Phase field simulations of grain growth in the presence of second-phase particles that evolve in time

Nele Moelans(1), Liesbeth Vanherpe(2), Bart Blanpain(1), Patrick Wollants(1)

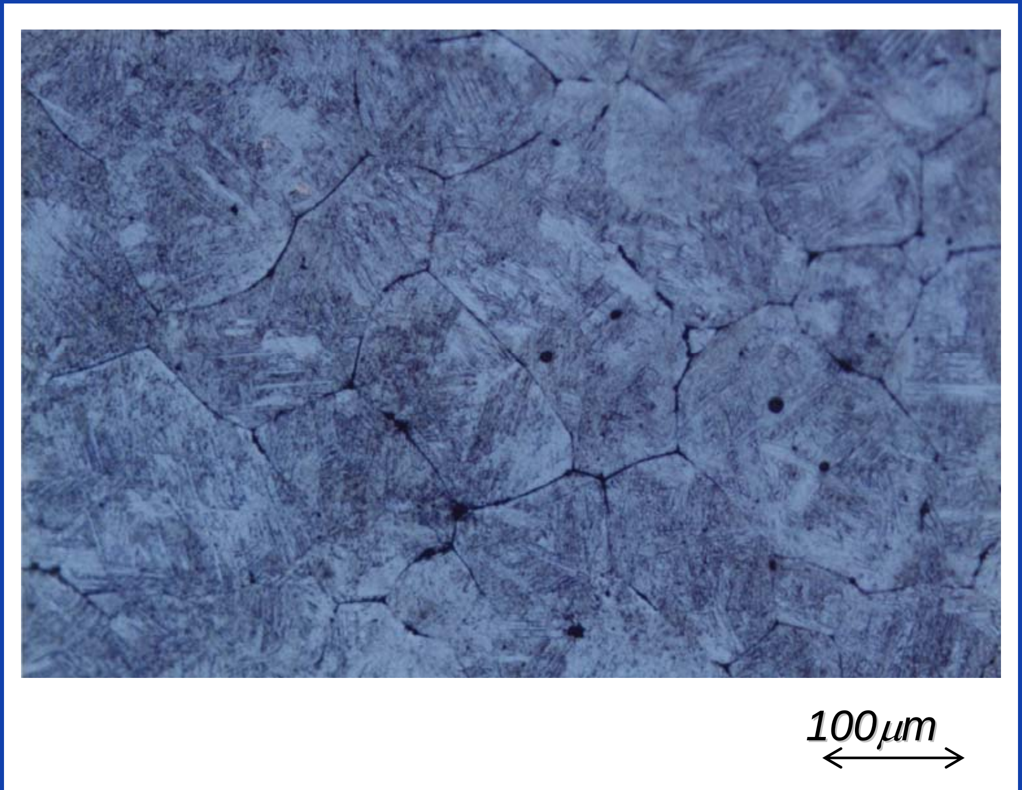
(1)Department of metallurgy and materials engineering, (2)Department of computer science, K.U.Leuven, Belgium

Outline

- Introduction on Zener pinning
- Phase field model for grain growth
- Three modelling approaches for Zener pinning + simulation results
- Conclusions and further research

Zener pinning: phenomenon

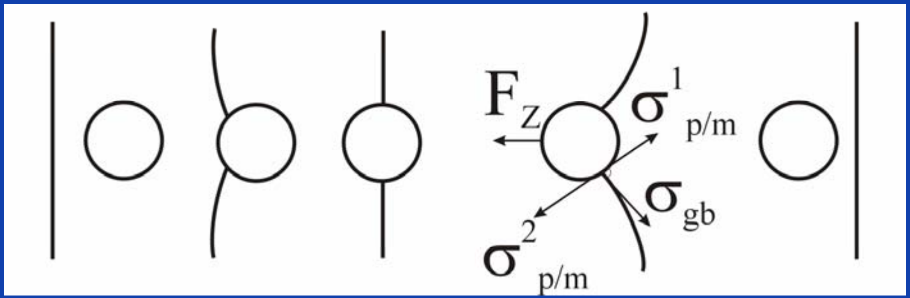
- **Polycrystalline structure with second-phase particles**

