Unraveling the nature of grain boundary migration by Potts model simulations

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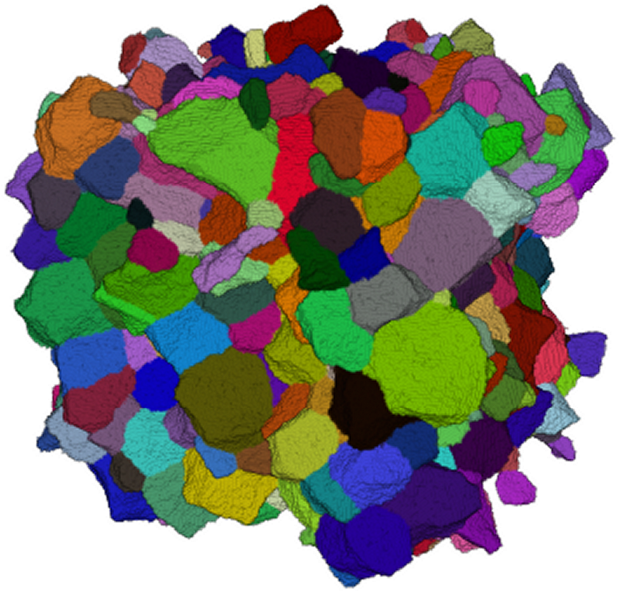
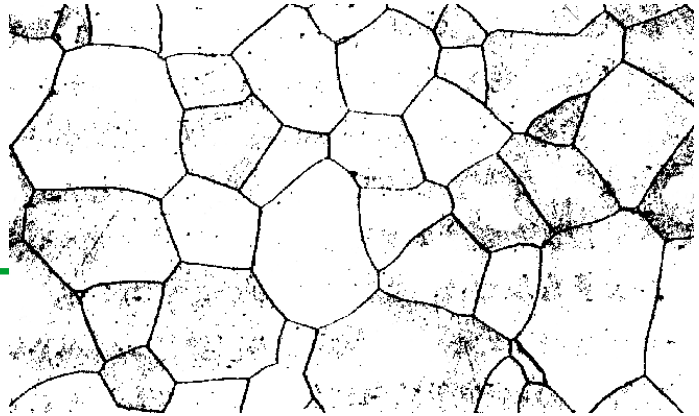
Outline



- Introduction
- Standard Monte Carlo Potts Model
  - History, Algorithms & Problems
  - Simulation of Grain Boundary Motion
- A Potts Model for Nanocrystalline Grain Growth
  - Size Effects in a Size-Invariant Simulation
- Going Back to 2D Grain Growth
  - Grain Boundary Migration in Graphene
- Summary and Outlook

Introduction



Importance of grain growth:

- most materials properties depend on grain size
  - Hall-Petch-effect: small grains = higher yield stress
- grain microstructure = important feature of poly-crystalline solids
- understanding & control = key to improve materials properties

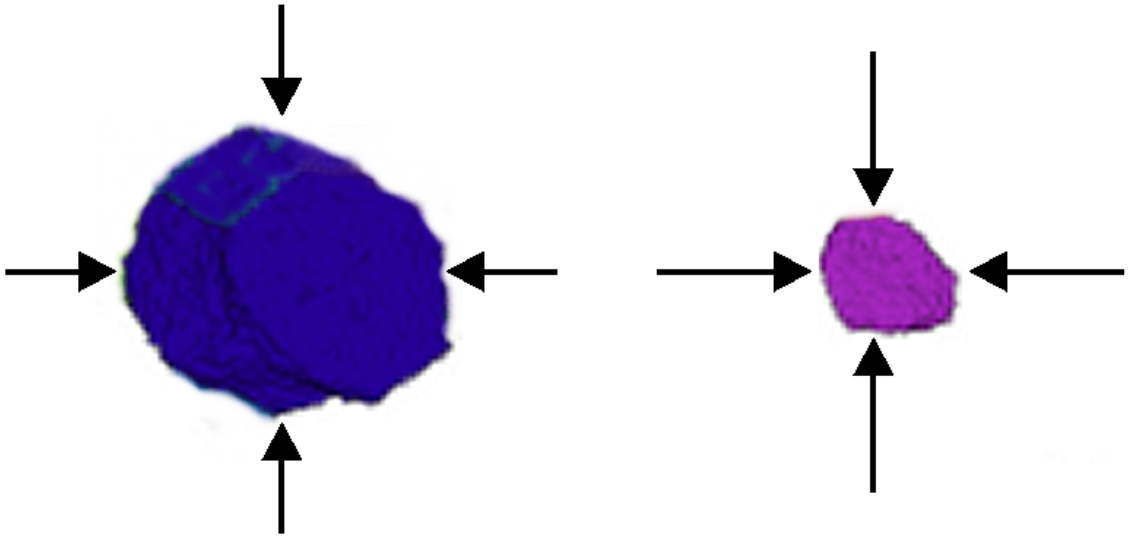
- Problem: thermally activated grain boundary migration
  - changing grain sizes

Introduction

Basic principles of grain growth:

- All grains of a polycrystalline material try to shrink!

  → thermodynamically: reduction of surface energy



- The smaller a grain is, the stronger it pushes its atoms to the neighboring grains.

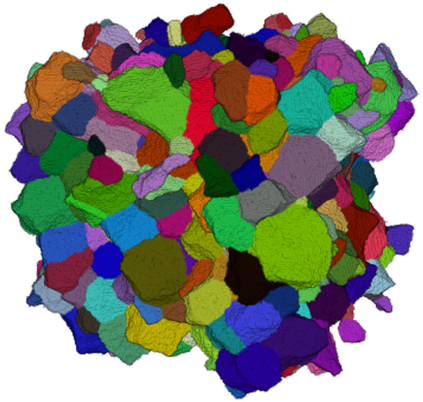
Introduction

Basic principles of grain growth:

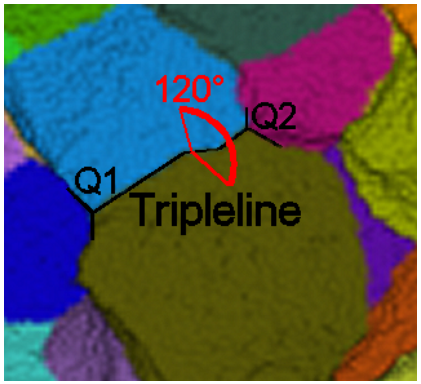
- We have a network of grain boundaries.

  → global: volume conservation

  → local: equilibrium at grain boundaries



versus



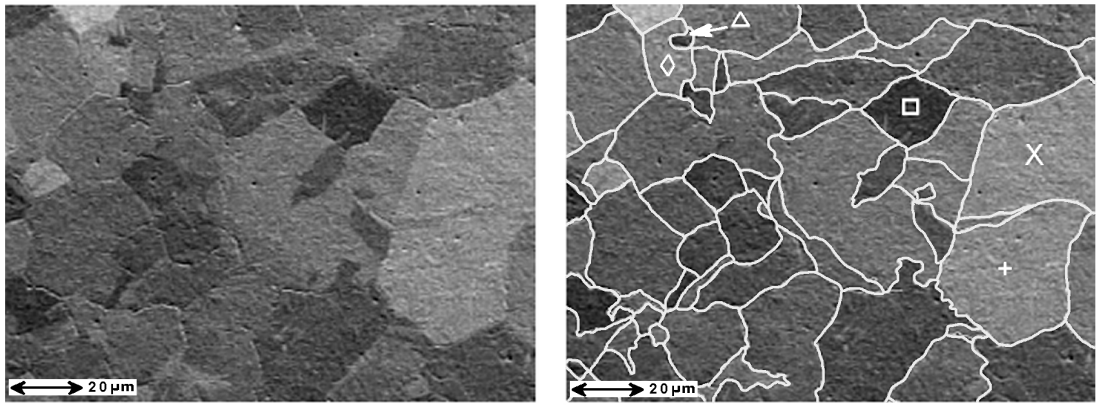
- Therefore, whether a grain will shrink or growth depends on its size and on its neighboring grains.

  → complex 3D problem

Introduction

Experimental observation of grain growth:

- SEM observation



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[I. Fielden: Mater. Sci. Forum 467-470 (2004) 875]

[D. Zöllner, I. Fielden, P. Streitenberger: Prac. Metallogr. 49 (2012) 428]

Introduction

What is known about normal grain growth:

- curvature driven kinetics
- follows parabolic growth law

$$\langle R\rangle^{1/n} = b\cdot t + \langle R\rangle_0^{1/n}$$

- shows self-similar scaling

$$F(R,t) = g(t)\cdot f(x), \quad \mathrm{g(t)} = \frac{N}{\langle R\rangle}, \quad x = \frac{R}{\langle R\rangle}$$

- rate of area resp. volume change
  - 2D: von Neumann-Mullins $\dot{A} = \frac{k\cdot\pi}{3}\cdot(s-6)$
  - 3D: MacPherson-Srolovitz $\dot{V} = -2\pi\cdot M\gamma\cdot\left(\mathcal{L}(R) - \frac{1}{6}\sum_{i=1}^{n} E_i(R)\right)$

Introduction

Why use mesoscopic computer simulations:

- bridge the gaps between experiments and theories
- give insight into fundamental physical processes
- give information on morphology and topology
- allow a far more precise manipulation of materials properties than can be realized experimentally
- can be understood as in-situ computer experiments

Standard Monte Carlo Potts Model

History:

- *Monte Carlo method*: all techniques of numerical mathematics using probabilistic methods to solve deterministic problems
- *first application in physics*: in solid states physics to model ferromagnetic materials → two spins
- 1952: generalisation by Potts to Q-states model
- 1984: applied by Anderson et al. to grain growth

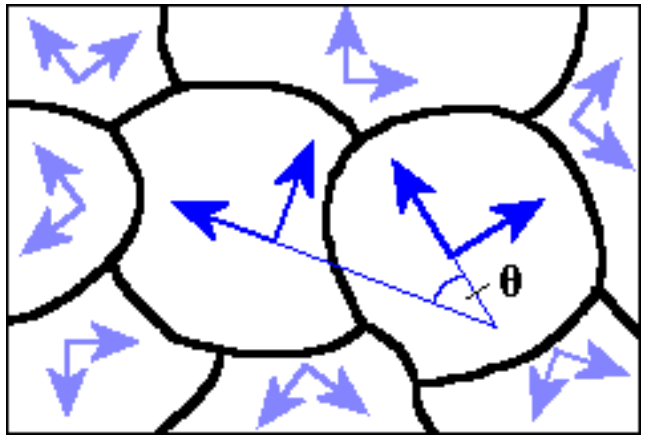
→ represents *curvature driven grain growth* and takes the *interaction of grains* into consideration *without using complex motion equations*

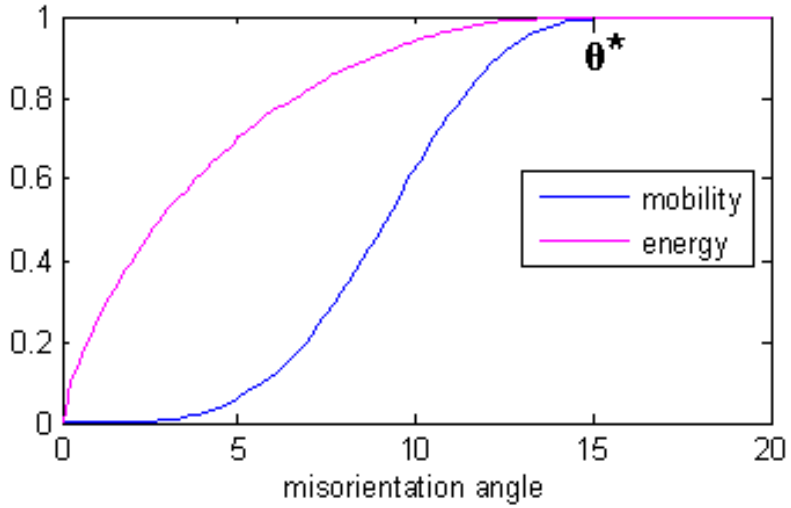
Standard Monte Carlo Potts Model

Algorithm - Parameters:

- grain boundary energy γ and mobility m depend only on misorientation angle θ between neighbouring grains

$$\gamma = \begin{cases} \frac{\theta}{\theta^*}\left(1 - \ln\frac{\theta}{\theta^*}\right) & \text{if } \theta \le \theta^* \\ 1 & \text{else} \end{cases} \qquad m = \begin{cases} 1 - \exp\left(-B\left(\frac{\theta}{\theta^*}\right)^n\right) & \text{if } \theta \le \theta^* \\ 1 & \text{else} \end{cases}$$



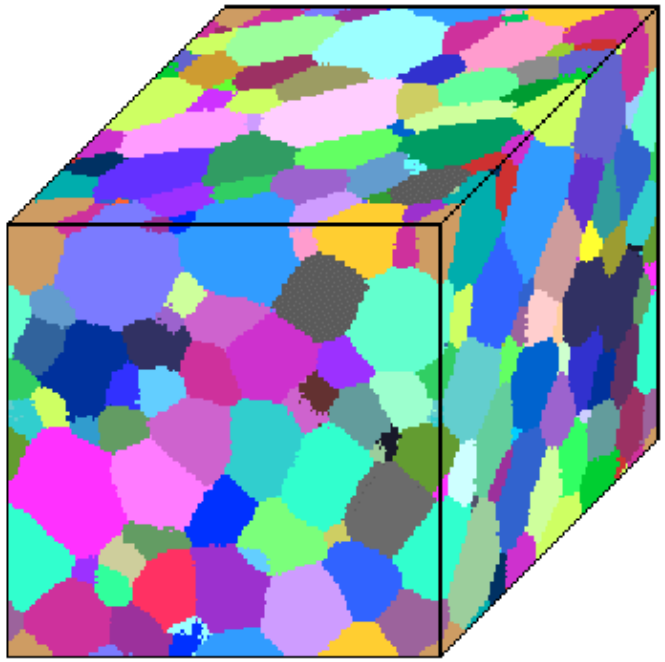


[D. Zöllner: *Monte Carlo Potts Model Simulation...* (2006); ISBN 3-8322-5633-4]

Standard Monte Carlo Potts Model

Algorithm - Parameters:

- cubic 3D lattice
- total $N > 200^3$ lattice points
- each lattice point has 26 nearest neighbours
- smallest size unit = Monte Carlo Unit (MCU) = one lattice point = represents a cluster of atoms of a grain
- smallest time unit = Monte Carlo Step (MCS) = N reorientation attempts

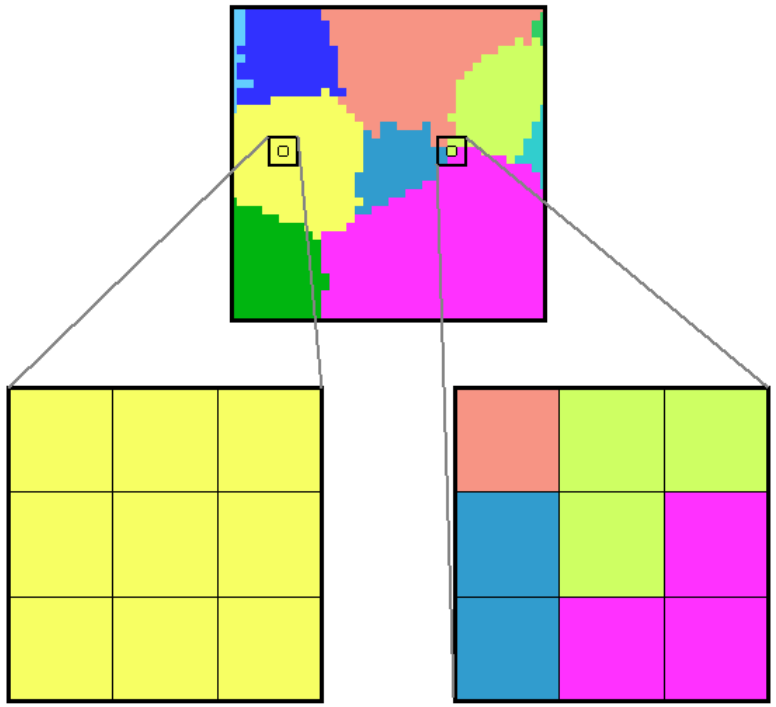


Standard Monte Carlo Potts Model

Algorithm:

1. probabilistic selection of a lattice point

- lattice point has orientation $Q\mu$



! grain boundary migration
→ atoms change orientation
from grain to neighboring grain

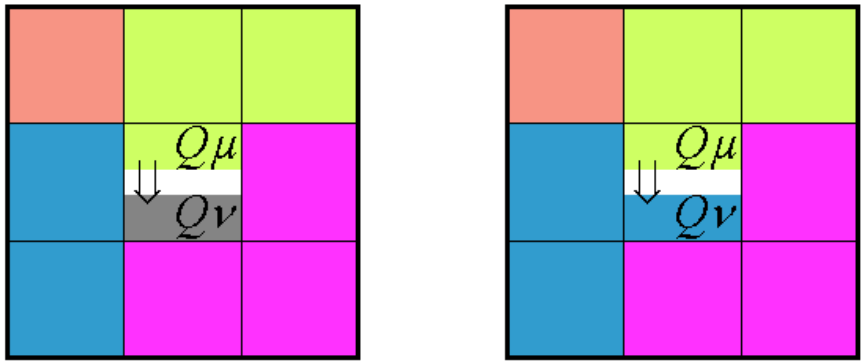
- lattice point on boundary → proceed with step 2
- else → terminate loop

Standard Monte Carlo Potts Model

Algorithm:

2. selection of new orientation Qv

- $Qv \neq Q\mu$



- assigned on probation
- consider only orientations from neighboring lattice points → no nucleation events!

