OpenPhase Solutions GmbH

OpenPhase Solutions

Microstructure simulation in metallic materials

Johannes Görler

The Company

- Start-up of **ICAMS, Ruhr-University Bochum**

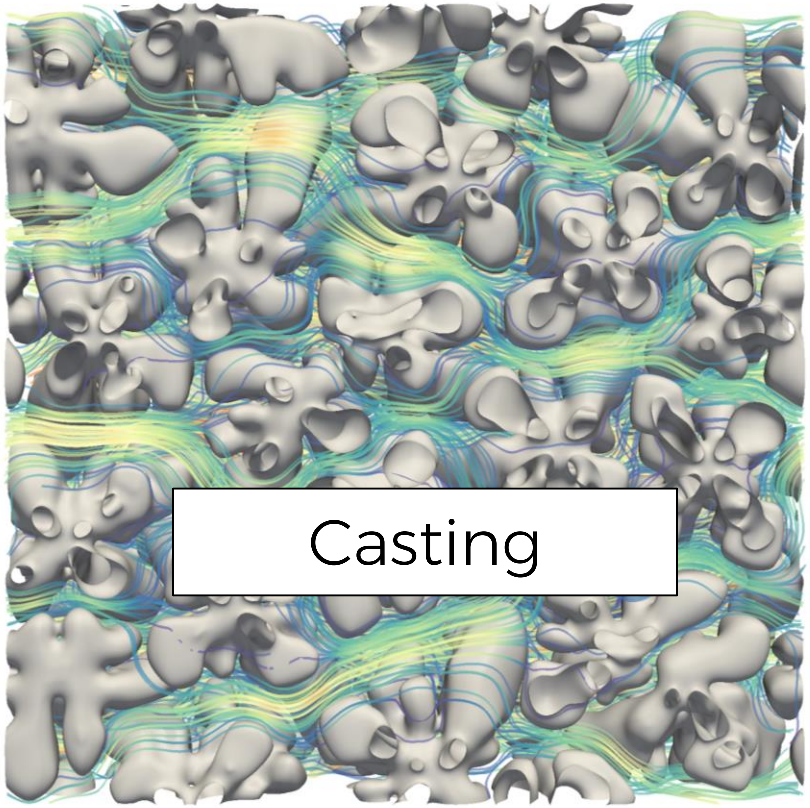
- Founded by four ICAMS scientists in 2018

OpenPhase Solutions GmbH

The Company

Goal: Provide innovative and accessible microstructure simulation solutions

- Multiphysics simulation suite
- Diverse applications and materials
- Cutting edge scientific development



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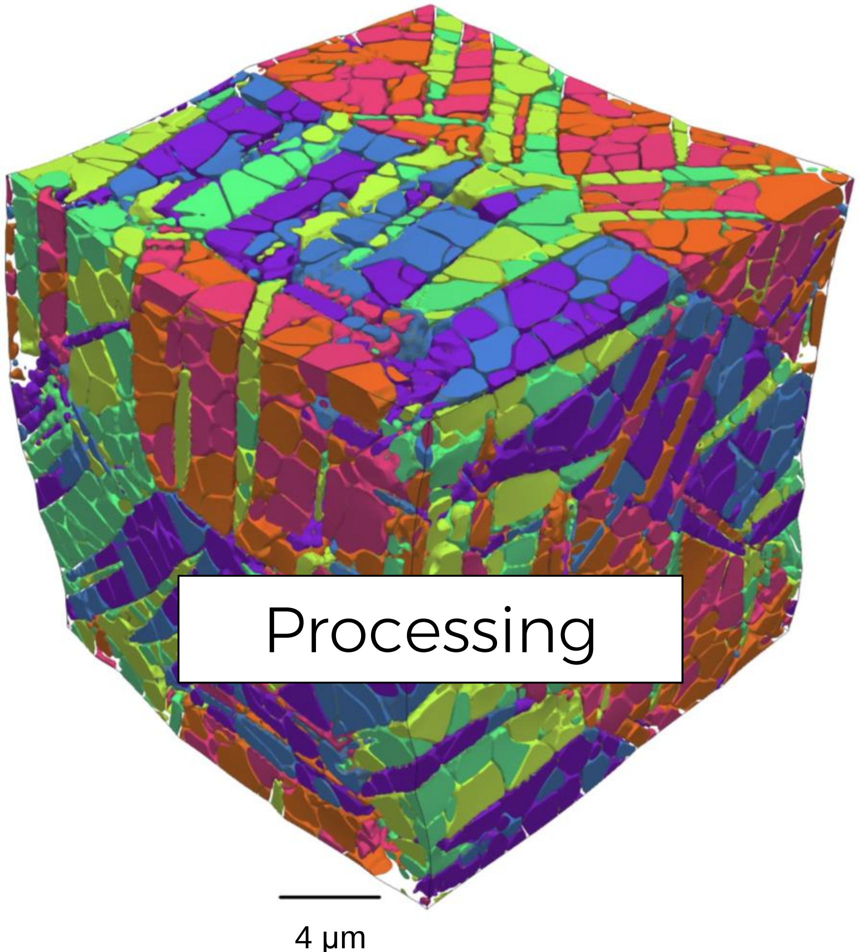
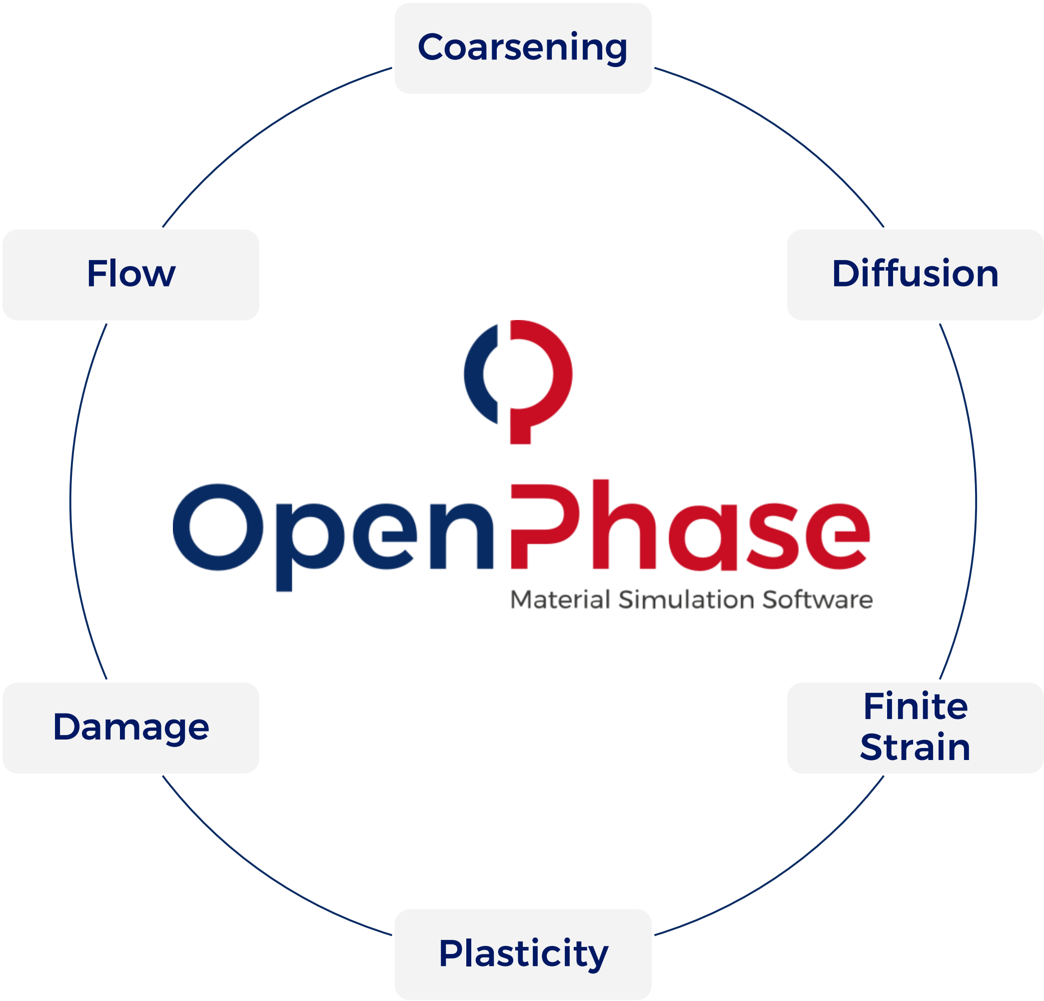
The Software

Obtain **microstructure and materials properties** from process parameters

- Mechanical properties
- Microstructure morphology
- Element distribution



The Software



Software library: > 50 man-years of research and development since 2009

Predictive power through:

- **Physics based** models
- Thermodynamic and kinetic **database** coupling

Thermo-Calc

Open Calphad

Gibbs Energies

Linearized Phase diagrams

Outline

- OpenPhase Products and Services
- Short introduction to the phase-field method
- Mg-Al casting simulation
- Coarsening of carbon nanotube reinforced aluminium
- Dynamic recrystallization in austenitic steel

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- **OpenPhase Products and Services**
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Our Products

Support

Training

Custom Solutions

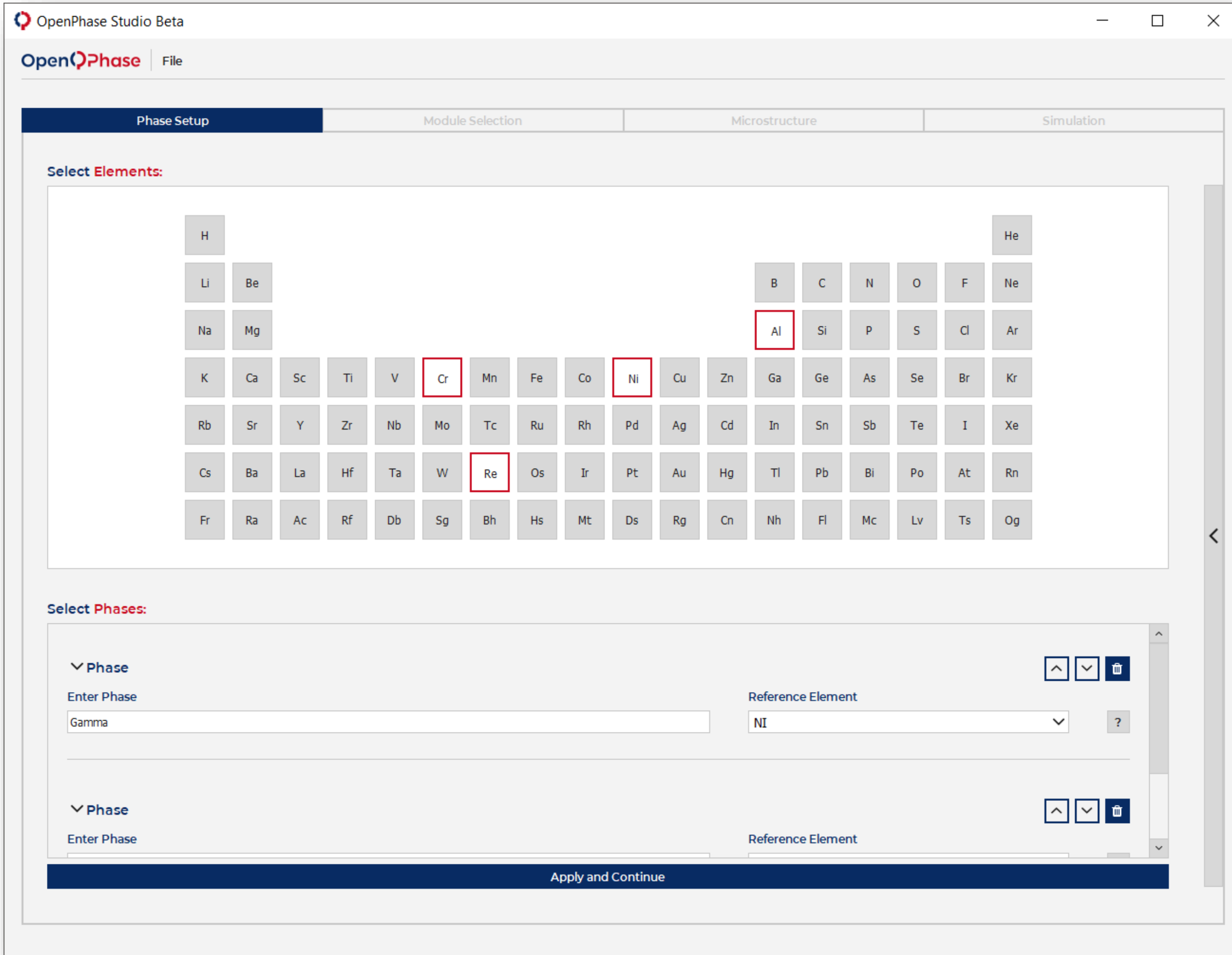
Software

- **OpenPhase Studio:** Full-featured simulation suite
- **OpenPhase Core:** powerful opensource Phase-field library

