Simulation and Kinetics of Grain-Boundary Nucleated Phase Transformations

E. A. Jägle[1], E. J. Mittemeijer[1,2]

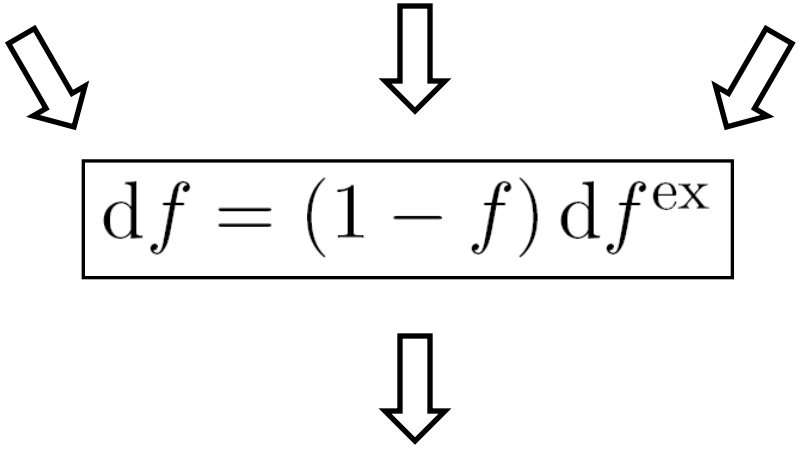
[1]Max Planck Institute for Metals Research, Stuttgart, Germany
[2]Institute for Materials Science, University of Stuttgart, Germany

PTM

2010-06-11

The framework for JMAK-like kinetics

nucleation model growth model temperature program

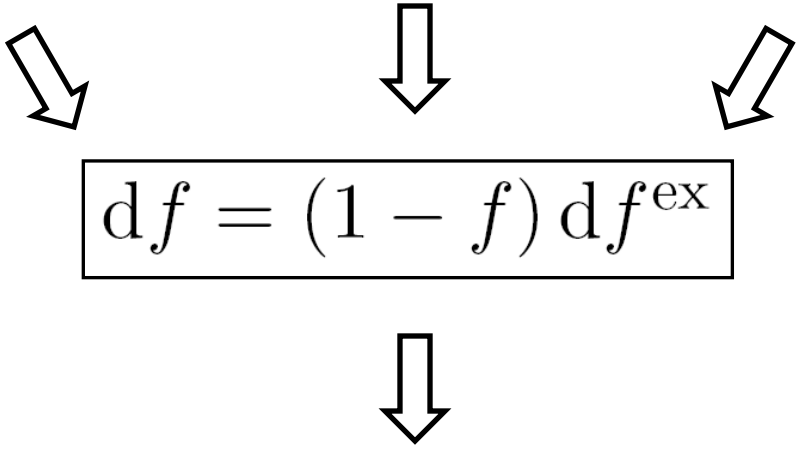


$$\boxed{\mathrm{d}f = (1-f)\,\mathrm{d}f^{\mathrm{ex}}}$$

kinetics, i.e. $f(t) = \frac{V(t)}{V_{\mathrm{tot}}}$

The framework for JMAK-like kinetics

nucleation model growth model temperature program



$$\boxed{\mathrm{d}f = (1-f)\,\mathrm{d}f^{\mathrm{ex}}}$$

kinetics, i.e. $f(t) = \frac{V(t)}{V_{\mathrm{tot}}}$

example: Johnson-Mehl-Avrami-Kolmogorov equation:

$$f(t) = 1 - \exp(-kt^n)$$

Restrictions of JMAK-like kinetics

$$\boxed{\mathrm{d}f = (1 - f)\,\mathrm{d}f^{\mathrm{ex}}}$$

[1] Bruna et al., *J. Appl. Phys.* **100** (2006) 054907 / [2] Godiksen et al., *Scripta Mater.* **58** (2008), 279

Restrictions of JMAK-like kinetics

$$\mathrm{d}f = (1 - f)\,\mathrm{d}f^{\mathrm{ex}}$$

hard impingement

violated e.g. if
diffusion fields overlap

e.g. Phase-Field
simulations[1]

[1] Bruna et al., *J. Appl. Phys.* **100** (2006) 054907 / [2] Godiksen et al., *Scripta Mater.* **58** (2008), 279

Restrictions of JMAK-like kinetics

$$\mathrm{d}f = (1 - f)\,\mathrm{d}f^{\mathrm{ex}}$$

hard impingement

violated e.g. if diffusion fields overlap

e.g. Phase-Field simulations[1]

equiaxed growth

violated e.g. if product phase grows as platelets

e.g. Monte-Carlo simulations[2] or Cellular Automata

[1] Bruna et al., *J. Appl. Phys.* **100** (2006) 054907 / [2] Godiksen et al., *Scripta Mater.* **58** (2008), 279

Restrictions of JMAK-like kinetics

$$\mathrm{d}f = (1 - f)\,\mathrm{d}f^{\mathrm{ex}}$$

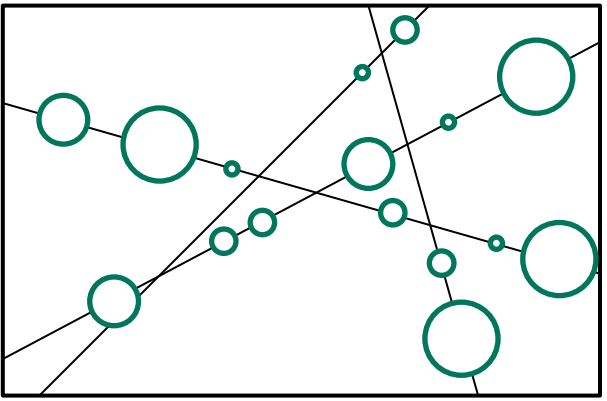
hard impingement	equiaxed growth	random nucleation
violated e.g. if diffusion fields overlap	violated e.g. if product phase grows as platelets	violated e.g. if nuclei form at grain boundaries (GBN)
e.g. Phase-Field simulations[1]	e.g. Monte-Carlo simulations[2] or Cellular Automata	?

[1] Bruna et al., *J. Appl. Phys.* **100** (2006) 054907 / [2] Godiksen et al., *Scripta Mater.* **58** (2008), 279

Approaches for kinetics with grain-boundary nucleation

1. modified impingement correction[4]: $\mathrm{d}f = (1-f)^{\xi}\,\mathrm{d}f^{\mathrm{ex}}$

2. Cahn's treatment[3]:



- random nucleation on randomly distributed planes
- on plane: $\mathrm{d}O = (1-f_O)\,\mathrm{d}O^{\mathrm{ex}}$
- between planes: $\mathrm{d}V = (1-f_V)\,\mathrm{d}V^{\mathrm{ex}}$

→Problem treatable by splitting one non-random process in two random processes

3. Geometrical Simulations

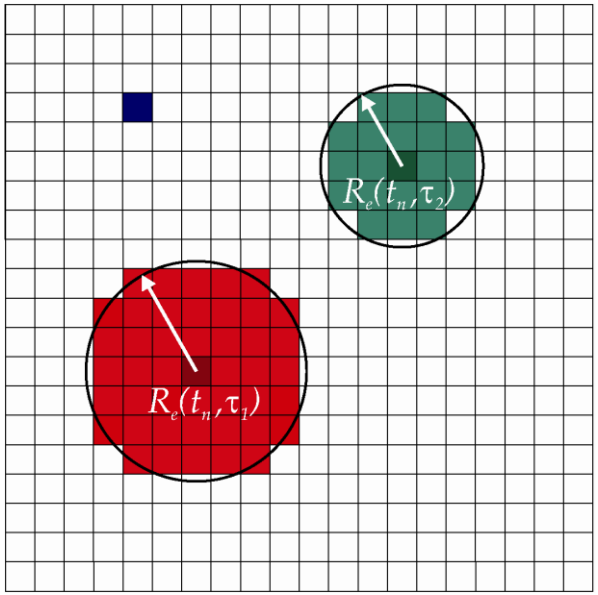
[3] J. W. Cahn, *Acta Metall.* **4** (1956) 449 / [4]Starink, *J. Mater. Sci.* **36** (2001) 4433

Geometrical simulations[5]

- use nucleation and growth rates, $\dot{N}$ and v, as in kinetic model
- discretise time and space (3D)
- assume hard impingement and interface-controlled growth

→ impingement automatically taken into account

$$t = t_n$$



⇨ very efficient simulation method

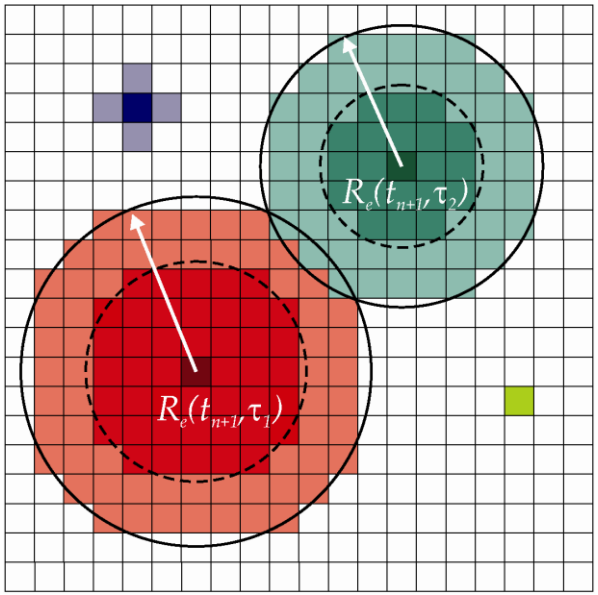
typically 700^3 voxel, >50k grains,
simulation time 5-10 min

Geometrical simulations[5]