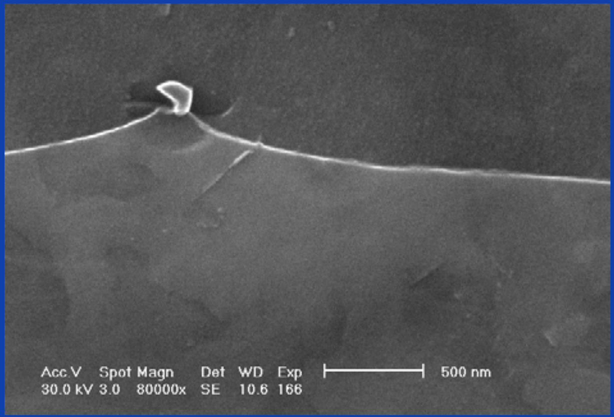


Fe-0.09 to 0.53 w% C-0.02 w% P containing Ce_2O_3 inclusions (M. Guo 1999)

Zener pinning: phenomenon

- **Second-phase particles exert back force on moving grain boundaries**
  - **Dimple-shape**





MnS precipitate in low-C steel

- **Mechanism for controlling the grain size**
  - ***NbC, AlN, TiN,... in HSLA-steels for small grain size***

Zener pinning: analytical theories

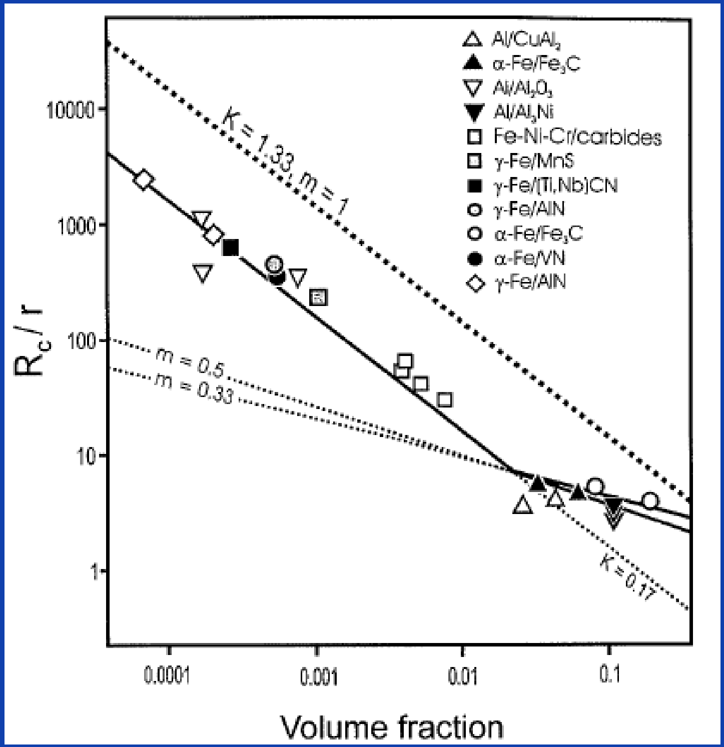
KATHOLIEKE UNIVERSITEIT LEUVEN

- **Zener type relation for limiting grain size**

$$\frac{\overline{R}_{\text{lim}}}{\overline{r}} = K \frac{1}{f_V^{\,m}}$$

- **Effect of**
  - **Particle shape**
  - **Interfacial properties**
  - **Particles distribution**