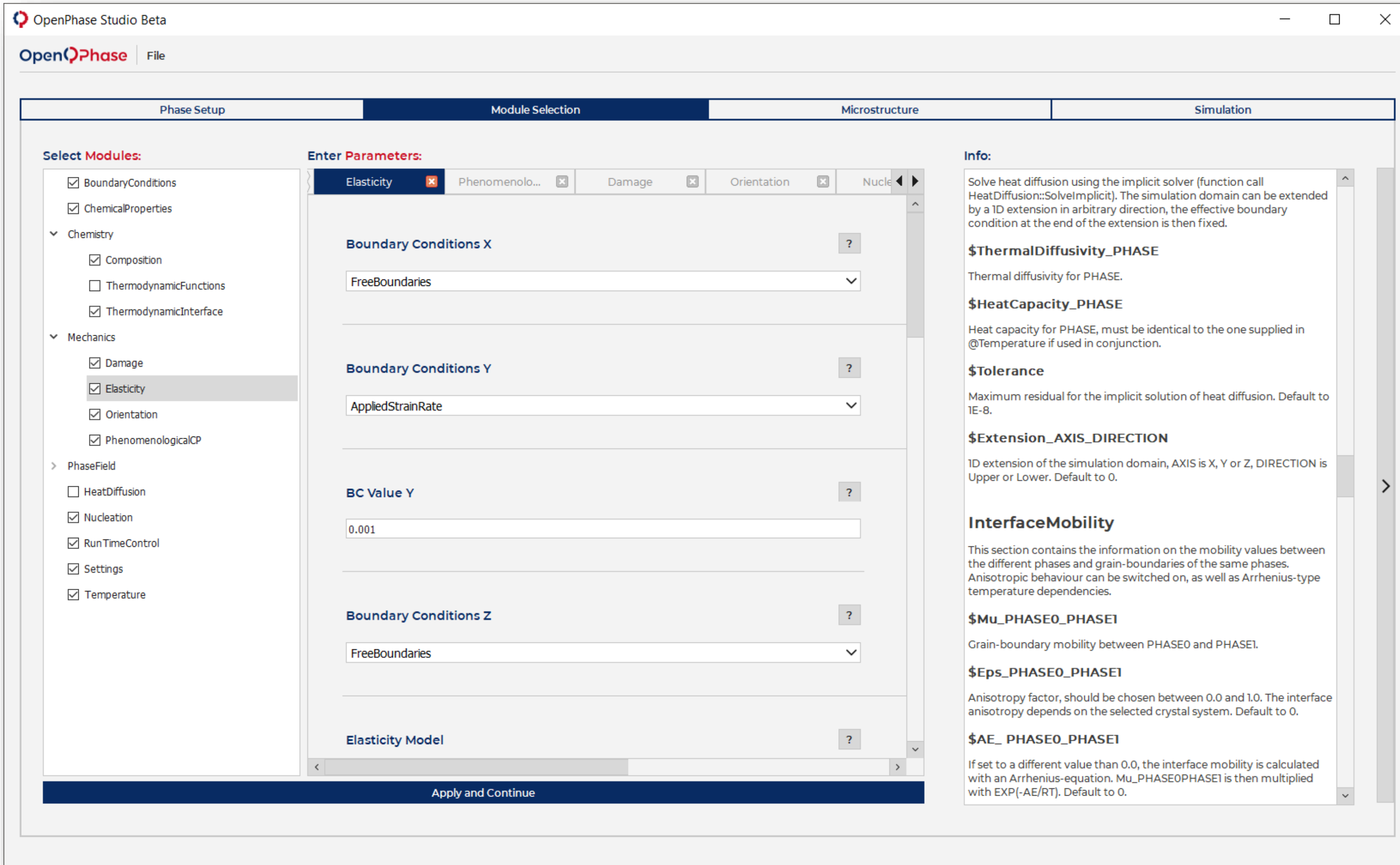
Based on OpenPhase Core, **OpenPhase Studio** provides:

- Intuitive **GUI** (Graphical User Interface)
- **Built-in analysis** of key properties
- **Presets** for quick and easy simulation setup
- Built-in **documentation** with context based navigation
- Windows and Linux versions available

OpenPhase Studio

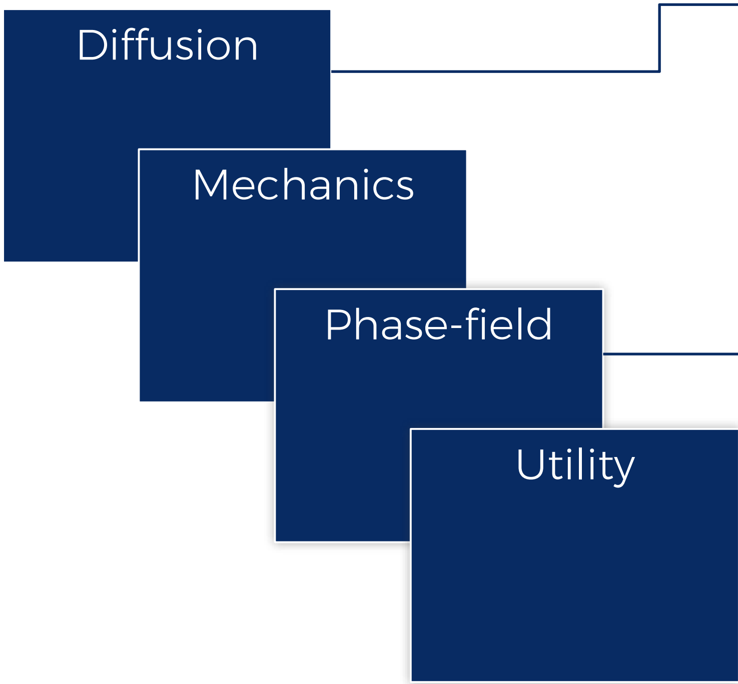


OpenPhase Studio



OpenPhase Core

Modules




```
DO.CalculatePhaseFieldIncrements(Phi, Sigma, Mu);
Timer.SetTimeStamp("Get PhiDot");
DF.GetDrivingForce(Phi, Cx, Tx, dG);
Timer.SetTimeStamp("Chemical Driving Force");
EP.SetEffectiveElasticConstants(Phi);
EP.SetEffectiveEigenStrains(Phi, Cx);

Timer.SetTimeStamp("Elastic Properties");
EP.CalculateChemicalPotentialContribution(Phi, DF);
Timer.SetTimeStamp("Elastic Chem Pot");

EP.CalculateDrivingForce(Phi, dG);
Timer.SetTimeStamp("Elastic Driving Force");
if(!(tStep % 10))
{
    ES.Solve(EP, BC, 1.0e-6, 10000.0, 1000, RTC.dt);
}
Timer.SetTimeStamp("Elastic Solver");
dG.Average(Phi, BC);
Timer.SetTimeStamp("Driving Force Average");
dG.MergePhaseFieldIncrements(Phi, Sigma, Mu);
Phi.NormalizeIncrements(BC, RTC.dt);
Timer.SetTimeStamp("Merge Velocities");
```

Simulation code

Our Products

Software

Training

Custom Solutions

Support

- Quick and reliable support
- Configure simulations, answer technical and scientific questions

Our Products

Software | **Support** | **Custom Solutions**

Training

- OpenPhase training is available for beginners and advanced users
- Immediately work productively with OpenPhase

Our Products

Software

Support

Training

Custom solutions

- Custom simulations
- Custom interfaces to other software
- Implementation of new models

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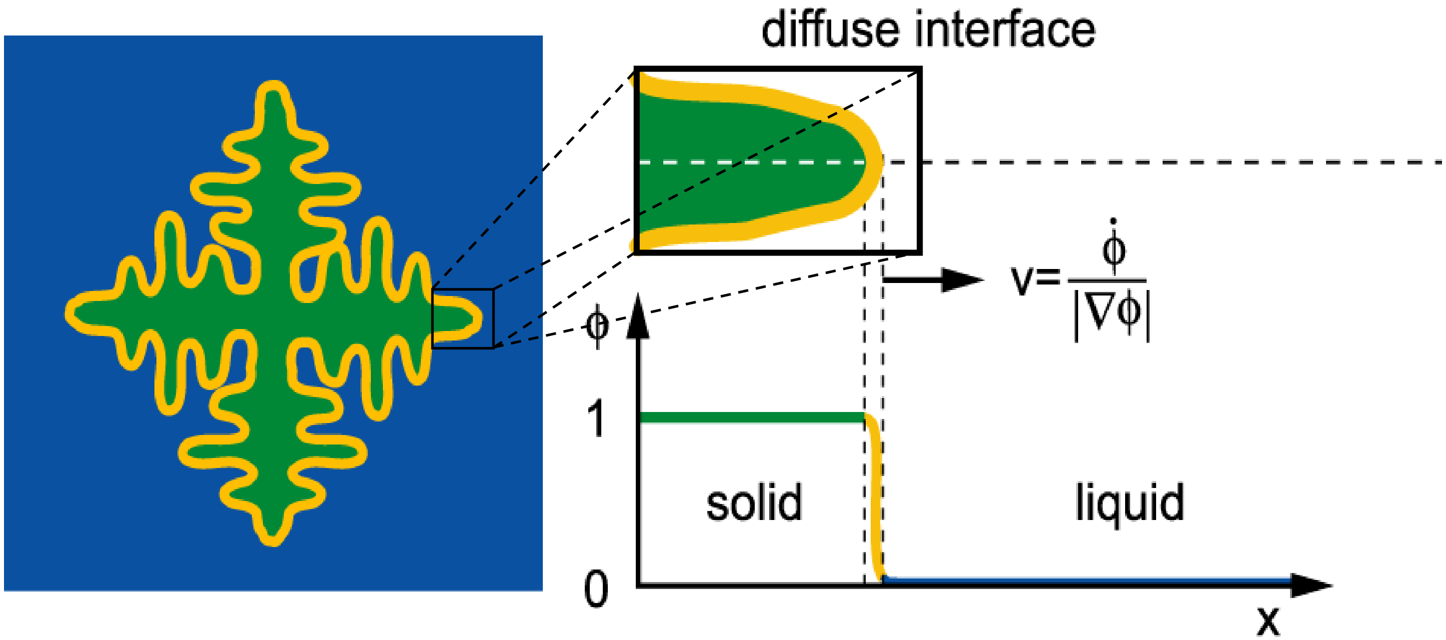
The Phase-Field Approach

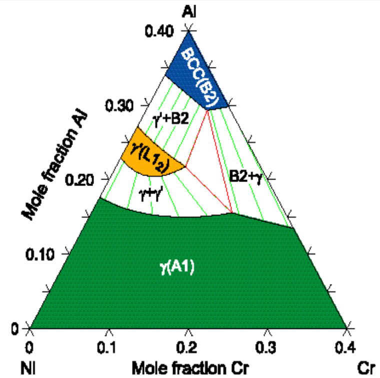


- Diffuse interface between the phases. The phase distribution in space is prescribed by the phase field function ϕ(x,t).
- The temporal evolution of ϕ (x,t) will be derived from the principle of minimization of Gibbs energy.