- use nucleation and growth rates, $\dot{N}$ and v, as in kinetic model
- discretise time and space (3D)
- assume hard impingement and interface-controlled growth

→ impingement automatically taken into account

$$t = t_{n+1}$$

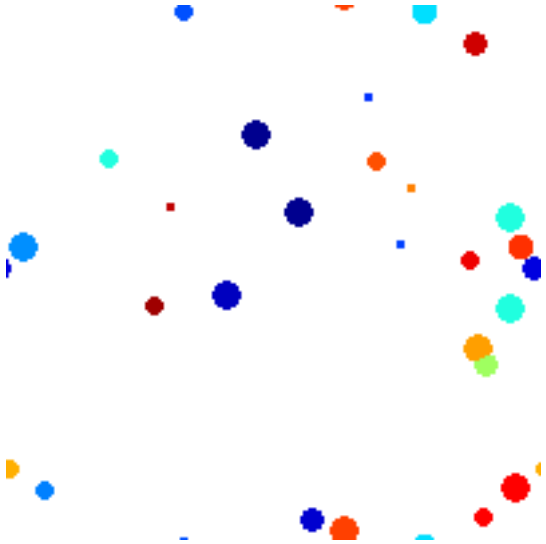


⇨ very efficient simulation method

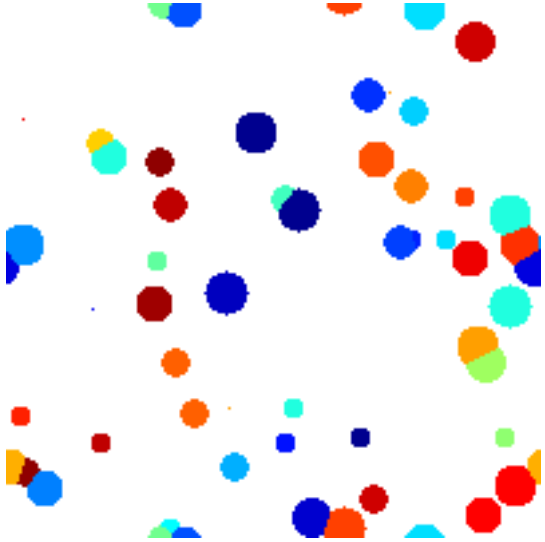
typically 700^3 voxel, >50k grains, simulation time 5-10 min

Simulation results – random bulk nucleation

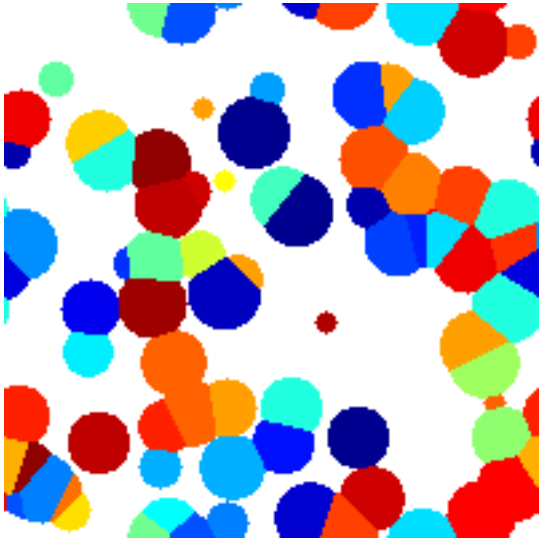
Simulation results – random bulk nucleation



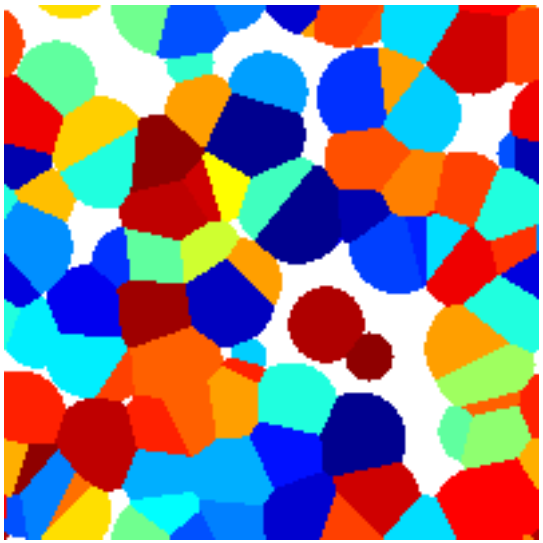
Simulation results – random bulk nucleation



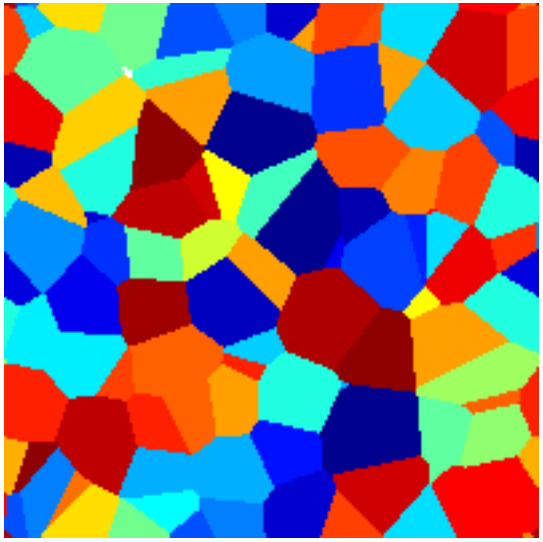
Simulation results – random bulk nucleation



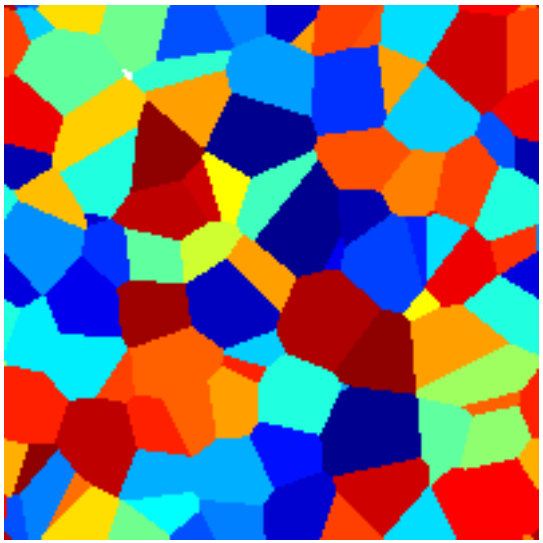
Simulation results – random bulk nucleation

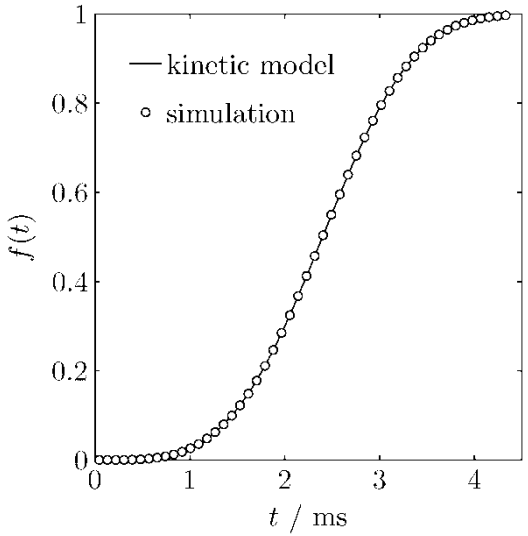


Simulation results – random bulk nucleation



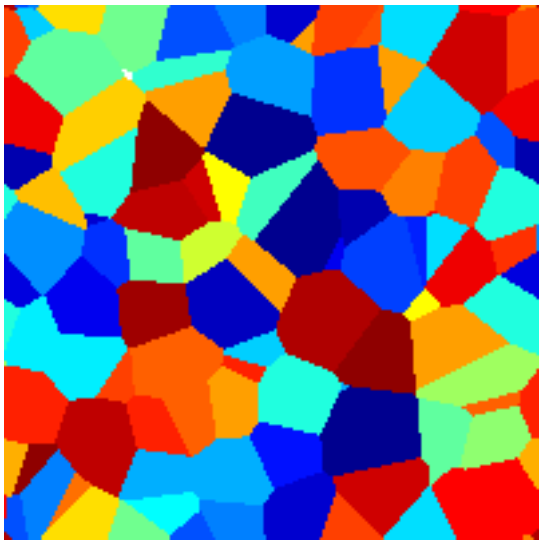
Simulation results – random bulk nucleation

