3D Phase Field Modelling of the Austenite Decomposition

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Background

Phase Field Modelling

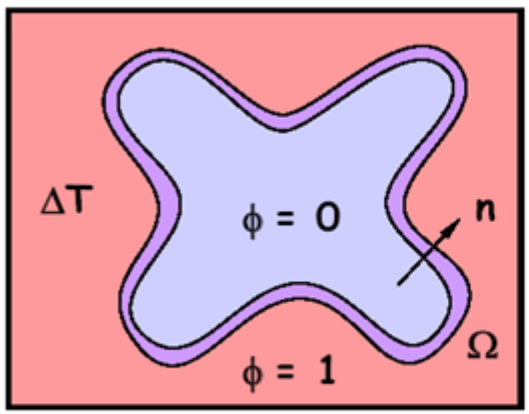
Modelling tool on the mesoscopic length scale

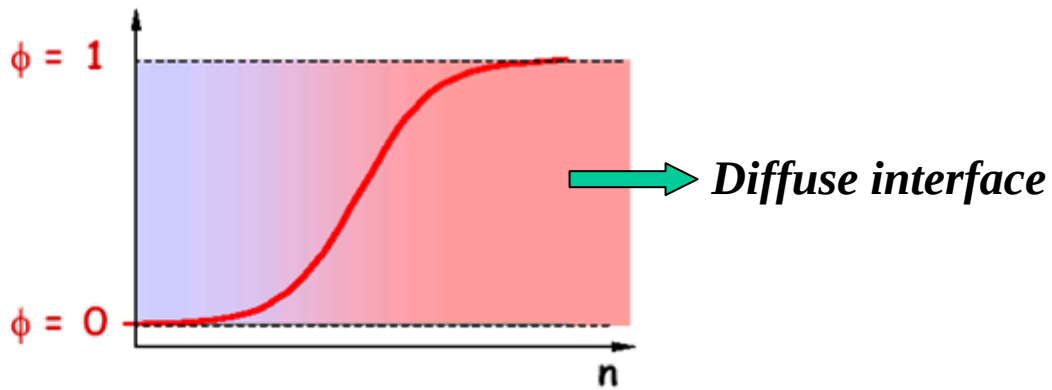
Phase field equation:

$$\frac{\partial \phi}{\partial t} = \mu\{\sigma[\nabla^2\phi - \frac{18}{\eta^2}(1-\phi)\phi(\frac{1}{2}-\phi)] + \frac{6\Delta G}{\eta}(1-\phi)\phi\}$$

μ, σ, ΔG: ***Material parameters***

η: ***Interface thickness***





- The phase field equation is coupled with the carbon diffusion equation to model the austenite/ferrite transformation

Background

PFM calculations of 3D phenomena frequently in 2D

3D PFM of austenite-ferrite transformation
$\Rightarrow$ Comparison with 2D results
$\Rightarrow$ Evaluation of 3D vs 2D calculations

Here, use of commercial code: MICRESS with multi-phase field approach

$$\frac{d\phi_i}{dt} = \sum_j \mu_{ij}\left[\sigma_{ij}\left(\phi_i\nabla^2\phi_j - \phi_j\nabla^2\phi_i + \frac{\pi^2}{2\eta_{ij}^2}(\phi_i - \phi_j)\right) + \frac{\pi}{\eta_{ij}}\sqrt{\phi_i\phi_j}\,\Delta G_{ij}\right]$$

Basic Assumptions

Investigated Case

- Fe-0.1wt%C-0.49wt%Mn
- Austenite grain size (EQAD) = 20μm
- Continuous cooling transformation (0.4 and 10K/s)

Assumptions

- Only carbon redistribution
- Carbon diffusion coefficients independent of carbon content
- Thermodynamics based on paraequilibrium
- Linearized phase diagram
- Carbon partitioning ratio in interface = equilibrium partitioning ratio

Parameters

Numerical parameters:

Interface thickness = 4 nodes, driving pressure averaging

Node size *x* and automatic time stepping such that convergency

Periodic boundary conditions

Maximum calculation domain size 165×165×165 nodes

Physical parameters (adjustable):

Interface mobility (pre-exponential term, μ_0)

Nucleation conditions (temperature range, nuclei distribution)