Standard Monte Carlo Potts Model

Algorithm:

3. calculation of energy

- given by Hamiltonian $$H = \gamma \cdot \sum_{i=1}^{N} \sum_{j=1}^{nn} \left(1 - \delta_{Q_i Q_j}\right)$$

  ! only one lattice point is considered at each trial

- hence: difference in energy simplified to

$$\Delta E = \gamma \cdot \sum_{j=1}^{nn} \left(\delta_{Q_j Q_\nu} - \delta_{Q_j Q_\mu}\right)$$

considering only nearest neighbors

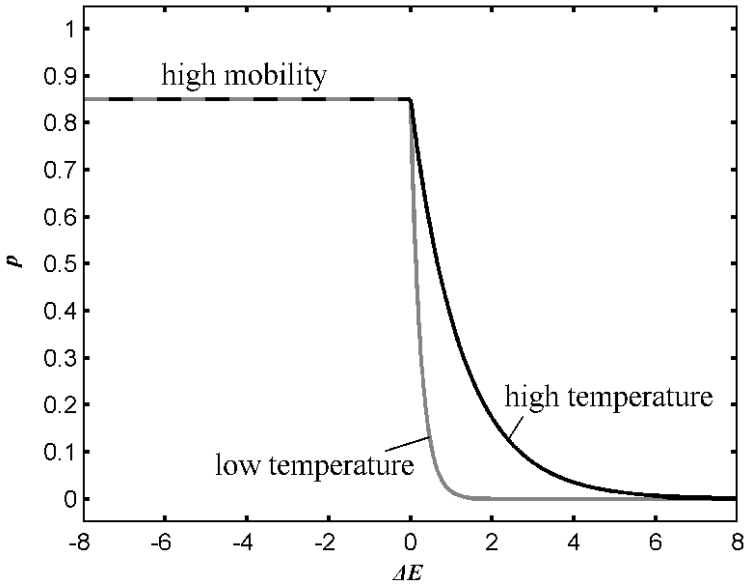
Standard Monte Carlo Potts Model

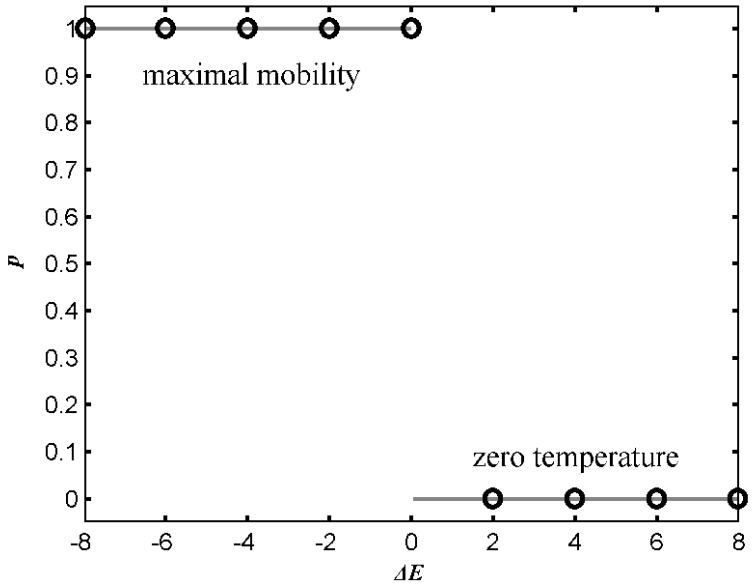
Algorithm:

4. selection of final orientation $Q\mu^*$

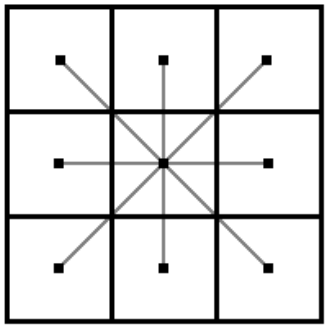
- chosen with probability

$$p = \begin{cases} m & \text{if } \Delta E \le 0 \\ m \cdot \exp\dfrac{-\Delta E}{k_B T} & \text{if } \Delta E > 0 \end{cases}$$





Standard Monte Carlo Potts Model

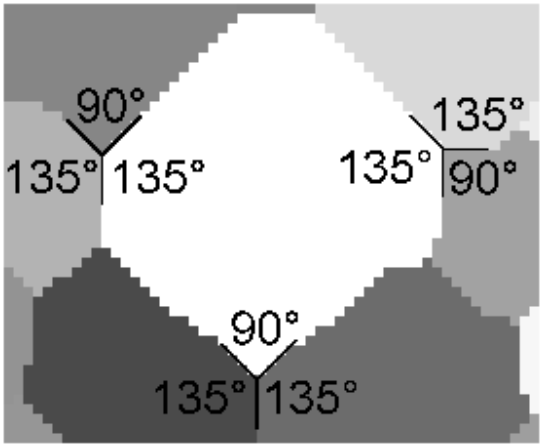


Problems:

1. choice of lattice

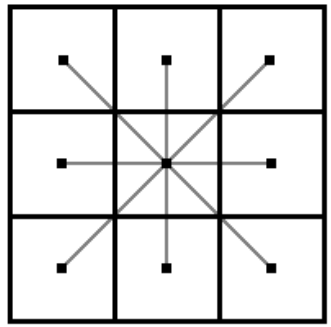
- in 2D: quadratic or triangular lattice
- quadratic lattice = easy implementation (*.bmp)

  → underlying lattice forces simulation results?



- Potts model = curvature driven kinetics
- energy minimized by decreasing boundary length
- driving force places boundaries along lattice facets

Standard Monte Carlo Potts Model



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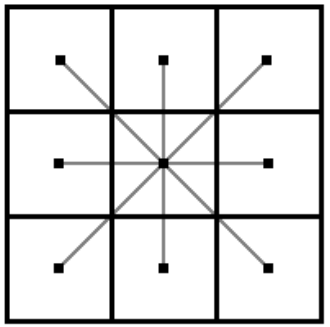
- solution:

1. increasing number of neighbor lattice points decreases energetic anisotropy of the lattice
2. introduction of simulation temperature $k_B T$ activates thermal fluctuations that roughens grain boundaries

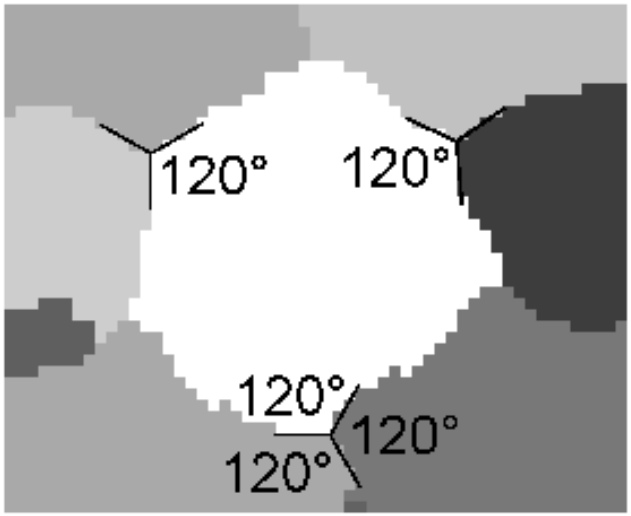
Standard Monte Carlo Potts Model



Problems:

1. choice of lattice

- in 2D: quadratic



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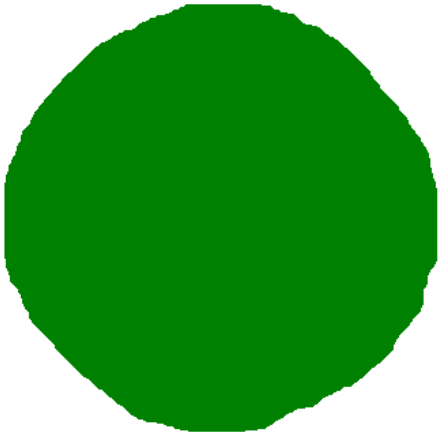
Standard Monte Carlo Potts Model

Problems:

2. choice of simulation temperature

- simulation temperature not related to real temperature
- usually found by trial and error



$k_B T =$ 0.0

Standard Monte Carlo Potts Model

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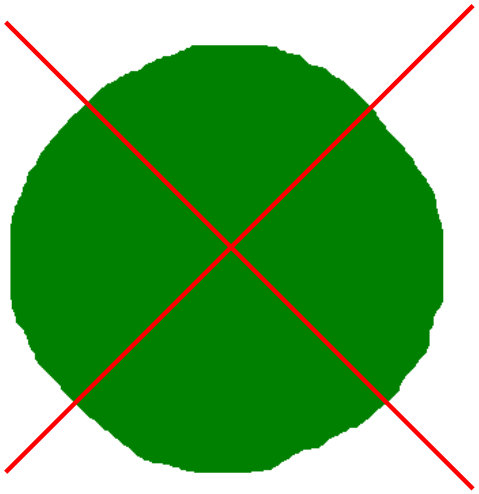

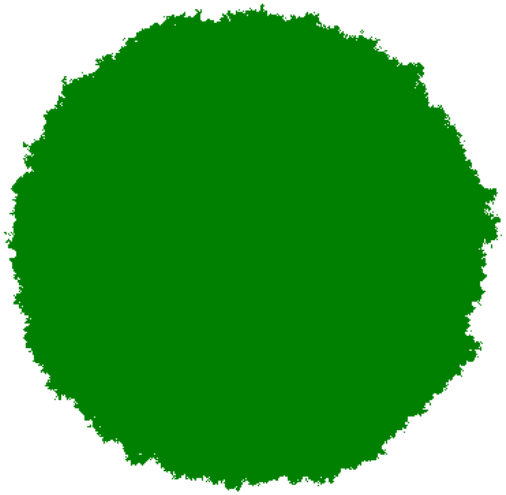

$k_BT =$ 0.0 2.4

Standard Monte Carlo Potts Model

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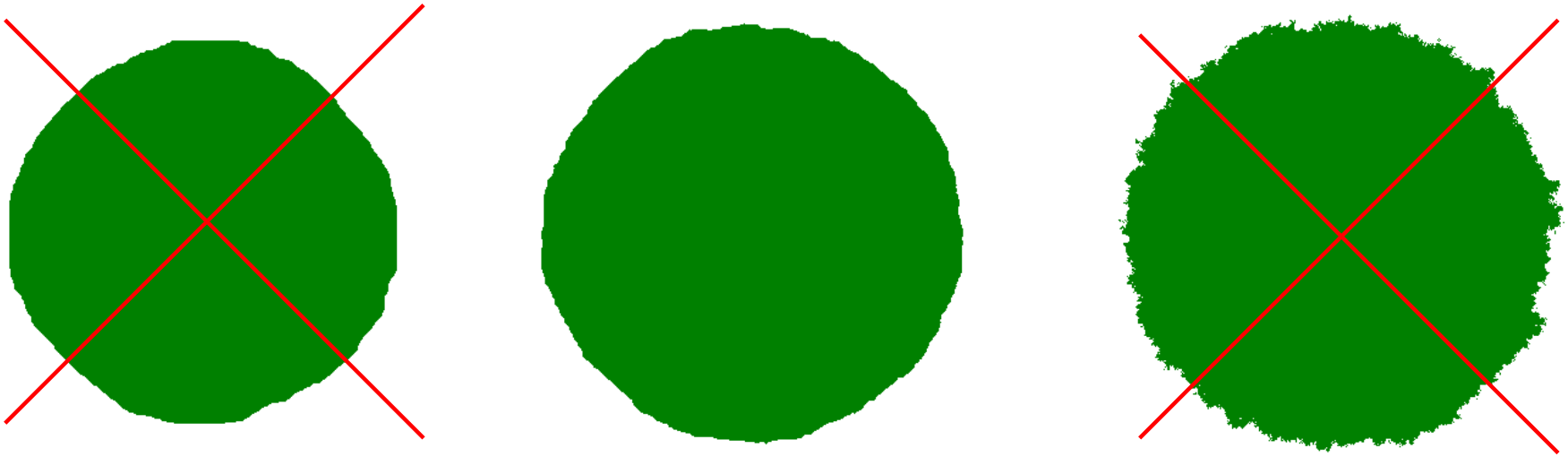


$k_B T =$ 0.0 0.6 2.4

Standard Monte Carlo Potts Model

Problems:

3. simulation runtime

- on standard PC (Intel® Core™2 Quad Q9650 CPU @ 3GHz with 3GB RAM)
  - three dimensional grain microstructure
  - 250^3 lattice points in size
  - 10,000 simulation time steps
- needs nearly 94 hours!

Standard Monte Carlo Potts Model

Problems:

3. simulation runtime

- solution:
- in recent years NVIDIA developed parallel computing architecture: Compute Unified Device Architecture
- CUDA allows programming of graphics processing units (GPUs) through standard programming languages (C)
  - GPUs have a parallel architecture
  - GPUs can compute many coexisting threads at the same time, rather than computing only a single thread

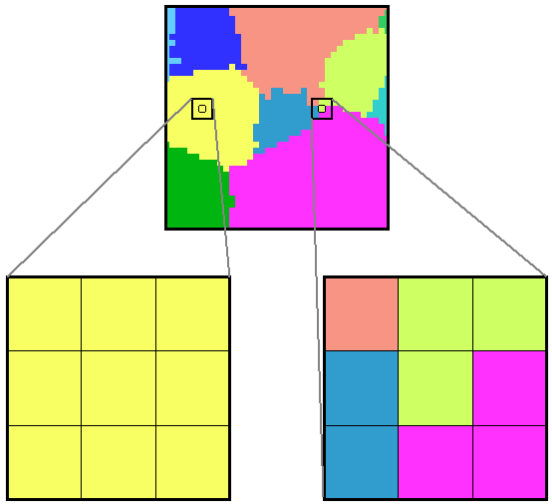
[S. Schäfer, D. Zöllner: CD-ROM Proceedings of the 6th Europ. Congr. on Comput. Meth. in Appl. Sci. and Eng. 2012; ISBN: 978-3-9502481-9-7]

Standard Monte Carlo Potts Model

Problems:

3. simulation runtime

- solution:



- drawback = lattice points not completely independent of each other!
- read from and write to the same lattice point?

  1. use two integer arrays
  2. introduce a checkerboard algorithm

Standard Monte Carlo Potts Model

Problems:

3. simulation runtime

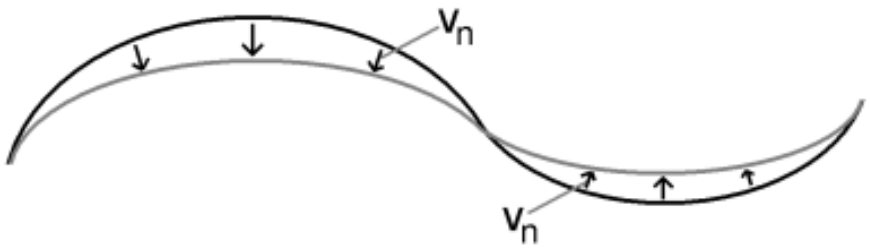
- solution:
- on a server with
  - two Intel® Xeon™ X5650 CPUs with 2.67GHz (12 cores) and
  - a Tesla™ C2050 graphic card from NVIDIA® with 448 cores) and 24GB RAM
- reduction of runtime down to approx. 18 minutes!