Multi-phase field method + diffusion + mechanics

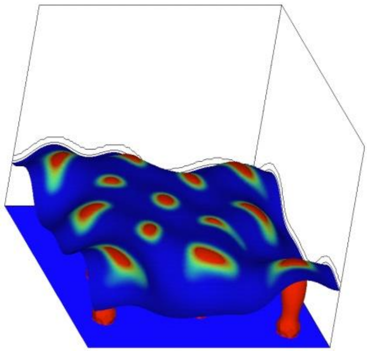
$$f = \sum_{\alpha,\beta} \frac{\sigma_{\alpha\beta}(\vec{n}_\alpha,\vec{n}_\beta)}{\eta_{\alpha\beta}} K^{\alpha\beta}(\Delta\phi_\alpha,\Delta\phi_\beta,\phi_\alpha,\phi_\beta) + \sum_\alpha \phi_\alpha f^\alpha(c_\alpha)$$

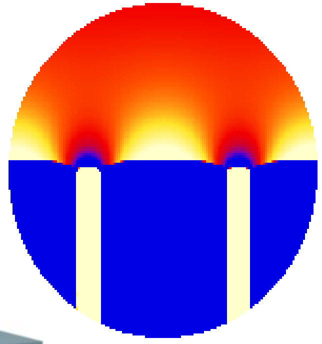
free energy functional



$$\dot{\phi}_\alpha = \frac{1}{n} \sum_\beta \mu_{\alpha\beta} \left(\frac{\delta f}{\delta\phi_\alpha} - \frac{\delta f}{\delta\phi_\beta} \right)$$

phase evolution



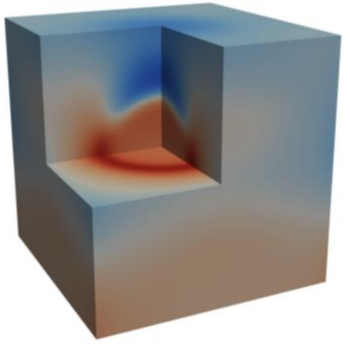


$$\dot{c}^i = \sum_k \nabla M^{ik} \nabla \frac{\partial f}{\partial c^i} = \sum_k \sum_\alpha \nabla D_\alpha^{ik} \nabla c_\alpha^k$$

diffusion

$$0 = \nabla \frac{\partial f}{\partial \varepsilon} = \nabla\sigma = \sum_\alpha \nabla \phi_\alpha C_\alpha \left(\varepsilon_\alpha - \varepsilon_\alpha^* - \varepsilon_\alpha^1 c_\alpha \right)$$

mechanical equilibrium



Implementation details

Phase field module

Phase field equation

$$\dot{\phi}_\alpha = -\sum_{\beta=1}^{N} \frac{\mu_{\alpha\beta}}{N}\left(\frac{\delta F}{\delta \phi_\alpha} - \frac{\delta F}{\delta \phi_\beta}\right);$$

Interfacial energy density

$$f^{GB} = \sum_{\alpha,\beta=1}^{N} \frac{4\sigma_{\alpha\beta}}{\eta_{\alpha\beta}}\left\{\frac{\eta^2_{\alpha\beta}}{\pi^2}\left|\nabla\phi_\alpha\right|\cdot\left|\nabla\phi_\beta\right| + \phi_\alpha\phi_\beta\right\}$$

Initialization module

Fluid dynamics module

Navier-Stokes equation

$$\frac{\partial}{\partial t}(\phi_l \vec{u}) + \nabla\cdot(\phi_l \vec{u}\vec{u}) = \nabla[\nu\nabla\cdot(\phi_l\vec{u})] - \frac{\phi_l}{\rho_0}\left[\nabla P + \frac{\partial\rho}{\partial c}\left(c_l - \langle c_l\rangle\right)\vec{g}\right] + h^*\frac{\nu(1-\phi_l)^2\phi_l\vec{u}}{\eta^2}$$

Modular structure dictated by the free energy contributions

interfacial elastic

$$F = \int_\Omega f^{GB} + f^{CH} + f^{EL} + \cdots$$

chemical etc..

Diffusion module

Advection-diffusion equation

$$\dot{\bar{c}} + \vec{u}\cdot\nabla(\phi_l\bar{c}_l) = \nabla\cdot\left(\sum_{\alpha=1}^{N} M\nabla\frac{\delta F}{\delta \bar{c}}\right) + \nabla\cdot\vec{j}_{at};$$

Chemical energy density

$$f^{CH} = \sum_{\alpha=1}^{N}\phi_\alpha f_\alpha(\bar{c}_\alpha) + \bar{\mu}\left(\bar{c} - \sum_{\alpha=1}^{N}\phi_\alpha\bar{c}_\alpha\right)$$

… other modules are being added by introducing new solvers

Elasticity module

Elastic equilibrium equation

$$0^i = \nabla^j\sigma^{ij} = \nabla^j\frac{\delta F}{\delta\varepsilon^{ij}};$$

Elastic energy density

$$f^{EL} = \frac{1}{2}\sum_{\alpha=1}^{N}\phi_\alpha\left(\varepsilon^{ij}_\alpha - \varepsilon^{*ij}_\alpha\right)C^{ijkl}_\alpha\left(\varepsilon^{kl}_\alpha - \varepsilon^{*kl}_\alpha\right)$$

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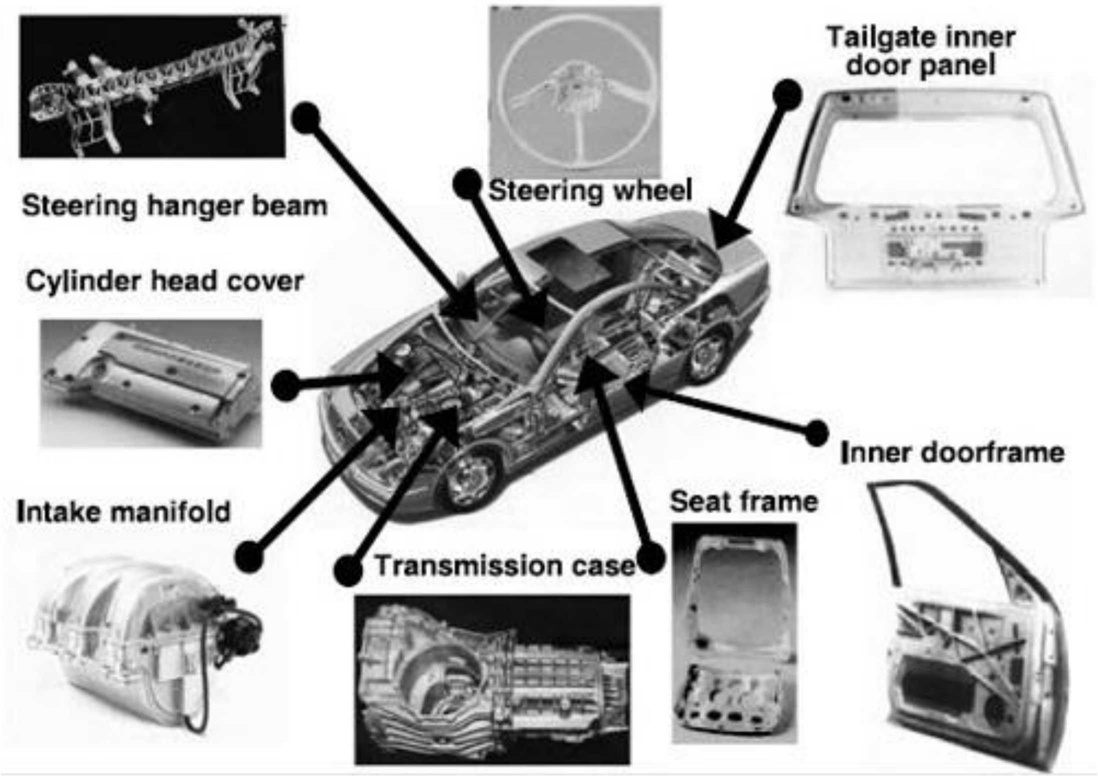
Mg-Al Alloys

- Low density structural materials
- Automotive applications
- Consumer electronics

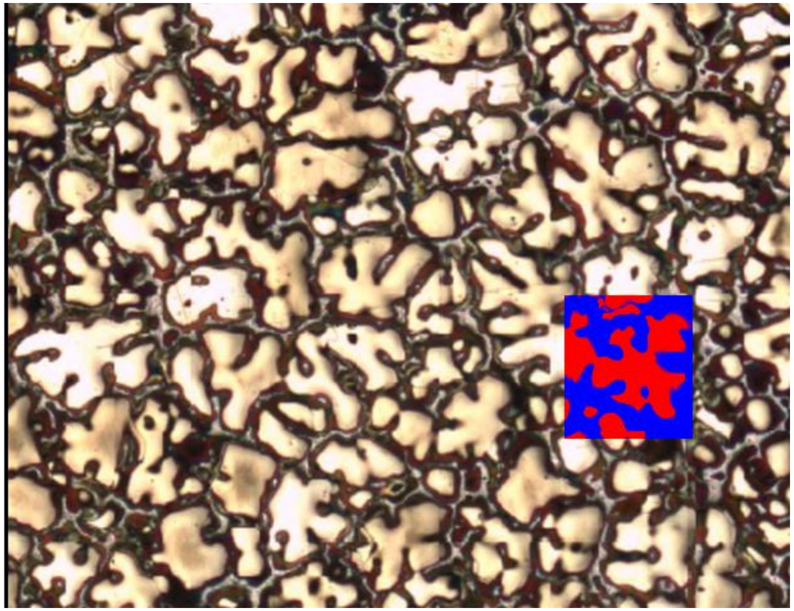
Element	Mg	Al	Fe
Density [g/cm³]	1.73	2.70	7.87



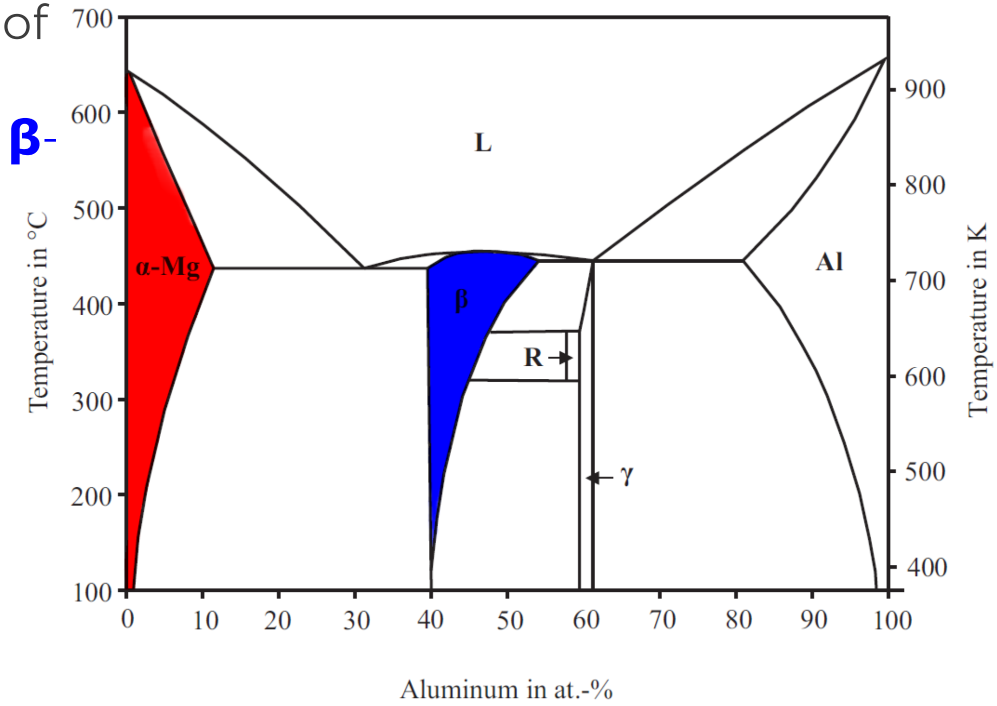
Key to Metals AG 2010

Mg-Al Microstructure and Thermodynamics

- Mg-Al alloys microstructure consist of **α**-phase (HCP-Mg dendrites) surrounded by closed shell $Mg_{17}Al_{12}$ **β**-phase
- properties depend on the microstructure



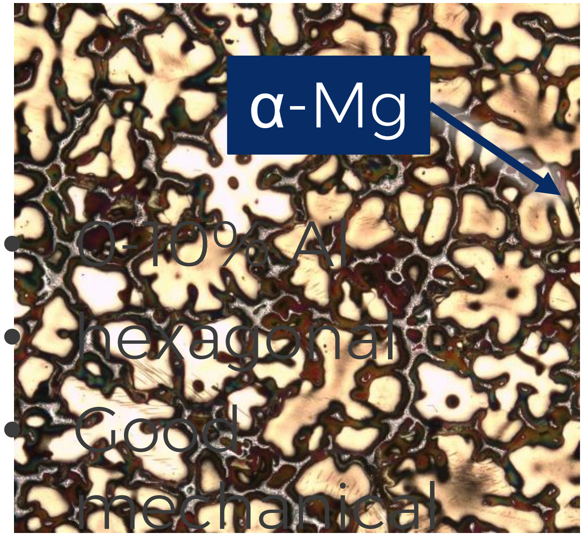
200µm



Goal:

- Optimize the solidification morphology to form a percolating **β**-phase around the primary **α**-phase