$\Rightarrow$ Shield time, shield distance

Conversion 2D → 3D

Grain sizes, nuclei densities

2D

$$N_0 \frac{\pi}{4} d^2 = fA$$

3D

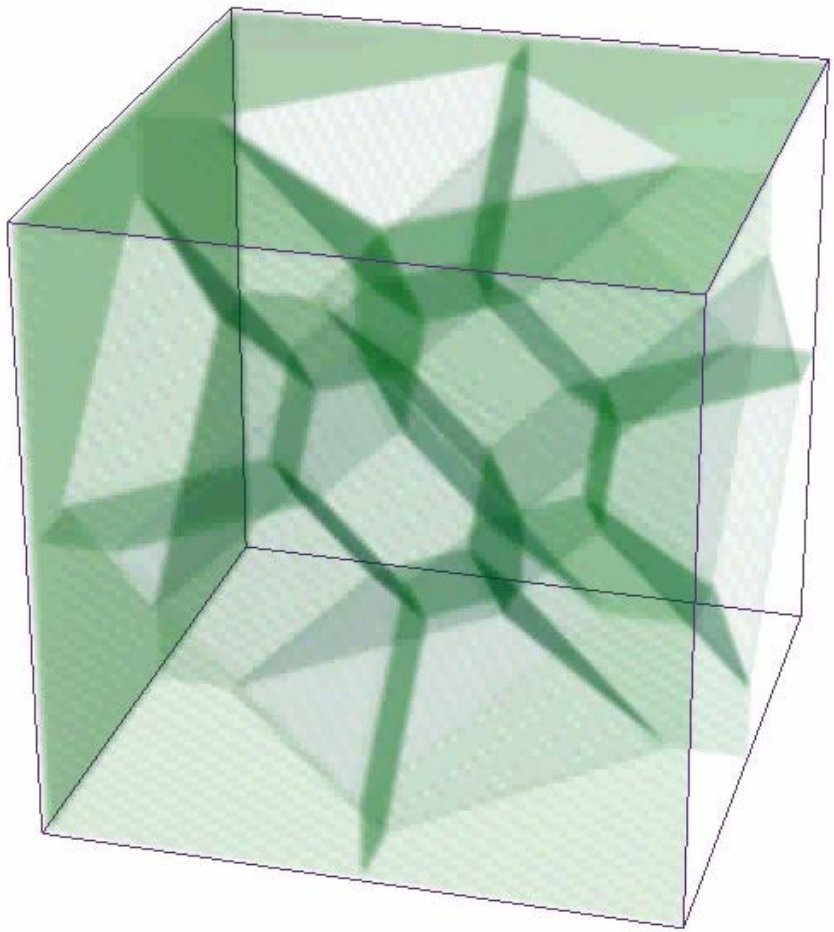
$$N \frac{\pi}{6} (1.2d)^3 = fV$$

$$\Downarrow$$