  << 94 hours

Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

1. curvature driven kinetics



- velocity of grain boundary

$$v_n = -k \cdot K$$

K = curvature; k = kinetic constant

- temporal change of area

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \oint_U v_n \mathrm{d}s$$

- for any closed plane curve (it can be shown)

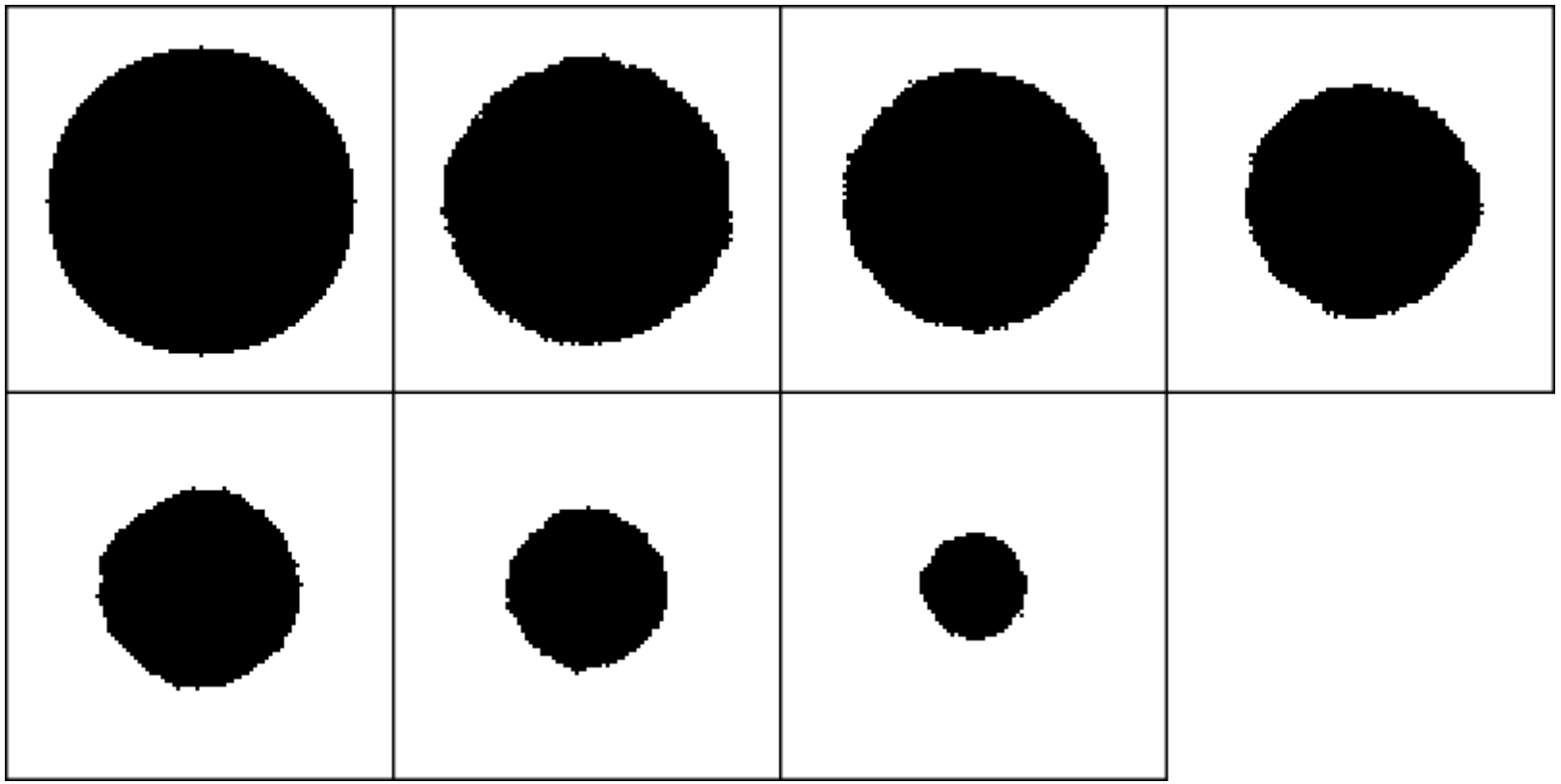
$$\oint_U K \cdot \mathrm{d}s = 2\pi$$

Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

1. curvature driven kinetics – simple case

- temporal change of area $A = -2\pi \cdot k \cdot t + A_0$



Standard Monte Carlo Potts Model

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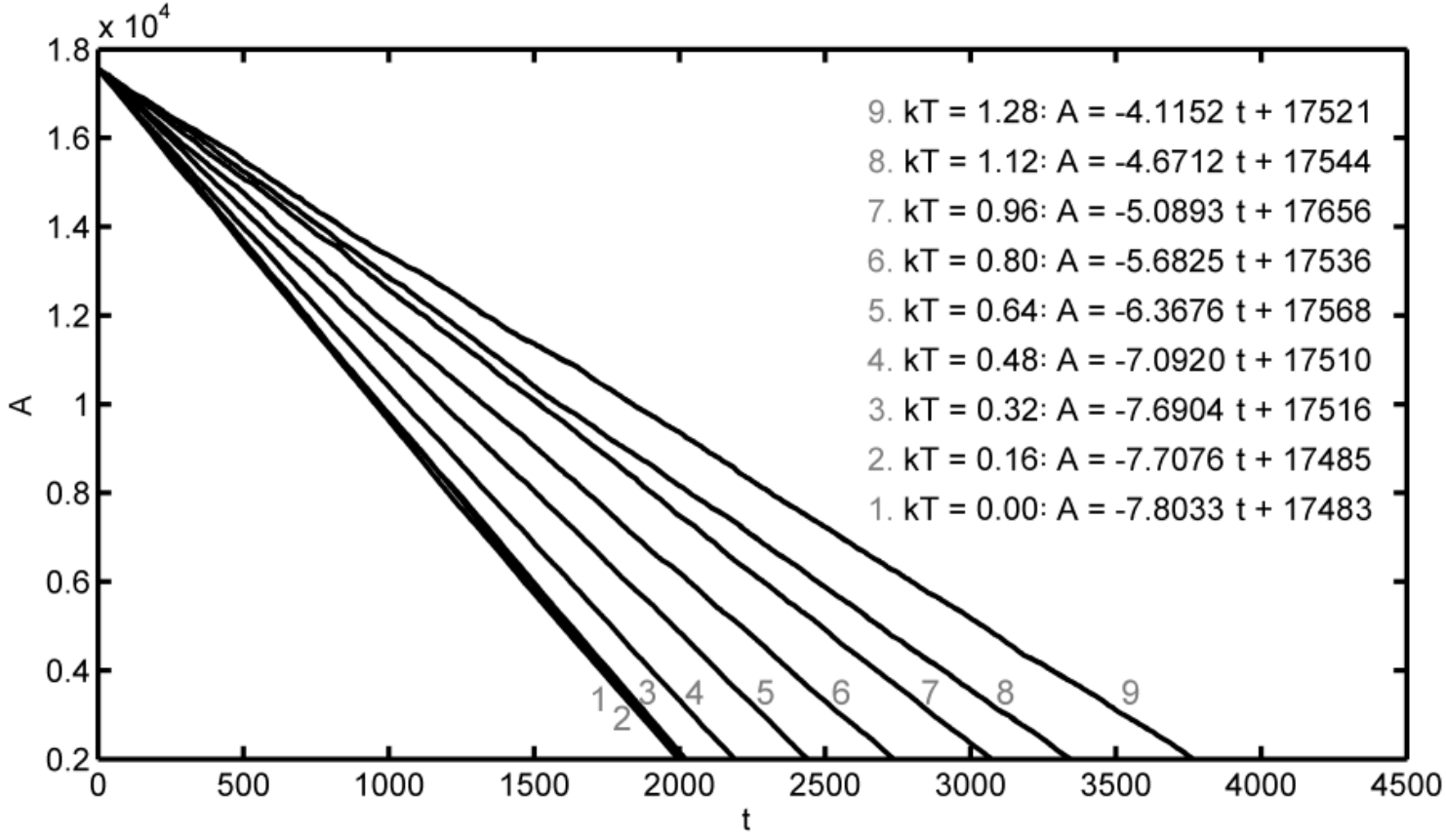


Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

2. ensemble of moving grain boundaries

remember?

- parabolic growth law

$$\langle R\rangle^{1/n} = b\cdot t + \langle R\rangle_0^{1/n}$$

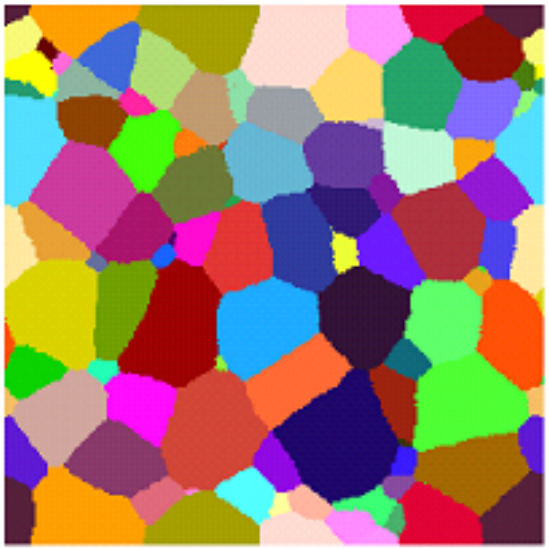
- self-similar scaling

$$F(R,t) = g(t)\cdot f(x), \quad \mathrm{g(t)} = \frac{N}{\langle R\rangle}, \quad x = \frac{R}{\langle R\rangle}$$

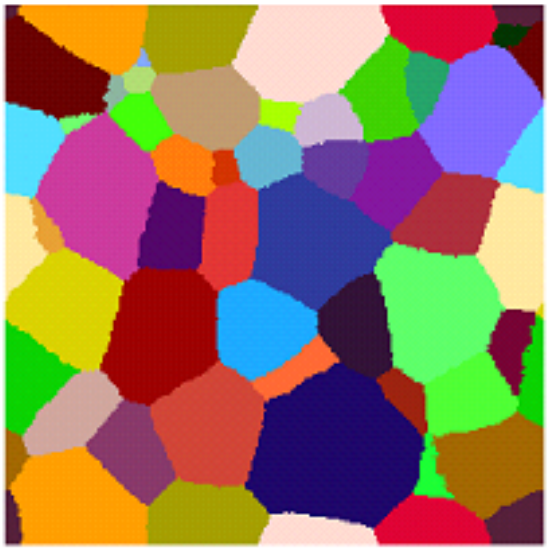
Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

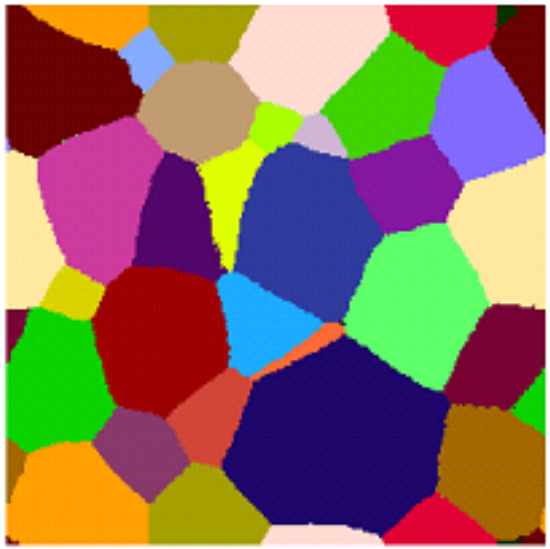
2. ensemble of moving grain boundaries



t = 1000



t = 2000

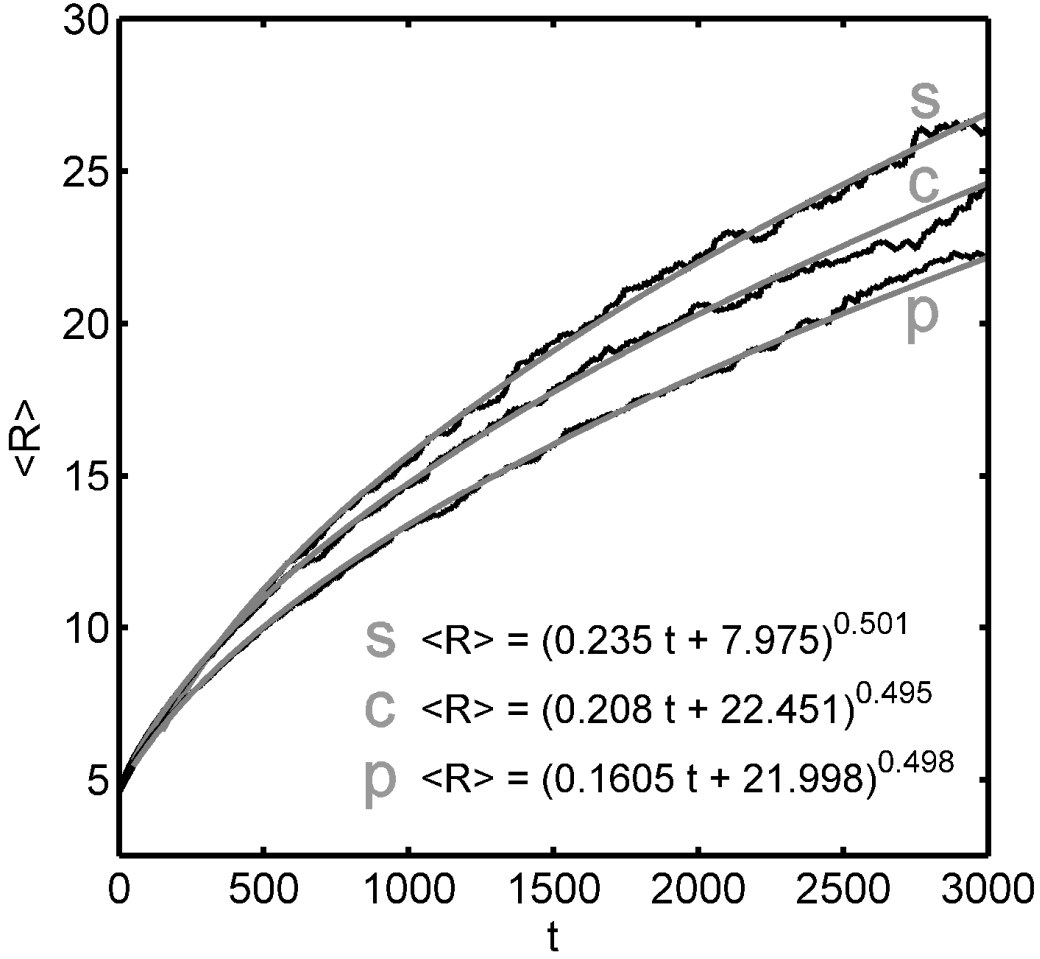


t = 3000

Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

2. ensemble of moving grain boundaries



- parabolic growth law

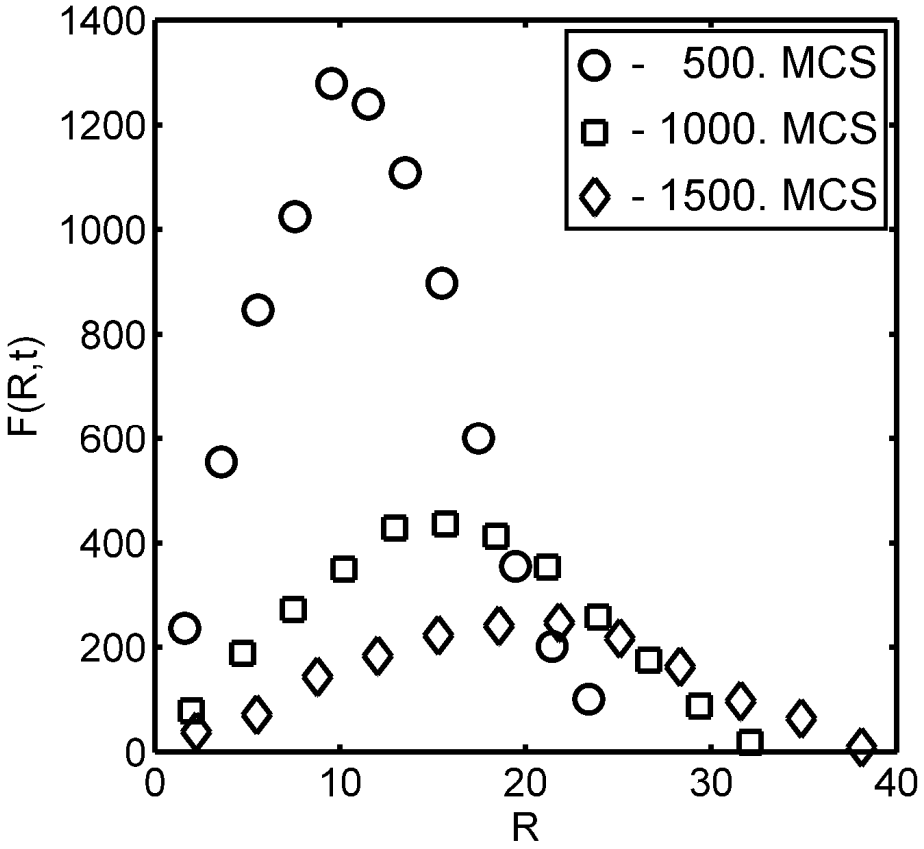
$$\langle R \rangle^{1/n} = b \cdot t + \langle R \rangle_0^{1/n}$$

- exponent n ≈ ½
- factor b depends on simulation type
- s = serial
- p = parallel
- c = checkerboard

Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

2. ensemble of moving grain boundaries

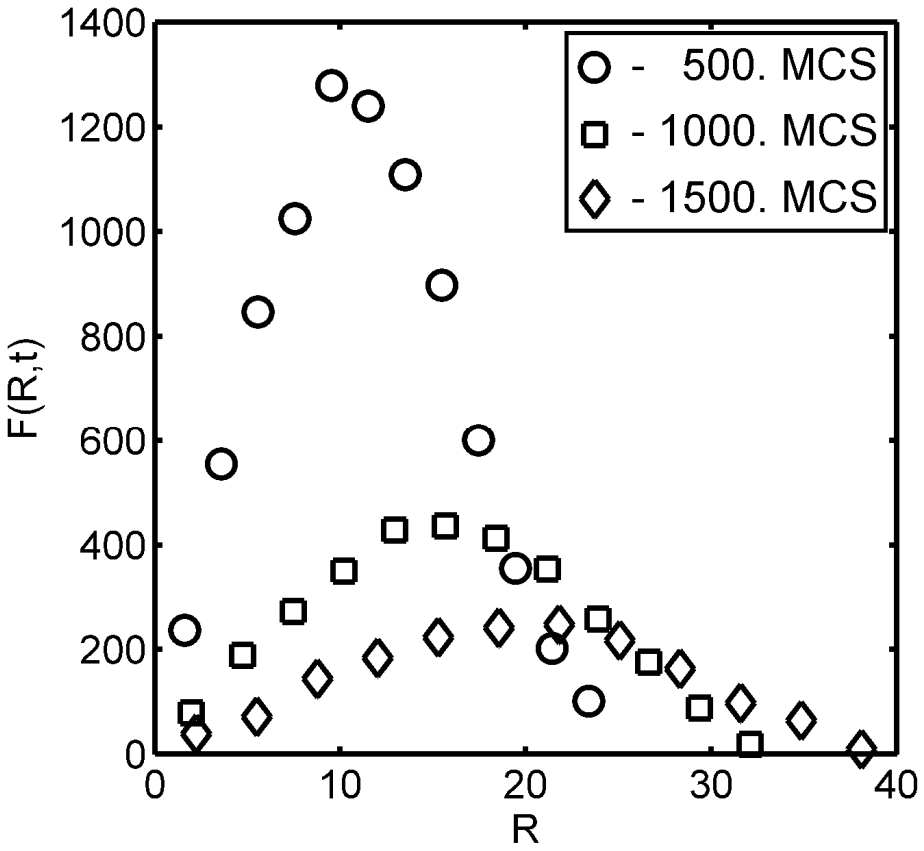


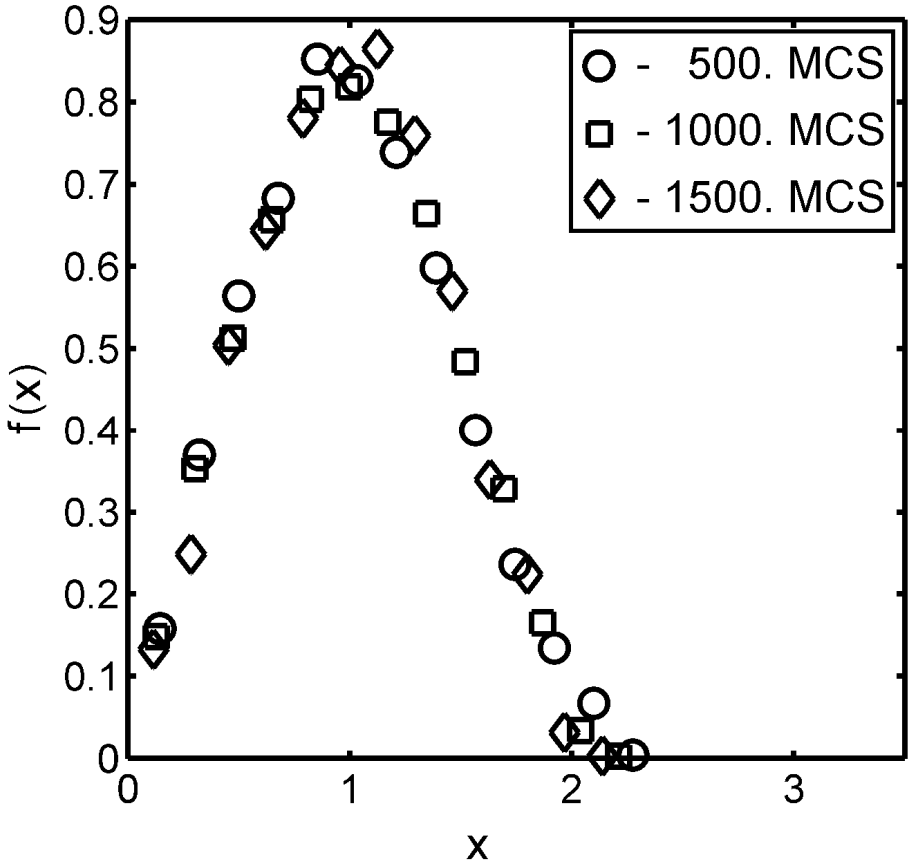
$$F(R,t) = g(t) \cdot f(x)$$

Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

2. ensemble of moving grain boundaries

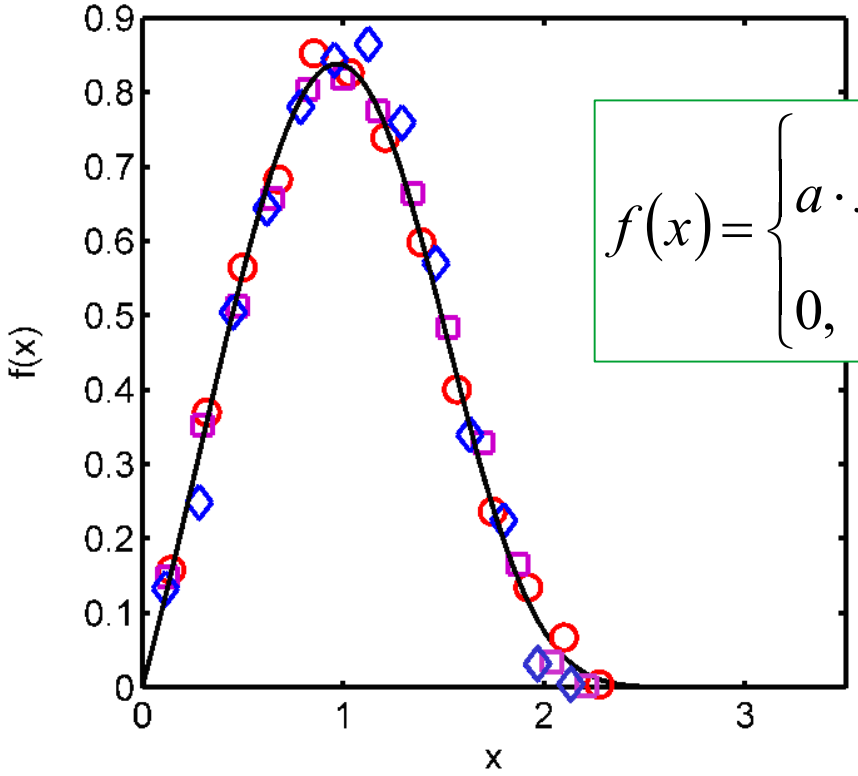




Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

2. ensemble of moving grain boundaries



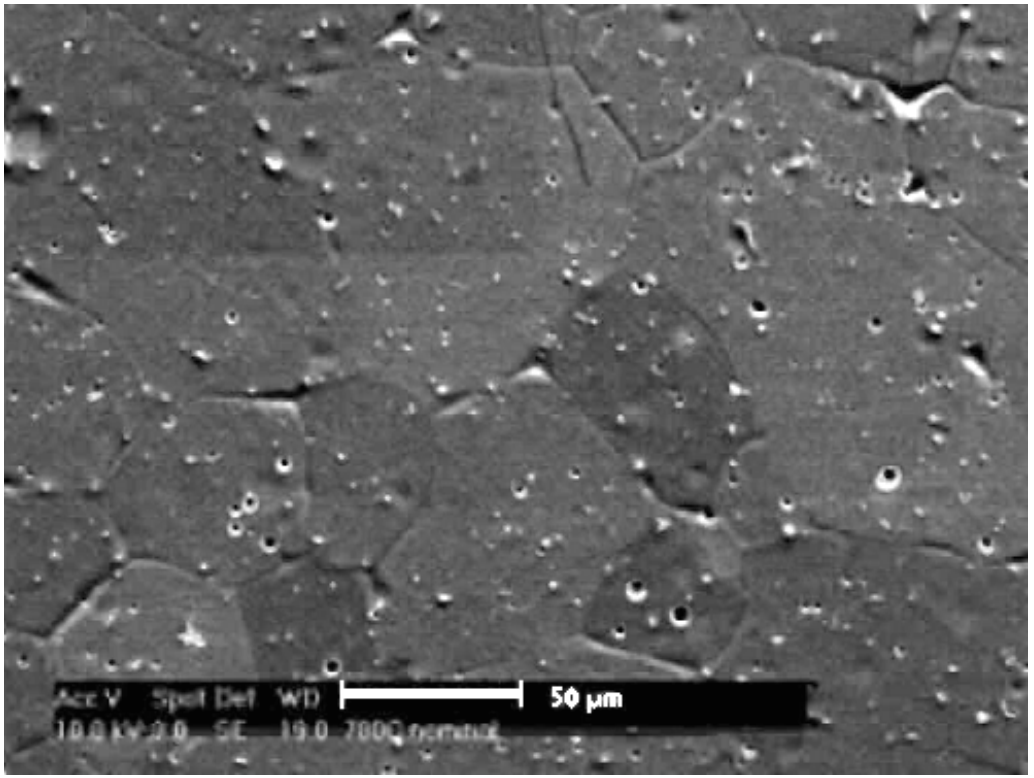
$$f(x) = \begin{cases} a \cdot x_0^a \cdot \exp(a) \cdot x \cdot (x_0 - x)^{-(a+2)} \cdot \exp\left(-\dfrac{a x_0}{x_0 - x}\right), & x \le x_0 \\ 0, & x > x_0 \end{cases}$$

[D. Zöllner, P. Streitenberger: Prac. Metallogr. 47 (2010) 618]

Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

3. individual growth kinetics



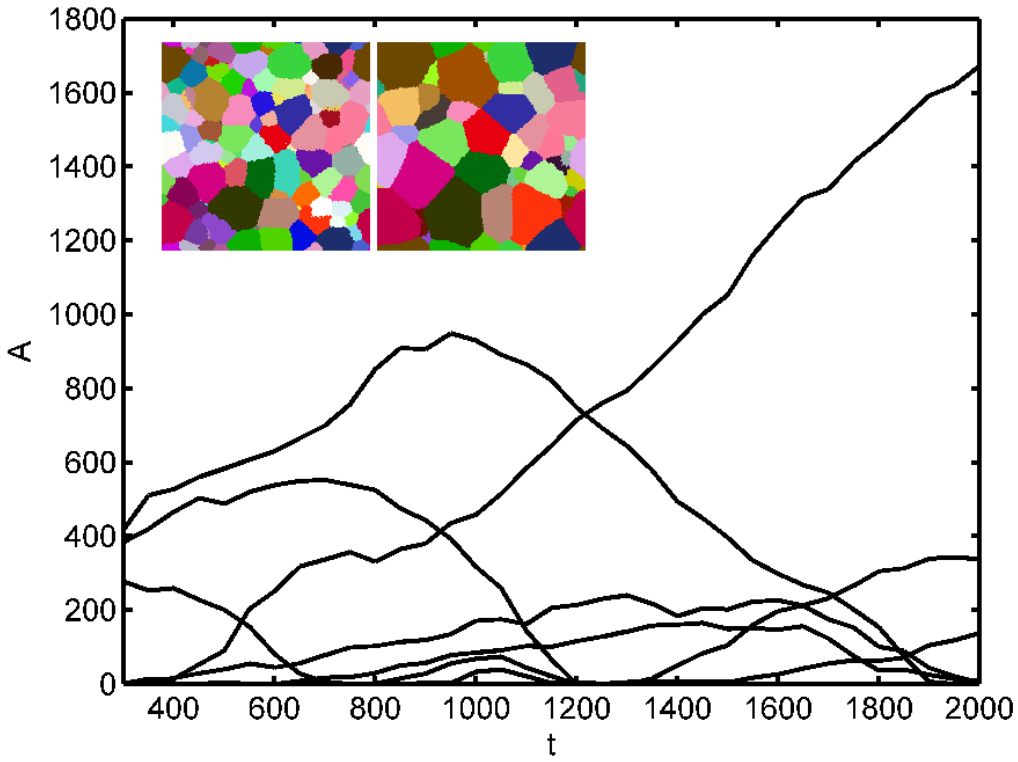
Aluminium at approx. 650°C
from in-situ real-time SEM

[D. Zöllner, P. Streitenberger, I. Fielden: Prac. Metallogr. 49 (2012) 428]

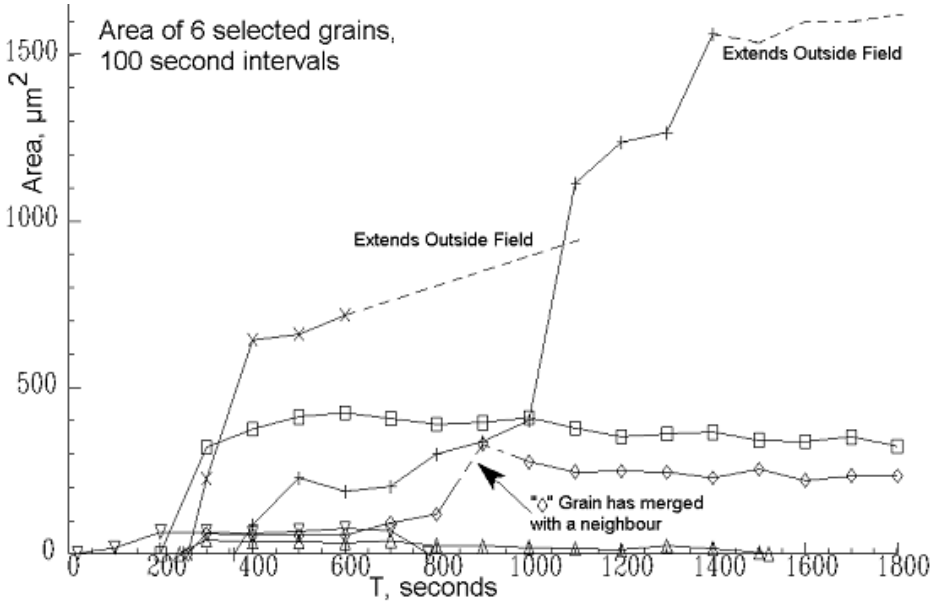
Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

3. individual growth kinetics



simulation (left) and real-time, in-situ image sequences (right) of evolving microstructures



Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

3. individual growth kinetics

$$\dot{R}(R,t) = \frac{dR}{dt} = \langle \dot{R} \rangle \cdot G(x)$$

Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

3. individual growth kinetics

$$\dot{R}(R,t) = \frac{dR}{dt} = \langle \dot{R} \rangle \cdot G(x)$$

$$R(z, x_i) = \langle R \rangle \cdot z \cdot \sqrt{\tau(z, x_i) + 1}$$

$$t(z, x_i) = \frac{\langle R \rangle^2}{2\gamma} \tau(z, x_i)$$

$$\tau(z, x_i) = \left\{ (x_0 - x_i)^{2a/D} \exp\left(\frac{2ax_0}{D(x_0 - x_i)} \right) \right\} \cdot \left\{ (x_0 - z)^{-2a/D} \exp\left(-\frac{2ax_0}{D(x_0 - z)} \right) \right\} - 1$$

Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

3. individual growth kinetics

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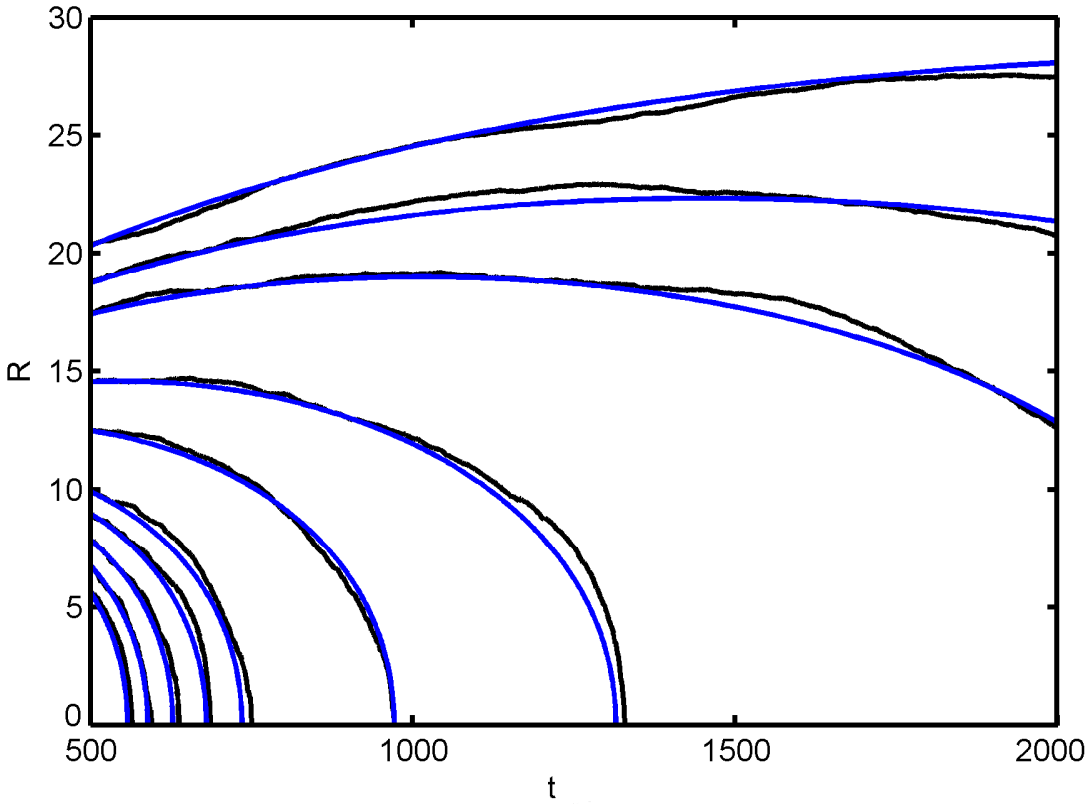

