Phase field simulations of the pinning effect of second-phase particles

Effect of particle shape, stability and interfacial properties

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

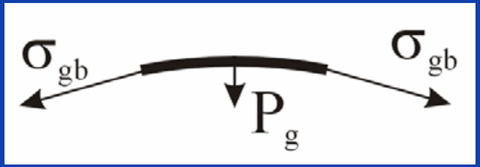
- Introduction on Zener pinning
- Phase field model for grain growth
- Three modeling approaches for Zener pinning
- Simulation results
- Conclusions and further research

KATHOLIEKE UNIVERSITEIT LEUVEN

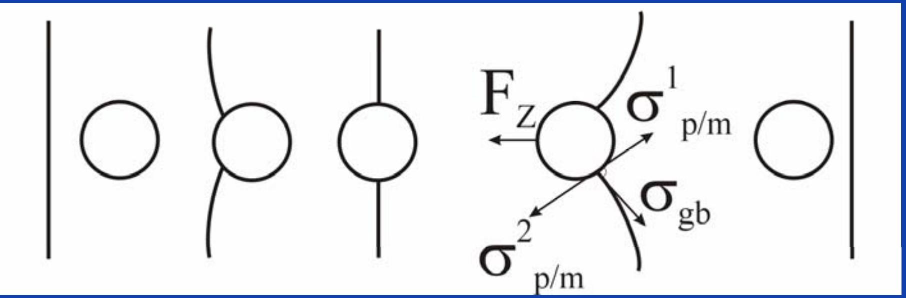
Zener pinning: phenomenon

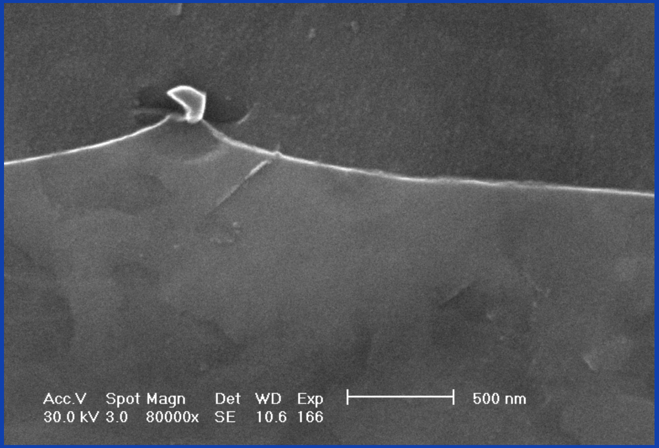
- **Grain growth in polycrystalline materials**
  - **Driving pressure for grain boundary movement:**

$$P_g = \frac{\alpha \sigma_{gb}}{\rho_1 + \rho_2}$$



- **Second-phase particles exert back force**
  - **Dimple-shape**





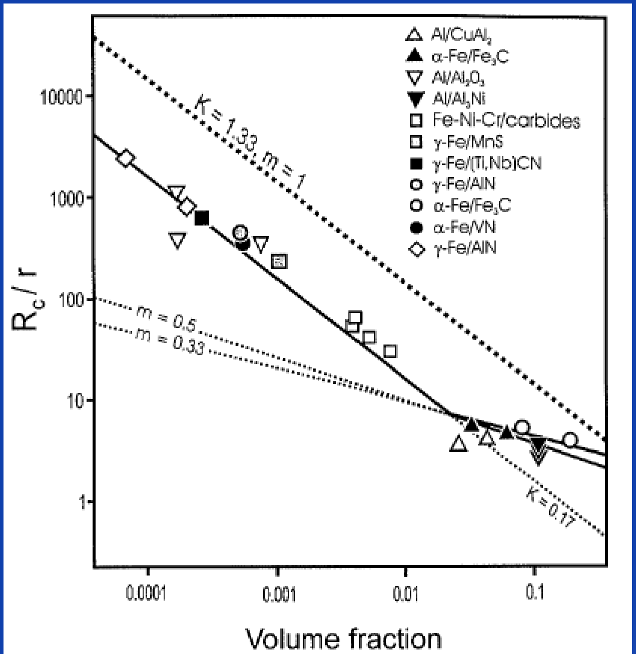
MnS precipitate in low-C steel

- **Mechanism for controlling grain size**
  - ***NbC, AlN, TiN,... in HSLA-steels for small grain size***
  - **Induce abnormal grain growth in thin films**