$$\frac{N_0}{N} = \frac{2}{3} (1.2)^3 d \frac{A}{V}$$

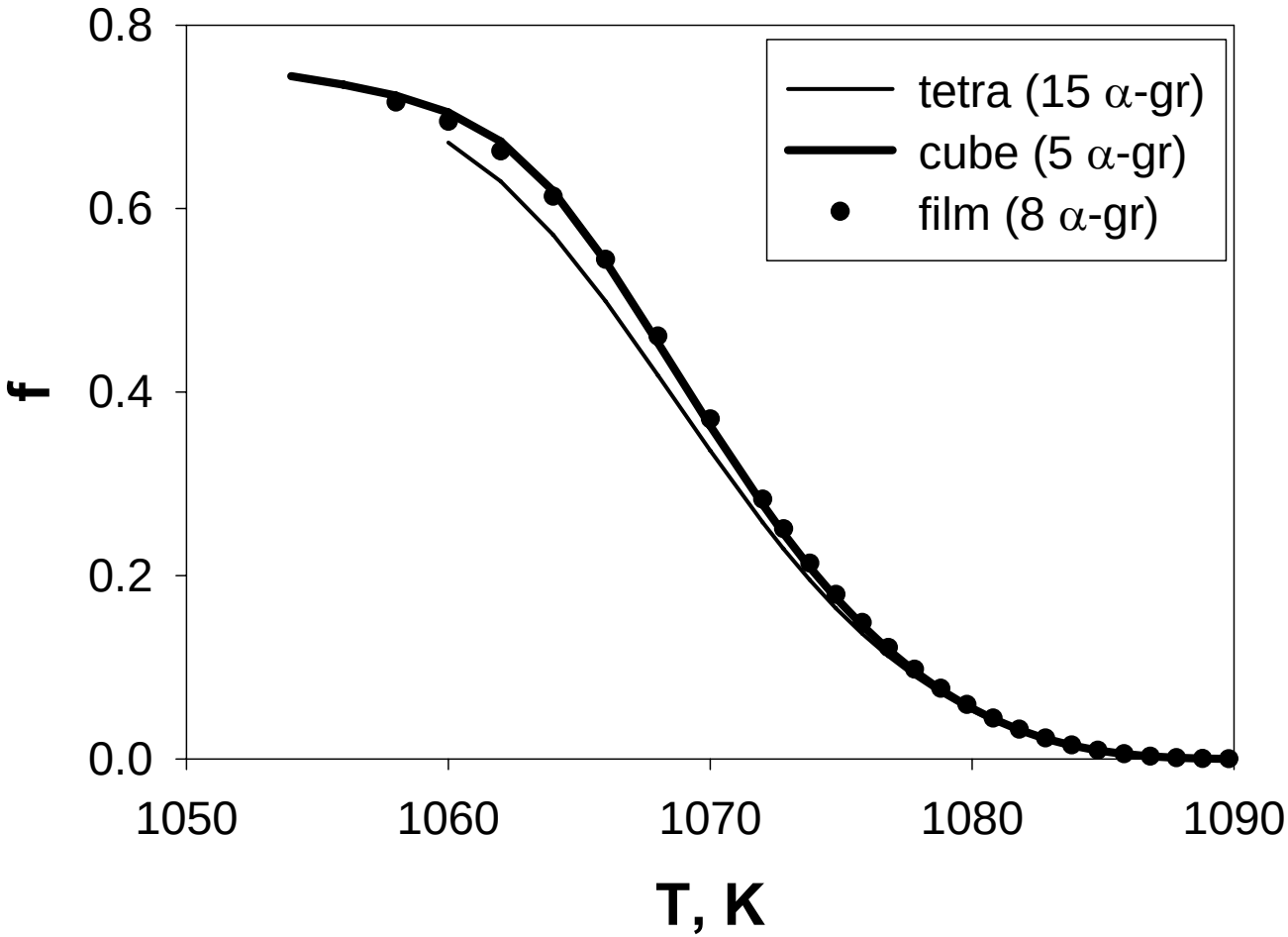
Nucleation at Triple Lines

0.4 K/s: Ferrite grain size = Austenite grain size

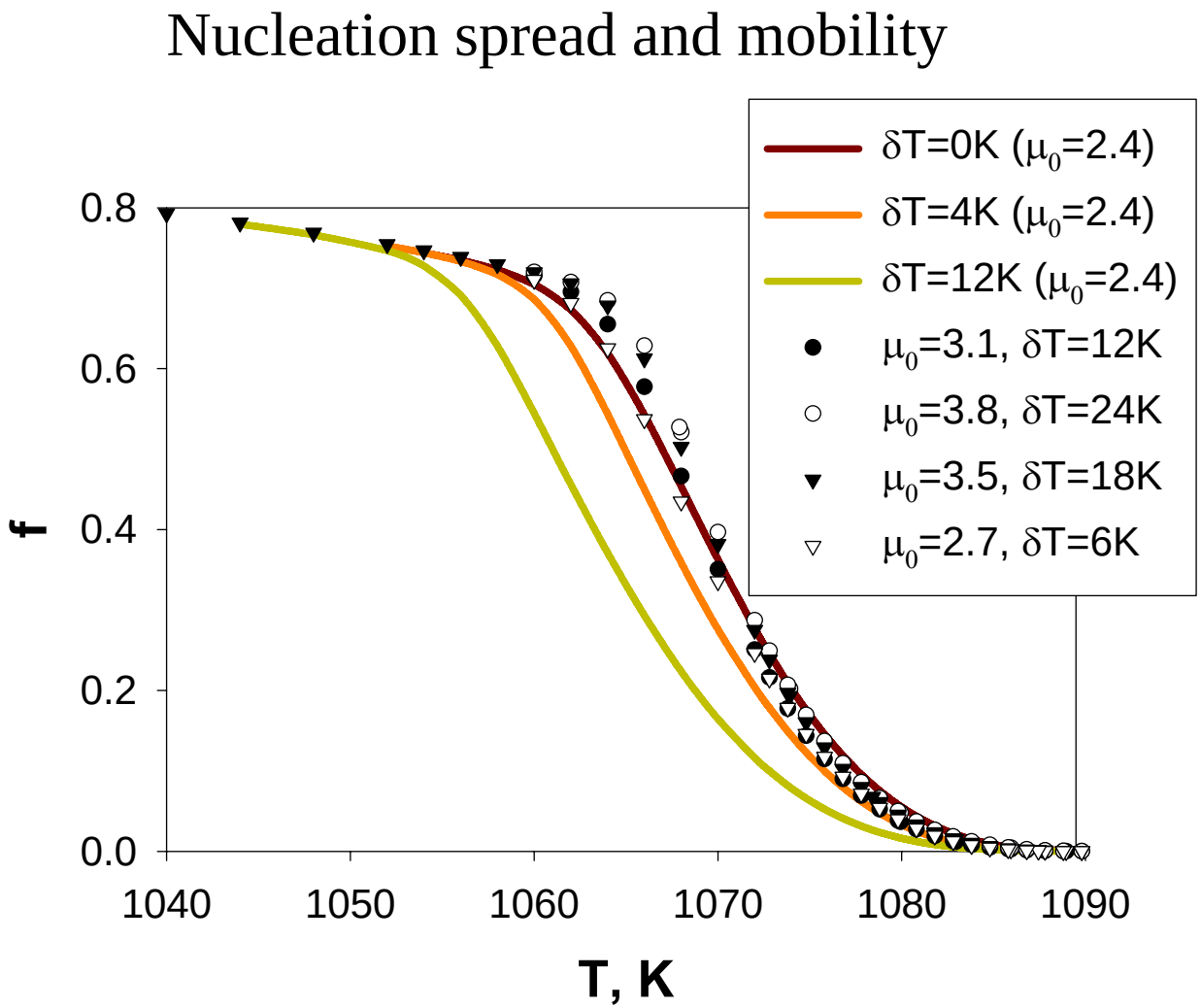


Nucleation at Triple Lines