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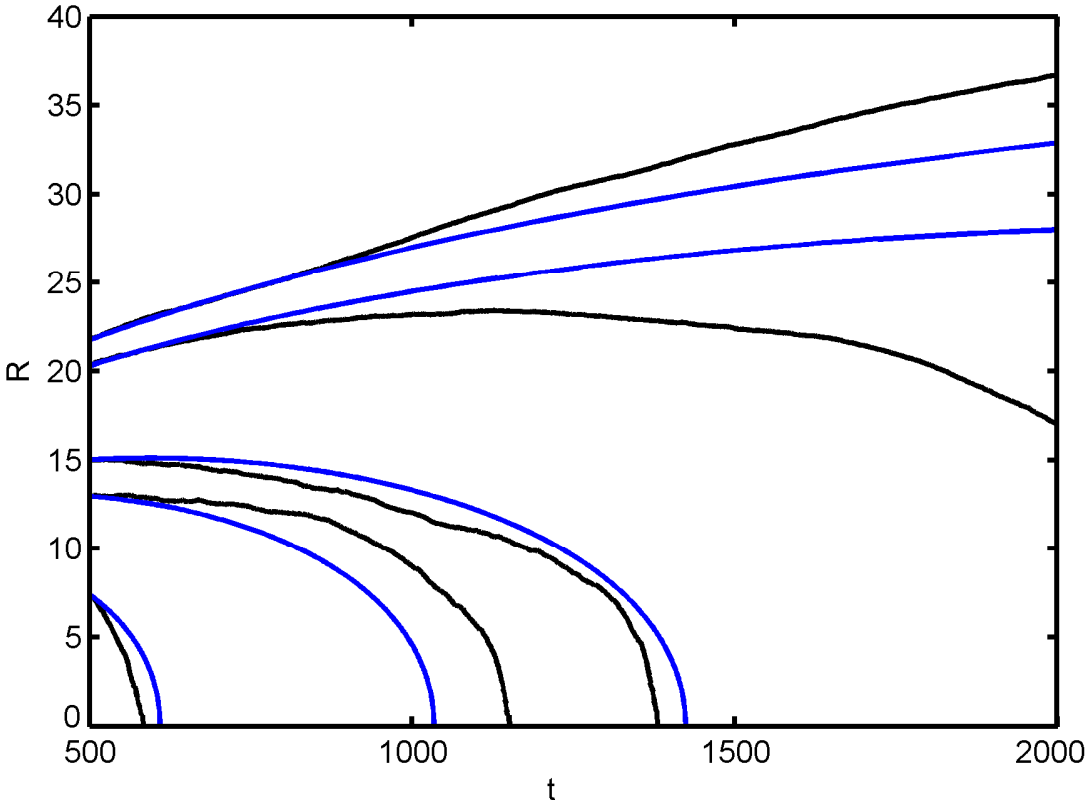

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Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

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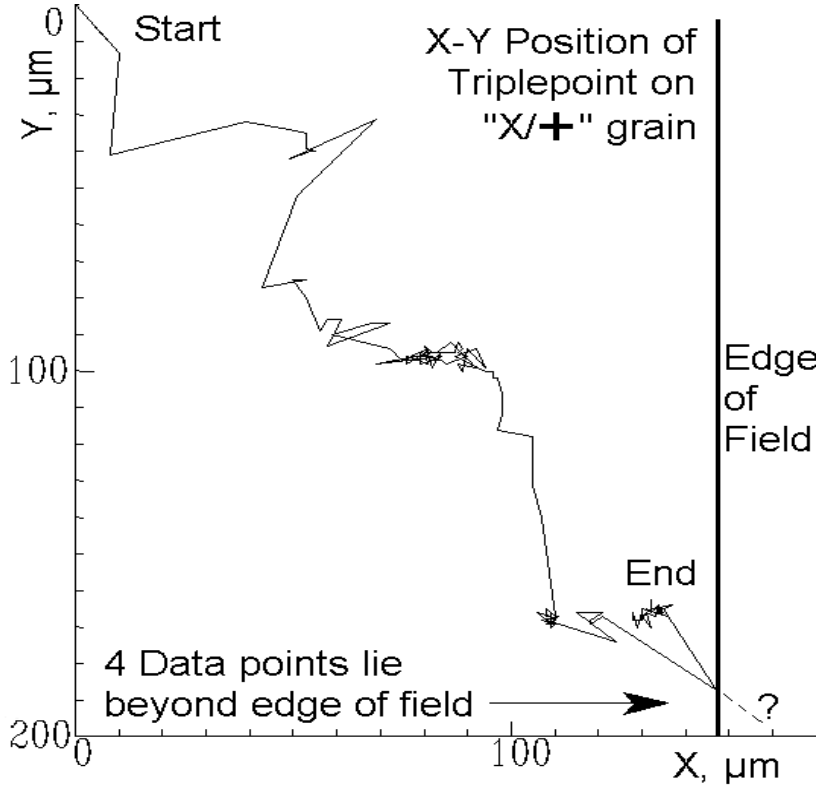
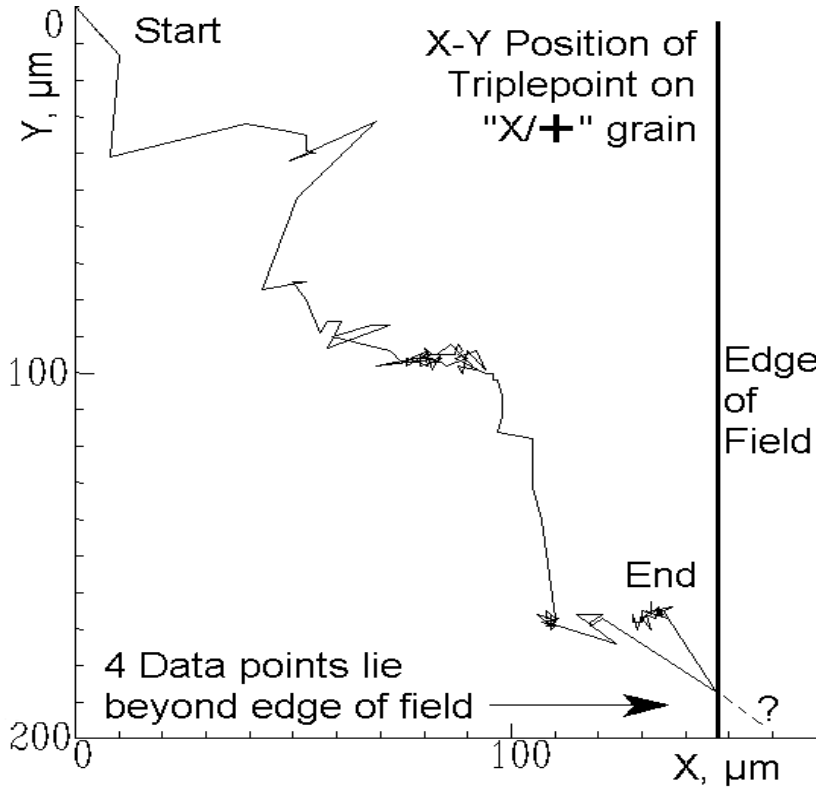


Track of triple point position at 10s intervals

Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

3. individual growth kinetics



Track of triple point position at 10s intervals

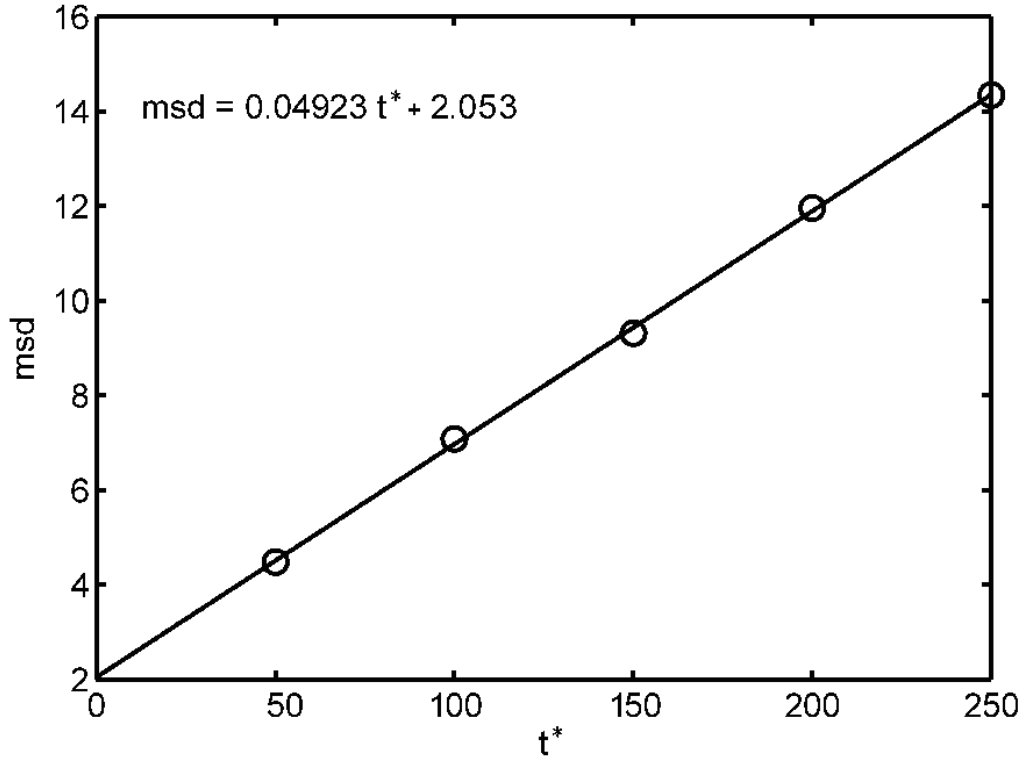
$$\widetilde{D} = \frac{msd}{6 \cdot t^*} = \frac{1}{3}\sum_{i=1}^{3} \frac{\langle \left(x_i - x_i\left(t^* = 0\right)\right)^2 \rangle}{2 \cdot t^*}$$

$$\langle R \rangle^{1/n} = \frac{6\widetilde{D}}{sd^2} \cdot t + \langle R \rangle_0^{1/n}$$

Standard Monte Carlo Potts Model

Simulation of grain boundary motion:

3. individual growth kinetics



- $\widetilde{D} = 0.0082$ MCU²/MCS
- sd = 0.429
  - it follows: b = 0.2672 MCU²/MCS
- average growth law: b = 0.2255 MCU²/MCS

A Potts Model for Nanocrystalline Grain Growth

A Potts Model for Nanocrystalline Grain Growth

What is different?

experiments on nanocrystalline materials

- high values of hardness and yield/fracture strength
- linear or exponential growth kinetics in contradiction to parabolic normal grain growth

experiment, theory and molecular dynamics simulation

- triple lines and quadruple points have **finite mobilities** different from adjoining boundaries

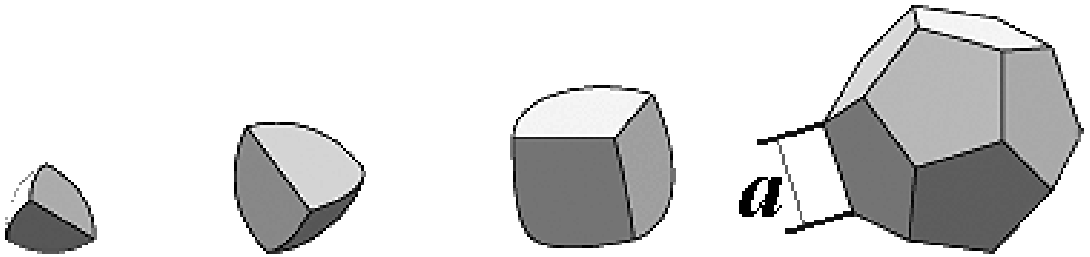
- failure of standard Potts model

A Potts Model for Nanocrystalline Grain Growth

theoretical predictions in nanocrystalline size range:

- principle expression

$$v = \frac{m_{gb}\gamma_{gb}K}{1 + \frac{m_{gb}}{am_{tl}} + \frac{m_{gb}}{a^2 m_{qp}}}$$



- from thermodynamic approach
  - → 1. normal grain growth
    2. triple line control
    3. quadruple point control

$$\langle R \rangle \sim \left\{ t^{1/2} \quad t \quad e^{t/\tau} \right\}$$

[G. Gottstein, L. Shvindlerman, Scripta Mater. 54 (2006) 1065]

[P. Streitenberger, D. Zöllner, Acta Mater. 59 (2011) 4235]

A Potts Model for Nanocrystalline Grain Growth

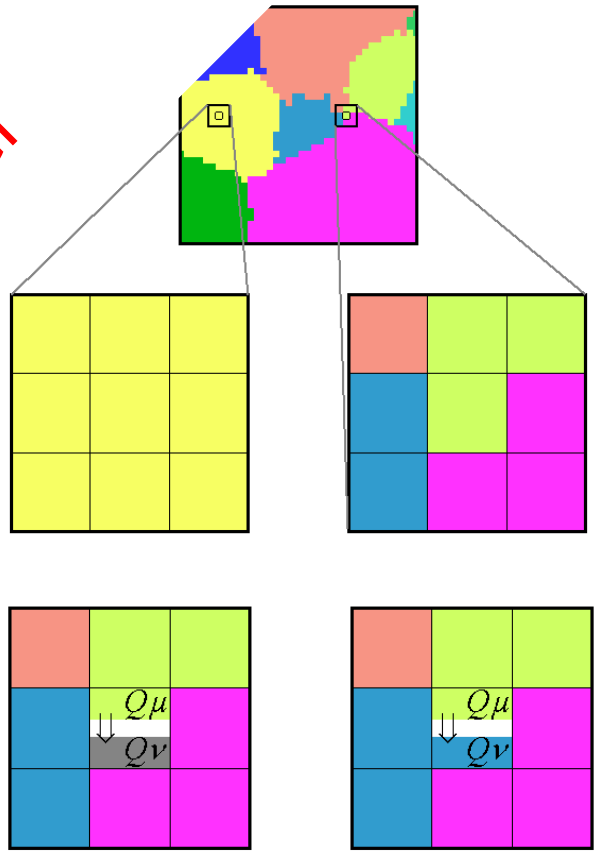
One Monte Carlo Step (MCS):

1. probabilistic selection of one MCU
2. selecting a new orientation Q_ν
3. $\Delta E = \gamma \cdot \sum_{j=1}^{nn} \left(\delta_{QjQ\nu} - \delta_{QjQ\mu} \right)$
4. selecting orientation wit

$$p = \begin{cases} m & \text{if } \Delta F \\ m \cdot \exp \dfrac{-\Delta E}{k_B T} & \text{if} \end{cases}$$

repeat N-times

standard Potts model



A Potts Model for Nanocrystalline Grain Growth

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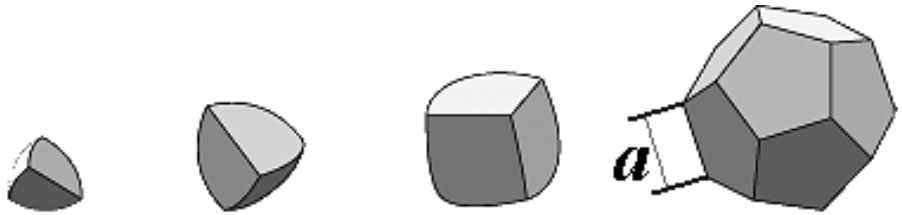
4. selecting orientation with

$$p = \begin{cases} m & \text{if } \Delta E \le 0 \\ m \cdot \exp \dfrac{-\Delta E}{k_B T} & \text{if } \Delta E > 0 \end{cases}$$



$$v = \frac{m_{gb} \gamma_{gb} K}{1 + \dfrac{m_{gb}}{a m_{tl}} + \dfrac{m_{gb}}{a^2 m_{qp}}}$$

