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The effect of second-phase particles on grain growth in thin films studied by phase field simulations

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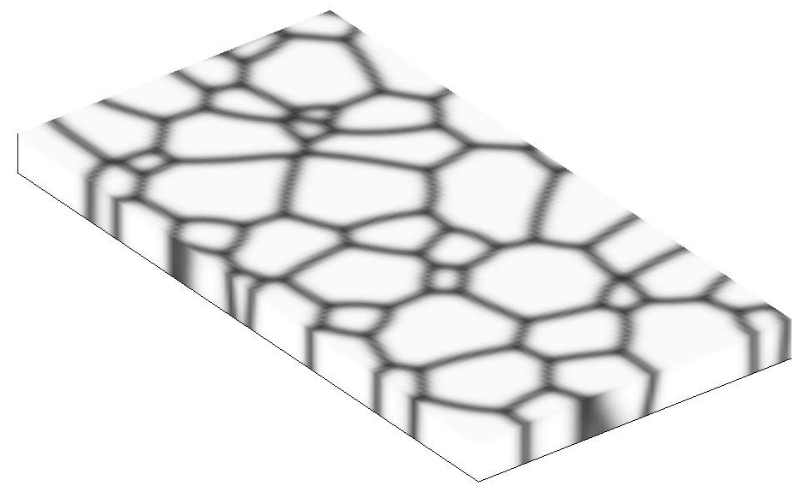
- Conclusions

Grain growth in thin films

- Bamboo structure
  - 3-D => 2-D grain growth
- Surface energy
  - Grooving
  - Anisotropy
- Particles



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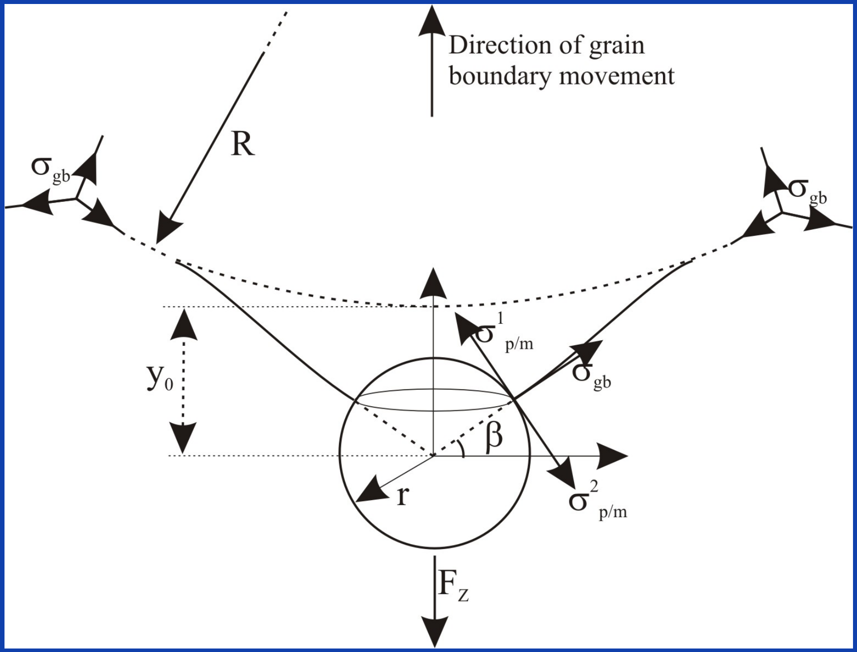
Zener pinning

- **Pinning force of a particle**
  - **3-D :** $F_Z = 2\pi r \sigma_{gb} \cos(\beta)\sin(\beta)$
  - **2-D :** $F_Z = 2\sigma_{gb} \sin(\beta)$
- **'Dimple shape'**
- **Final grain size:** $\frac{\overline{R_{\lim}}}{\overline{r}} = \frac{b}{f_V^{\alpha}}$
  - **3-D :** $\alpha \cong 1$
    $b = 2/3, b = 4/9, \ldots$
  - **2-D :** $\alpha \cong 0.5$
    $1.2 < b < 1.7$