Effect of initial austenite microstructure

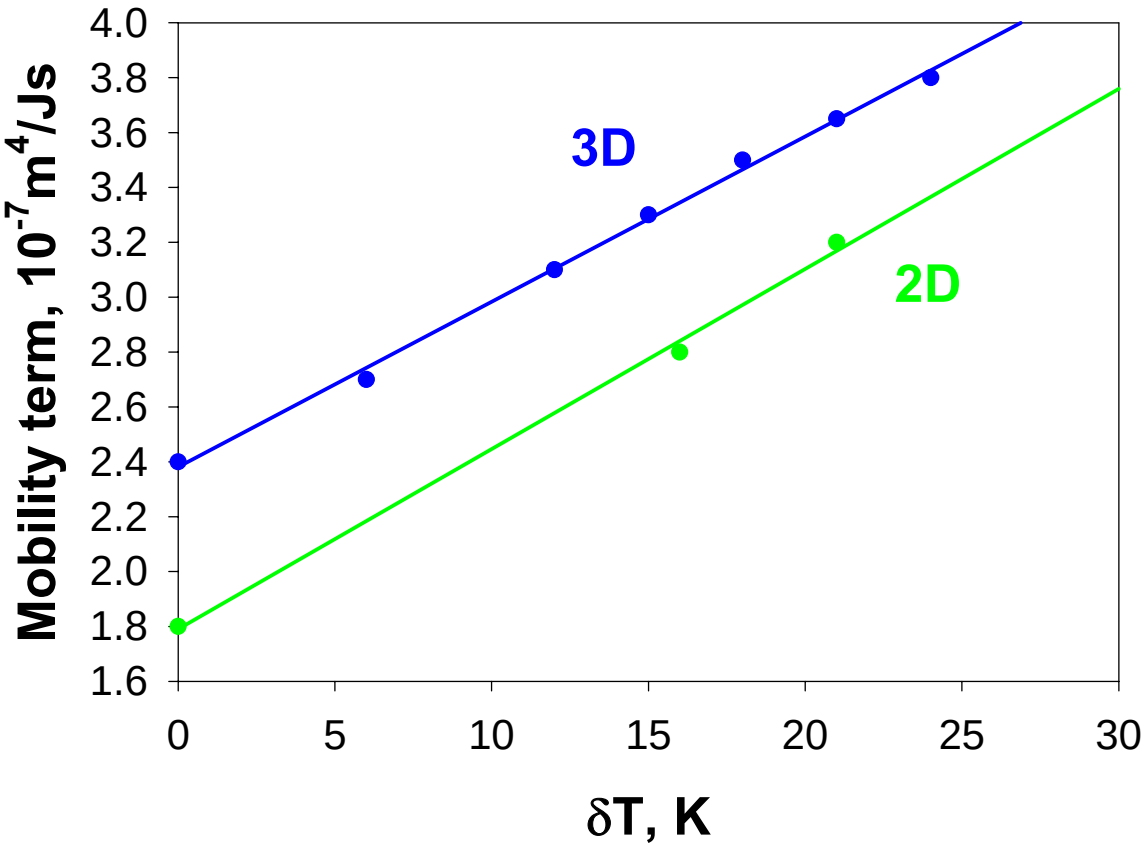


Nucleation at Triple Lines



Nucleation at Triple Lines

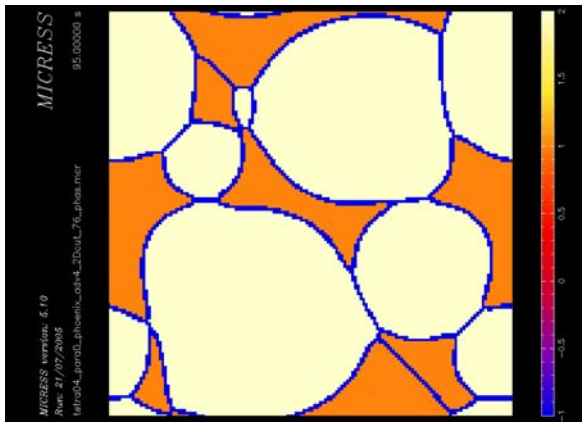
3D vs 2D mobility results

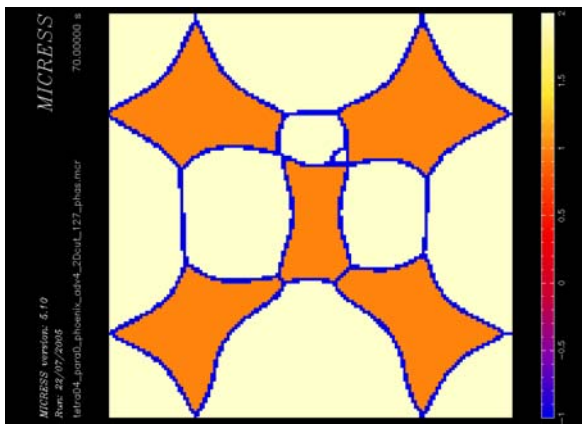