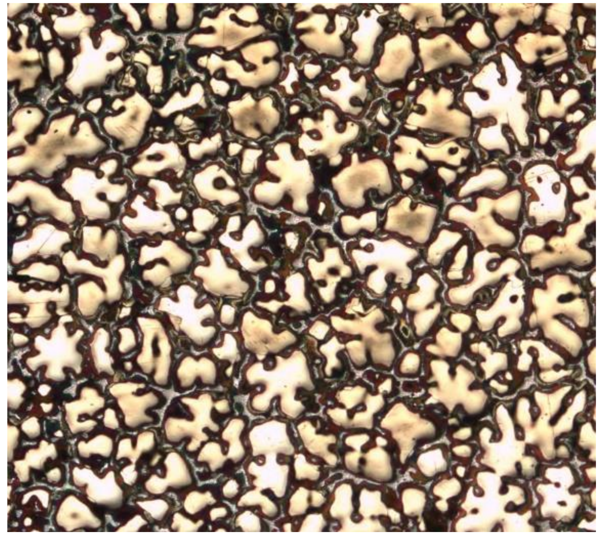
Effect of cooling rate on solidification microstructure



- 0-10% Al
- hexagonal
- Good mechanical properties

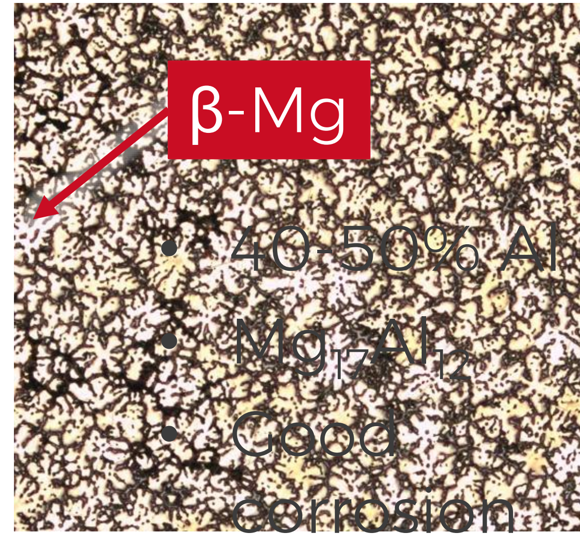
furnace control

- coarse microstructure
- connected eutectic regions



air cooling

Mg-5at.%Al



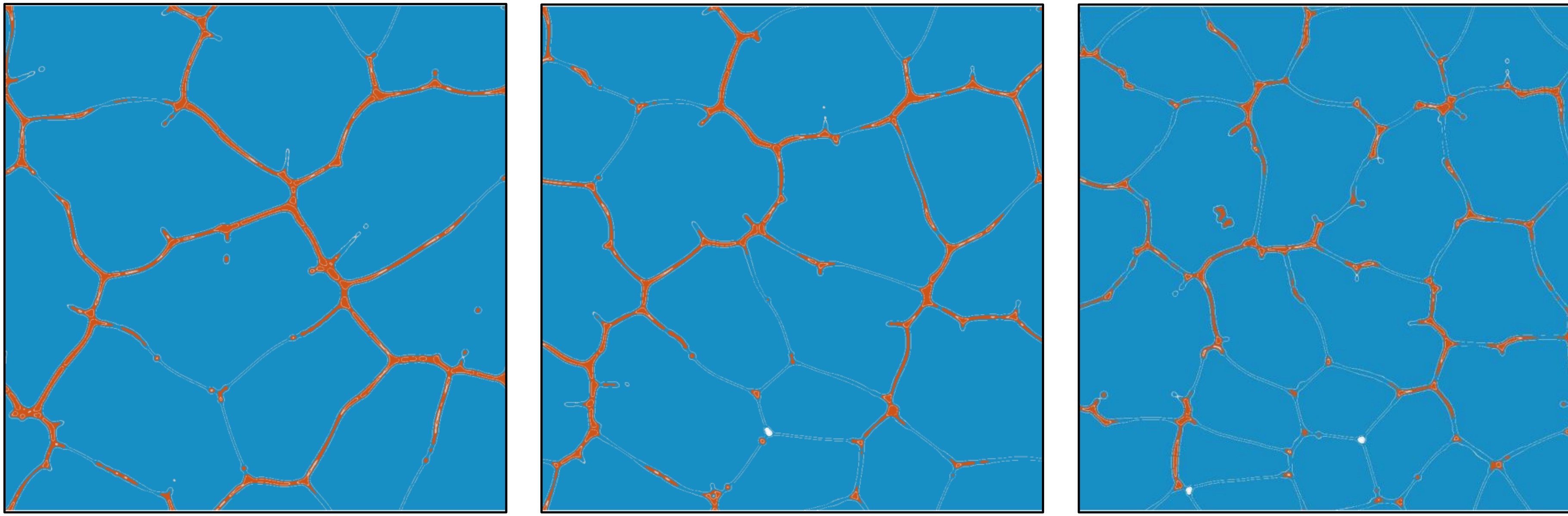
- 40-50% Al
- $Mg_{17}Al_{12}$
- Good corrosion properties

water cooling

- fine microstructure
- dispersed eutectic regions

Effect of cooling rate on solidification microstructure

5 K/s   15 K/s   25 K/s



slower cooling

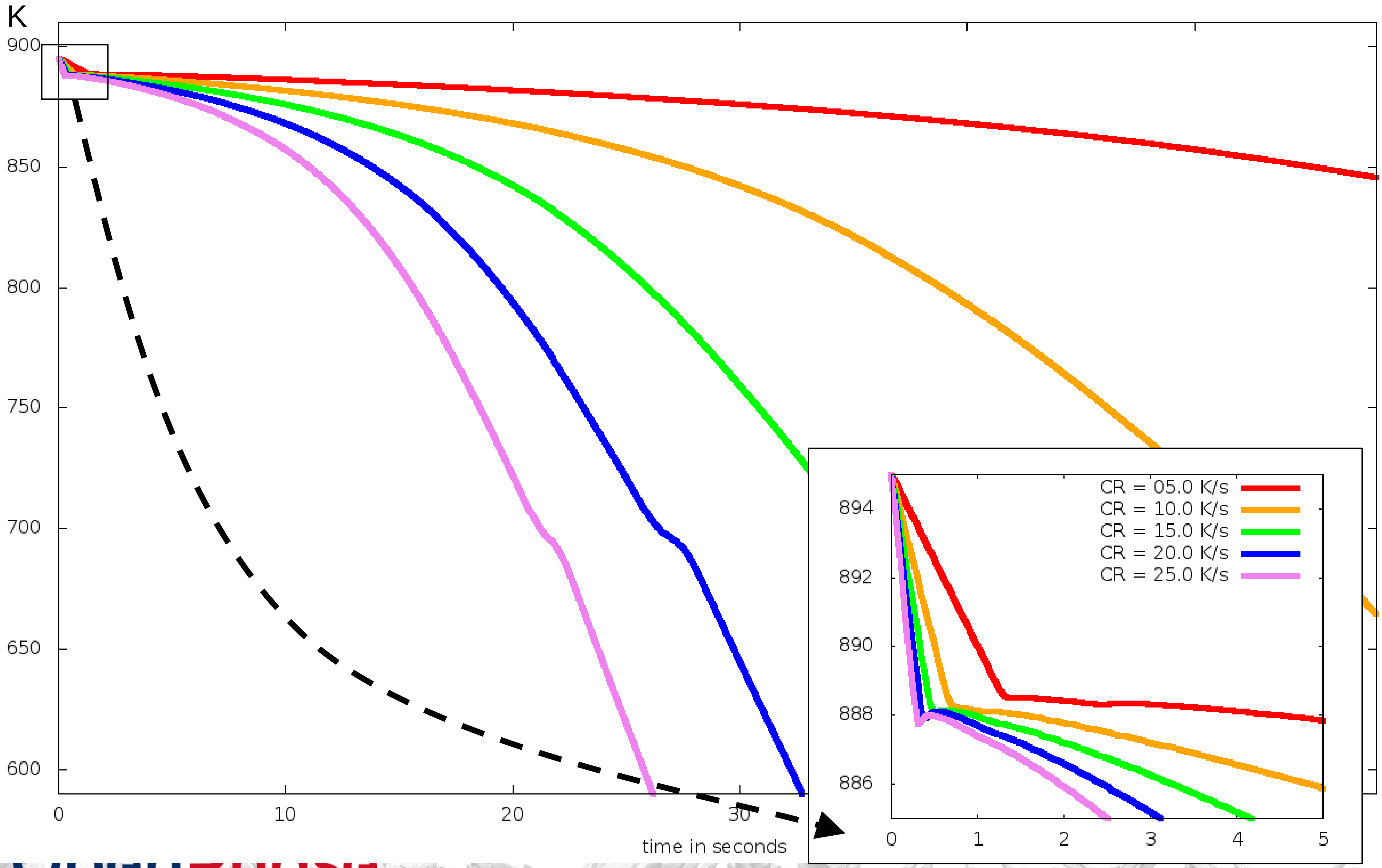
finer microstructure

α-Mg

β-Mg

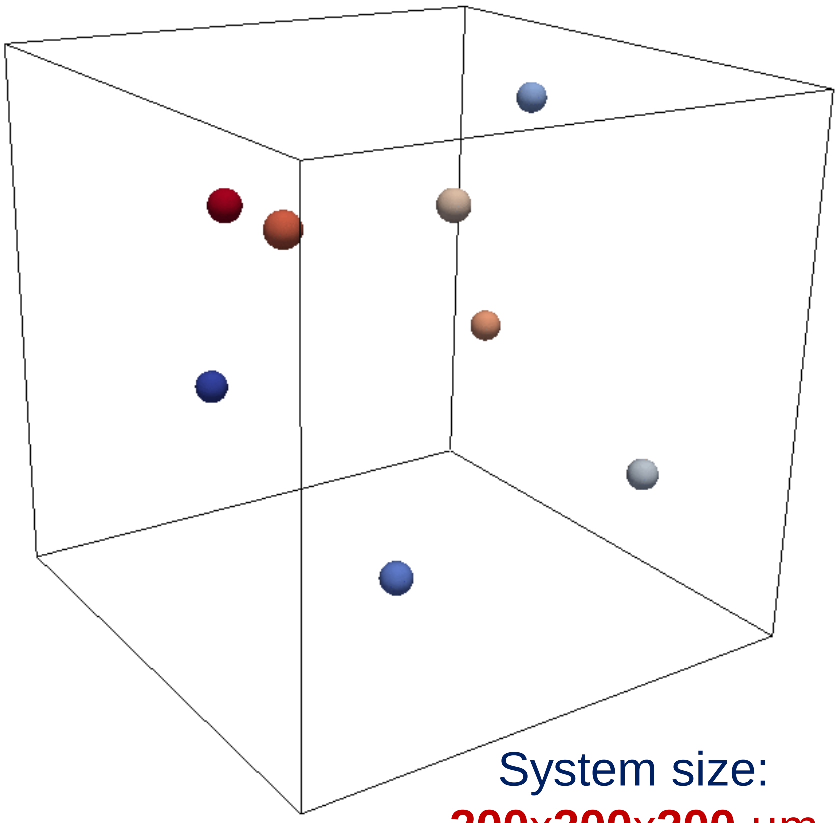
200µm

Cooling curves



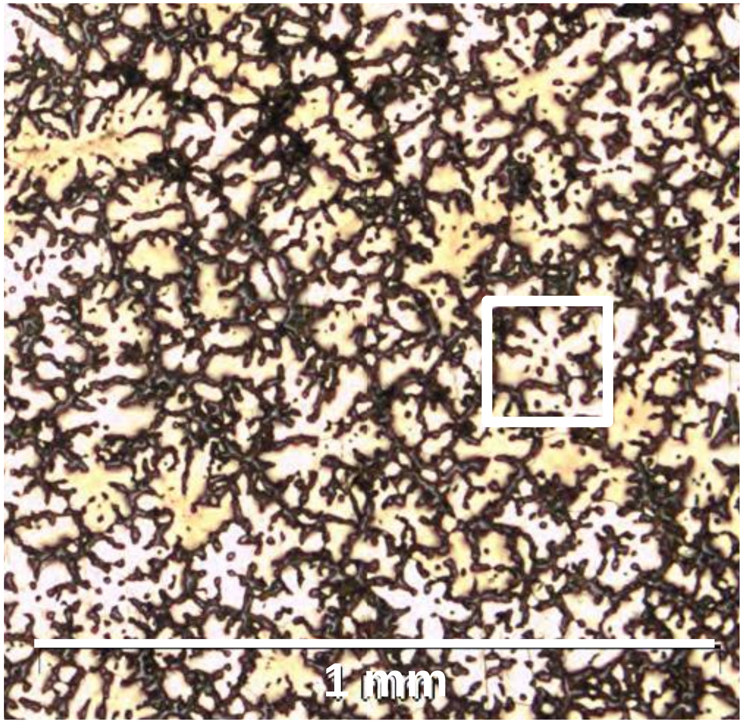
Simulation examples: Mg-Al solidification