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Phase field model

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

- **Phase field variables:**

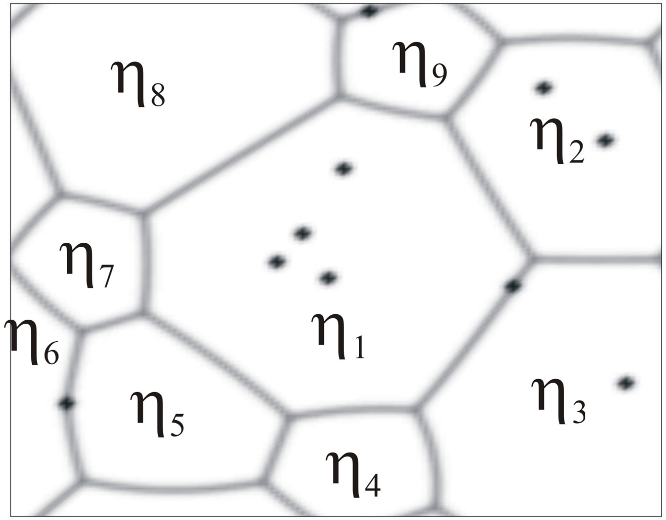
$$\eta_1, \eta_2, \ldots, \eta_i, \ldots, \eta_p$$

- **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**

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

- **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)**

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

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Model parameters

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

with

$$f = m\left(\sum_{i=1}^{p}\left(\frac{\eta_i^4}{4}-\frac{\eta_i^2}{2}\right)+\sum_{i=1}^{p}\sum_{j\neq i}^{p}\eta_i^2\eta_j^2 + \varepsilon\Phi\sum_{i=1}^{p}\eta_i^2\right)$$

- **Grain boundary energy :** $0.39\sqrt{\kappa m}$
- **Interfacial thickness :** $\propto \sqrt{\frac{\kappa}{m}}$
- **Grain boundary velocity :** $V = \kappa L(\lambda_1 + \lambda_2)$
  - **=>** $\kappa L = M^* = M\sigma_{gb}$ **(reduced mobility)**
- **Interfacial energy particles :** $f(\varepsilon)\sqrt{\kappa m}$

2-D simulations

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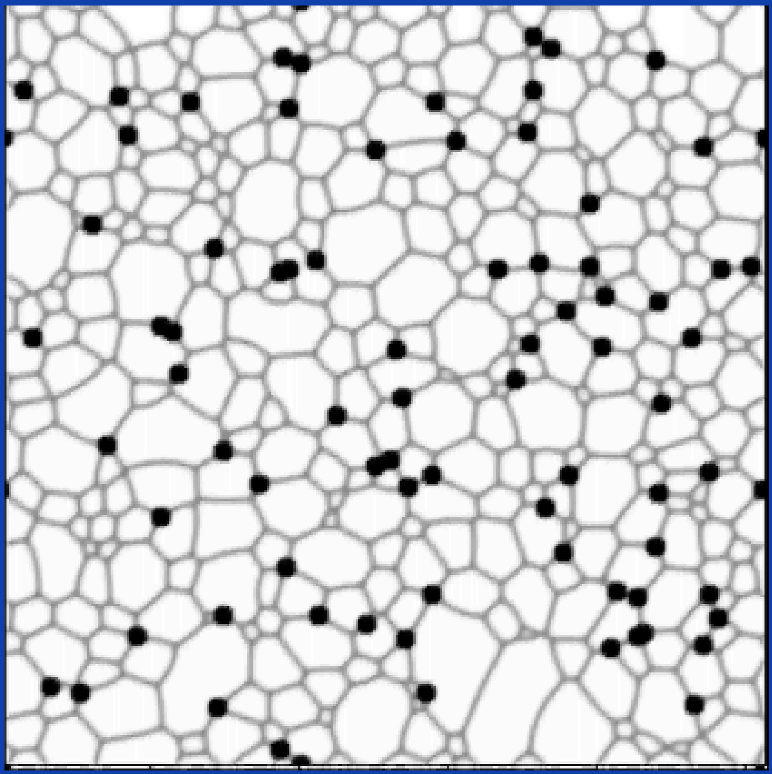
- **Parameters**

  $\kappa = 0.5, L = 1, m = 1, \varepsilon = 1$

- **Particle size**
  - **Final grain size :** $\overline{R_{\lim}} = \left(\frac{b}{f_a^{\alpha}} \right) r$
  - **Diffuse interfaces**