Zener pinning: analytical theories

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

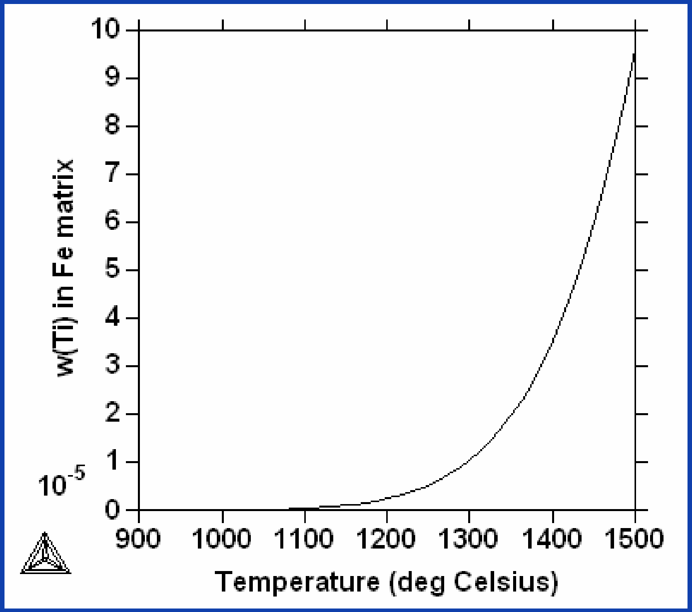
- **Zener relation for limiting grain size**
  - **Spherical incoherent particles**
  - **Position of particles and particles are not correlated**
- **Modifications for**
  - **Particle shape**
  - **Interacial properties**
  - **Interaction between grain boundaries and particles**
- **No consensus on parameters *K* and *b***
  - **Exact description for local interaction**
  - **Approximations required for the number of particles that contribute**



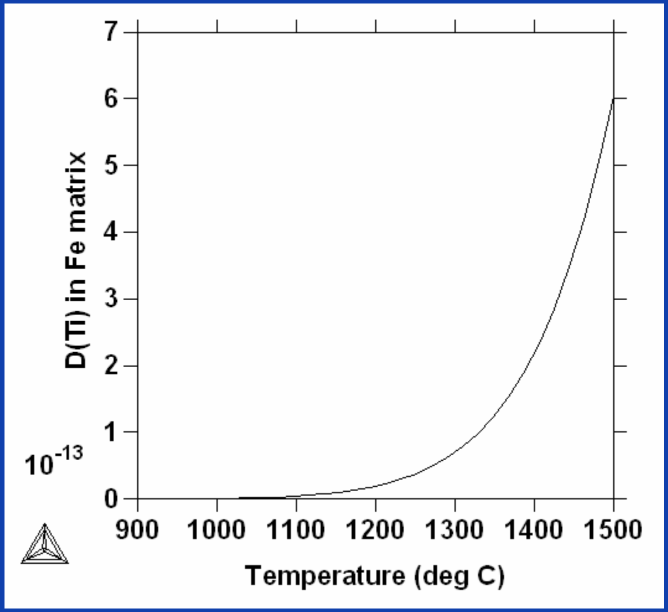
Comparison with experimental data (Manohar, ISIJ Int.,1998)