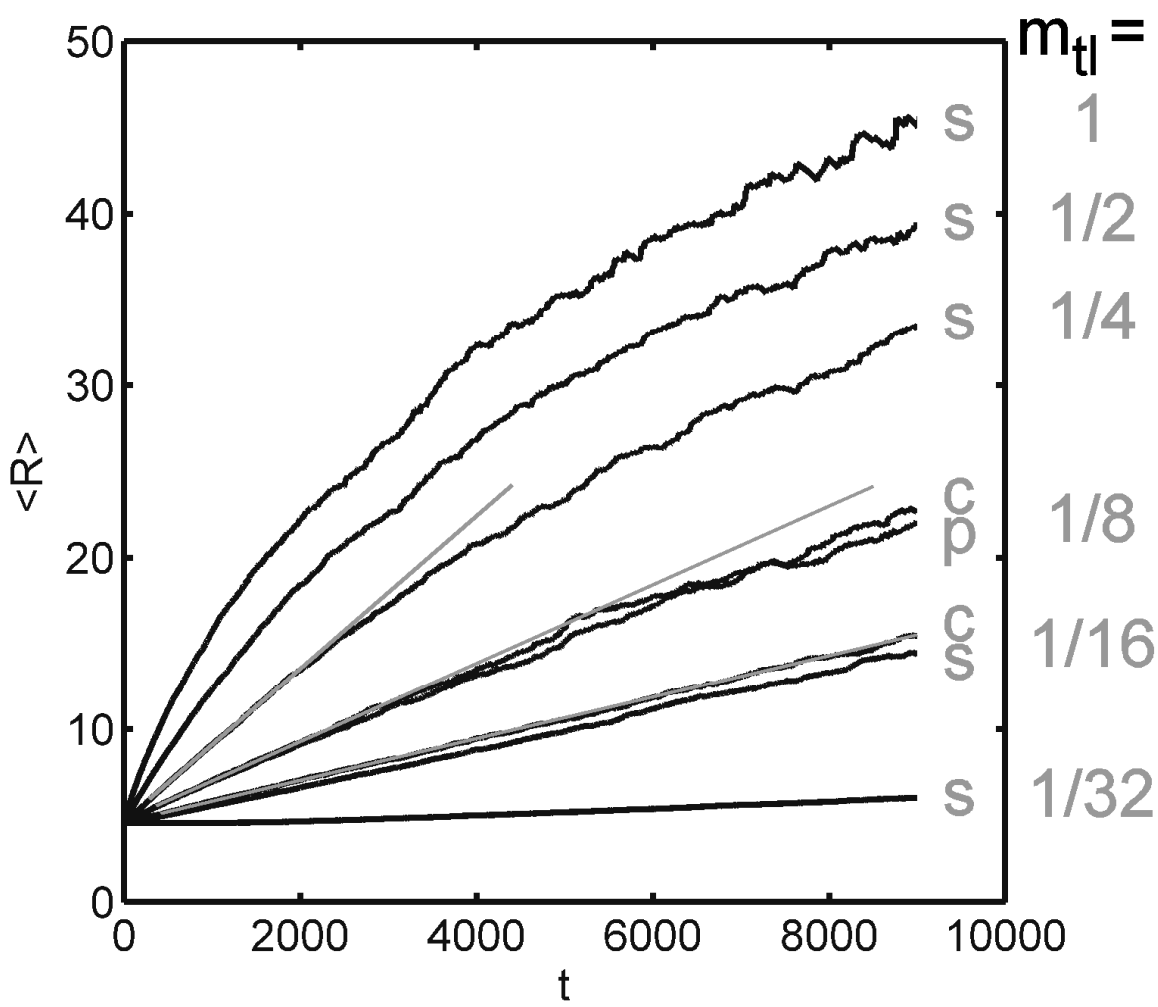
include separate mobilities for all grain features

repeat N-times

[D. Zöllner: Comput. Mater. Sci. 50 (2011) 2712]

A Potts Model for Nanocrystalline Grain Growth

triple junction control:



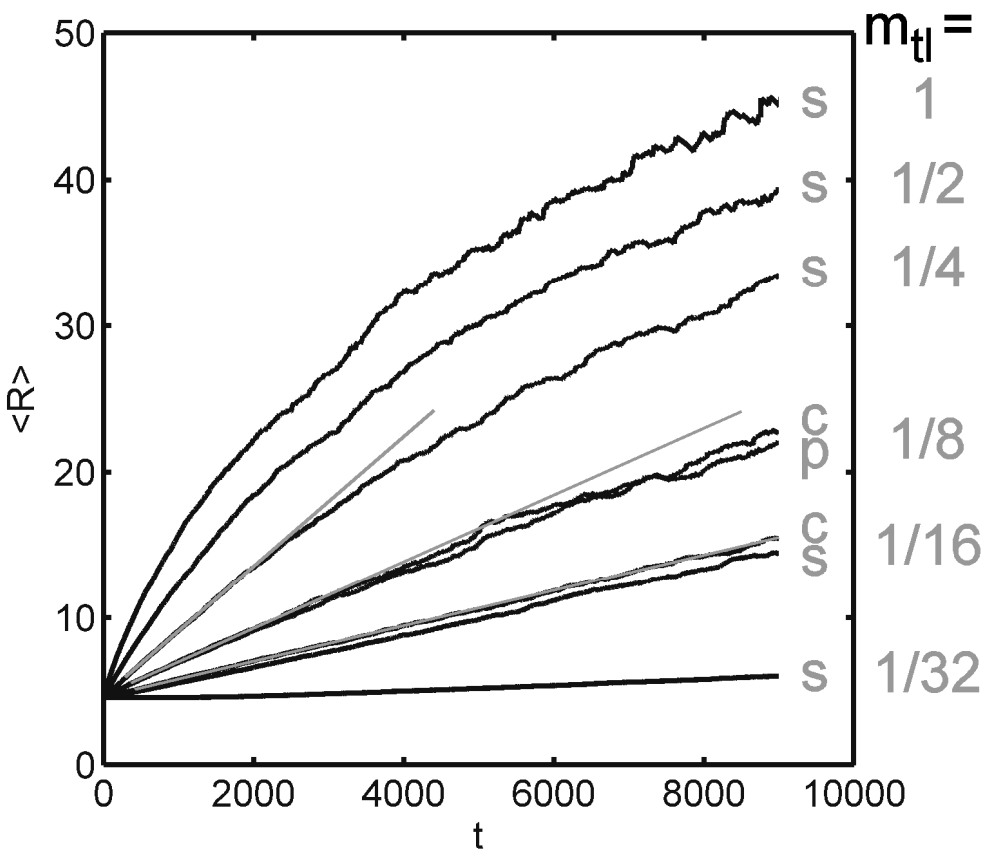
m_{gb} = 1 and m_{tl} = m_{qp} = {1, 1/2, 1/4, 1/8, 1/16}

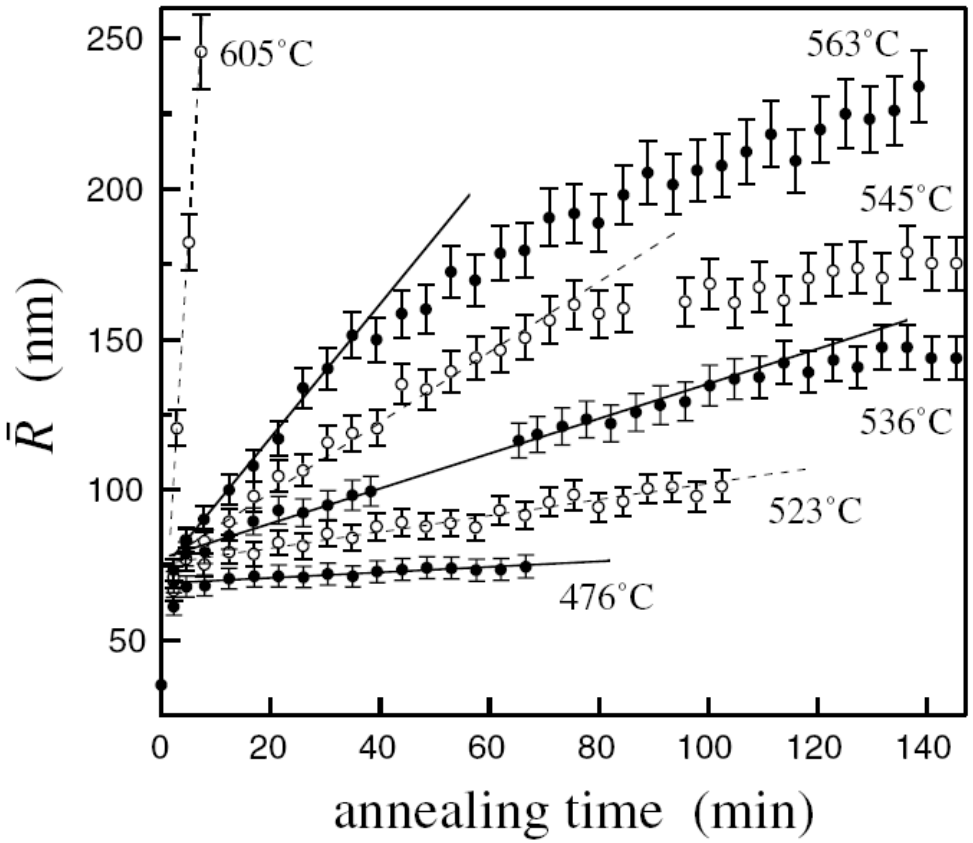
$$\langle R \rangle \sim \left(t^{1/2} \boxed{t} e^{t/\tau} \right)$$

- kinetics changes from parabolic to linear
- kinetics does not depend on the simulation type

A Potts Model for Nanocrystalline Grain Growth

triple junction control:

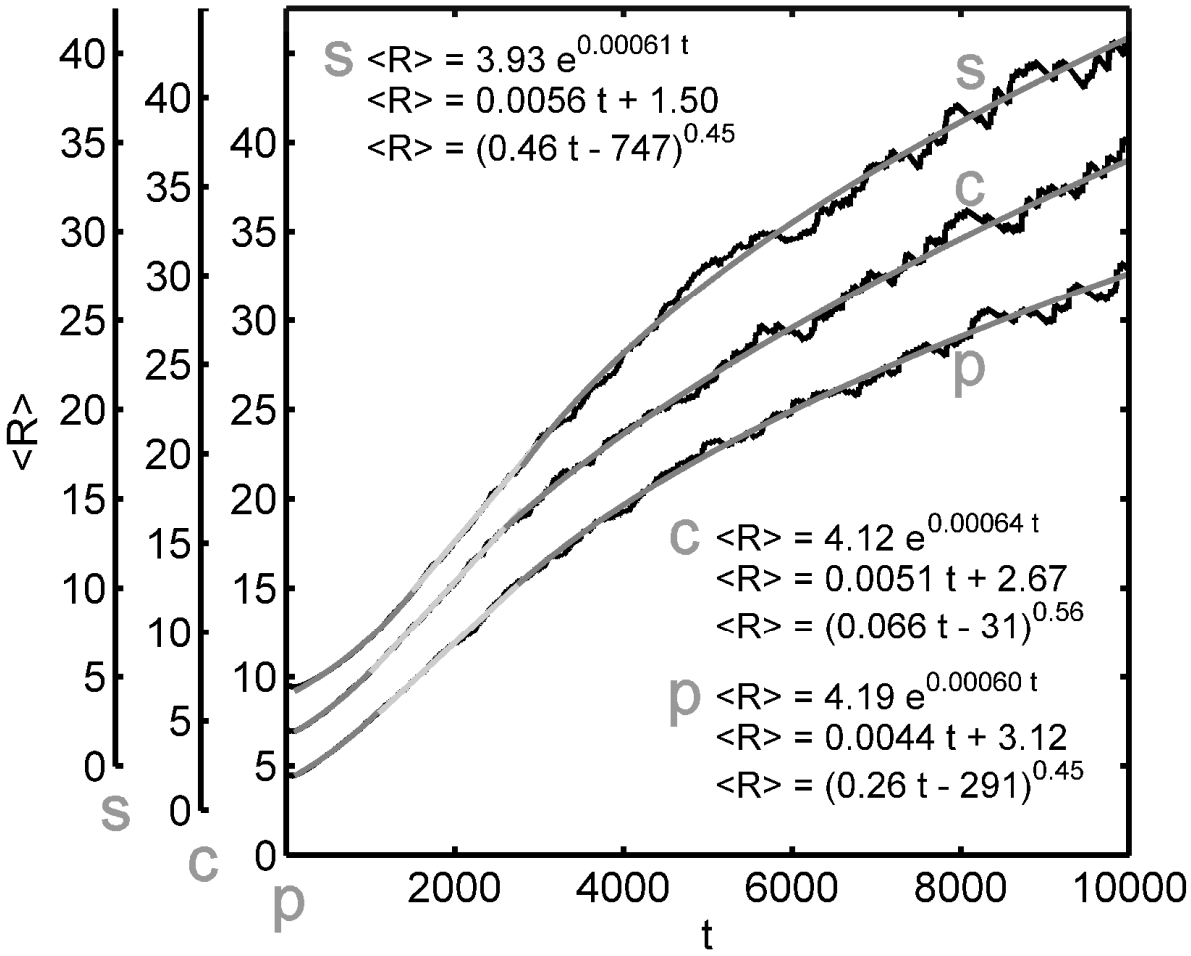




[C.E. Krill III, L. Helfen, D. Michels, H. Natter, A. Fitch, O. Masson, R. Birringer: Phys. Rev. Lett. 86 (2001) 842]

A Potts Model for Nanocrystalline Grain Growth

quadruple junction control:



$m_{gb} = m_{tl} = 1$ and

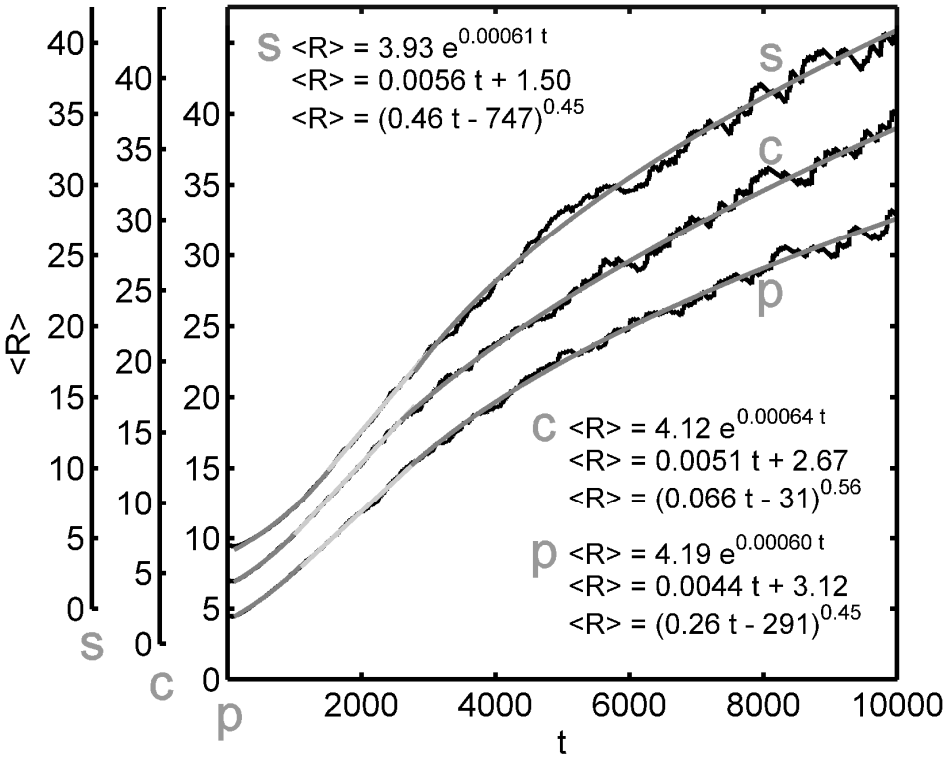
$m_{qp} < 1$

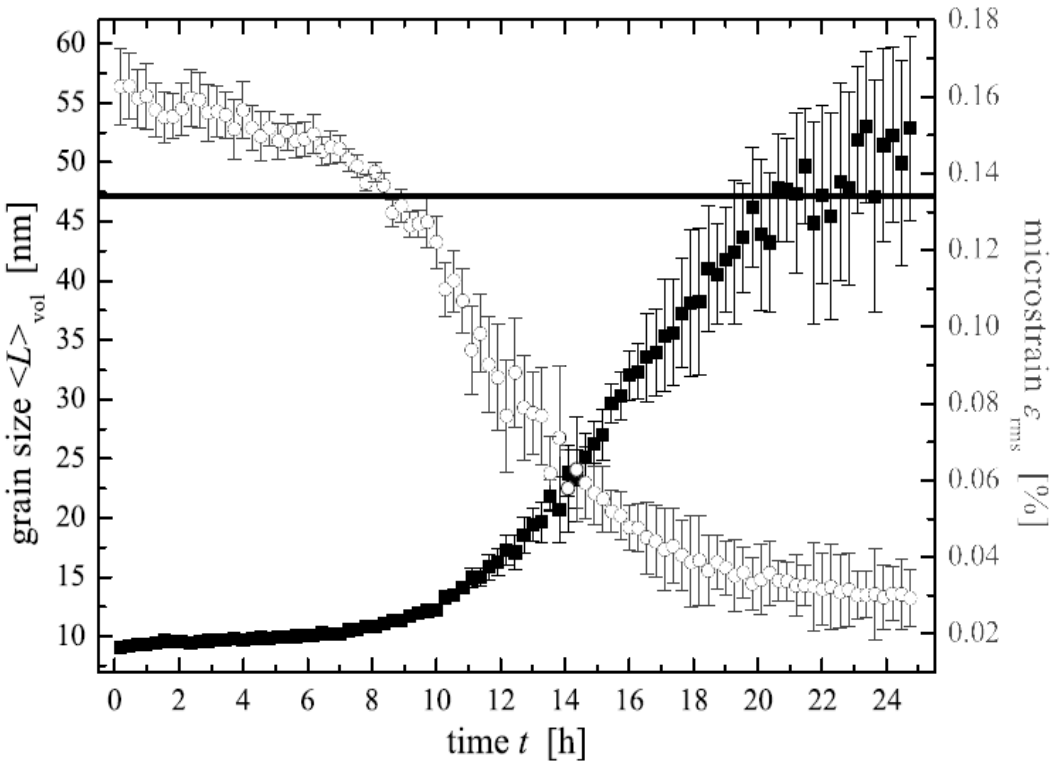
$$\langle R \rangle \sim \left(t^{1/2} \quad t \quad e^{t/\tau} \right)$$

- exponential growth behavior for early annealing times
- long-time annealing → linear & parabolic