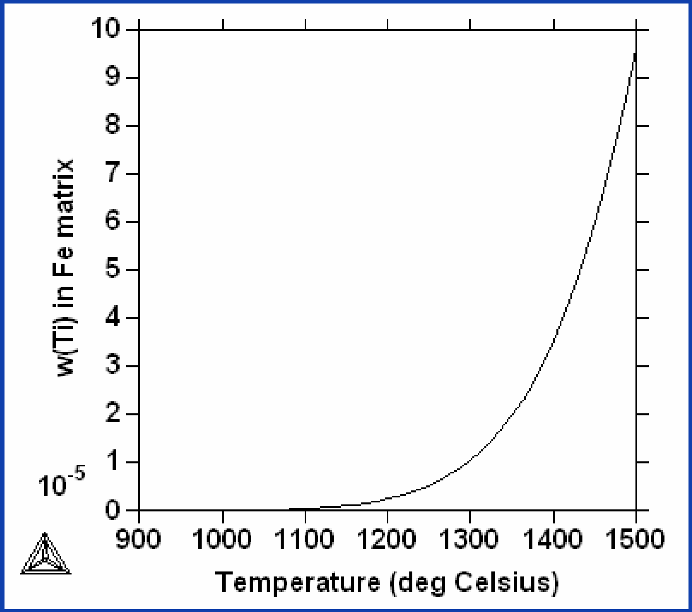
- **No consensus on parameters *K* and *m***
  - **Exact description for local interaction**
  - **Approximations required for the number of particles that contribute**



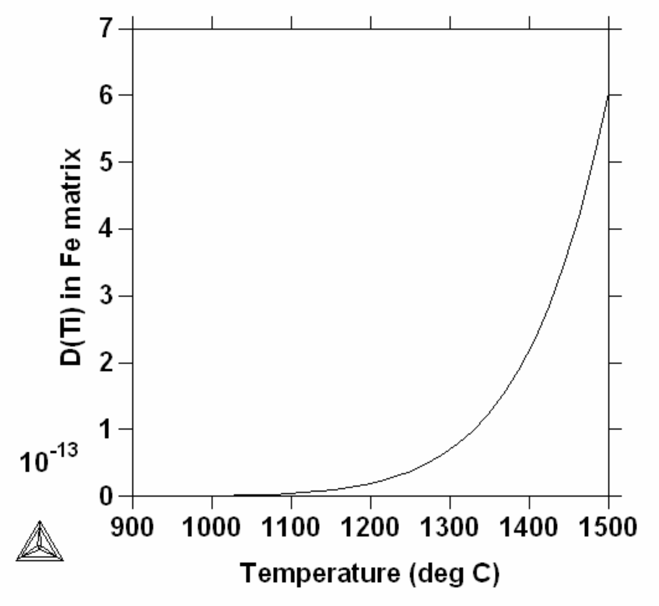
Comparison with experimental data (Manohar, ISIJ Int.,1998)

Evolution and stability of the particles

- **Grain coarsening temperature**
  - **Particle coarsening and dissolution for $T>T_{gc}$**
  - **E.g TiN particles in austenitic low-alloyed steels**