Evolution and stability of the particles

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

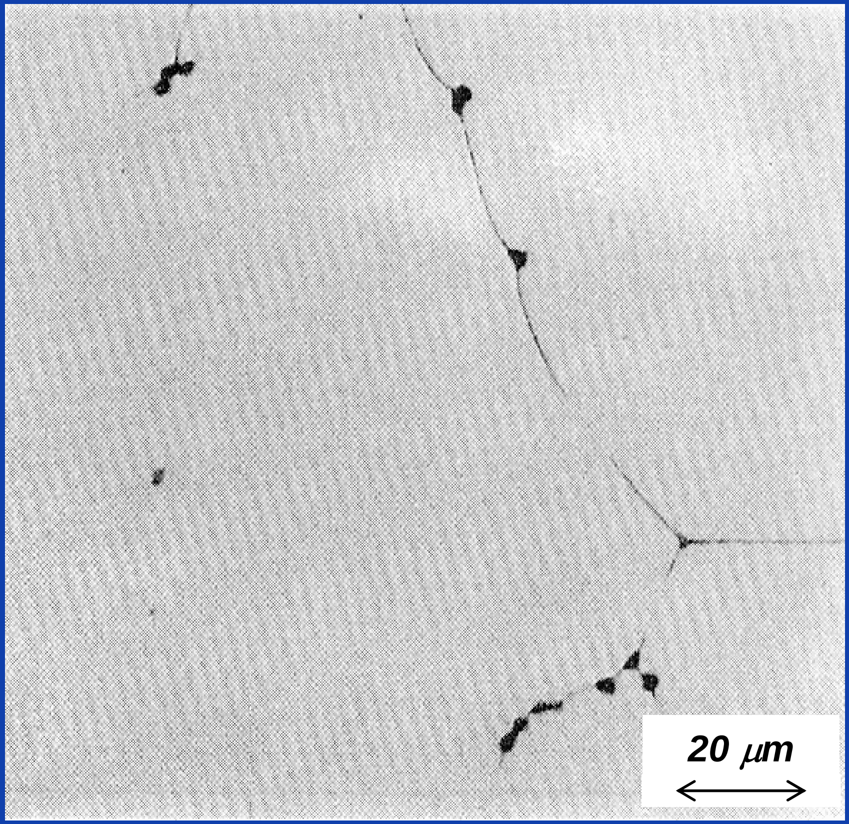


Solubility Ti in austenitic matrix



Diffusivity Ti in austenitic matrix

Experimental observation



- Fe-0.09 to 0.53 w% C-0.02 w% P containing Ce_2O_3 inclusions
  - PhD – work M. Guo (1999)
  - Pinned austenite grain boundaries
  - Specialized and time-consuming work

Simulations

- No assumptions on the number of grain boundary-particle interactions are required (+)
- Exact material properties and conditions are known (+)
  - Simplifies interpretation of results
- Relatively easy to adapt material parameters and conditions (+)
- Computationally intensive (-)
  - Particles can be more than 100 times smaller than grains
  - Large grain assemblies for reliable statistics