Nucleation at Triple Lines

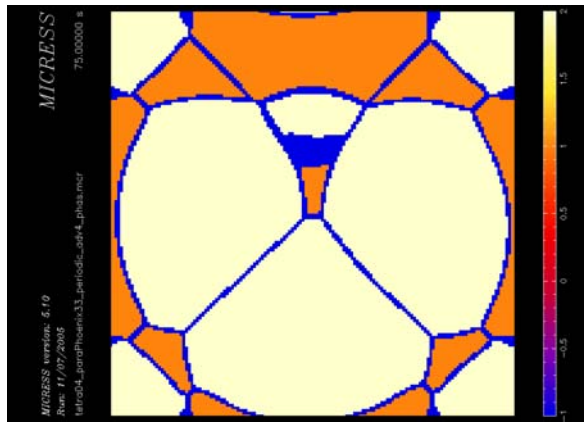
Comparison 3D – 2D for δT=18K

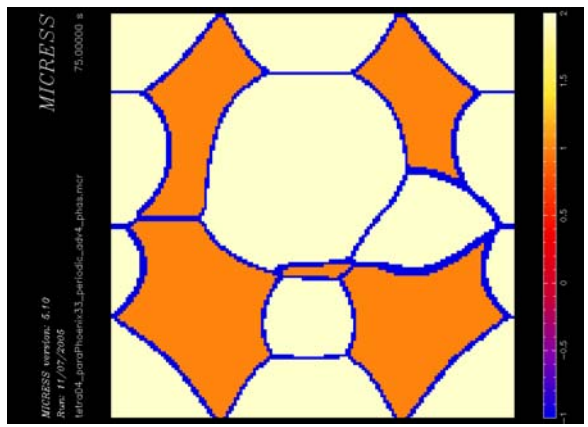
2D





3D





TL + Interface Nucleation

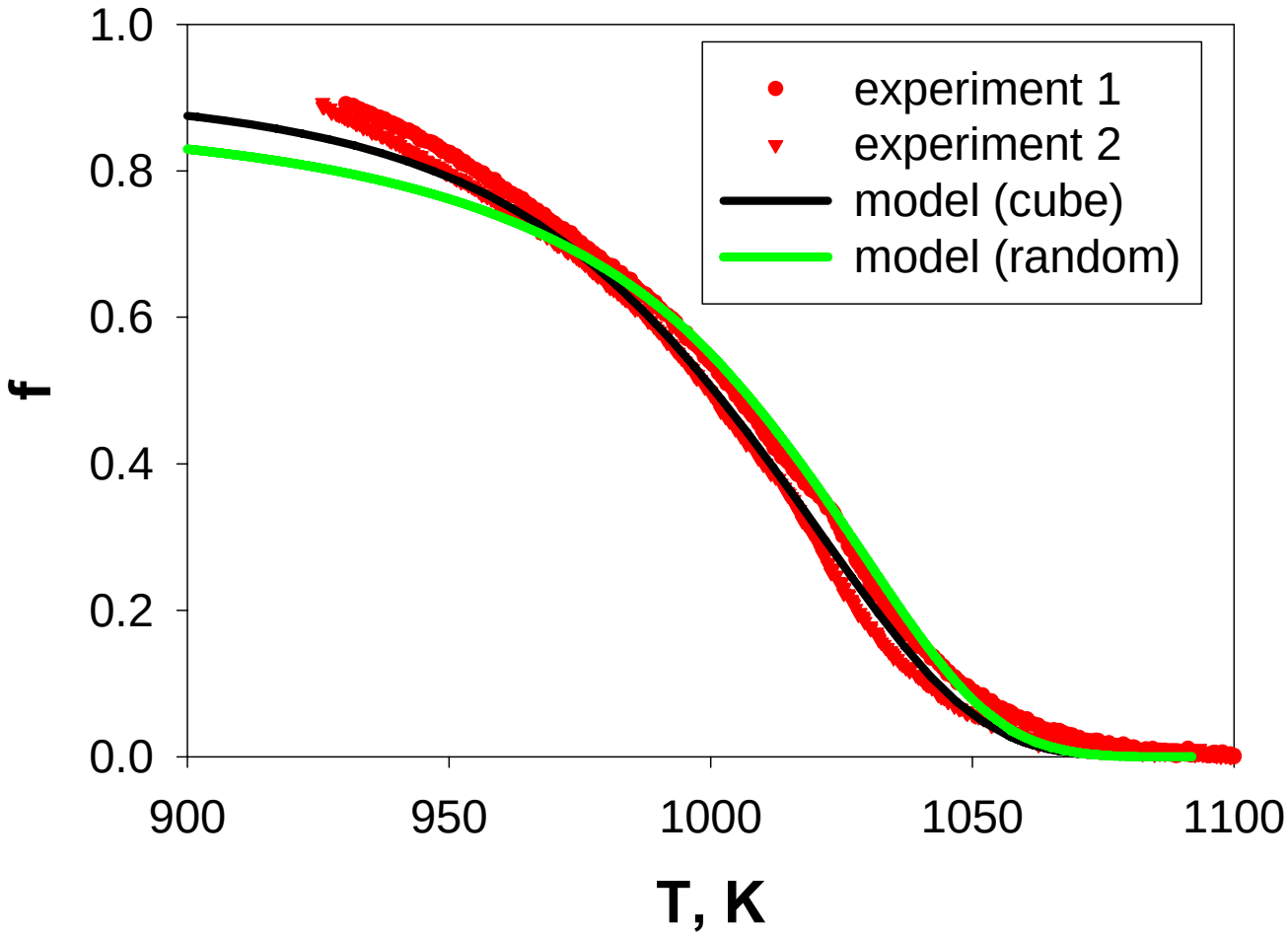
10 K/s