- **Numerical solution**
  - **Semi-implicit fourier spectral method**

- **Initial microstructure**
  - **$R_0 = 0$**
  - **$R_0 > 0$**



$r = 3, f_a = 0.04, \overline{R_0} = 0$

2-D : Final grain size

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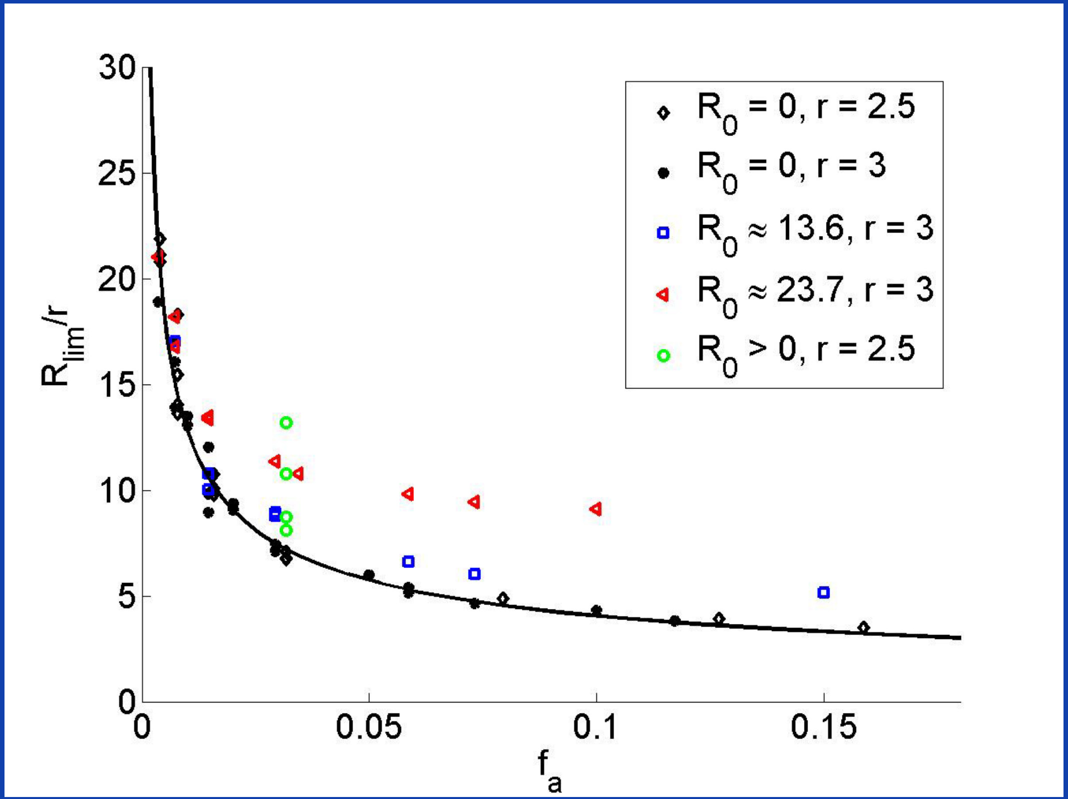
- $R_0 = 0$

$$\frac{\overline{R_{\lim}}}{r} = \frac{1.28}{f_a^{0.5}}$$

- $R_0 > 0$

For high f_a, large R_0

$$\overline{R_{\lim}} \cong \overline{R_0}$$



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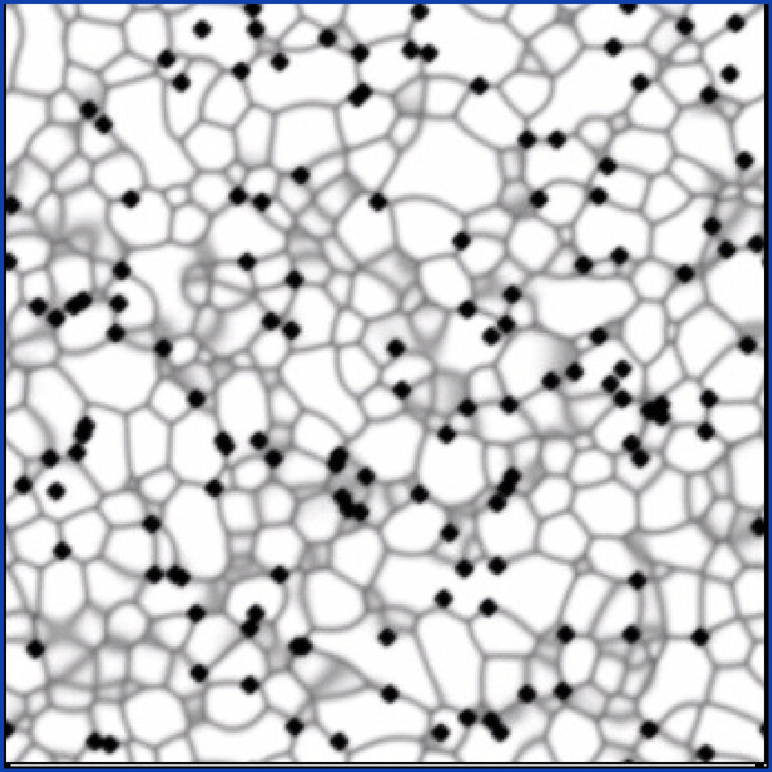
3-D simulations