Simulation
(cooling rate 10 K/s)



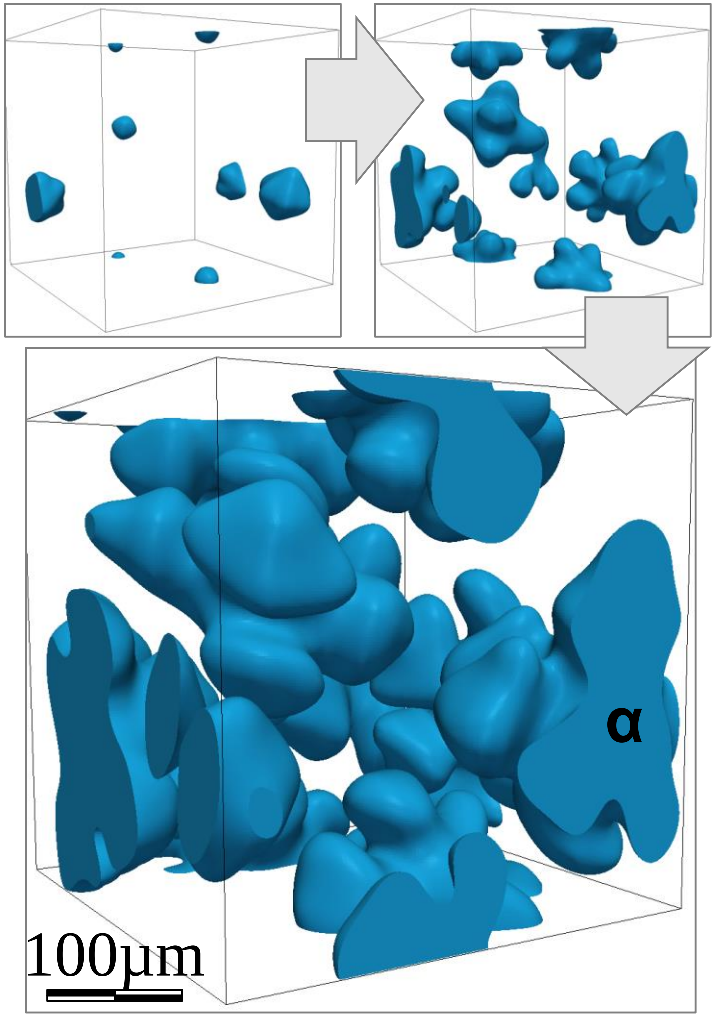
System size:
200x**200**x**200** µm

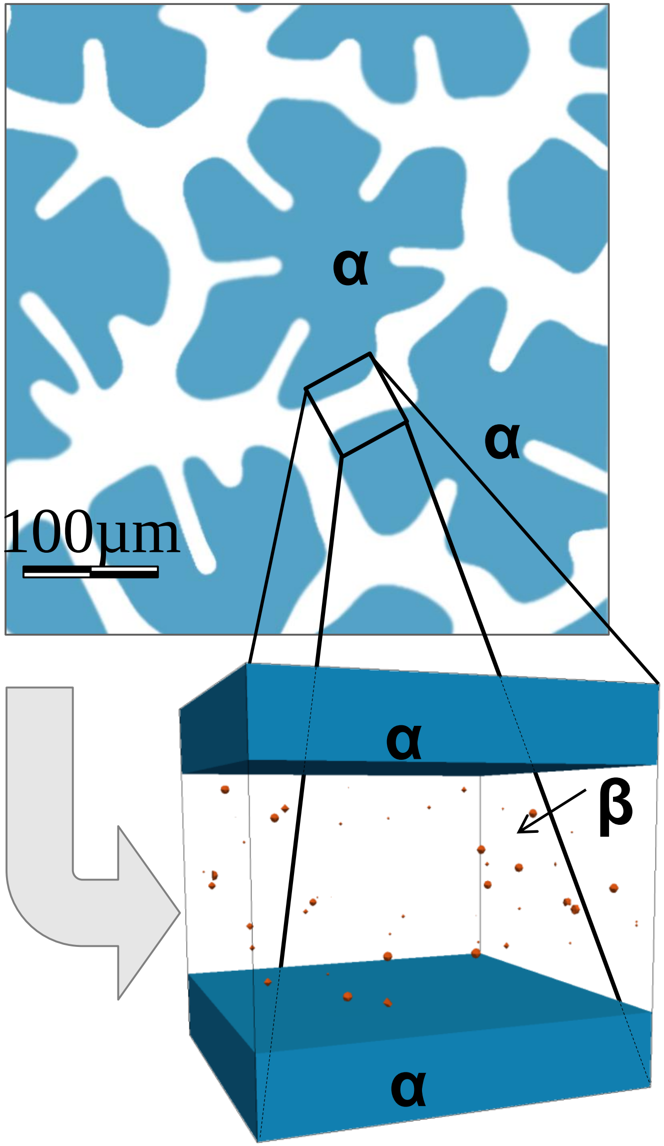
Experiment
(cooling rate 10 K/s)



courtesy of D. Hoeche

3D anisotropic alpha phase nucleation and growth





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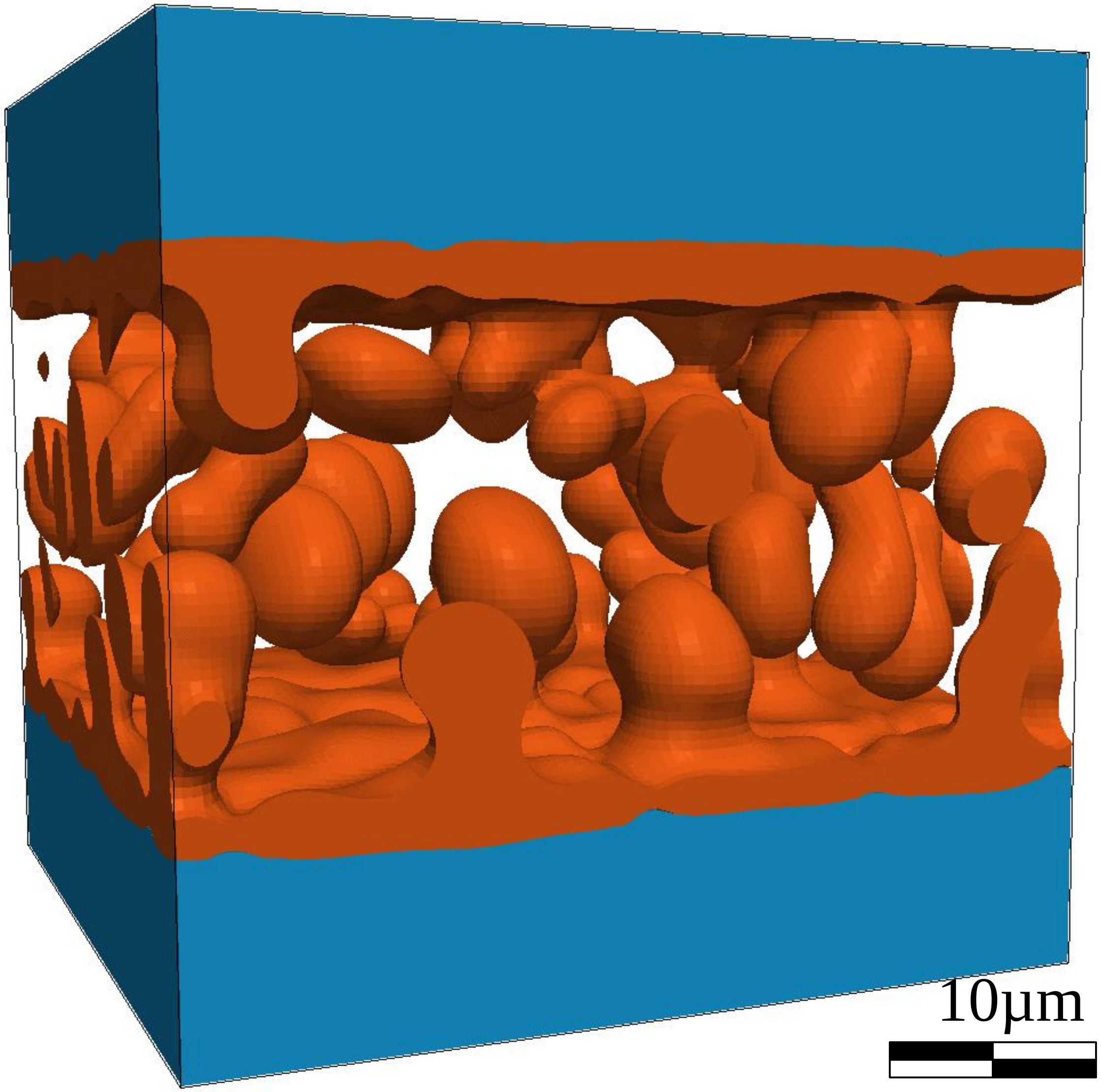
Sequential Eutectic Nucleation Modeling



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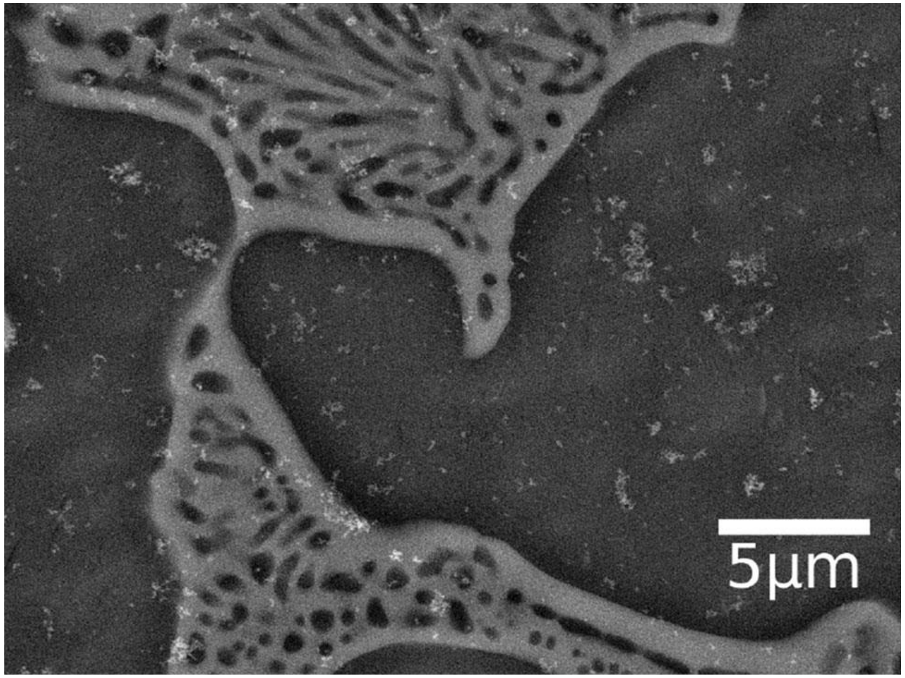
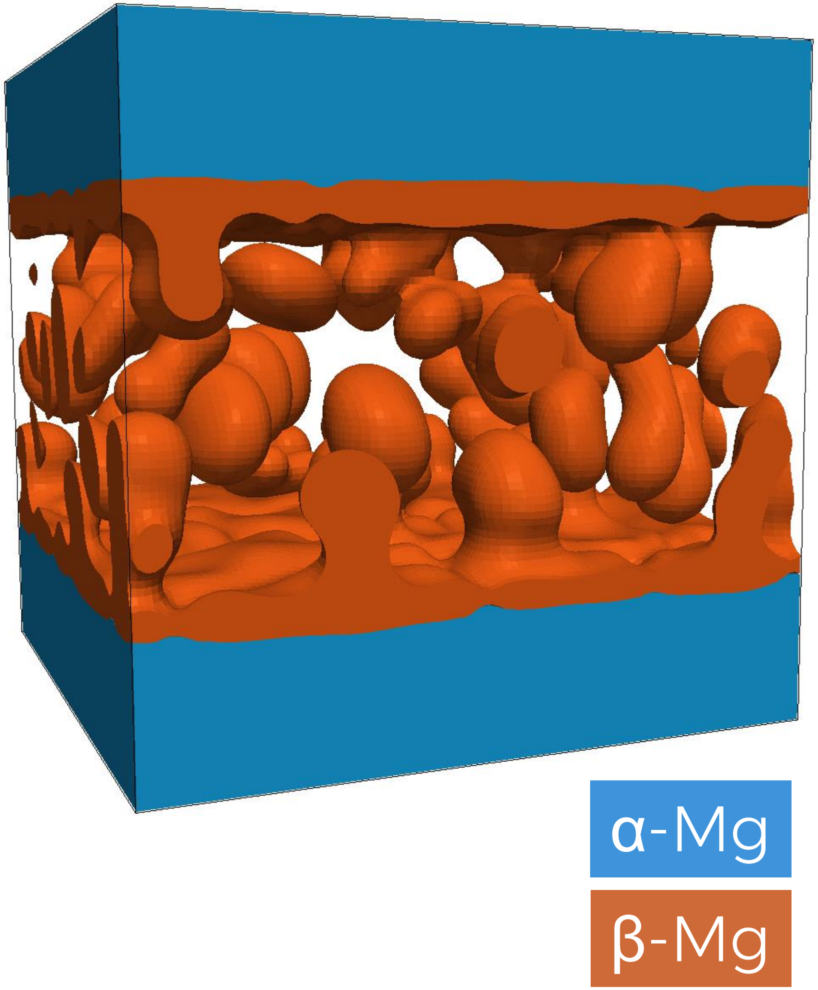
Evolution of microstructure during solidification