Substantial ferrite grain refinement to 9 μm
⇒ Additional nucleation modes active
⇒ Nucleation at triple lines (TL) and interfaces

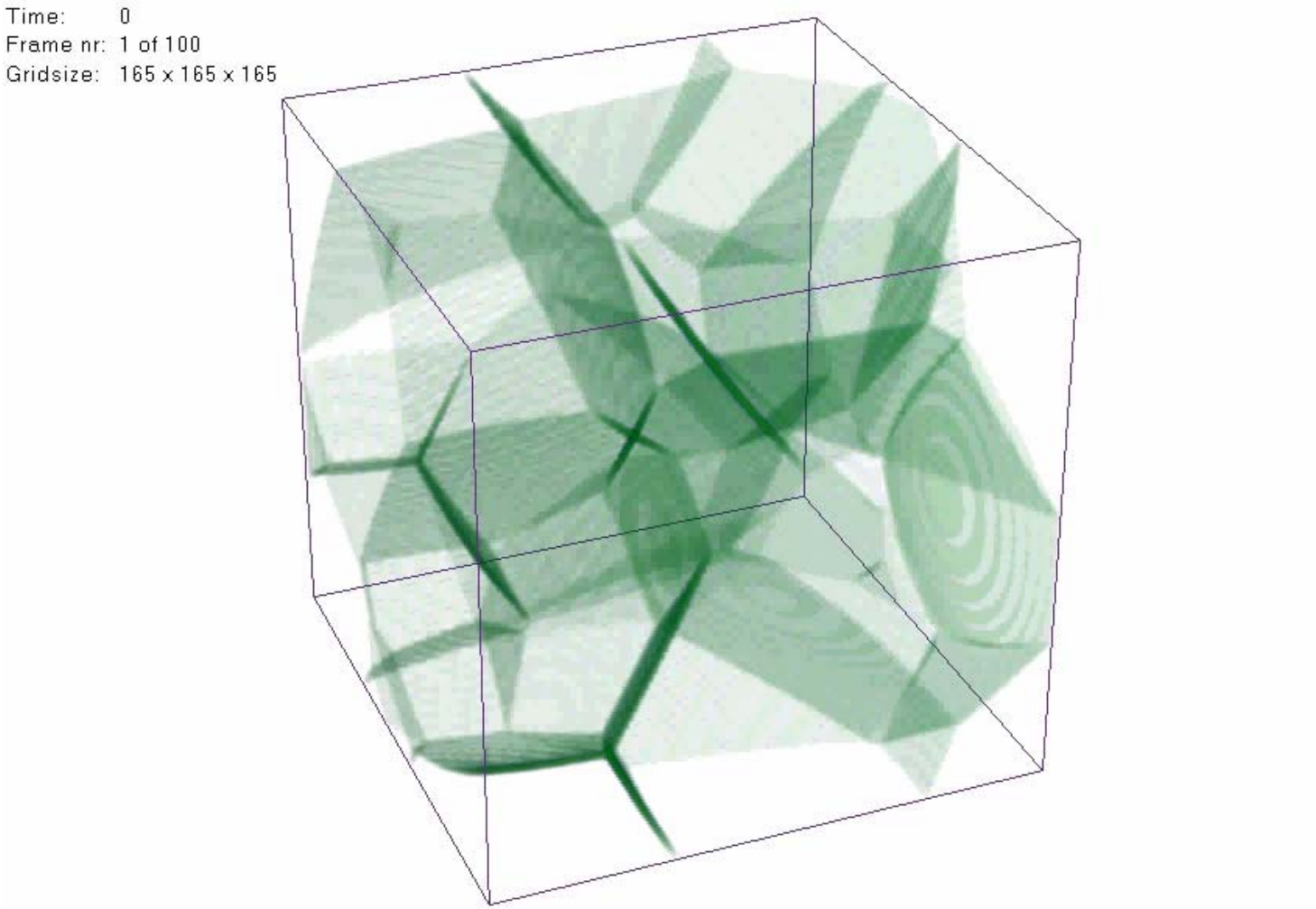
Transformation temperatures lower than for 0.4 K/s
⇒ Finer node size required (0.2 vs 0.3 μm)