- **Numerical solution**
  - **// film**
    - **2-D Fourier spectral method**
  - **⊥ film**
    - **Finite differences**
      - **Dirichlet : drag effect**
      - **Neumann**
- **3-D effect**
  - **Position of particles**
  - **Film thickness**



$$r = 3, f_a = 0.05, l = 21$$

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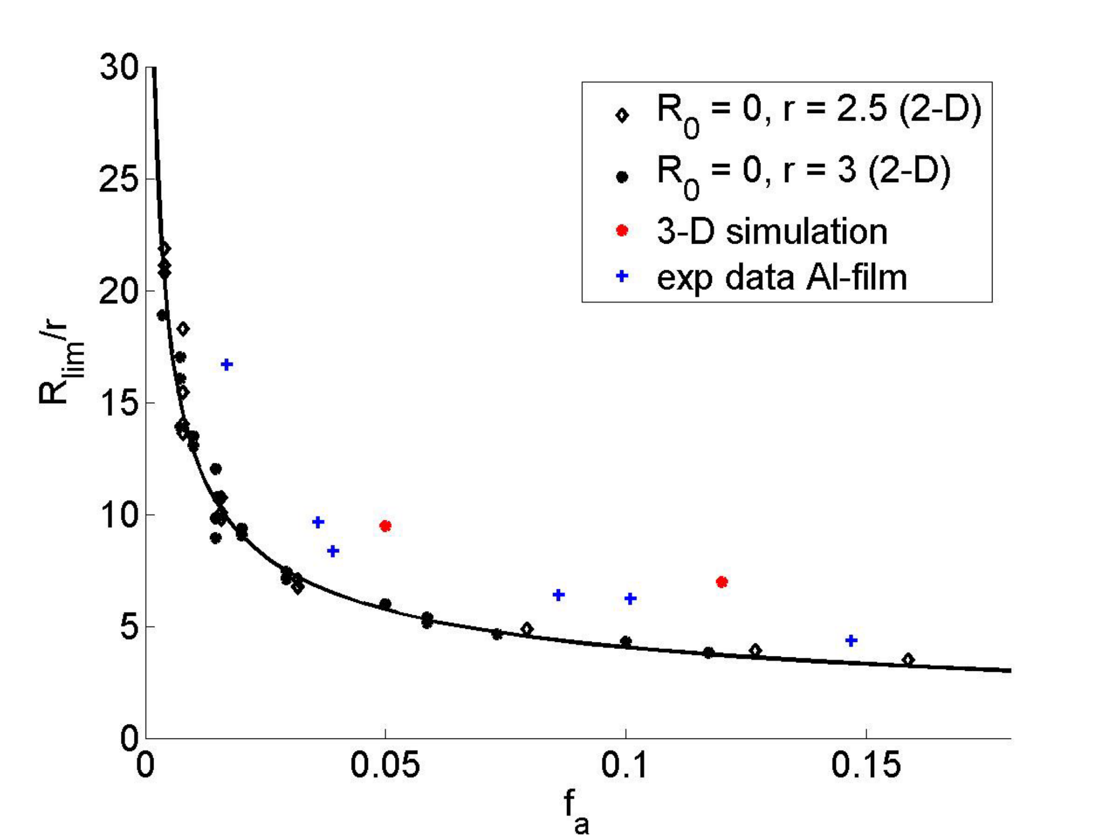
Comparison 2-D and 3-D results

- **Thin Al-films**
  - **Bamboo-structure**
  - **$CuAl_2$-particles in middle of film**
  - **r ≅ 1/7 film thickness**



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

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Conclusions

- 2-D and 3-D phase field simulations of grain growth in thin films containing second-phase particles were performed
- 2-D simulations => importance of R_0
- 3-D simulations => particles introduce 3-D effect
- Important parameters
  - Ratio of particle size and film thickness
  - Position of particles

End

Thank you for your attention !

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