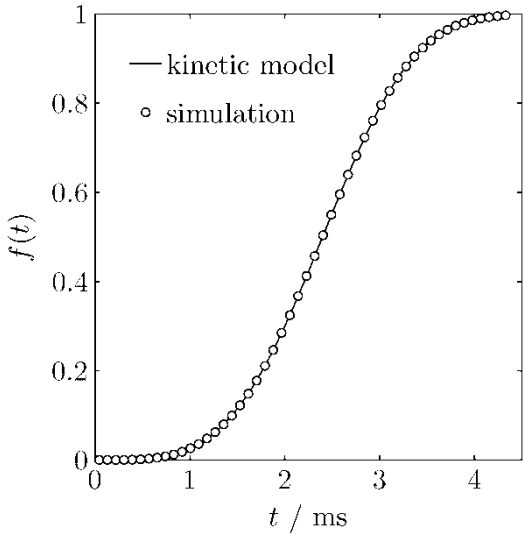


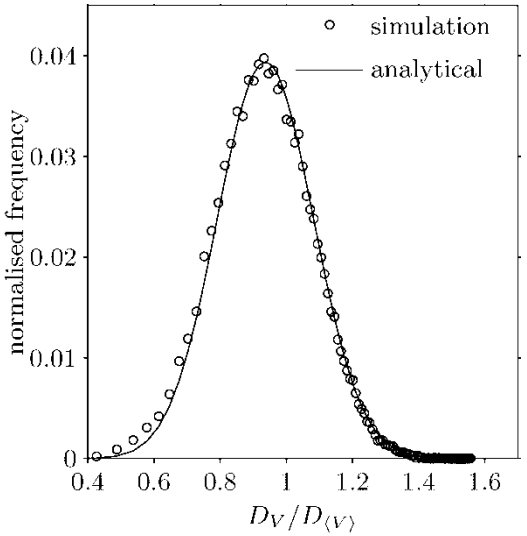


kinetics

Simulation results – random bulk nucleation

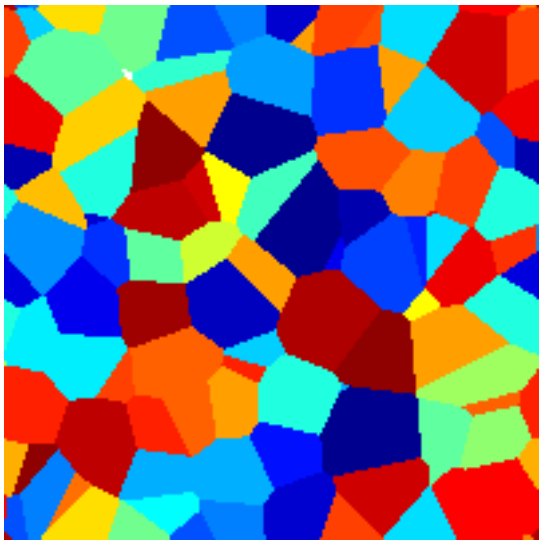


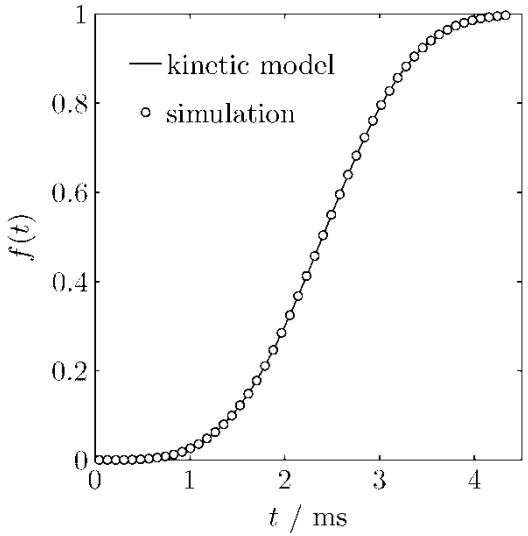


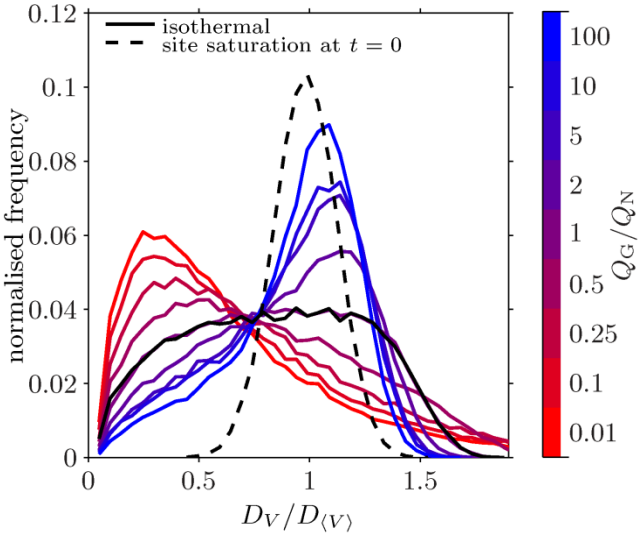


grain-size distribution (GSD)

Simulation results – random bulk nucleation

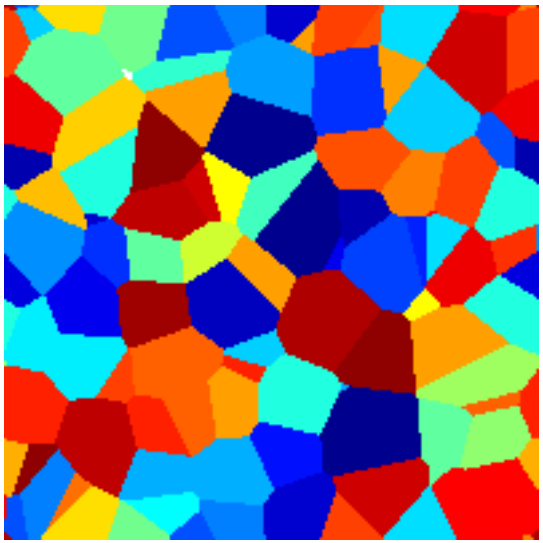


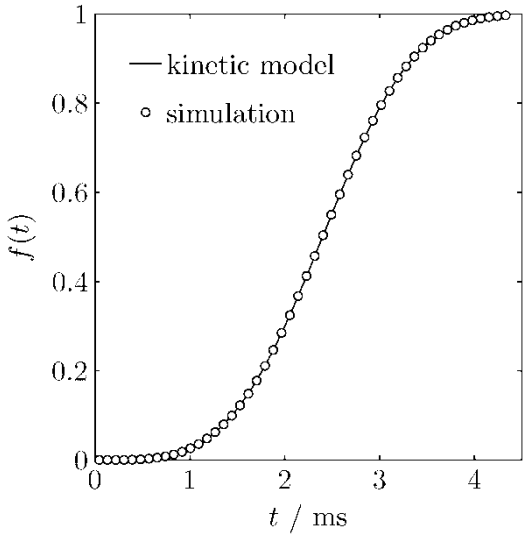


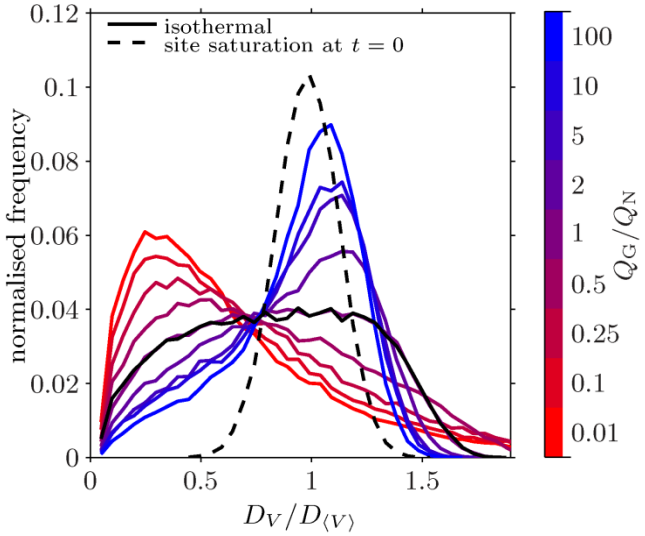


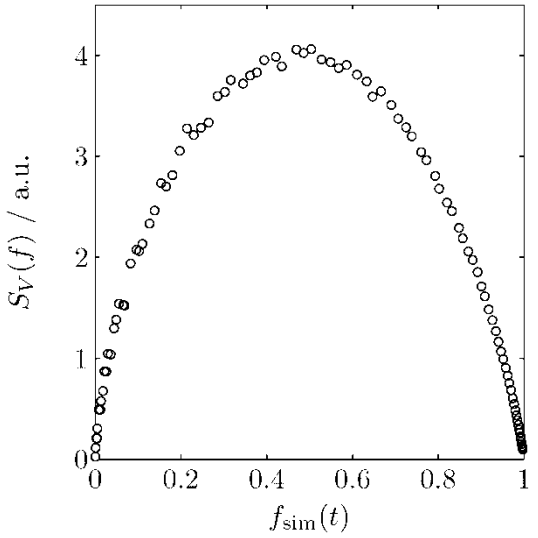
grain-size distribution (GSD)