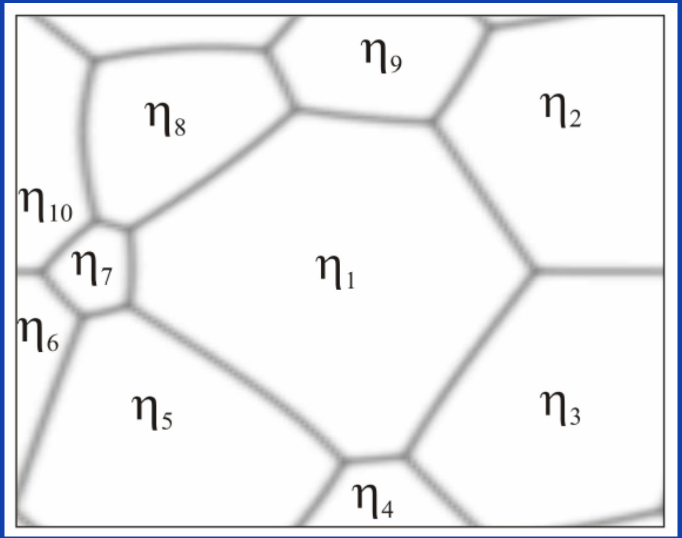
Grain growth model

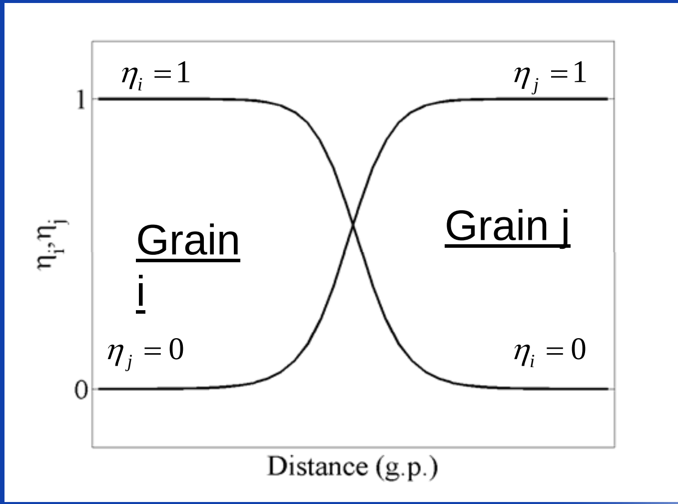
- **Based on models of Chen and Yang (1994), Fan and Chen (1997) and Kazaryan et al. (2000)**
- **Polycrystalline microstructure**

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

- **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)**

KATHOLIEKE UNIVERSITEIT LEUVEN

Three approaches for modeling Zener pinning

- Spatially dependent parameter Φ in free energy
  - Constant particle distribution
- Coupling with a Cahn-Hilliard equation
  - Φ is treated as a conserved field variable
  - Qualitative description of the evolution of the particles
- Multi-phase field approach + coupling with diffusion equation
  - Φ is treated as a non-conserved field variable
  - Composition field gives local composition
  - Quantitative treatment of phase stabilities, interfacial properties and kinetics

Possibilities ↗

Complexity and computational requirements ↗

Spatially dependent parameter

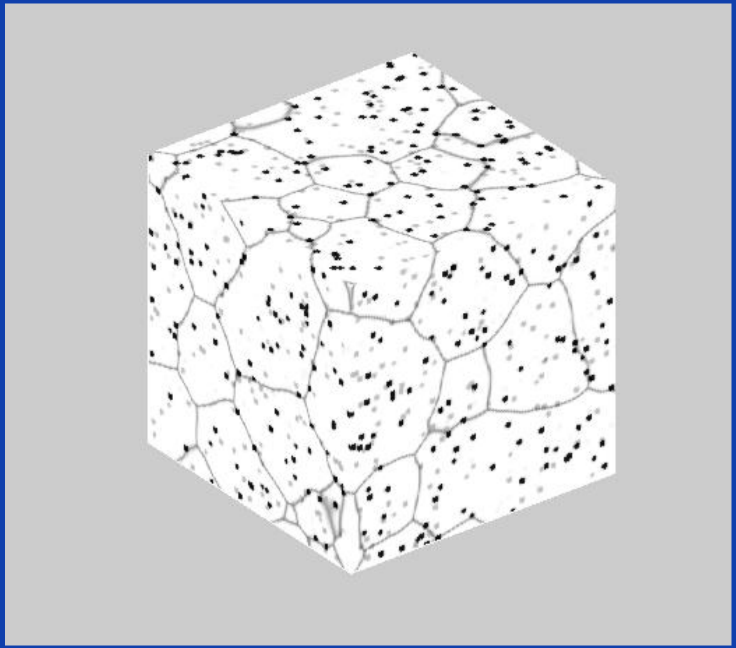
- **Minima free energy**
  - **Φ=1** $(\eta_1, \eta_2, \ldots, \eta_p) = (0, 0, \ldots, 0)$
  - **Φ=0** $(\eta_1, \eta_2, \ldots, \eta_p) = (1, 0, \ldots, 0), (0, 1, \ldots, 0), \ldots (0, 0, \ldots, 1),$
    $(-1, 0, \ldots, 0), \ldots$

- **Advantages**
  - **Particles can be small**
  - **Efficient and easy implementation**
    - **Semi-implicit Fourier-spectral method**