A Potts Model for Nanocrystalline Grain Growth

quadruple junction control:

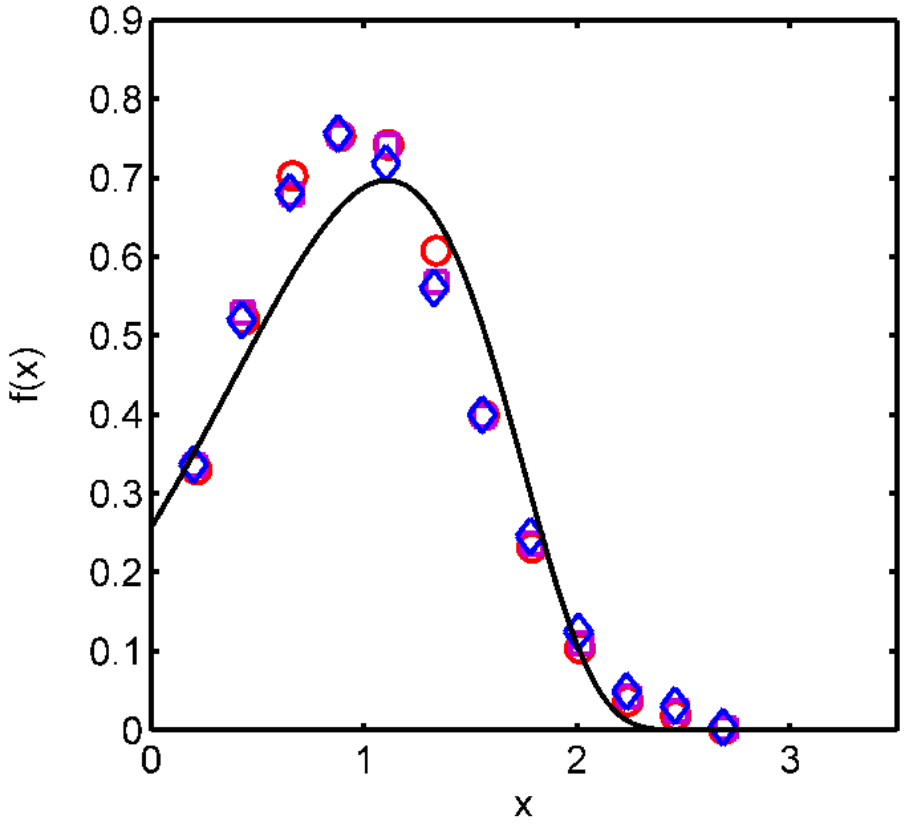


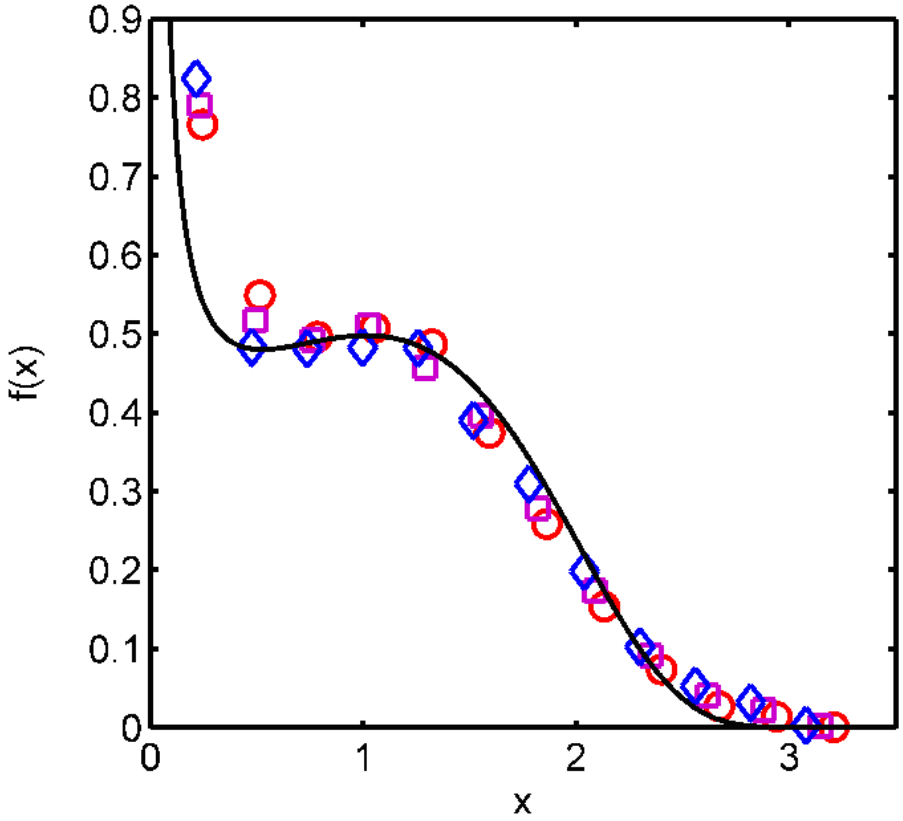


[M. Ames, J. Markmann, R. Karos, A. Michels, A. Tschöpe, R. Birringer: Acta Mater. 56 (2008), p. 4255]

A Potts Model for Nanocrystalline Grain Growth

triple line control vs. quadruple point control:





[P. Streitenberger, D. Zöllner, Acta Mater. 59 (2011) 4235]

Going back to 2D Grain Growth

Going back to 2D Grain Growth

What for?

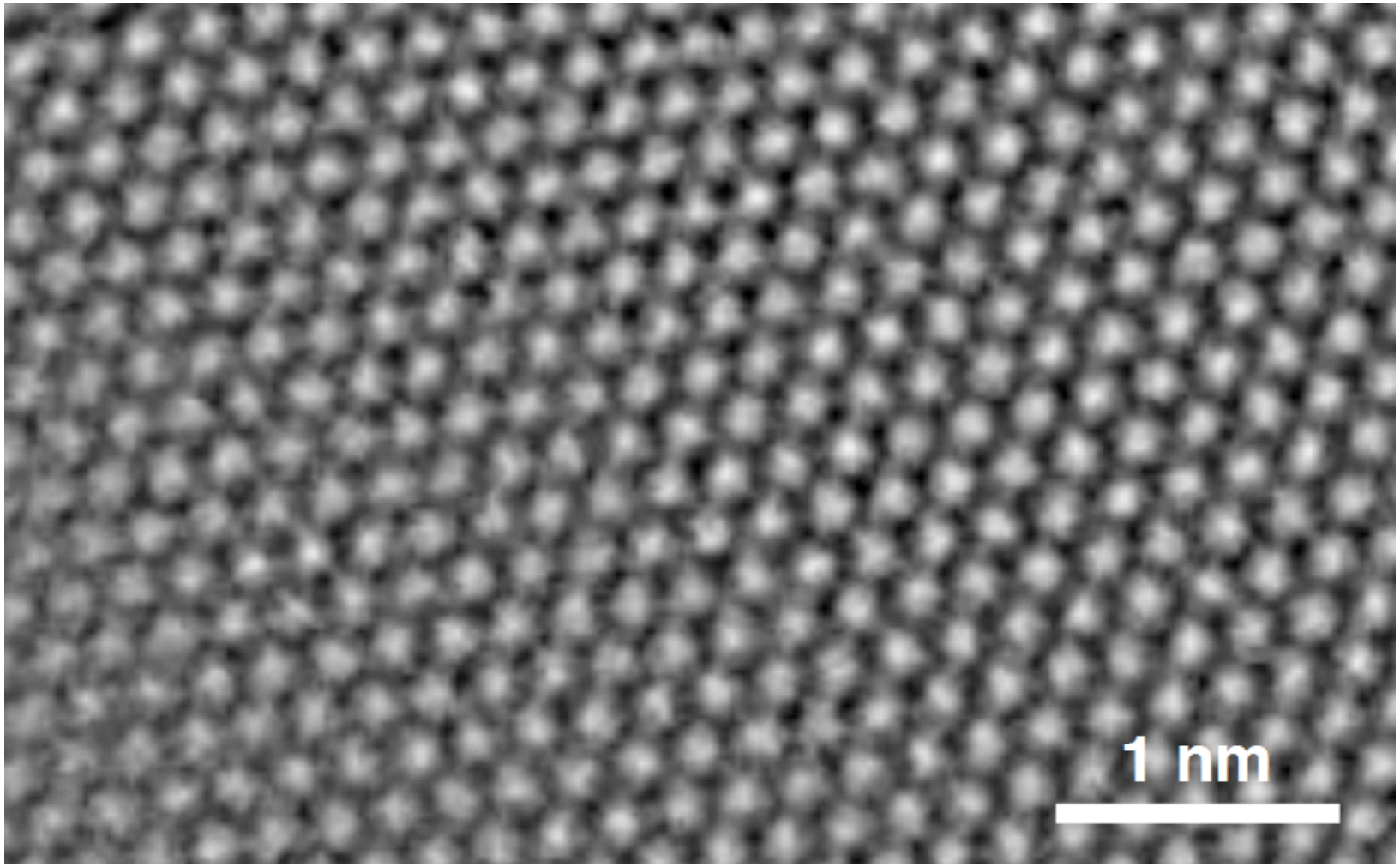
1. Independent of all the new knowledge that has been gained on grain boundary migration and grain growth in the end the motion of grain boundaries is still a complex 3D problem.

2. The dynamics of the individual atoms at the grain boundaries can not be captured (neither temporally nor spatially) by current experimental characterization techniques.

Going back to 2D Grain Growth

Where?

- solution: graphene

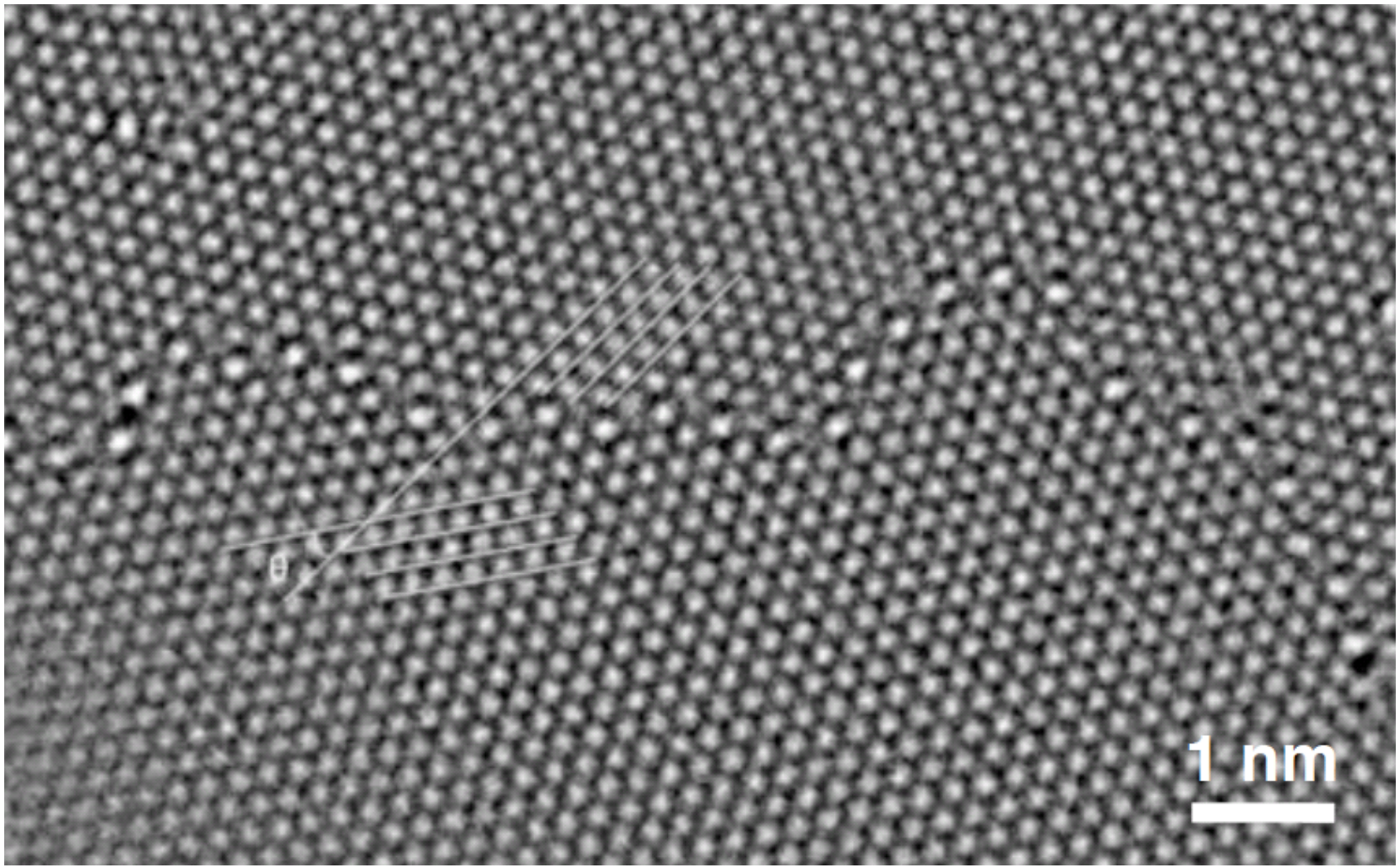


[Kurasch, Kotakoski, Lehtinen, Skákalová, Smet, Krill, Krasheninnikov, Kaiser: Nano Letters 12 (2012) 3168]

Going back to 2D Grain Growth

Where?

- solution: polycrystalline graphene



Going back to 2D Grain Growth

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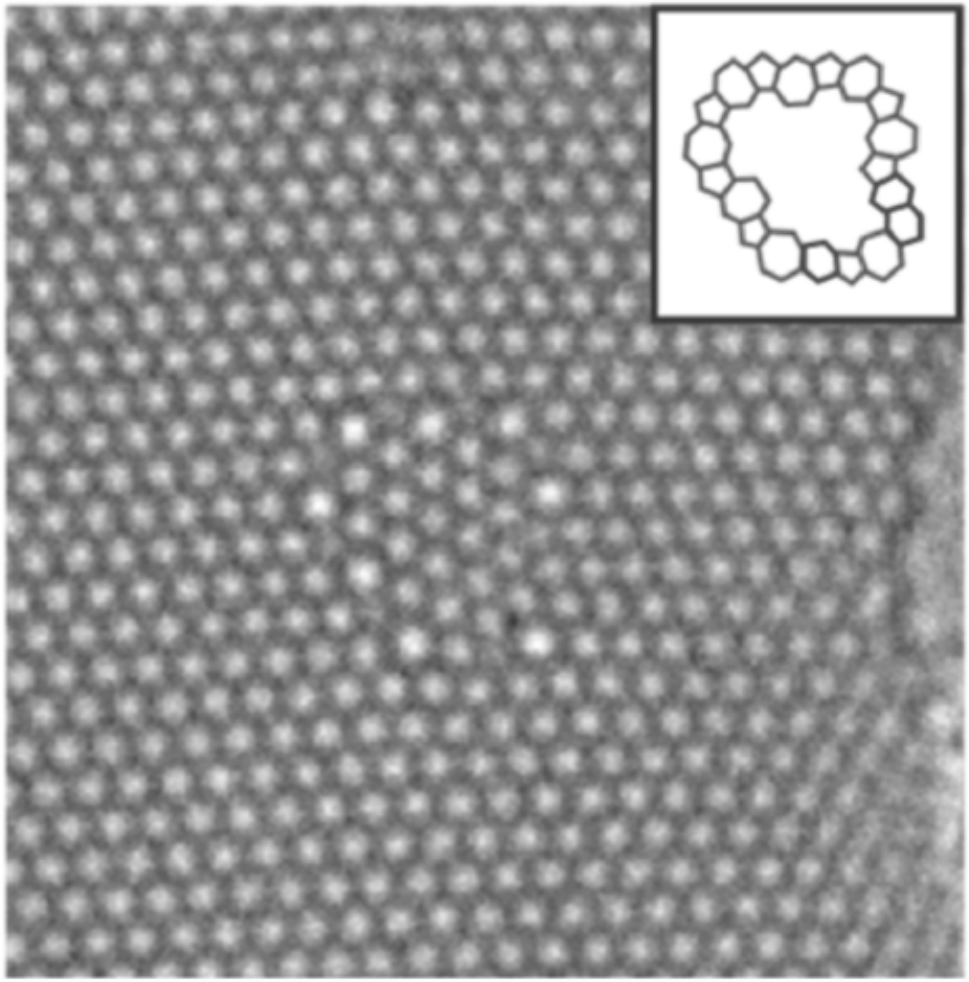
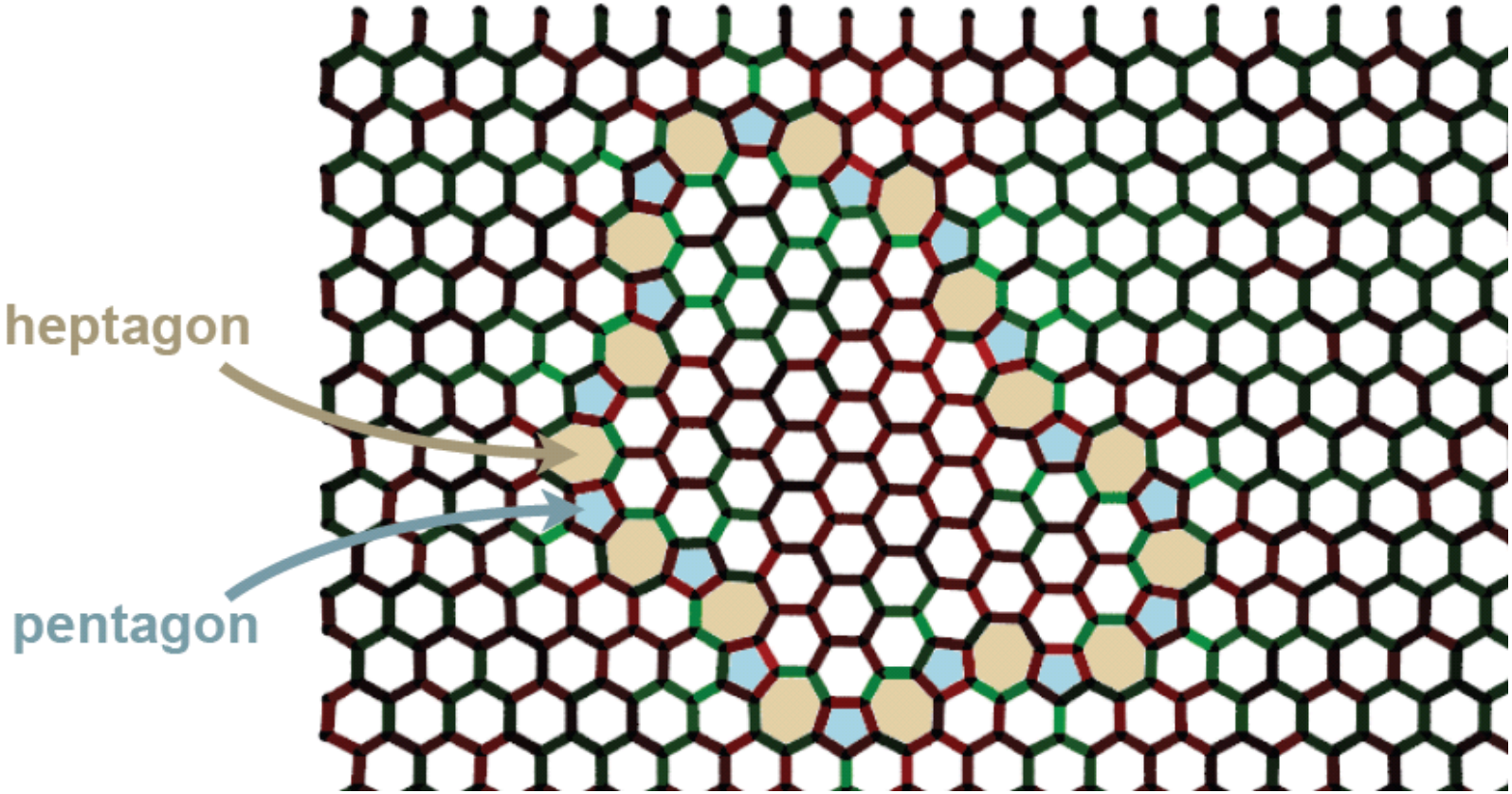