Solubility Ti in austenitic matrix



Diffusivity Ti in austenitic matrix

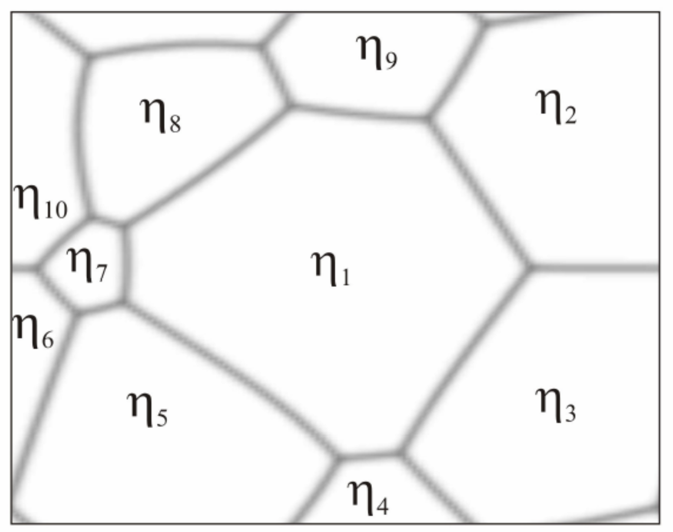
Grain growth model

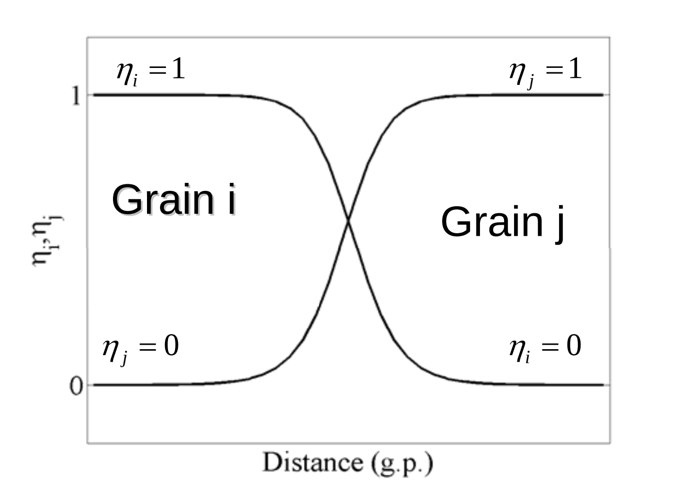
- **Based on models of Chen and Yang (1994), Fan and Chen (1997) and Kazaryan et al. (2000)**
- **Polycrystalline microstructure**

$$\eta_1, \eta_2, \ldots, \eta_i(\vec{r}, t), \ldots, \eta_p$$

- **Grain i of matrix-phase**

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





Grain growth model

- **Free energy**

$$F = \int_V \left[m \left(\sum_{i=1}^{p} \left(\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2} \right) + \sum_{i=1}^{p} \sum_{j<i}^{p} \gamma_{i,j} \eta_i^2 \eta_j^2 \right) + \frac{\kappa(\eta)}{2} \sum_{i=1}^{p} (\vec{\nabla} \eta_i)^2 \right] dV$$

- **Temporal evolution: Ginzburg-Landau equation**

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

- **Parameter assessment**
  - **For each interface:** $\kappa_{i,j}, \gamma_{i,j}, m, L_{i,j}$
  - **Related to interfacial energy ($\sigma_{i,j}$), interfacial mobility ($\mu_{i,j}$) and interfacial width (ε)**

Three approaches for modelling Zener pinning

- Spatially dependent parameter Φ in free energy
  - Constant particle distribution
- Coupling with a Cahn-Hilliard equation
  - Qualitative description of the evolution of the particles
- Multi-phase field approach + coupling with diffusion equation
  - Quantitative treatment of phase stabilities, interfacial properties and kinetics