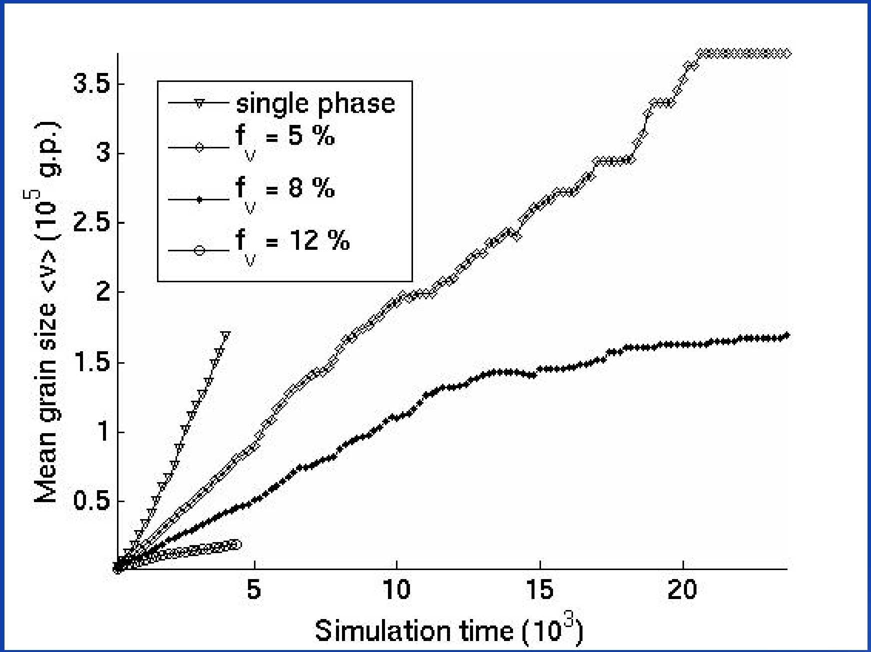
- **Shortcomings**
  - **Properties of the particles are ignored**

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*



$r=3, f_V=0.05$



Coupling with Cahn-Hilliard equation

- Φ is treated as conserved field variable
  - E.g. scaled composition variable

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

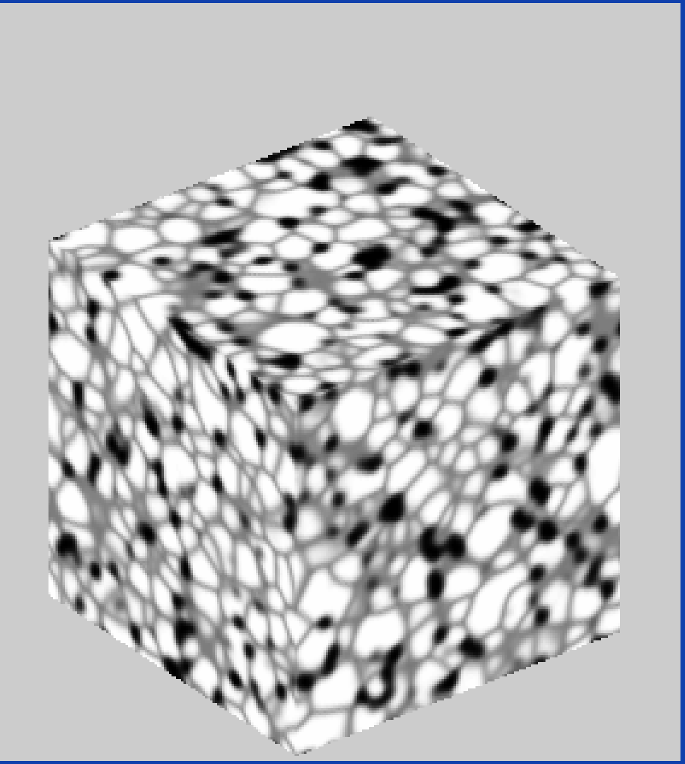
  - Cahn-Hilliard equation for evolution of Φ