Monas, A., Shchyglo, O., Höche, D., Tegeler, M., & Steinbach, I. (2015). Dual-scale phase-field simulation of Mg-Al alloy solidification. *IOP Conference Series: Materials Science and Engineering*, *84*, 012069. https://doi.org/10.1088/1757-899X/84/1/012069

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Nano-grained Al with carbon nanotubes

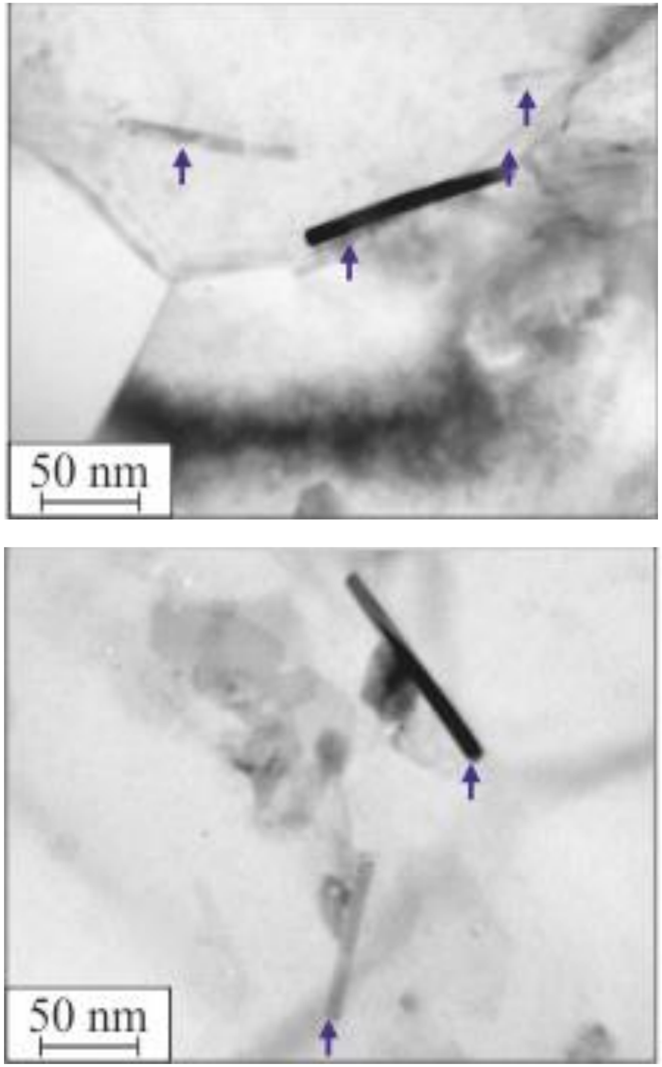
Secondary-phase particles

- interact with grain boundary
- Zener drag slows down grain growth

Carbon Nanotubes

- small size, low density, stable structure
- research interest: comparison to spherical particles

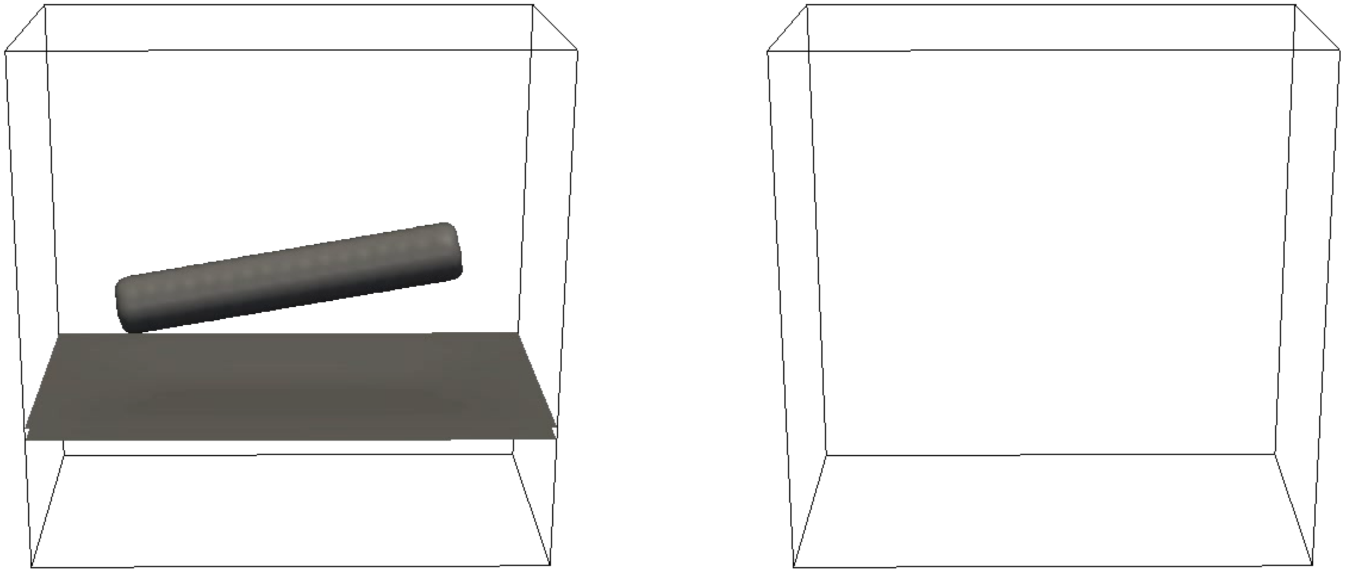
Courtesy of Bayer MaterialScience



Phase-field study of zener drag and pinning of cylindrical particles in polycrystalline materials, Schwarze et al., Acta Materialia, 106 (2016)