Possibilities ↗

Complexity and computational requirements ↗

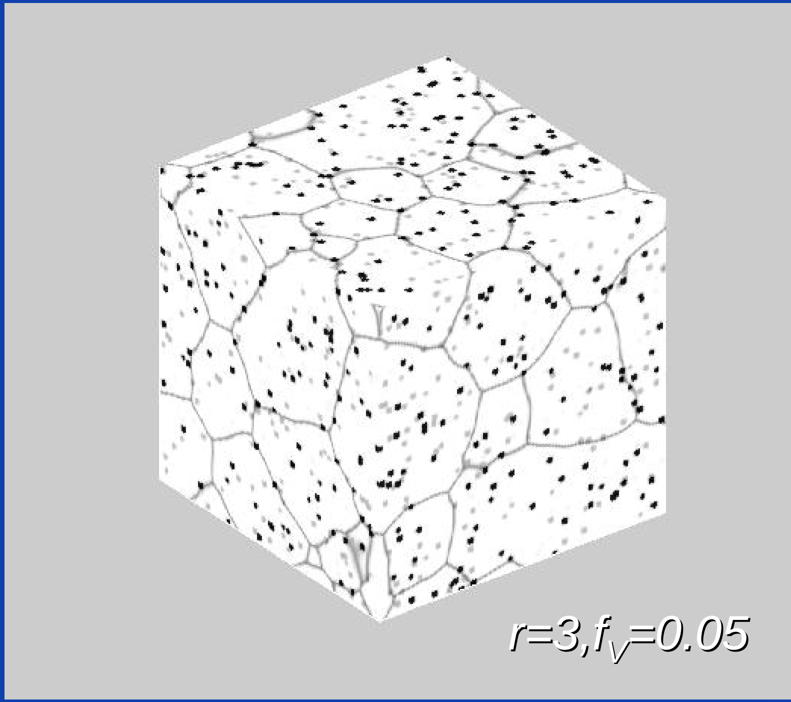
Spatially dependent parameter

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

- **Minima free energy**
  - **Φ=1** $(\eta_1, \eta_2, \ldots, \eta_p) = (0, 0, \ldots, 0)$
  - **Φ=0** $(\eta_1, \eta_2, \ldots, \eta_p) = (1,0,\ldots,0), (0,1,\ldots,0), \ldots (0,0,\ldots,1),$
    $(-1, 0, \ldots, 0), \ldots$
- **Advantages**
  - **Particles can be small**
  - **Efficient and easy implementation**
    - **Semi-implicit Fourier-spectral method**
- **Shortcomings**
  - **Properties of the particles are ignored**

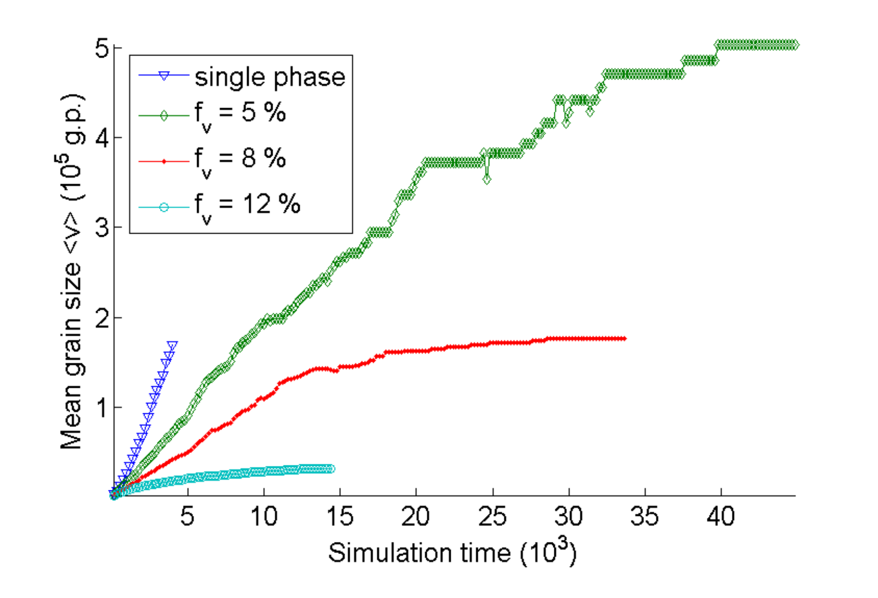
Spatially dependent parameter

- **Large-scale 3D simulations for high f_V**
- **Bounding box algorithm (Phd L. Vanherpe)**
  - **Equations for η_i are only solved for grain *i***
  - **1 processor (2gb RAM): system size *256x256x256***

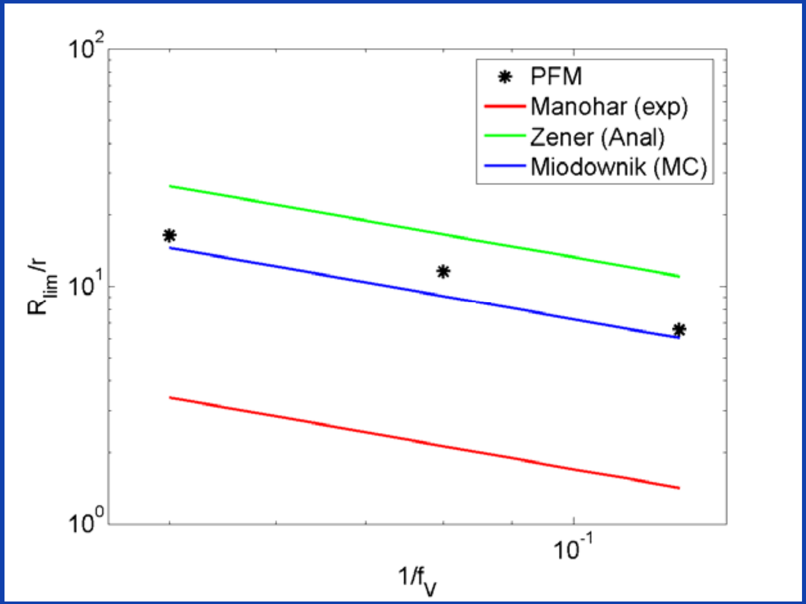


Spatially dependent parameter

- **Temporal evolution**



- **Limiting grain size** $\frac{\overline{R}_{\text{lim}}}{\overline{r}} = K \frac{1}{f_V^{\,m}}$



