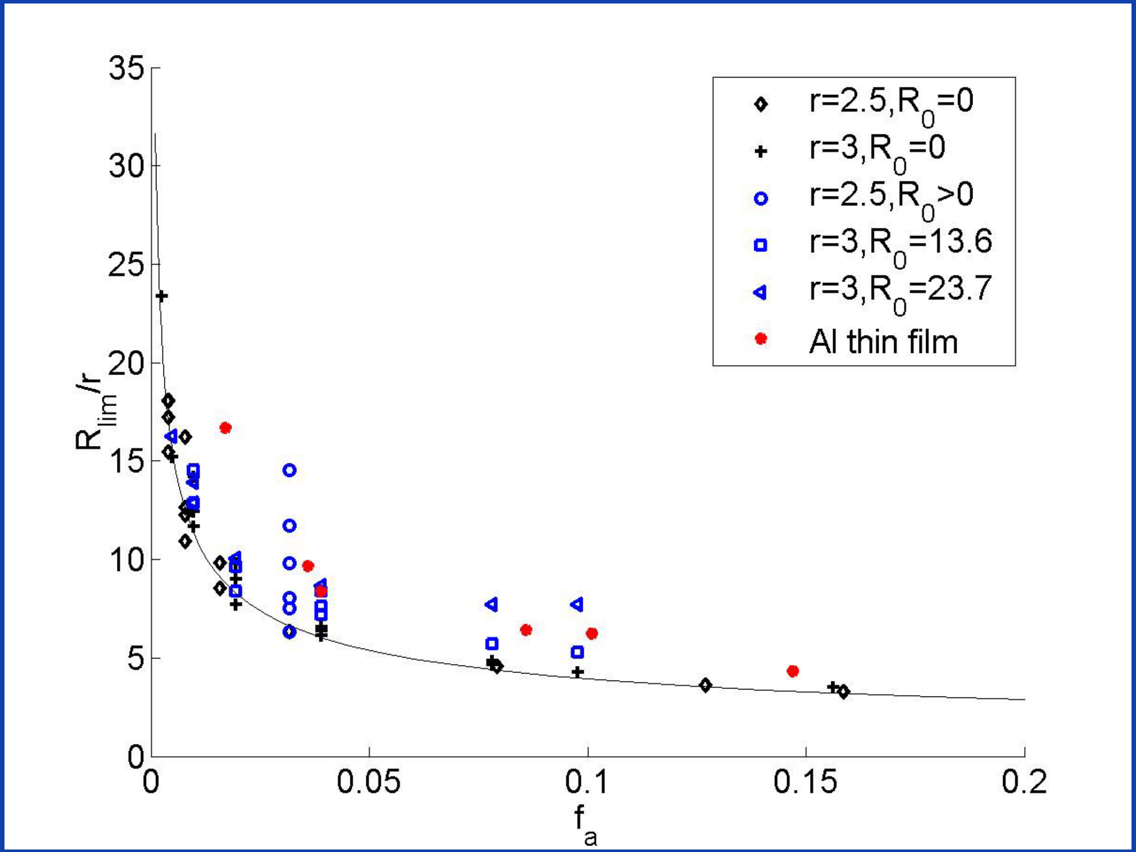
Role initial grain size

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



Comparison with experiment

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



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

Conclusions

- Zener pinning was studied as a function of
  - Particles size
  - Number of particles
  - Initial microstructure
- Long computation times even for simple materials
- Further study of ‘dimple shape’ and dynamic behavior of the grain boundaries is necessary

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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.*, 2005, in press.
- N. Moelans, B. Blanpain, P. Wollants, "Phase field simulations of grain growth in 2-dimensional polycrystalline systems containing finely dispersed incoherent second-phase particles", in preparation.
- Available on http://www.ulyssis.org/~nele/

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