TL + Interface Nucleation

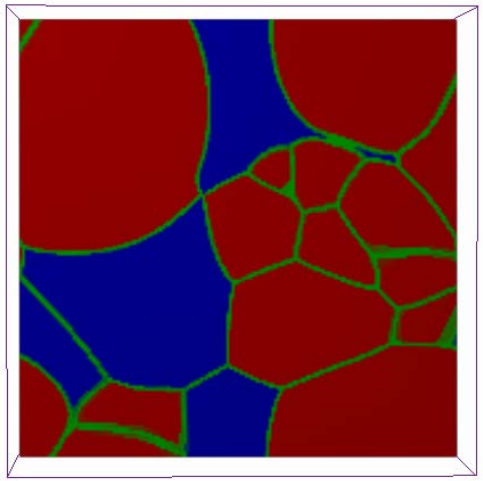
δT=16K/14K and μ_0=24×$10^{-7}$$m^4$/Js

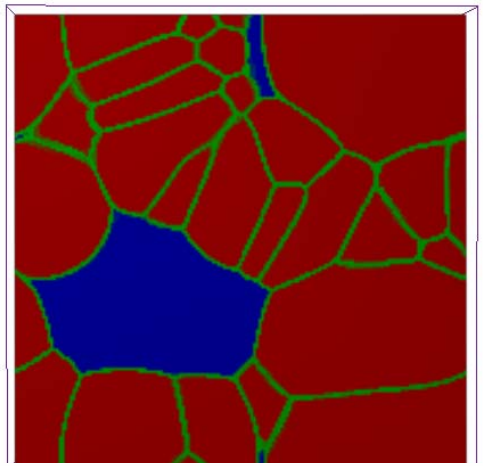


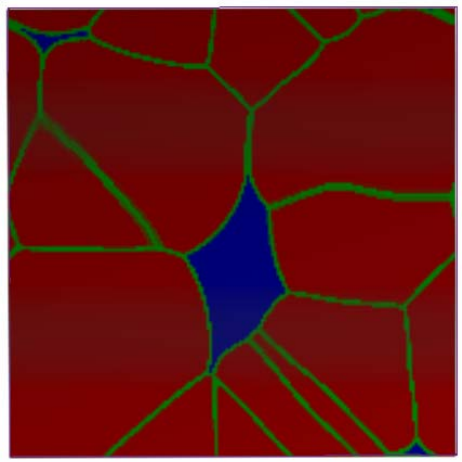
TL + Interface Nucleation

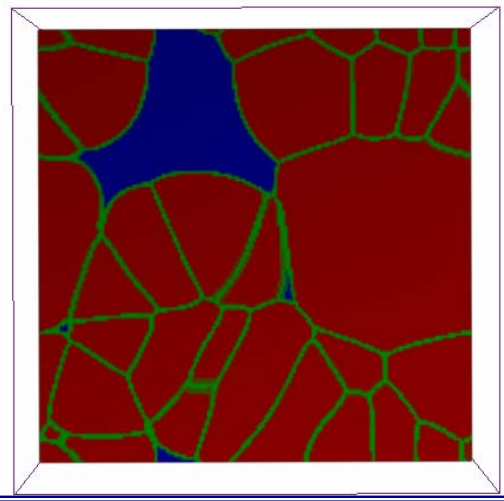


TL + Interface Nucleation



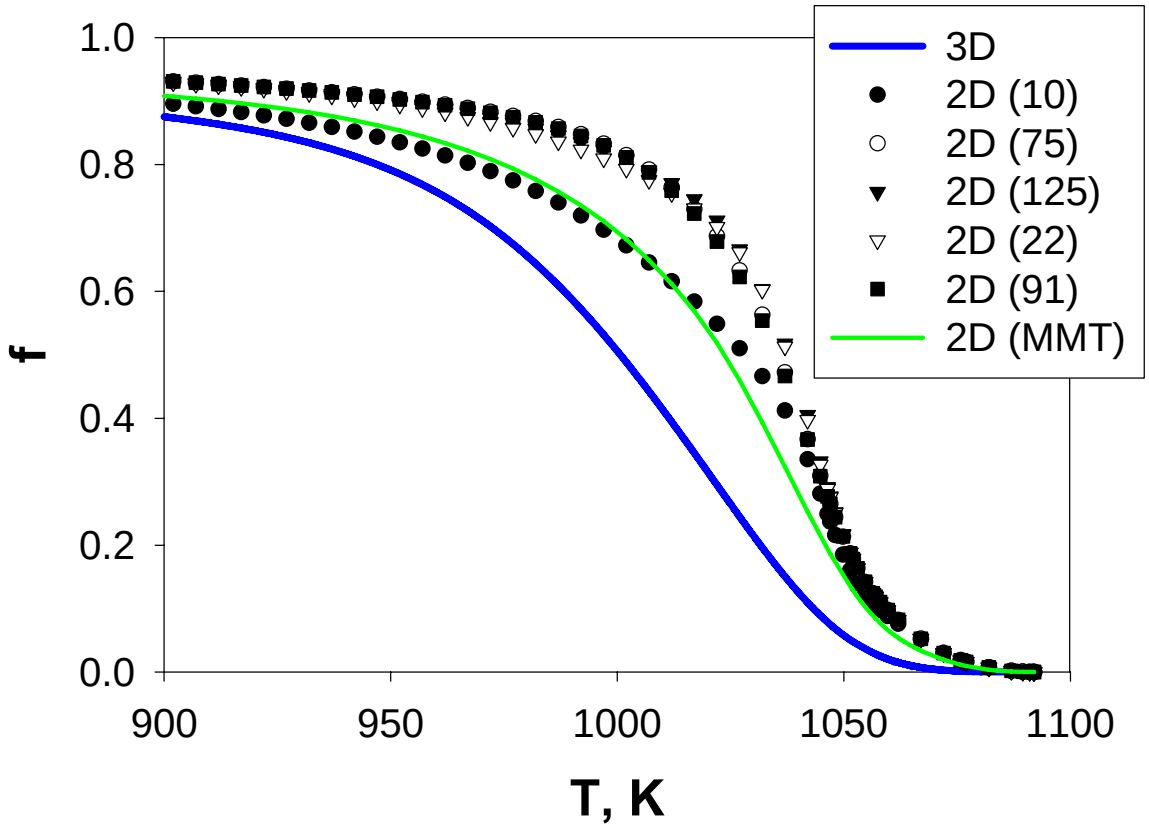






TL + Interface Nucleation

Comparison 3D – 2D for cube structure

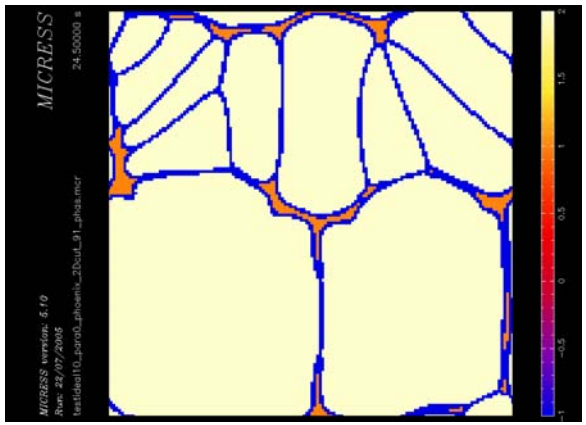


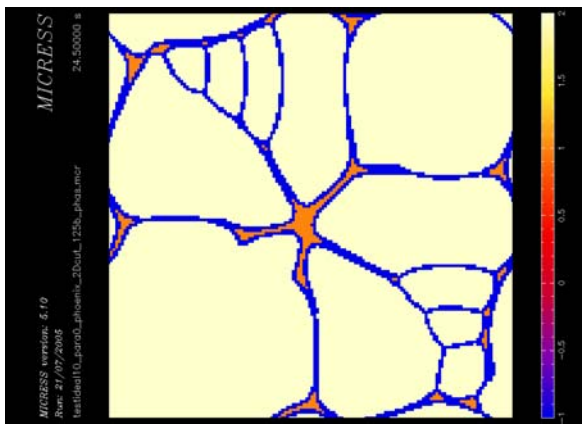
Nucleation temperatures:
1092-1076 K (TP) + 1072-1057 K (interfaces)