Carbon nanotube drag – simulations

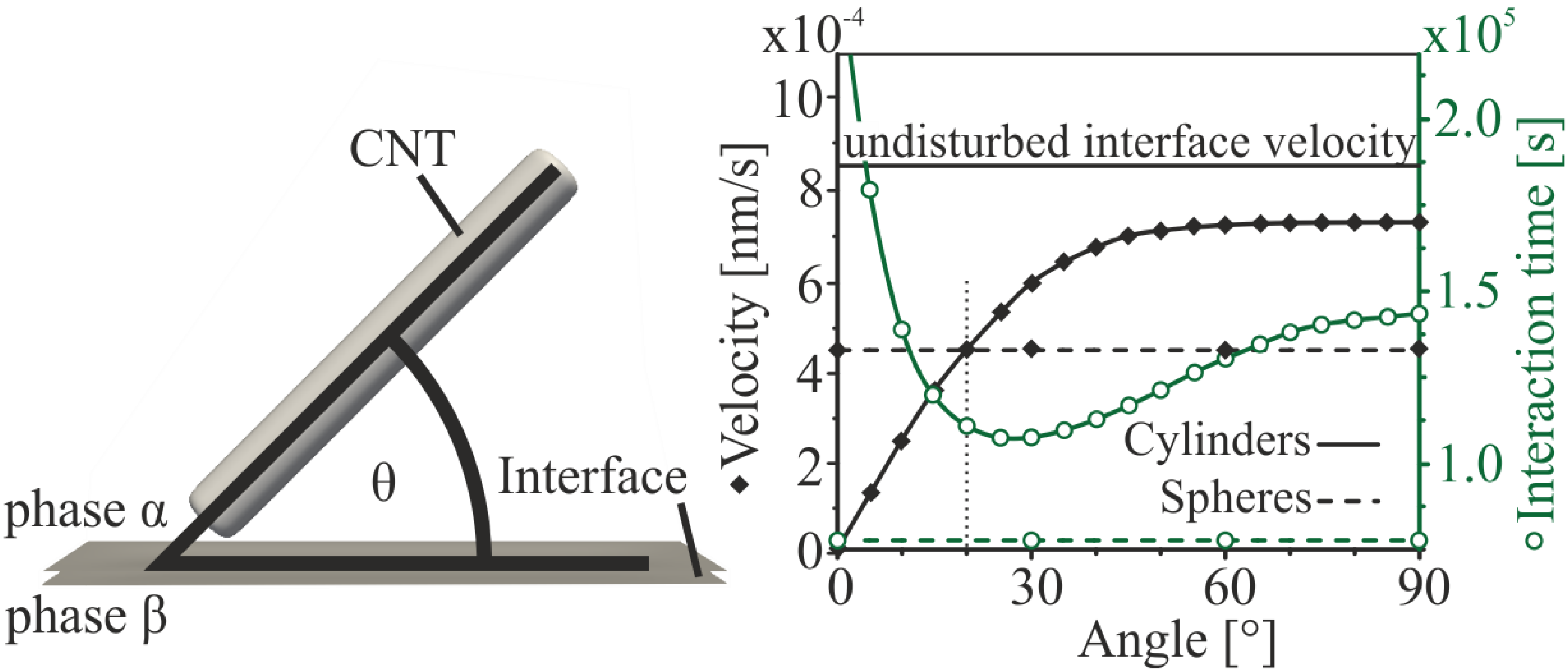
Single grain boundary behaviour



box size: 150x150x60 grid cells

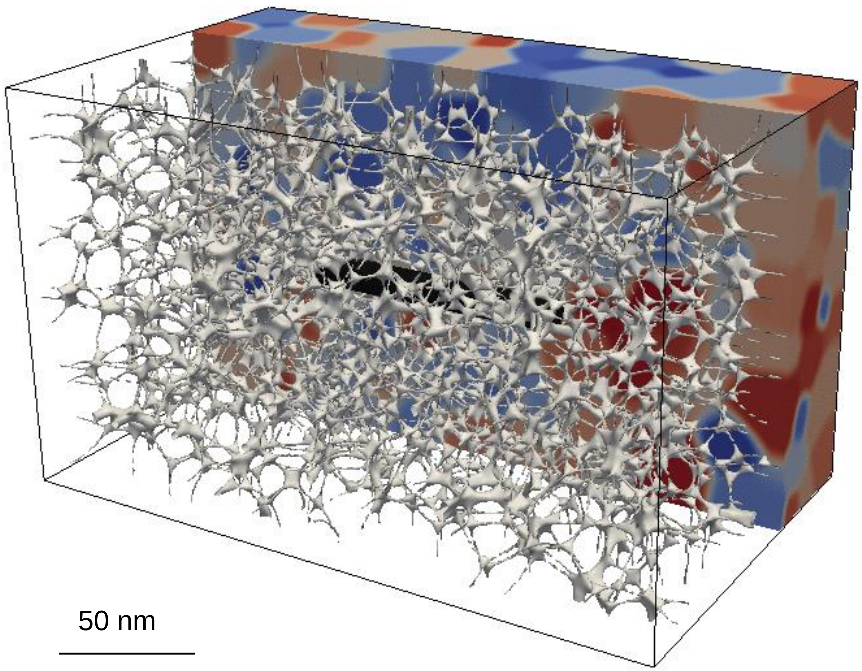
Carbon nanotube drag – simulations

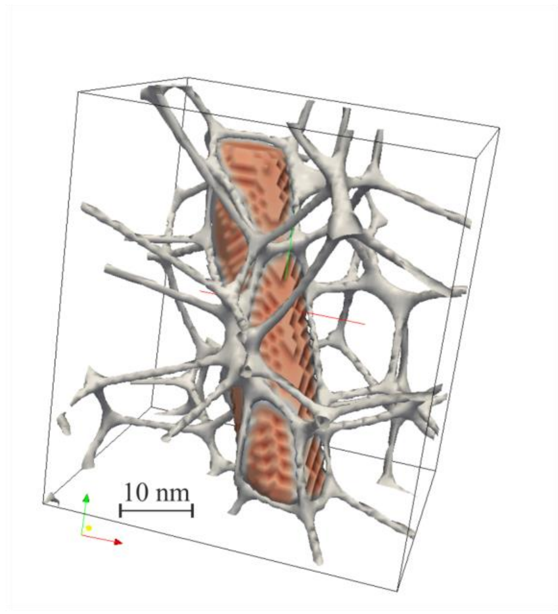
Single grain boundary behaviour



Carbon nanotube drag – simulations

The grain boundaries form a cage around the tube

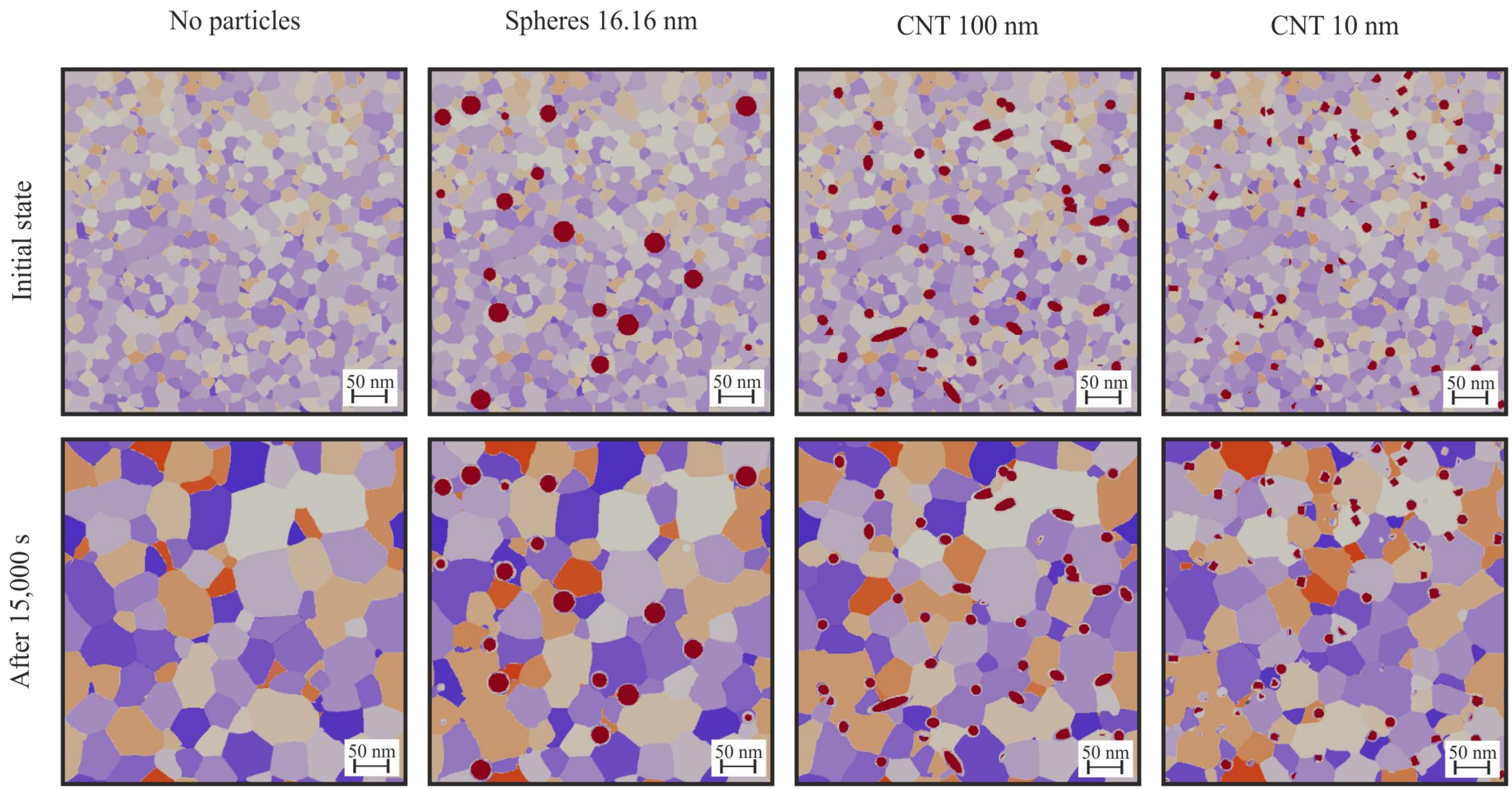




box size: 250x150x150 grid cells

Interaction of elongated particles with grain-boundaries

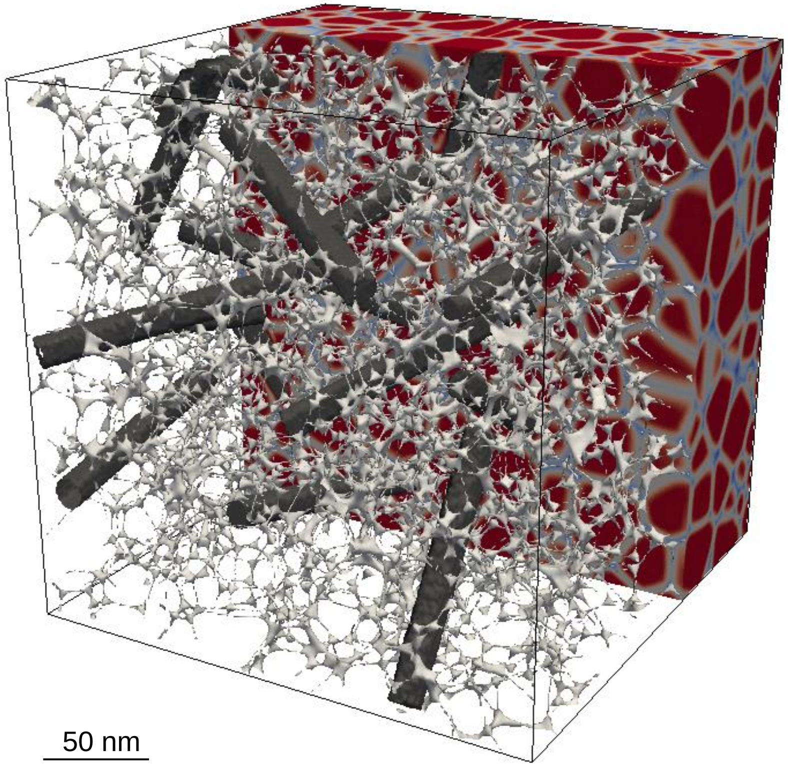
Different types of particles, constant volume fraction

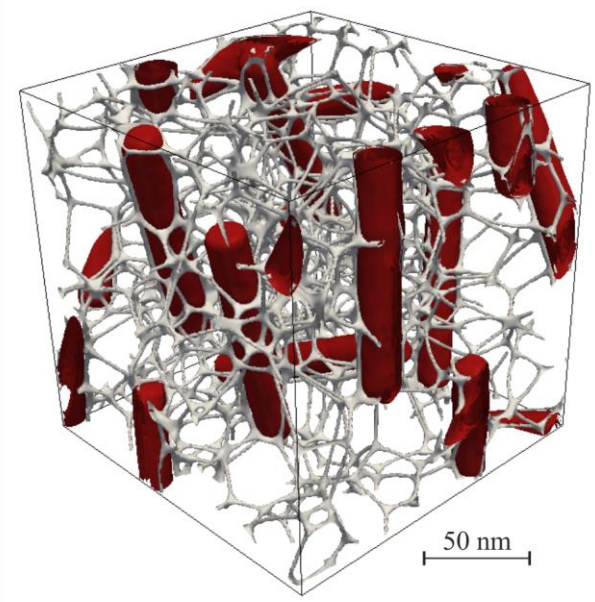


box size: 512^3 grid cells

Carbon nanotube drag – simulations

The grain boundaries form a cage around the tube





box size: 200^3 grid cells

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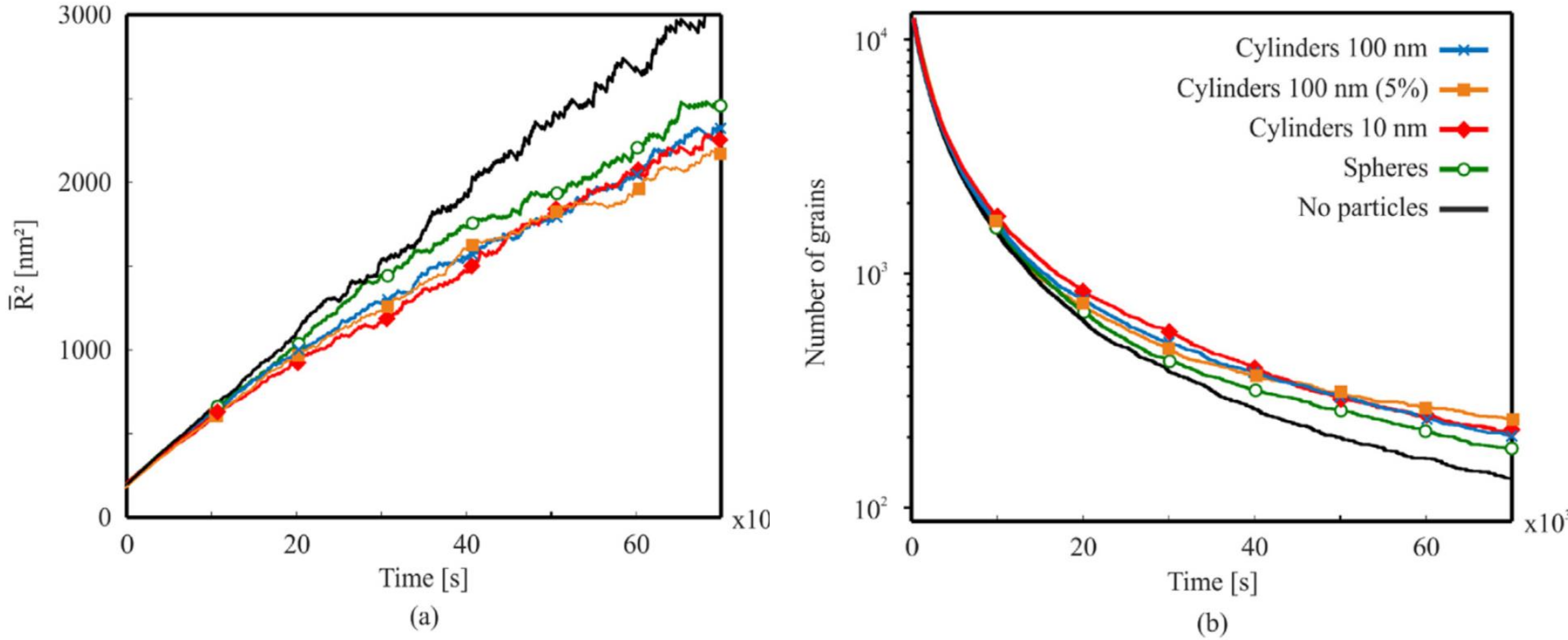
Carbon nanotube drag – simulations



Comparison to spherical particles and tubes with different length but same global volume fraction

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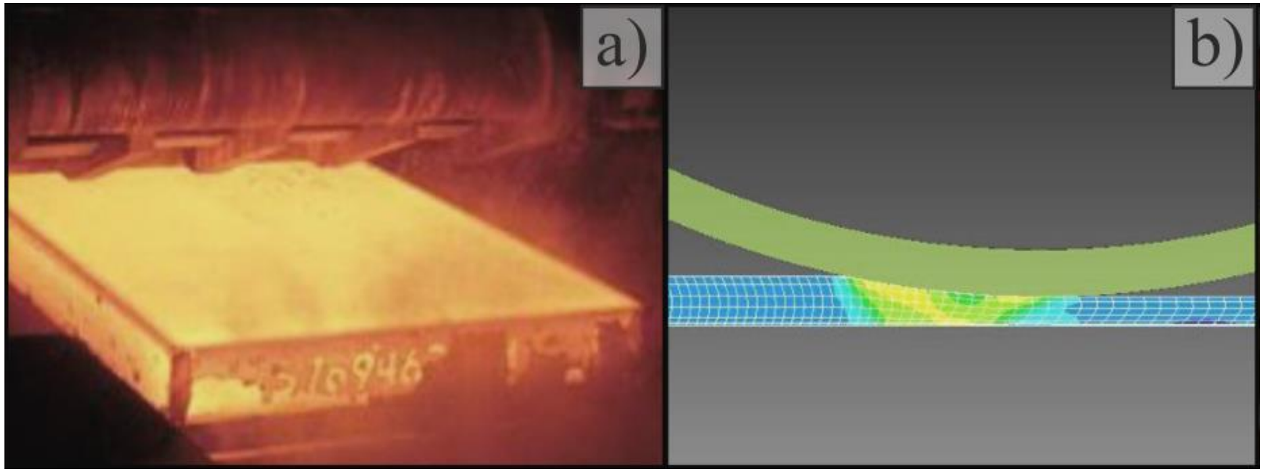
Dynamic recrystallization in austenitic steel