- **Close to Monte Carlo results**

  m ≈ 1

  K ≈ 3/4

Coupling with Cahn-Hilliard equation

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

- Φ is treated as conserved field variable, e.g.
  - Cahn-Hilliard equation for evolution of Φ

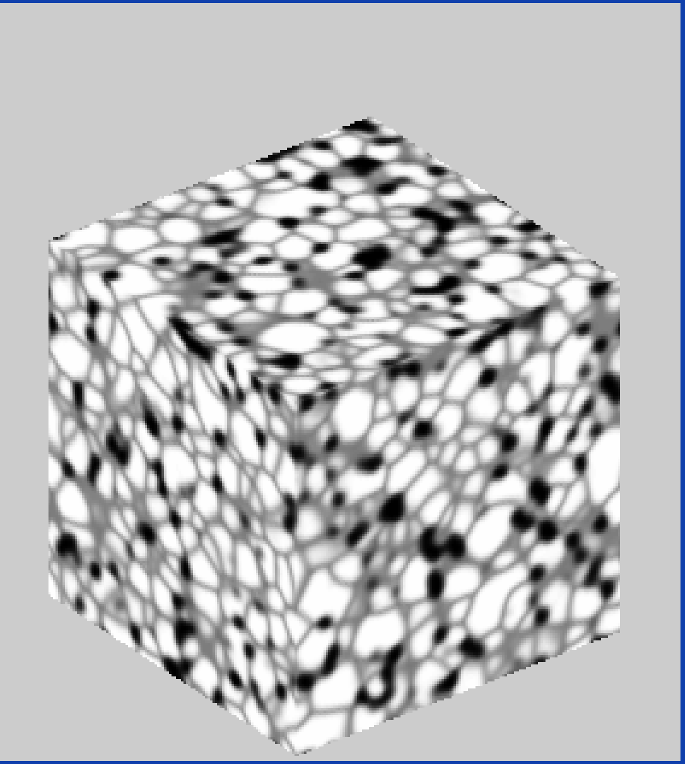
$$\Phi = \frac{c - c_{matrix}}{c_{particle} - c_{matrix}}$$

$$\frac{\partial \Phi(\vec{r},t)}{\partial t} = \vec{\nabla} \bullet M \vec{\nabla} \frac{\partial F}{\partial \Phi(\vec{r},t)}$$

- Advantages
  - Particles evolve in time
  - Relatively easy and efficient implementation
    - Semi-implicit Fourier-spectral method
- Shortcomings
  - Only for diffusion limited processes
  - Grain boundary segregation exagerated