- 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

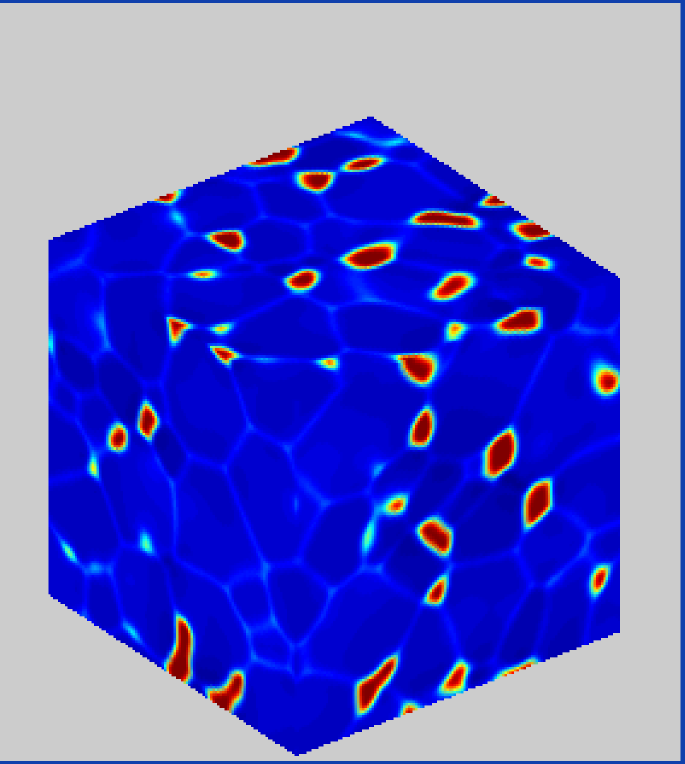
Coupling with Cahn-Hilliard equations

- **Evolution grain structure**



f_V=0.12, L=10M

- **Distribution Φ**



- **Grain boundary segregation exagerated**

KATHOLIEKE UNIVERSITEIT LEUVEN

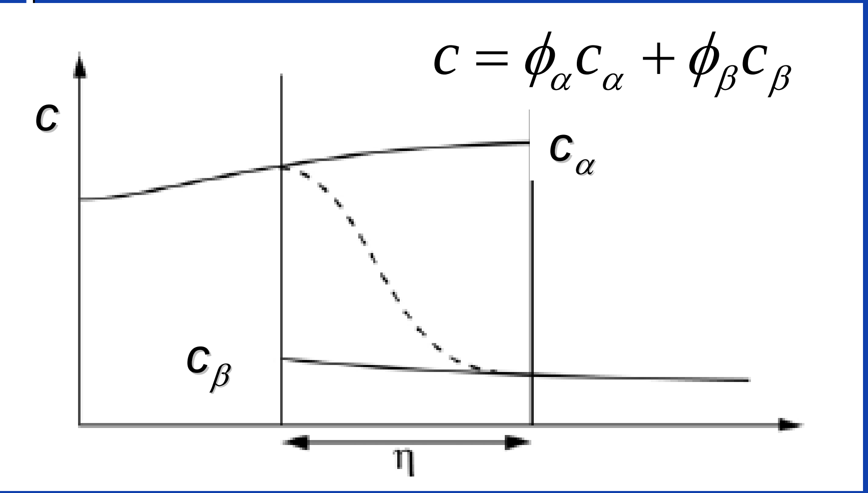
Coupling with multi-phase field approach

- Φ non-conserved field variable, composition field *c*
  - Interface consists of 2 phases
    - with for each component