Simulation results – random bulk nucleation



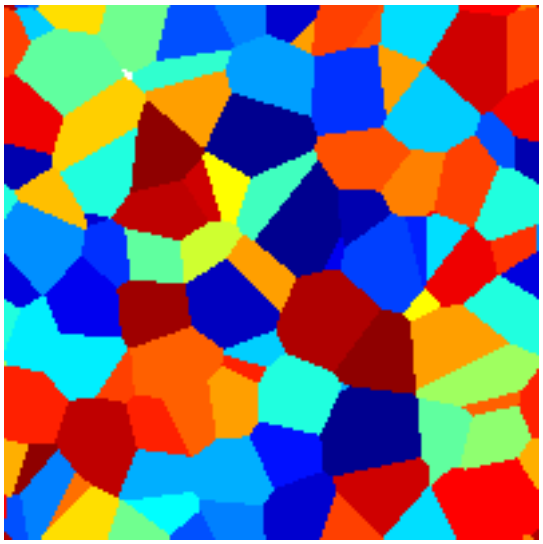


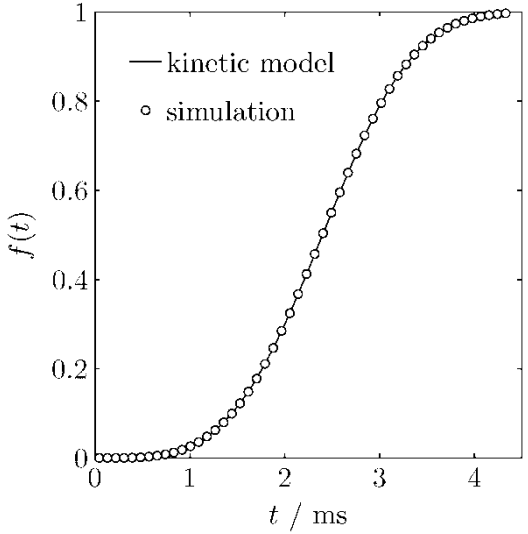


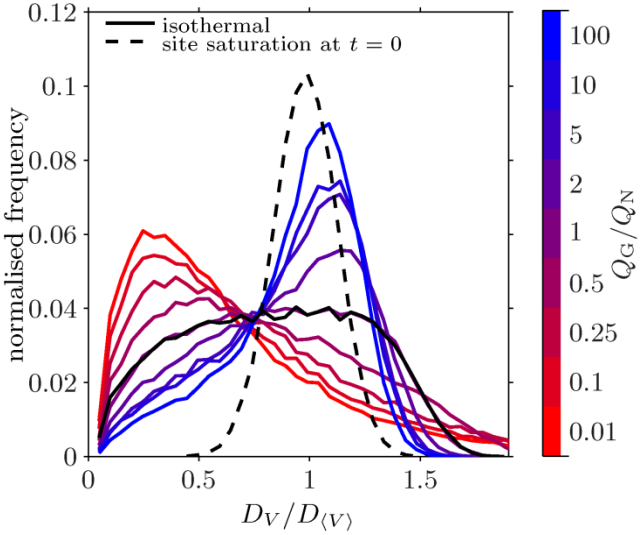


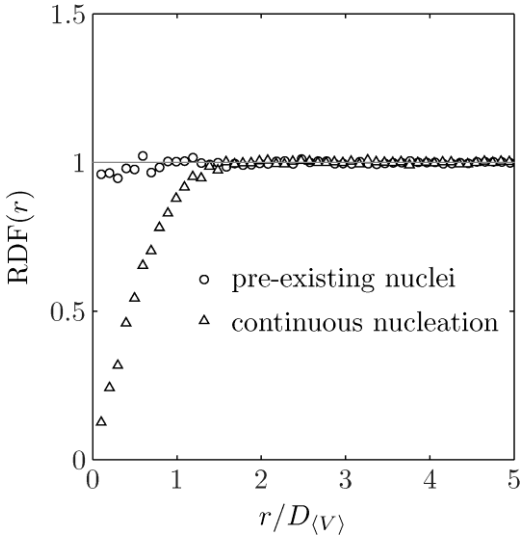
microstructural path

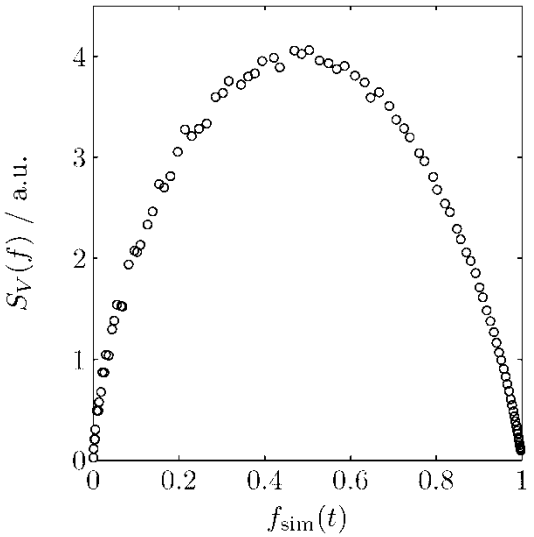
Simulation results – random bulk nucleation







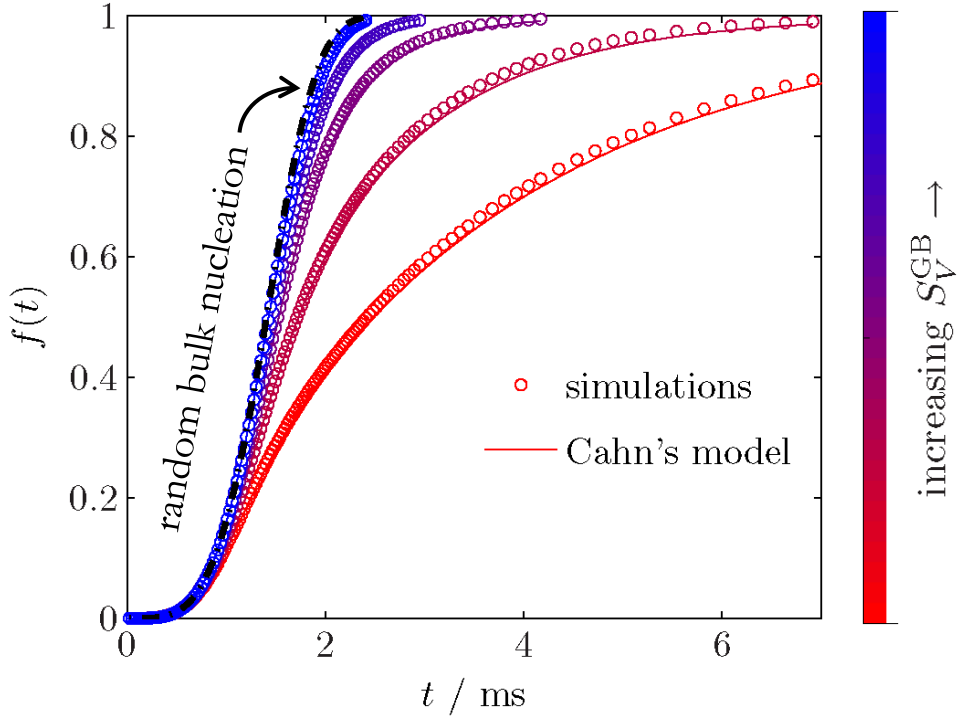


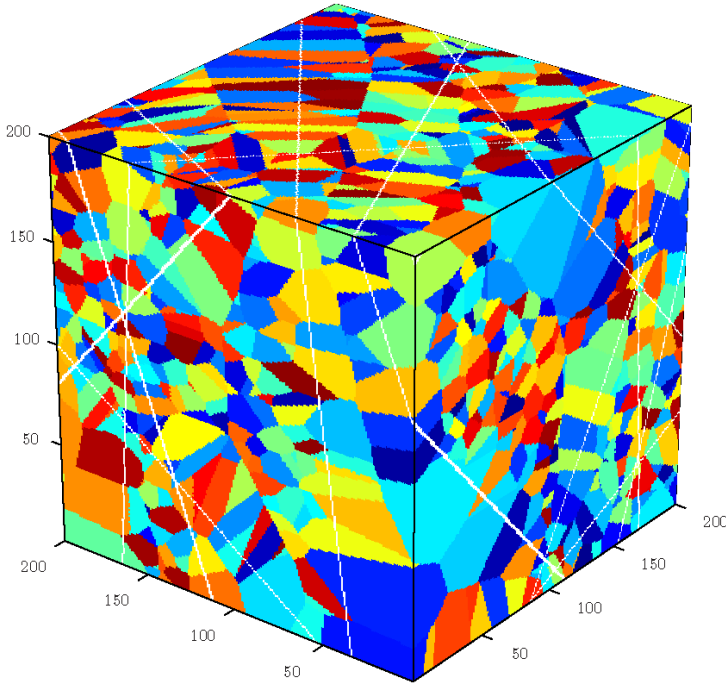


radial distribution function (RDF)

Simulation results – Cahn's model (random planes)

random nucleation on randomly distributed planes:

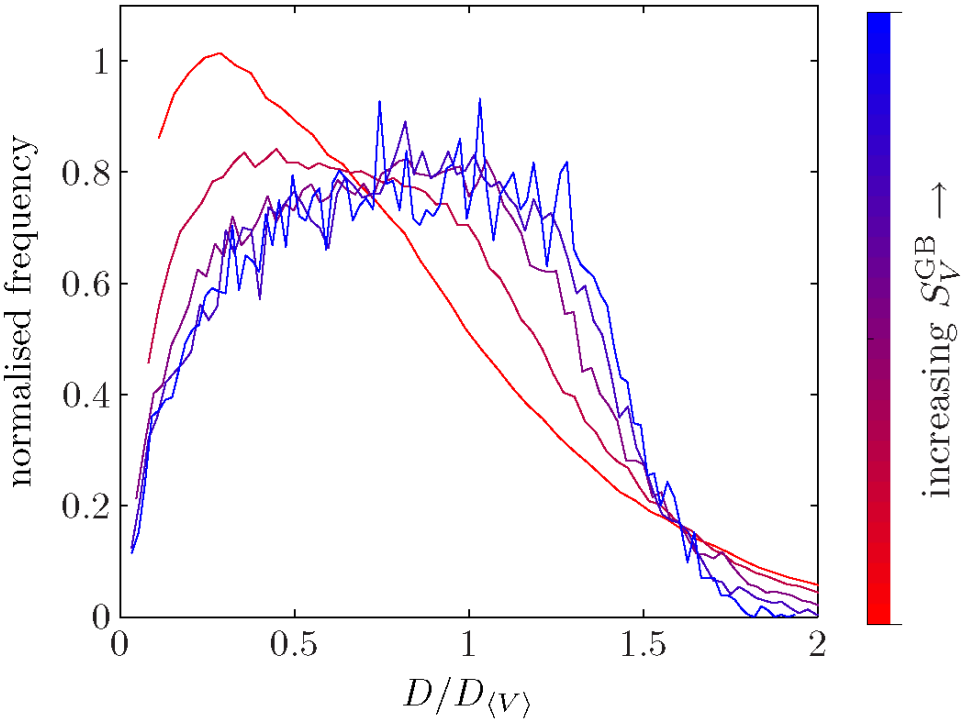


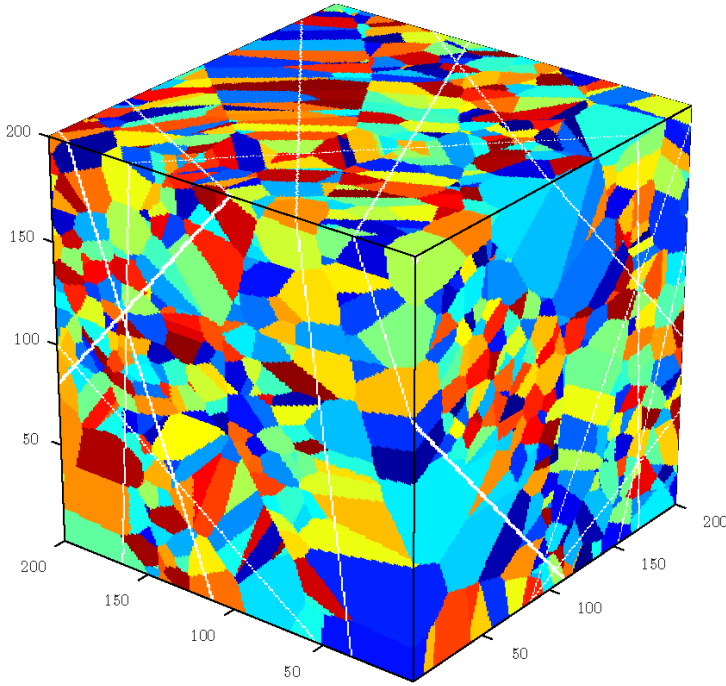


- deviation from JMAK if S_V^{GB} small / if parent GS > product GS
- kinetics: slower than JMAK
- GSD: higher number of small grains, broader
- reason: nucleation sites are strongly correlated

Simulation results – Cahn's model (random planes)

random nucleation on randomly distributed planes:

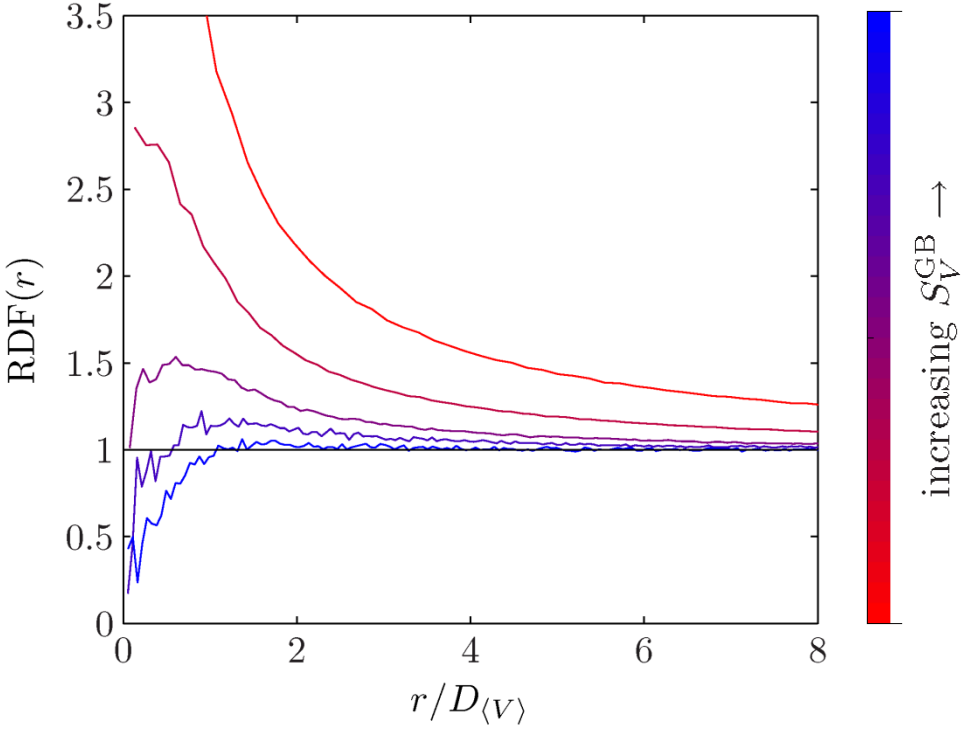


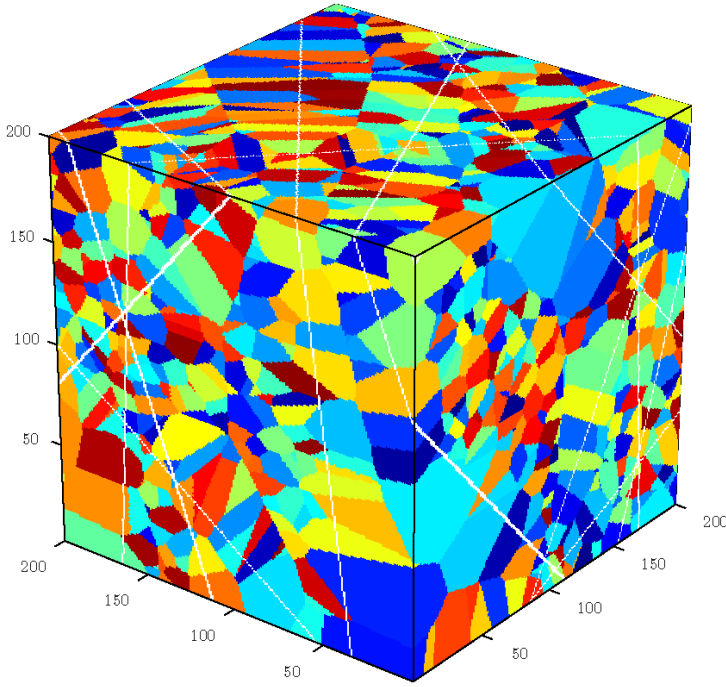


- deviation from JMAK if S_V^{GB} small / if parent GS > product GS
- kinetics: slower than JMAK
- GSD: higher number of small grains, broader
- reason: nucleation sites are strongly correlated

Simulation results – Cahn's model (random planes)

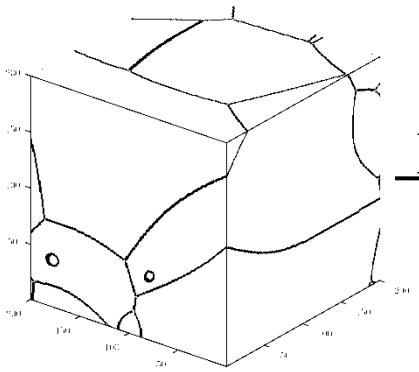
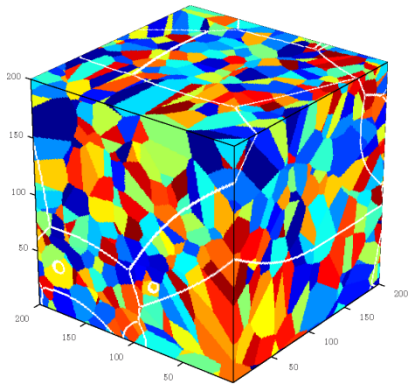
random nucleation on randomly distributed planes:





- deviation from JMAK if S_V^{GB} small / if parent GS > product GS
- kinetics: slower than JMAK
- GSD: higher number of small grains, broader
- reason: nucleation sites are strongly correlated

Grain-boundary nucleation: general approach

random, bulk nucleation → (parent kinetics) →  → (parent → product kinetics) → 

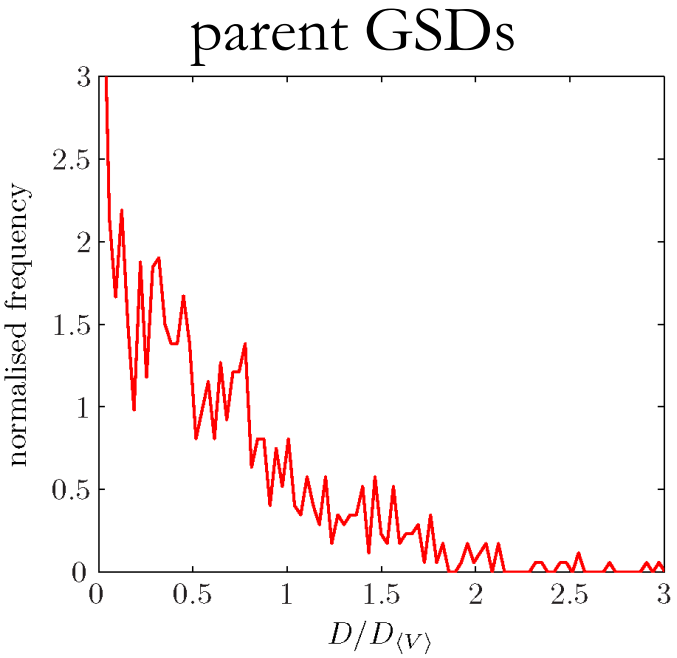
parent microstructure

product microstructure

1. influence of the parent microstructure
2. influence of the parent → product kinetics
3. kinetic models for GBN transformations

1. Influence of the parent microstructure

test various parent microstructures, keep all else identical:



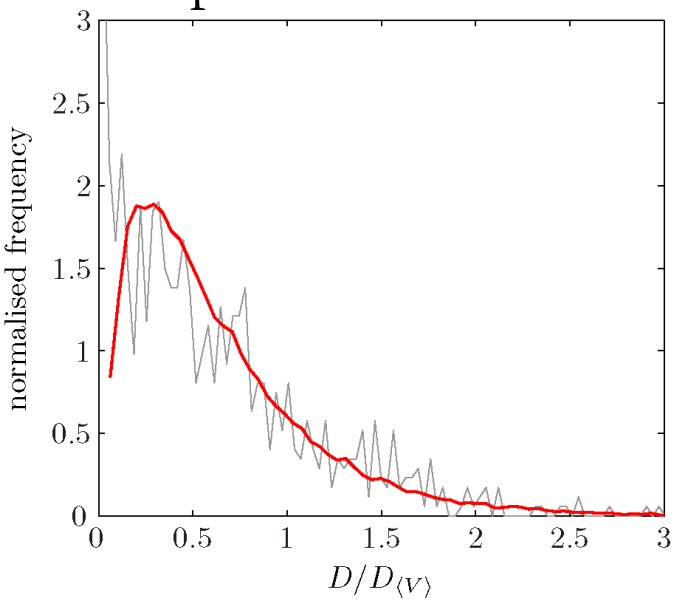
1. random nucleation on random planar GBs (Cahn's model)
2. random nucleation on *nonrandom* GBs
   - iso*chronal*, cont. nucl., $Q_G/Q_N = 0.01$
   - iso*thermal*, continuous nucleation
   - iso*chronal*, cont. nucl., $Q_G/Q_N = 100$
   - pre-existing nuclei
   - result of grain growth simulation (MC)

parent → product kinetics: continuous nucleation, isothermal transformation

1. Influence of the parent microstructure

test various parent microstructures, keep all else identical:

parent GSDs



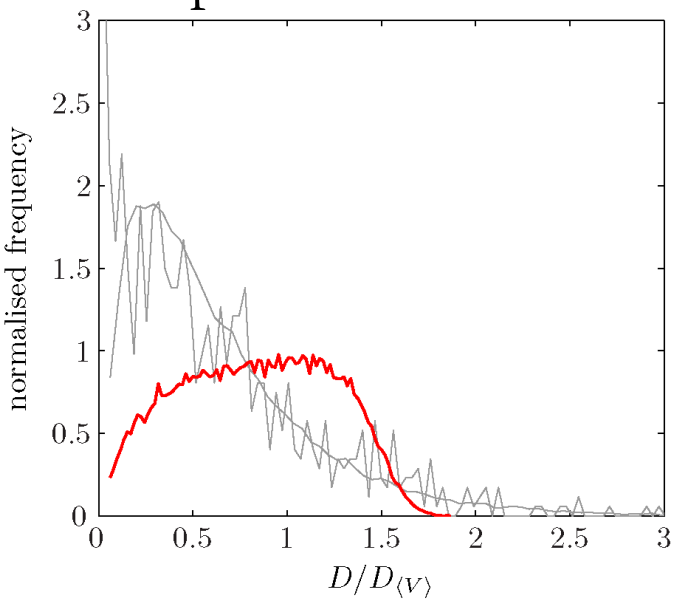
1. random nucleation on random planar GBs (Cahn's model)
2. random nucleation on *nonrandom* GBs
   - iso*chronal*, cont. nucl., $Q_G/Q_N = 0.01$
   - iso*thermal*, continuous nucleation
   - iso*chronal*, cont. nucl., $Q_G/Q_N = 100$
   - pre-existing nuclei
   - result of grain growth simulation (MC)

parent → product kinetics: continuous nucleation, isothermal transformation

1. Influence of the parent microstructure

test various parent microstructures, keep all else identical:

parent GSDs



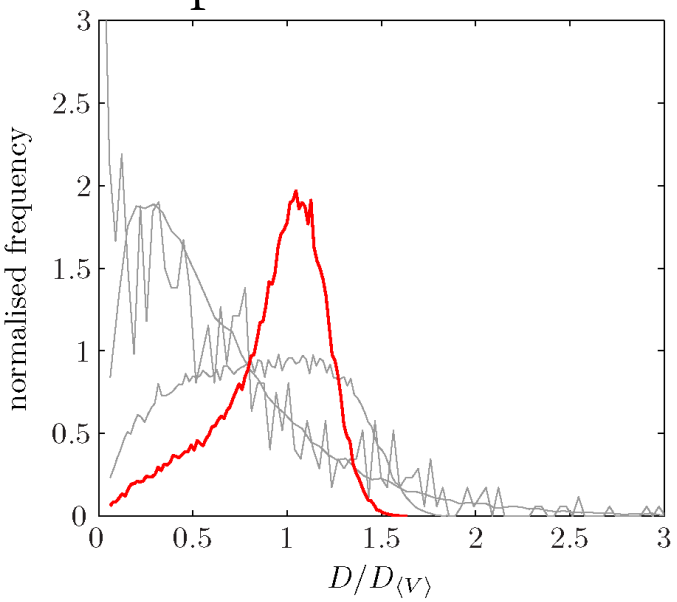
1. random nucleation on random planar GBs (Cahn's model)
2. random nucleation on *nonrandom* GBs
   - iso*chronal*, cont. nucl., $Q_G/Q_N = 0.01$
   - iso*thermal*, continuous nucleation
   - iso*chronal*, cont. nucl., $Q_G/Q_N = 100$
   - pre-existing nuclei
   - result of grain growth simulation (MC)

parent → product kinetics: continuous nucleation, isothermal transformation

1. Influence of the parent microstructure

test various parent microstructures, keep all else identical:

parent GSDs



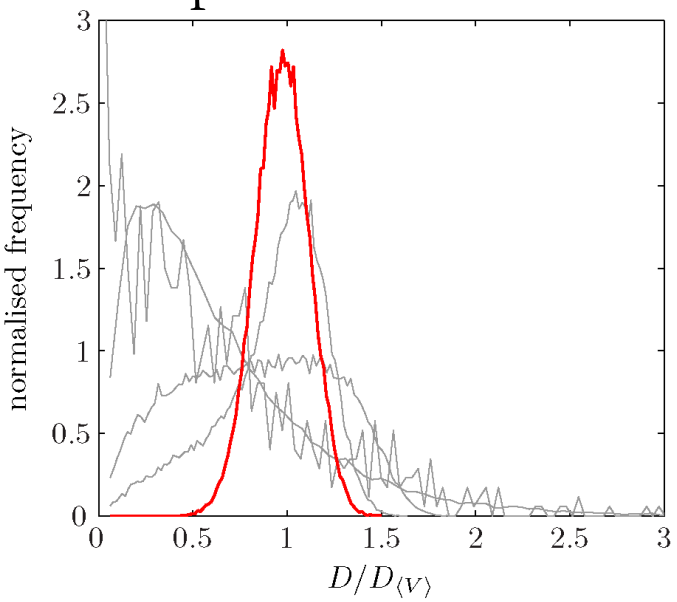
1. random nucleation on random planar GBs (Cahn's model)
2. random nucleation on *nonrandom* GBs
   - iso*chronal*, cont. nucl., $Q_G/Q_N = 0.01$
   - iso*thermal*, continuous nucleation
   - iso*chronal*, cont. nucl., $Q_G/Q_N = 100$
   - pre-existing nuclei
   - result of grain growth simulation (MC)

parent → product kinetics: continuous nucleation, isothermal transformation

1. Influence of the parent microstructure

test various parent microstructures, keep all else identical:

parent GSDs



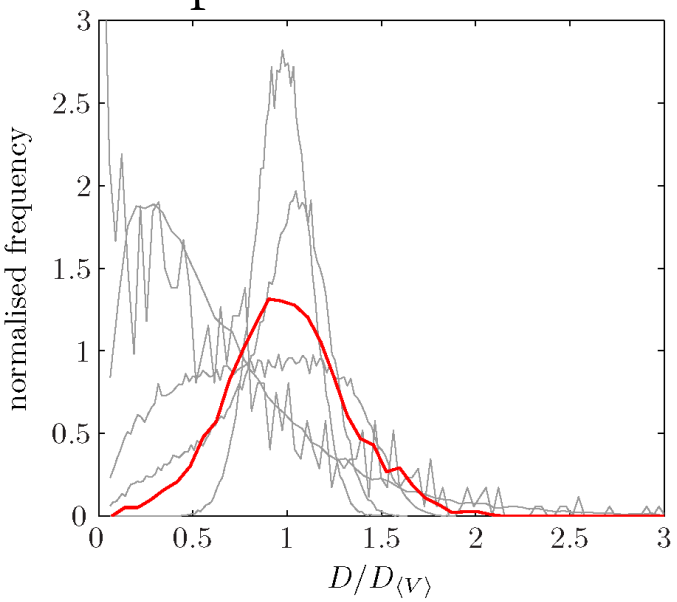
1. random nucleation on random planar GBs (Cahn's model)
2. random nucleation on *nonrandom* GBs
   - iso*chronal*, cont. nucl., $Q_G/Q_N = 0.01$
   - iso*thermal*, continuous nucleation
   - iso*chronal*, cont. nucl., $Q_G/Q_N = 100$
   - pre-existing nuclei
   - result of grain growth simulation (MC)

parent → product kinetics: continuous nucleation, isothermal transformation

1. Influence of the parent microstructure

test various parent microstructures, keep all else identical:

parent GSDs

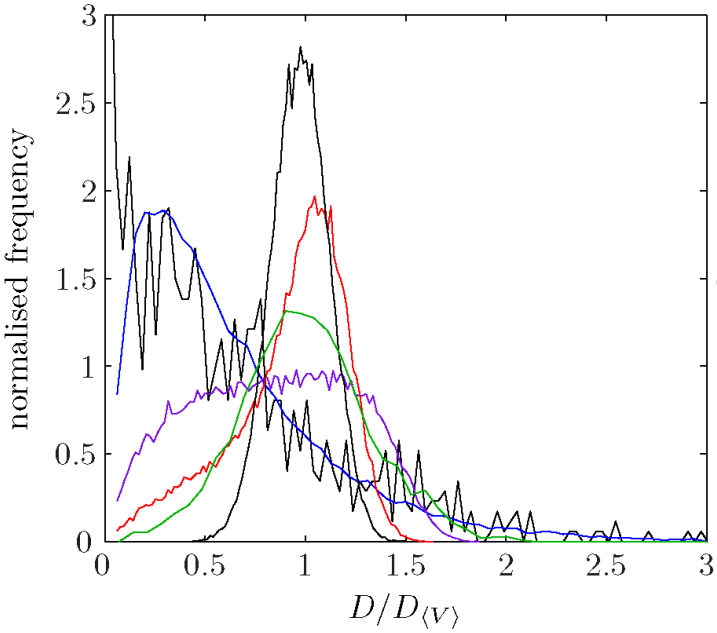


1. random nucleation on random planar GBs (Cahn's model)
2. random nucleation on *nonrandom* GBs
   - iso*chronal*, cont. nucl., $Q_G/Q_N = 0.01$
   - iso*thermal*, continuous nucleation
   - iso*chronal*, cont. nucl., $Q_G/Q_N = 100$
   - pre-existing nuclei
   - result of grain growth simulation (MC)

parent → product kinetics: continuous nucleation, isothermal transformation

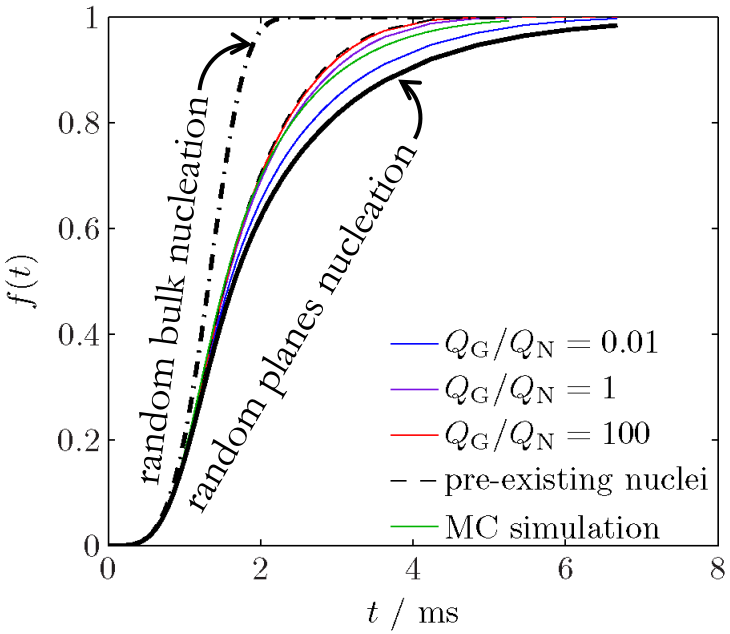
1. Influence of the parent microstructure

parent GSDs



parent → product

kinetics

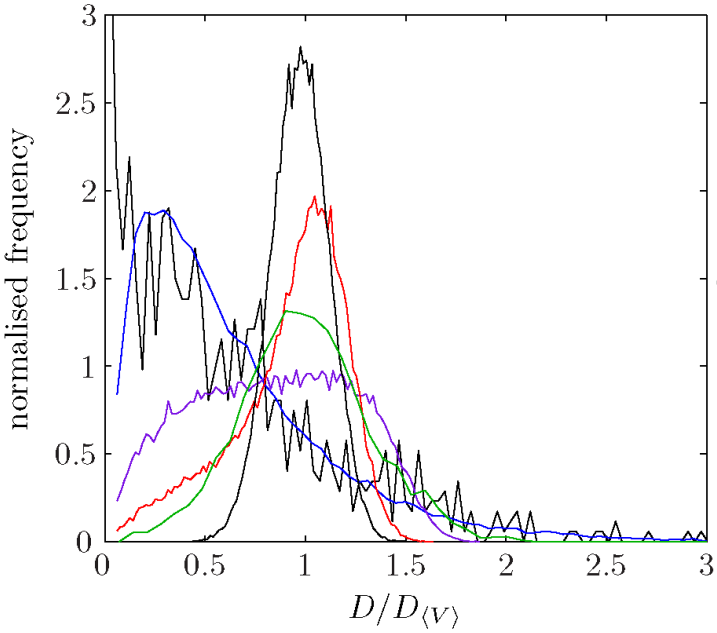


⇨ transformed fraction: random planes < simulation < random, bulk

⇨ strongest deviation from random, bulk nucleation kinetics if parent microstructure has a broad GSD with many small grains

1. Influence of the parent microstructure

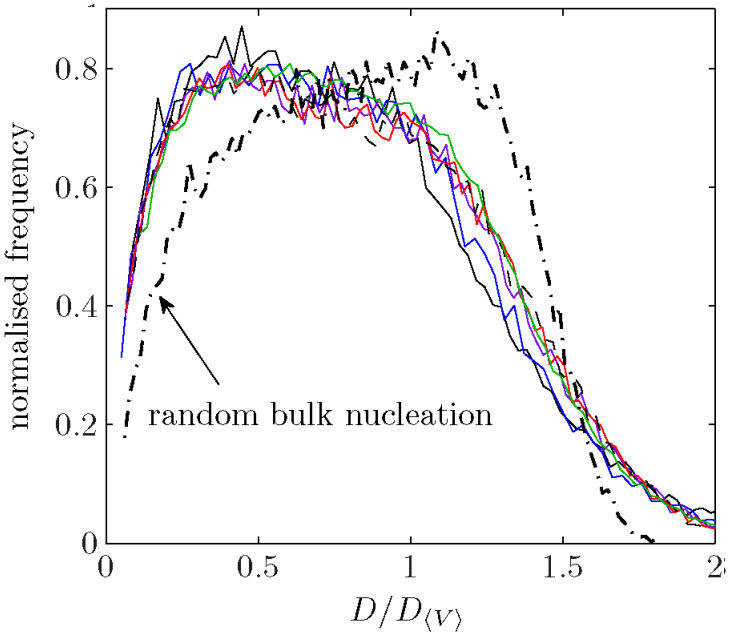
parent GSDs



parent → product

kinetics

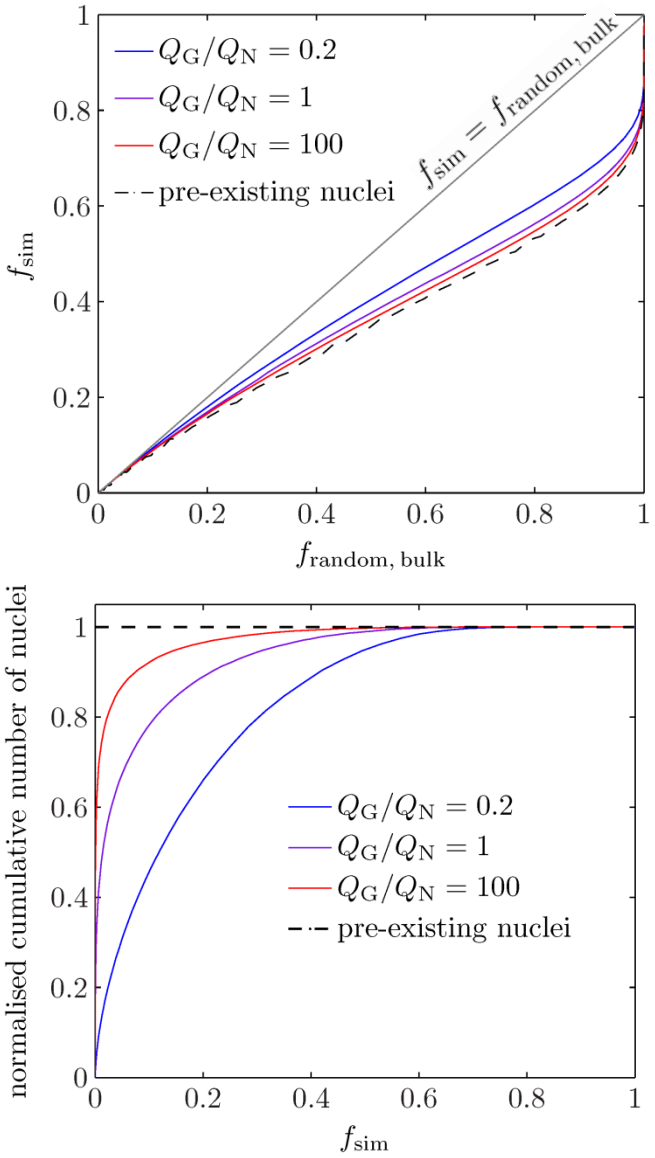
product GSDs



⇨ transformed fraction: random planes < simulation < random, bulk

⇨ strongest deviation from random, bulk nucleation kinetics if parent microstructure has a broad GSD with many small grains

2. Influence of the parent → product kinetics



parent microstructure:
random, bulk nucleation, pre-existing nuclei

simulations using various parent → product kinetics:

- pre-existing nuclei
- continuous nucleation, iso*thermal*
- cont. nucl., iso*chronal*, $Q_G/Q_N = 100$
- cont. nucl., iso*chronal*, $Q_G/Q_N = 0.2$

⇨ strongest deviation from random, bulk nucleation if nucleation predominantly at the beginning of the transformation

3. Kinetic models for GBN transformations

fitting various models to simulated data (known inputs):

1. JMAK impingement: $\mathrm{d}f = (1-f)\,\mathrm{d}f^{\mathrm{ex}}$
2. modified JMAK impingement: $\mathrm{d}f = (1-f)^{\xi}\,\mathrm{d}f^{\mathrm{ex}}$
3. Cahn's model: $\mathrm{d}O = (1-f_O)\,\mathrm{d}O^{\mathrm{ex}}$ and $\mathrm{d}V = (1-f_V)\,\mathrm{d}V^{\mathrm{ex}}$
4. modified Cahn model: $\mathrm{d}O = (1-f_O)\,\mathrm{d}O^{\mathrm{ex}}$ and $\mathrm{d}V = (1-f_V)^{\xi}\,\mathrm{d}V^{\mathrm{ex}}$