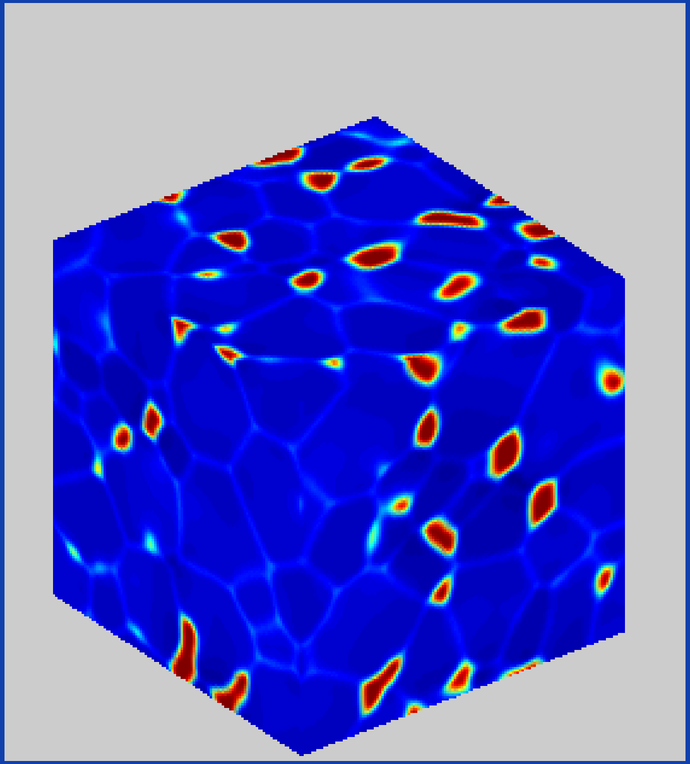
Coupling with Cahn-Hilliard equations

- **Evolution grain structure**



f_V=0.12, L=10M

- **Distribution Φ**

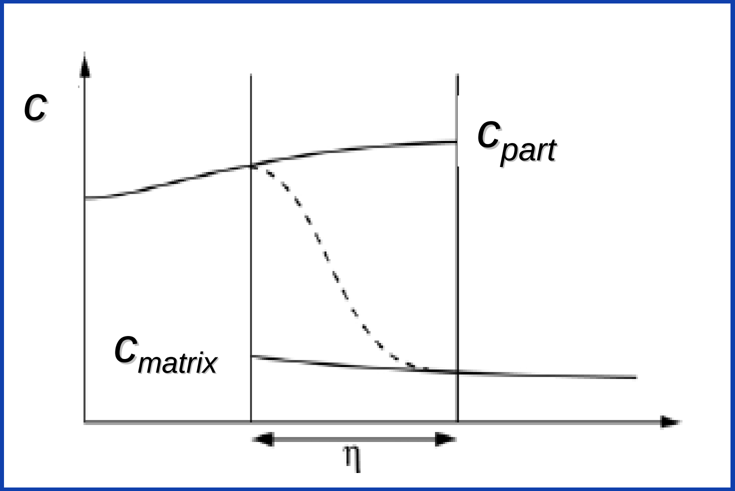


- **Grain boundary segregation exagerated**

Coupling with multi-phase field approach

- **Φ non-conserved field variable + composition field *c***
- **Interface consists of 2 phases**
  - **Local phase fractions**

$$\phi_{part} = \frac{\Phi^2}{\Phi^2 + \sum_i \eta_i^2}, \qquad \phi_{matrix} = \frac{\sum_i \eta_i^2}{\Phi^2 + \sum_i \eta_i^2}$$



Steinbach, Physica D, 127 (2006) 153-160

  - **Equal chemical potentials** $\mu_{part} = \mu_{matrix}$
  - **Local composition** $c = \phi_{part} c_{part} + \phi_{matrix} c_{matrix}$
- **Diffusion equation**

$$\dot{c} = \nabla \cdot \sum_{\alpha,\beta} \phi_\alpha M_\alpha \nabla \frac{\partial f_\alpha}{\partial c_\alpha}$$

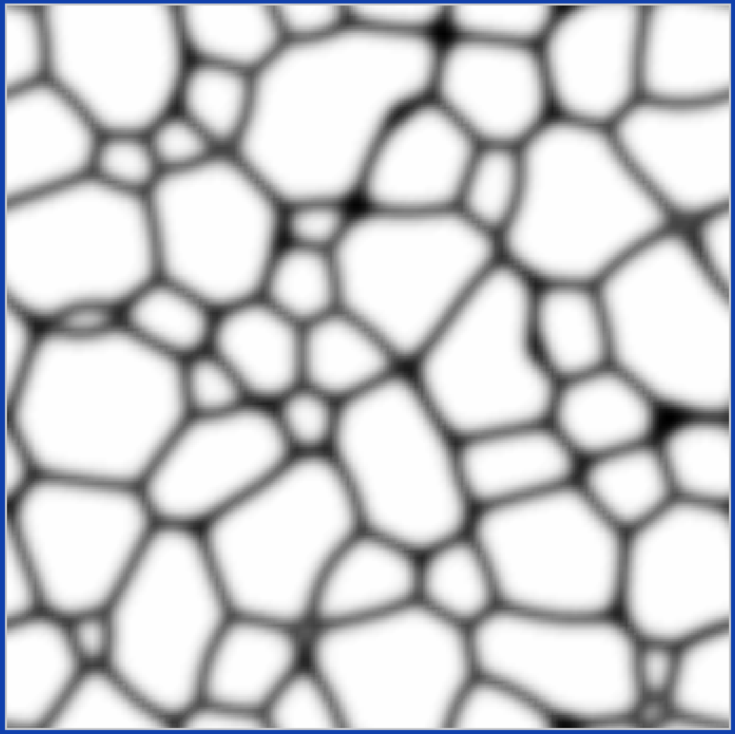
Coupling with multi-phase field approach