$$\mu_\alpha = \mu_\beta$$

  - Diffusion equation

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



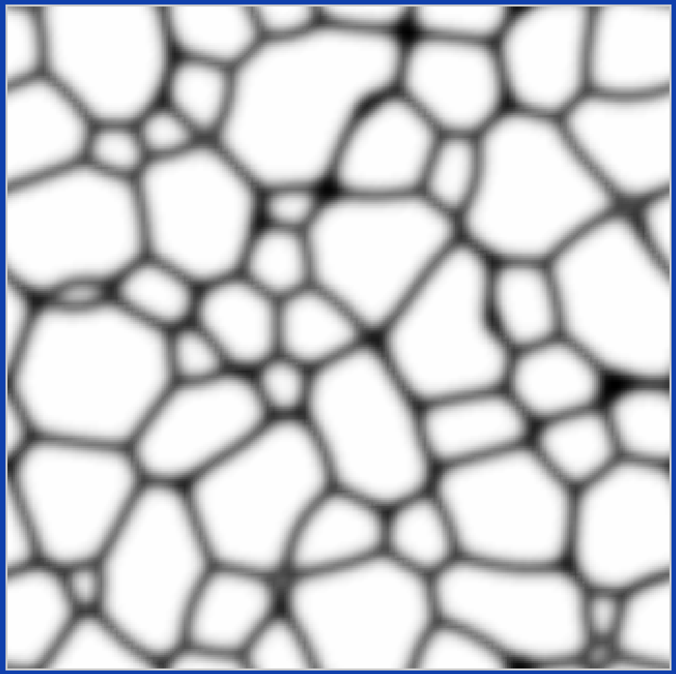
Steinbach, Physica D. 127 (2006) 153-160

- Advantages
  - Interfacial and bulk properties are decoupled
  - Extendable to multi-phase systems

- Shortcomings
  - Computationally intensive
  - Grain boundary segregation is neglected
  - Artificial wetting

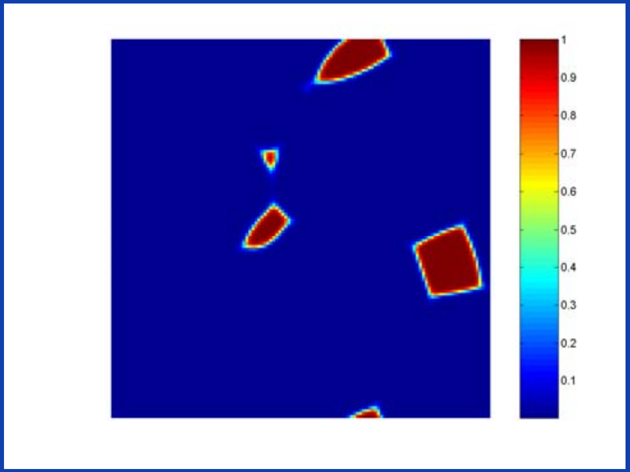
Coupling with multi-phase field approach

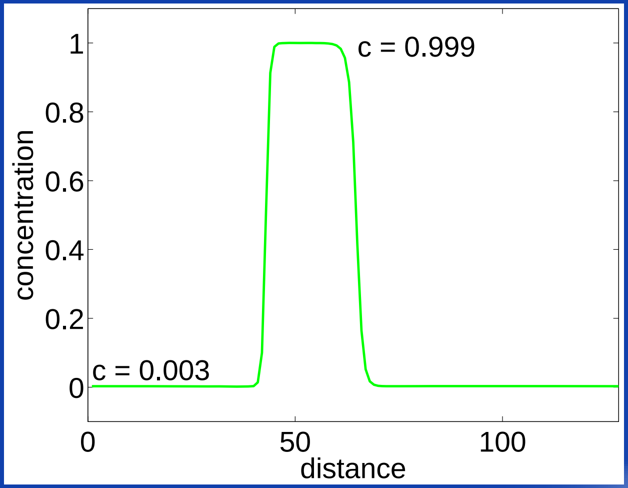
- **Evolution grain structure**



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

- **Composition profile**





KATHOLIEKE UNIVERSITEIT LEUVEN

Conclusions

- The effect of second-phase particles on grain growth is still not understood
- Simulation studies are important for a better understanding
- 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

Future research

- Further validation of the three modeling approaches
- Orientation dependence of interfacial energy of the particles
- Systematic studies of particular phenomena for 3D structures
- Towards quantitative simulations for real alloy systems

End

- Thank you for your attention!

- Acknowledgment:
  - 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 (operational since May 2005)

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