3. Kinetic models for GBN transformations

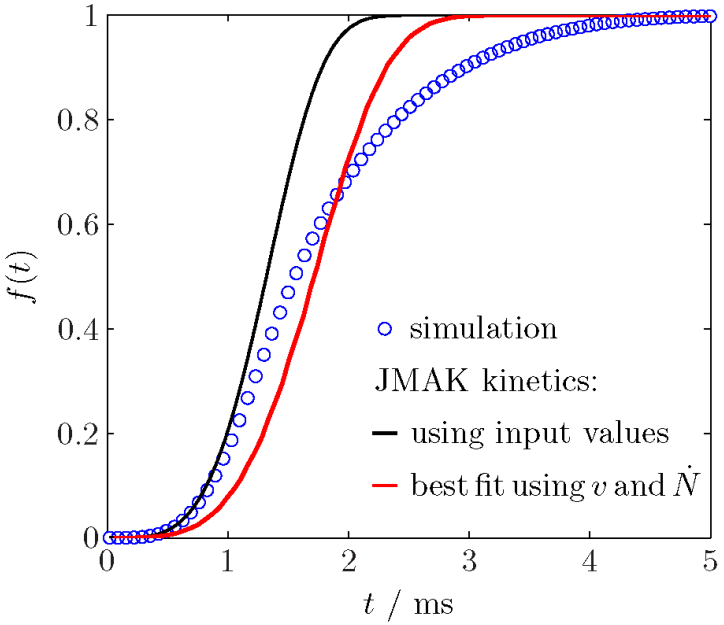
fitting various models to simulated data (known inputs):

1. JMAK impingement
2. modified JMAK impingement
3. Cahn's model
4. modified Cahn model

3. Kinetic models for GBN transformations

fitting various models to simulated data (known inputs):

1. JMAK impingement → no fit using $\dot{N}$ and v
2. modified JMAK impingement
3. Cahn's model
4. modified Cahn model



3. Kinetic models for GBN transformations

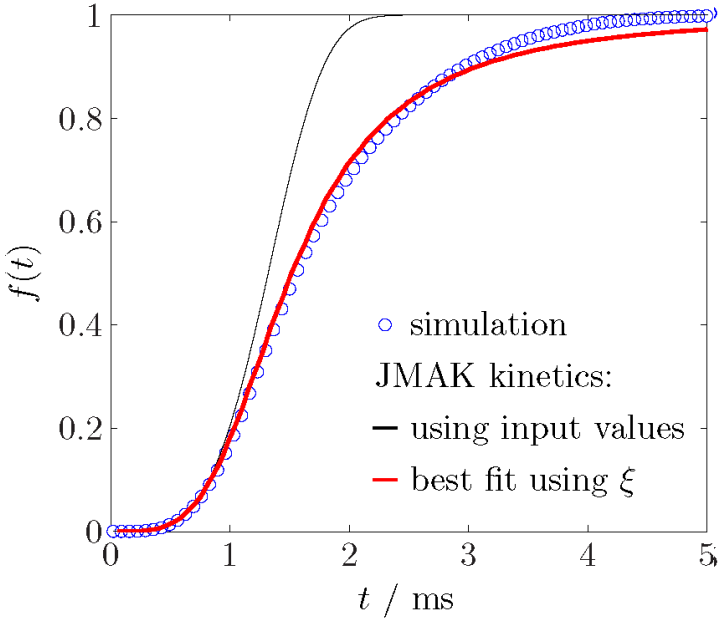
fitting various models to simulated data (known inputs):

✘ 1. JMAK impingement → no fit using $\dot{N}$ and v

✓ 2. modified JMAK impingement → good fit using ξ

3. Cahn's model

4. modified Cahn model



3. Kinetic models for GBN transformations

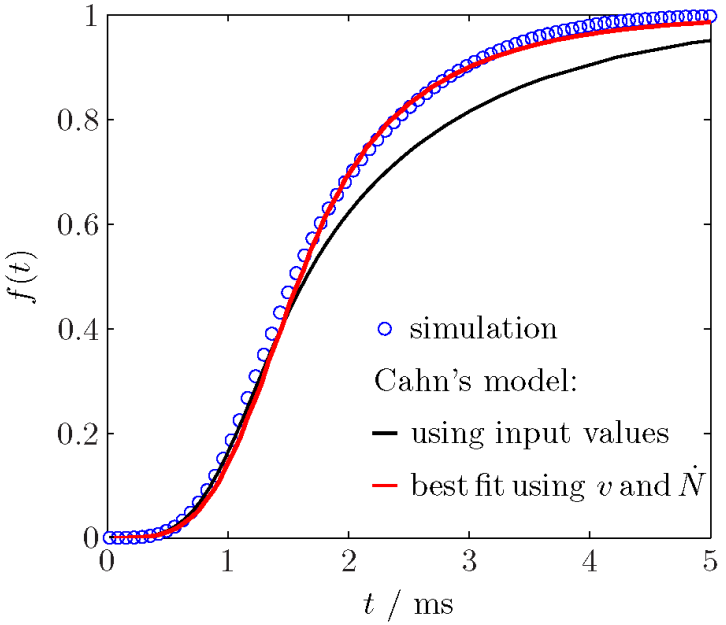
fitting various models to simulated data (known inputs):

✘ 1. JMAK impingement → no fit using $\dot{N}$ and v

✓ 2. modified JMAK impingement → good fit using ξ

✘ 3. Cahn's model → good fit, but incorrect results

4. modified Cahn model



3. Kinetic models for GBN transformations

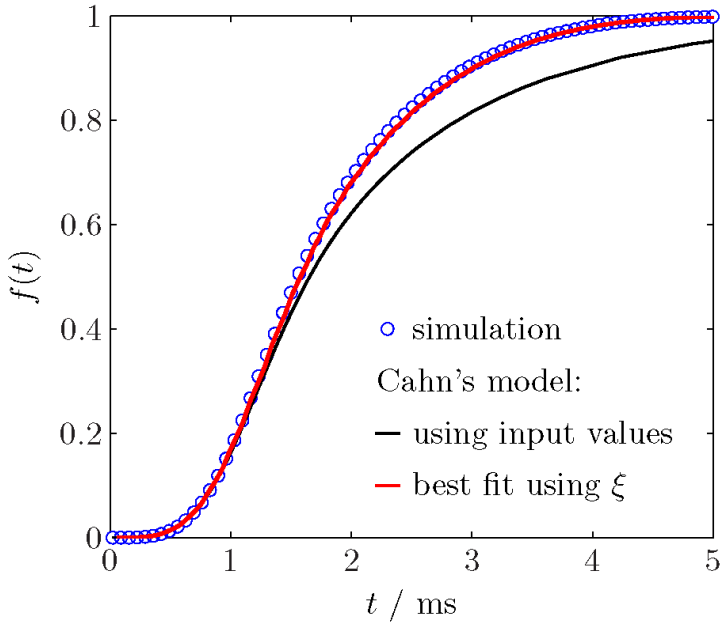
fitting various models to simulated data (known inputs):

✘ 1. JMAK impingement → no fit using $\dot{N}$ and v

✓ 2. modified JMAK impingement → good fit using ξ

✘ 3. Cahn's model → good fit, but incorrect results

✓ 4. modified Cahn model → good fit using ξ



3. Kinetic models for GBN transformations

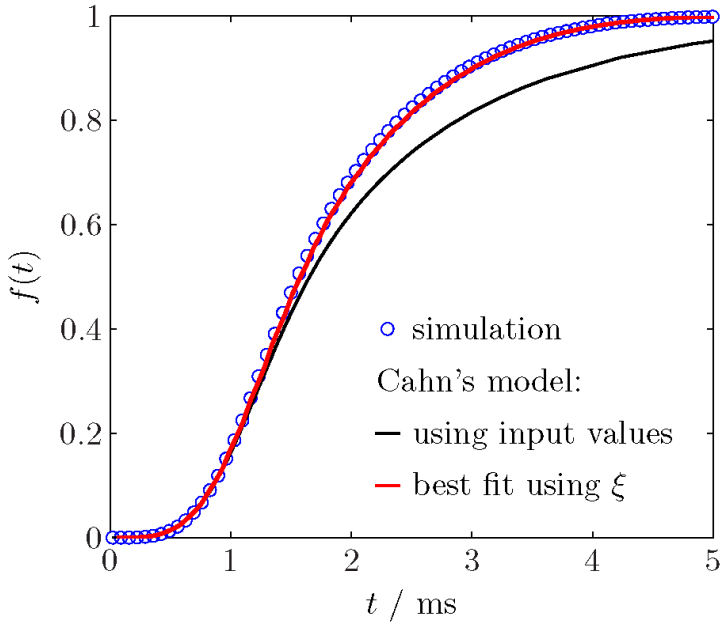
fitting various models to simulated data (known inputs):

✘ 1. JMAK impingement → no fit using $\dot{N}$ and v

✓ 2. modified JMAK impingement → good fit using ξ

✘ 3. Cahn's model → good fit, but incorrect results

✓ 4. modified Cahn model → good fit using ξ



⇨ modified impingement correction required to describe simulated kinetics

Conclusions

- geometrical simulations are a useful tool to study phase-transformation kinetics and microstructure
- Grain-boundary nucleation kinetics:
  - random planes nucleation < simulation < random, bulk nucleation
- transformation most influenced by GB nucleation if
  - parent microstructure has broad GSD with many small grains
  - nucleation takes place predominantly at the beginning of the transformation
- modified impingement correction required to describe simulated kinetics