- Advantages
  - Interfacial and bulk properties are decoupled
    - $\Rightarrow$ Quantitative approach
  - Extendable to multi-phase systems

- Shortcomings
  - Computationally intensive
  - Grain boundary segregation is neglected

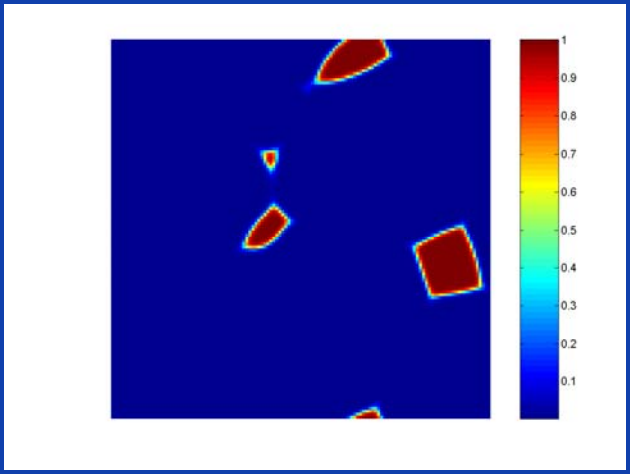
Coupling with multi-phase field approach

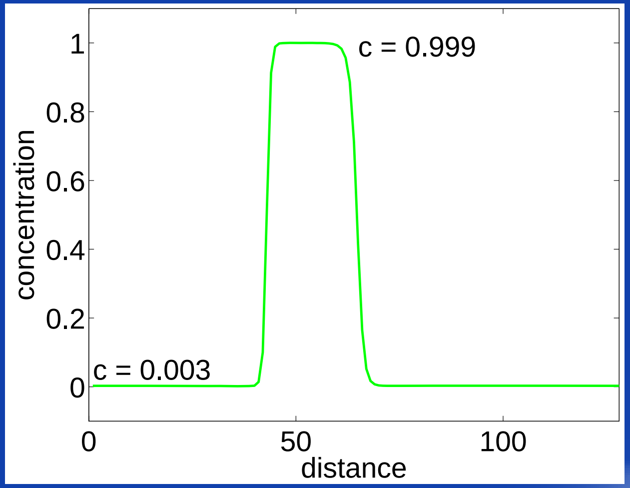
- **Evolution grain structure**



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

- **Composition profile**





Conclusions + Outlook

KATHOLIEKE UNIVERSITEIT LEUVEN

- **Conclusions**
  - **Three phase field models that account for the effect of second-phase particles on grain growth have been discussed**
    - **Particle distribution is constant in time**
    - **Qualitative treatment of particle evolution**
    - **Quantitative treatment of particle evolution and interfacial properties**

- **Outlook**
  - **Further validation and optimization of the models**
  - **Orientation dependence of interfacial energy of the particles**
  - **Systematic studies of particular grain growth phenomena in 3D**
  - **Towards quantitative simulations for real alloy systems**

Acknowledgments

- **Nele Moelans is Postdoctoral Fellow of the Research Foundation - Flanders (FWO-Vlaanderen)**
- **Simulations were performed on the HP-computing infrastructure of the K.U.Leuven**

- **More information on *http//nele.studentenweb.org***