Challenges:

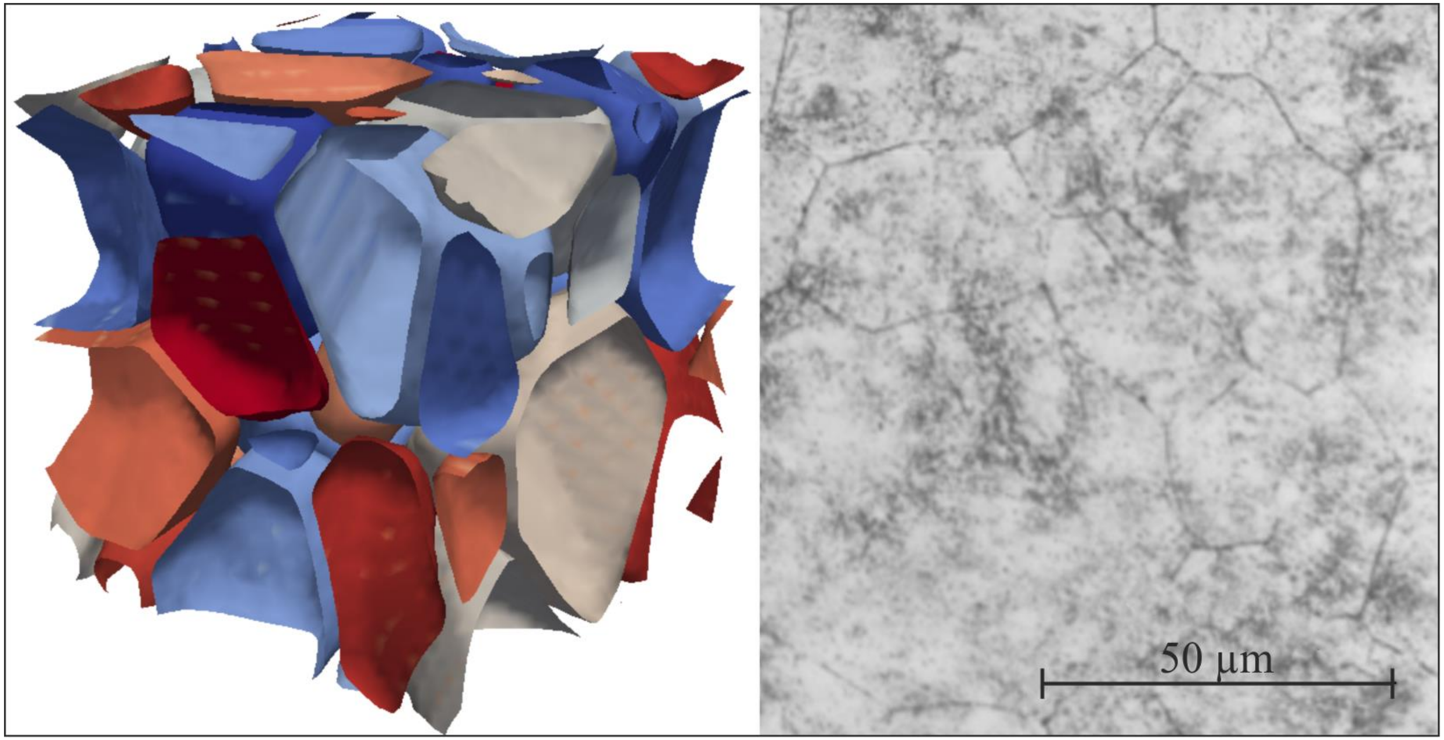
- Nucleation and grain growth depending on local dislocation density
- Large deformation combined with phase transformation



Dissertation Jan Hiebeler, thyssenkrupp
Jan Hiebeler et al. MATEC Web of Conferences **80**, 01003 (2016)

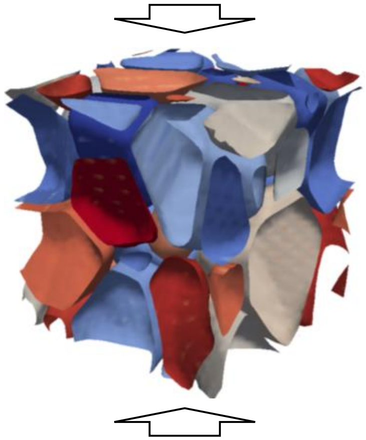
Initial condition

- Reference volume with 20 µm average grain size to match experimental conditions



Boundary conditions and model assumptions

Periodic boundary conditions and uniaxial compression in z-direction



Phenomenological crystal plasticity model with

- Hardening
- Recovery

Nucleation condition dependent on local hardening rate

Coarsening and growth of recrystallized grains driven by reduction of stored deformation energy

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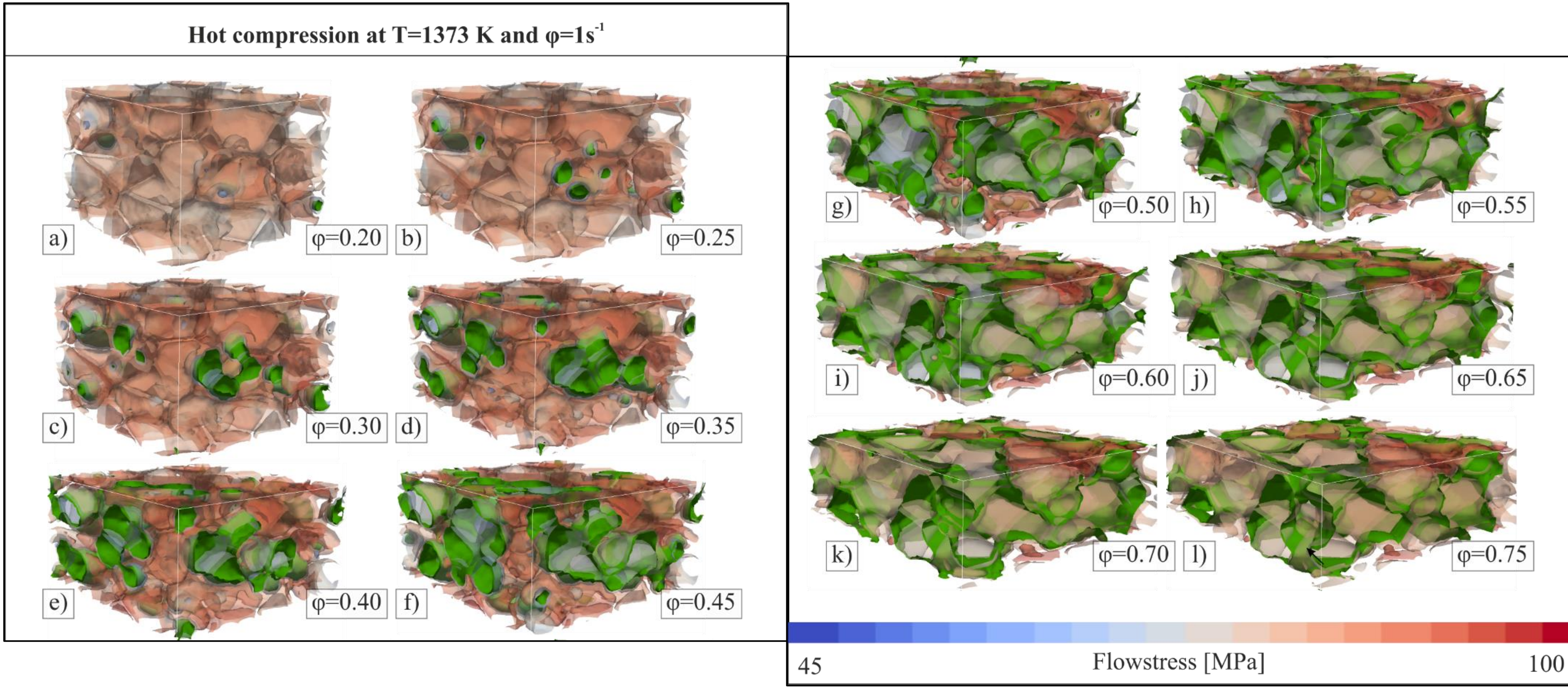
3-dimensional simulation: 75% reduction



Color corresponds to effective flow stress. Recrystallized grains are indicated in green.

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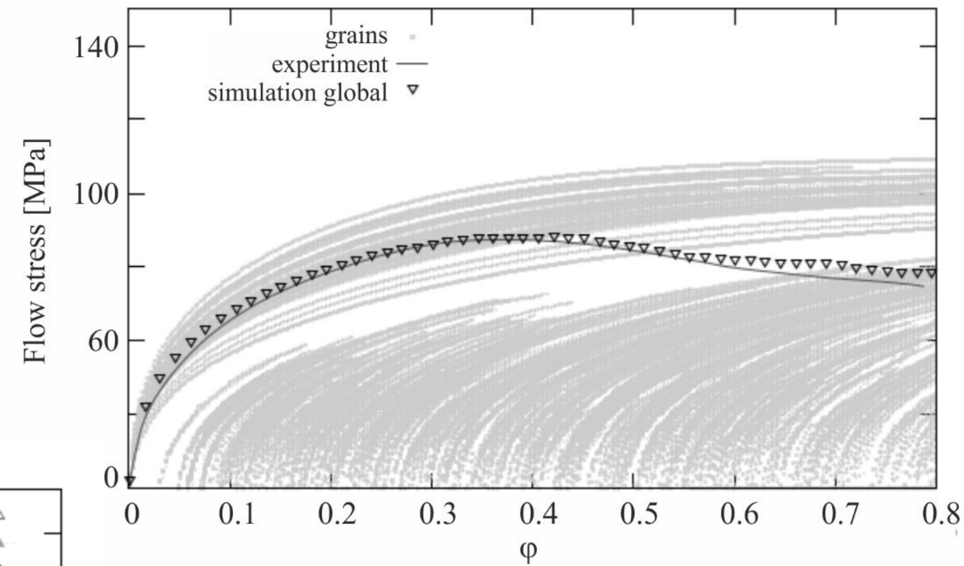
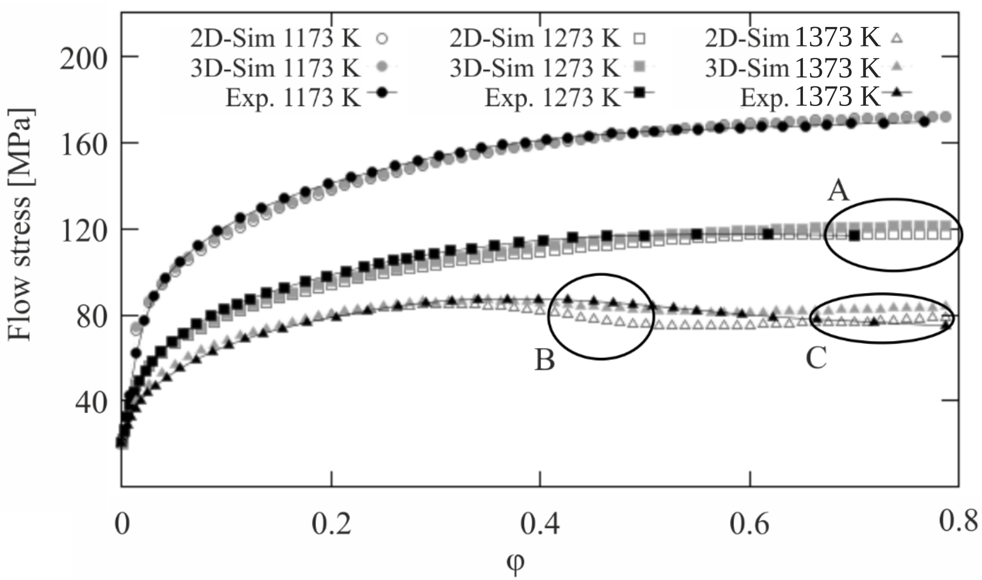
3-dimensional simulation: 80% reduction



Flow stress in individual grains and average flow stress

Variation of temperature: Experiment versus theory



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Conclusion

- Phase-Field Method is quite universal
- PFM applies to diffusive timescales and continuum description of matter
- PFM is a handy tool to investigate correlations of different mechanisms controlling microstructure evolution
  - Transport and morphology
  - Nucleation and growth
  - Mechanical and diffusive dissipation
- PFM evaluates macroscopic material properties during production and service considering evolving microstructures