TL + Interface Nucleation

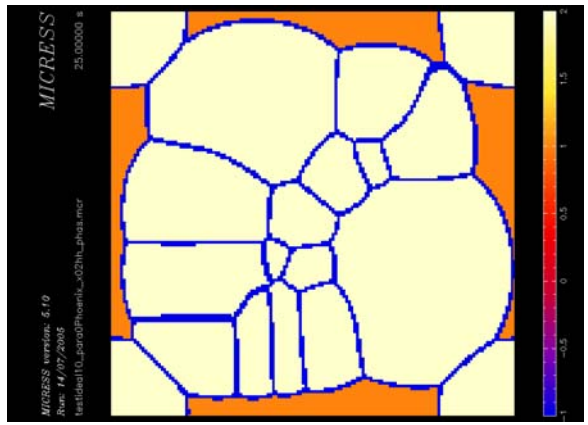
Comparison 3D – 2D

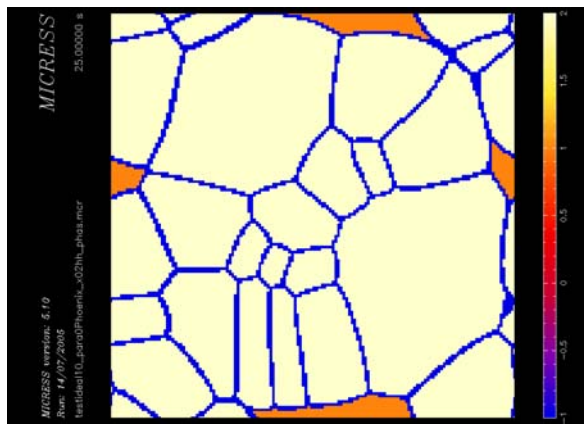
2D





3D

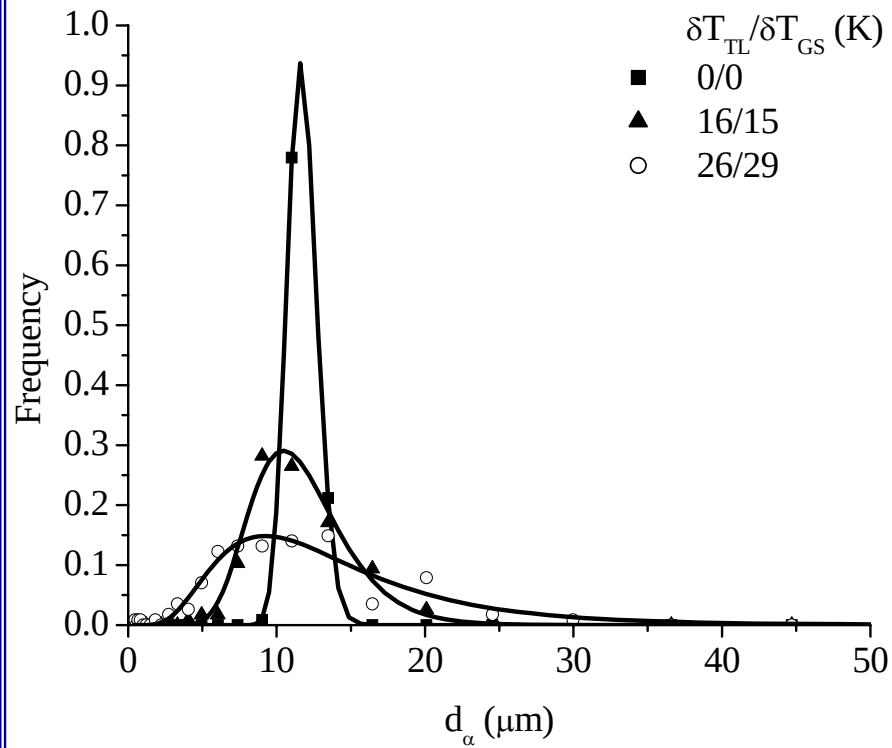




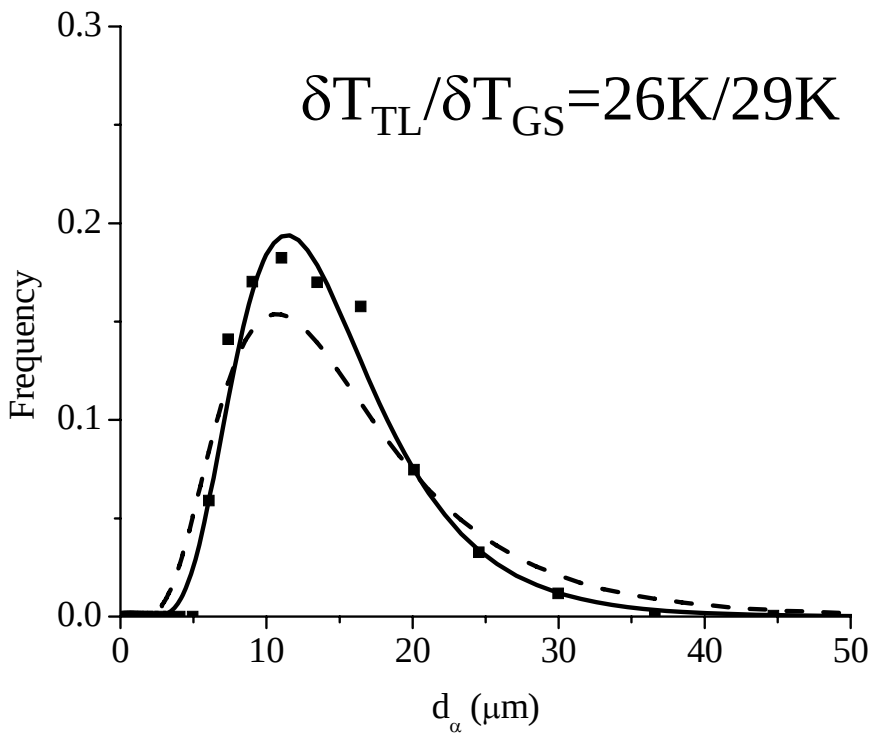
TL + Interface Nucleation

Use grain size distribution to determine μ_o-δT combination

Simulation



Comparison with experiment



Summary

3D PFM predicts more realistic final microstructures

3D transformation “slower” than 2D due to different growth geometries

$\Rightarrow$ 3D mobilities approximately 30% larger

Challenges:

Control of complex nucleation modes with MICRESS

Intermediate microstructures (e.g. ferrite film)

Statistical relevance of 3D calculations

Ongoing/Future Work

Comparison of 3D PFM with single grain and spherical shell models

Analysis of mixed-mode character

Evaluation of temperature dependence of mobility

Application to deformation induced ferrite transformation

Application to austenite formation

Ongoing/Future Work

What can we learn from PFM?

- **Effective mobility as a function of nucleation conditions**
- **Evaluation of solute drag and/or diffusion of substitutional elements**
- **Transition from restrictive equilibria (e.g. paraequilibrium) to full equilibrium (orthoequilibrium)**

Ongoing/Future Work

Evaluation of Role of Alloying Elements

- $\gamma \rightarrow \alpha$ **transformation: Connect PFM with solute drag model by describing effective mobility as a function of temperature and velocity**
- $\alpha \rightarrow \gamma$ **transformation: Considering long-range diffusion of substitutional elements in vicinity of interface (small domain size?, fast diffusion paths?)**