Going back to 2D Grain Growth

How?

- irradiation with 80 keV electrons



[J. Kotakoski, A.V. Krasheninnikov, U. Kaiser, J. C. Meyer: Phys. Rev. Lett. 106 (2011) 105505]

Going back to 2D Grain Growth

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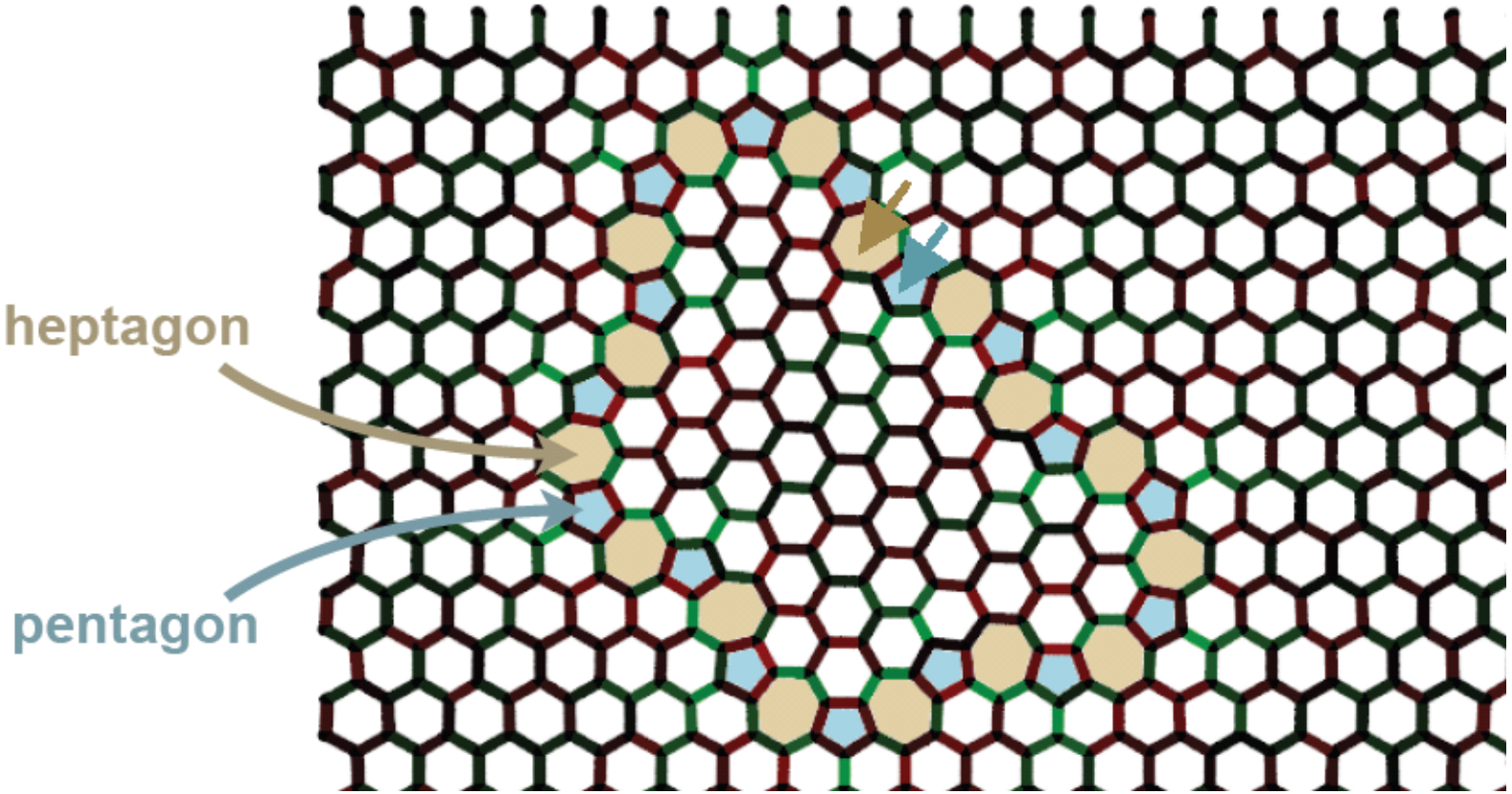

Going back to 2D Grain Growth

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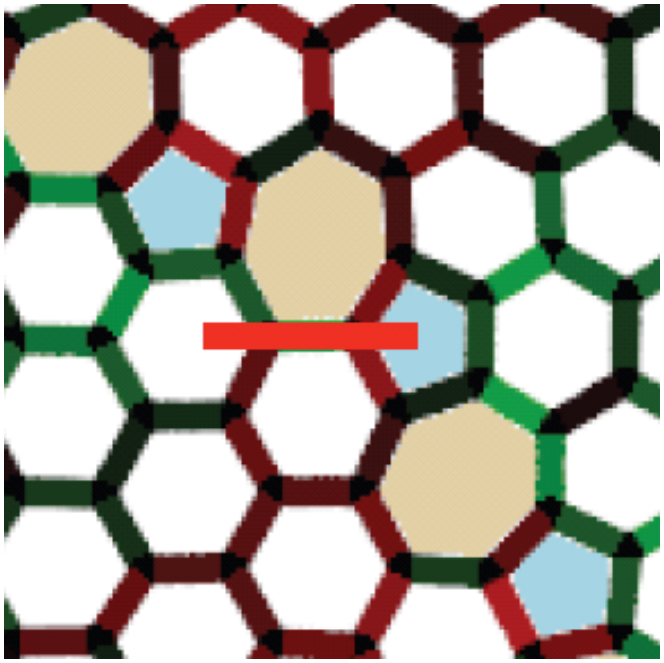
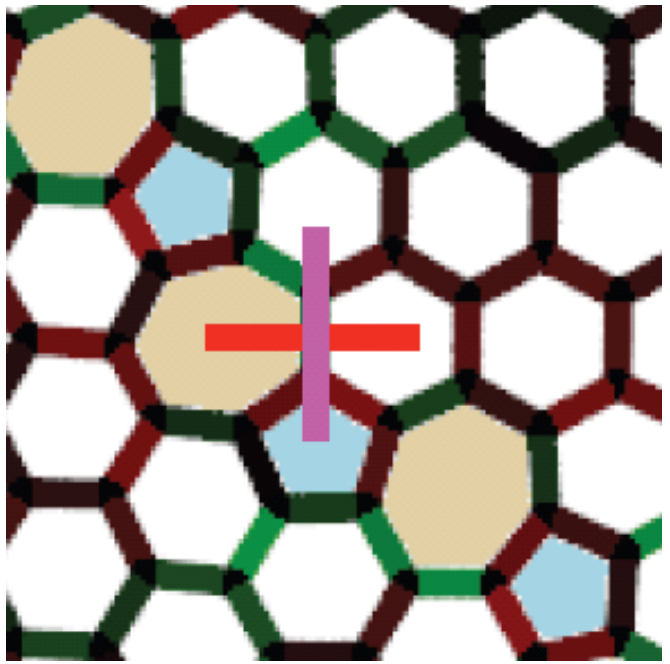
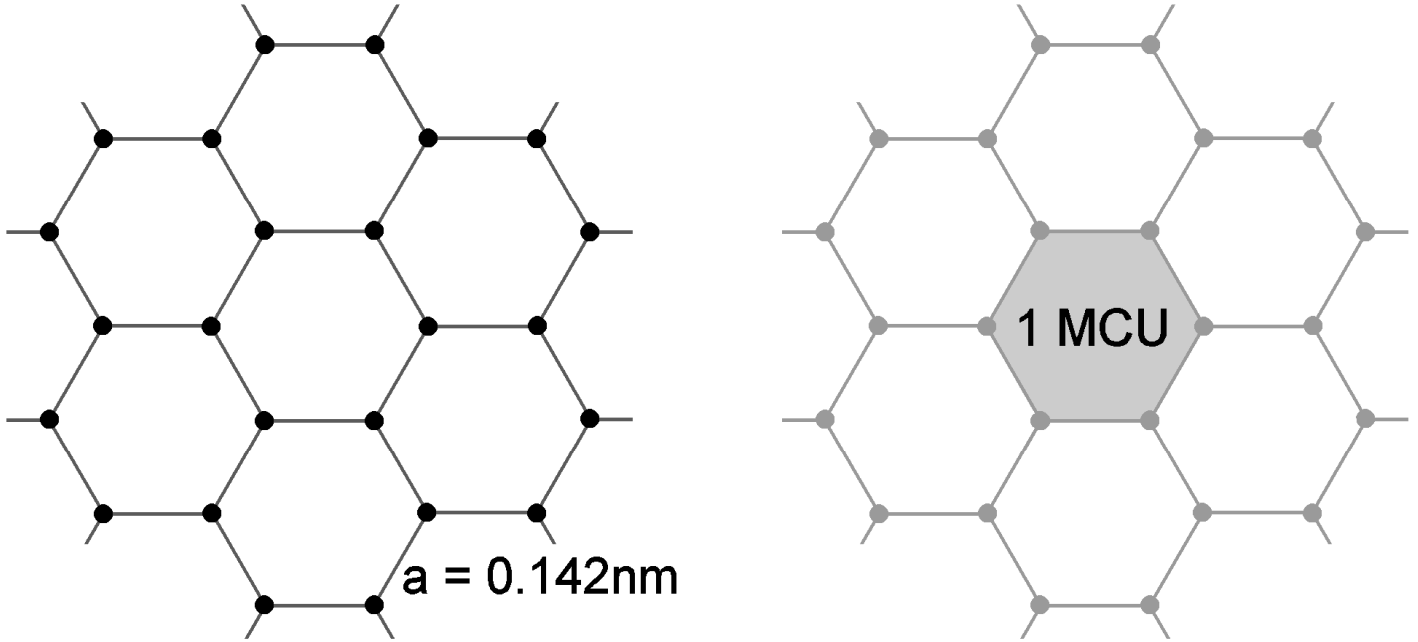




Going back to 2D Grain Growth

2D Potts model simulation:

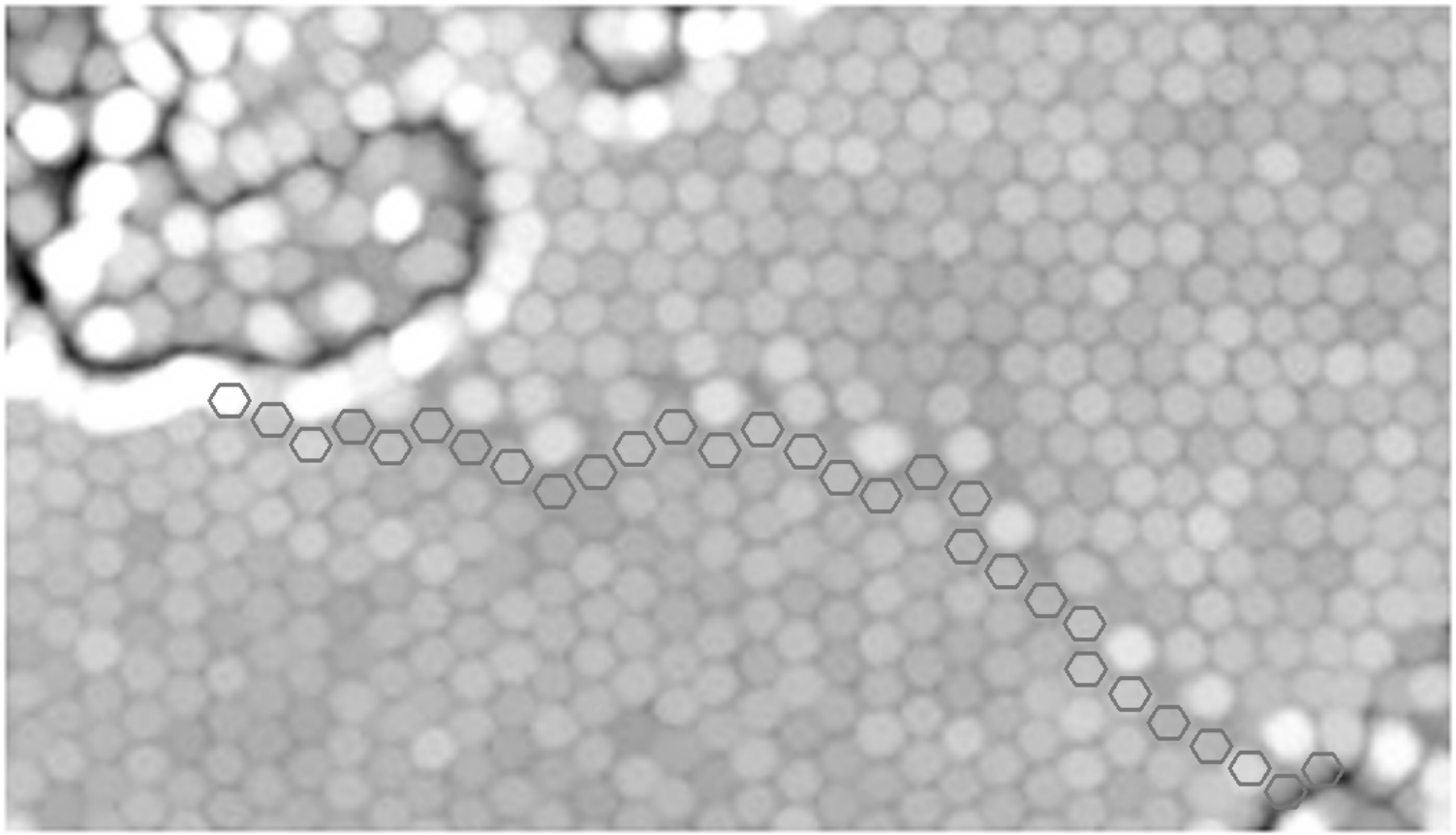


a b

- one problem:
  - experiment: two grains = two lattice orientations
  - simulation: two grains = one underlying lattice

Going back to 2D Grain Growth

2D Potts model simulation: grain boundary migration



[S. Kurasch, J. Kotakoski, O. Lehtinen, V. Skákalová, J. Smet, C.E. Krill III, A.V. Krasheninnikov, U. Kaiser: Nano Letters 12 (2012) 3168]

Going back to 2D Grain Growth

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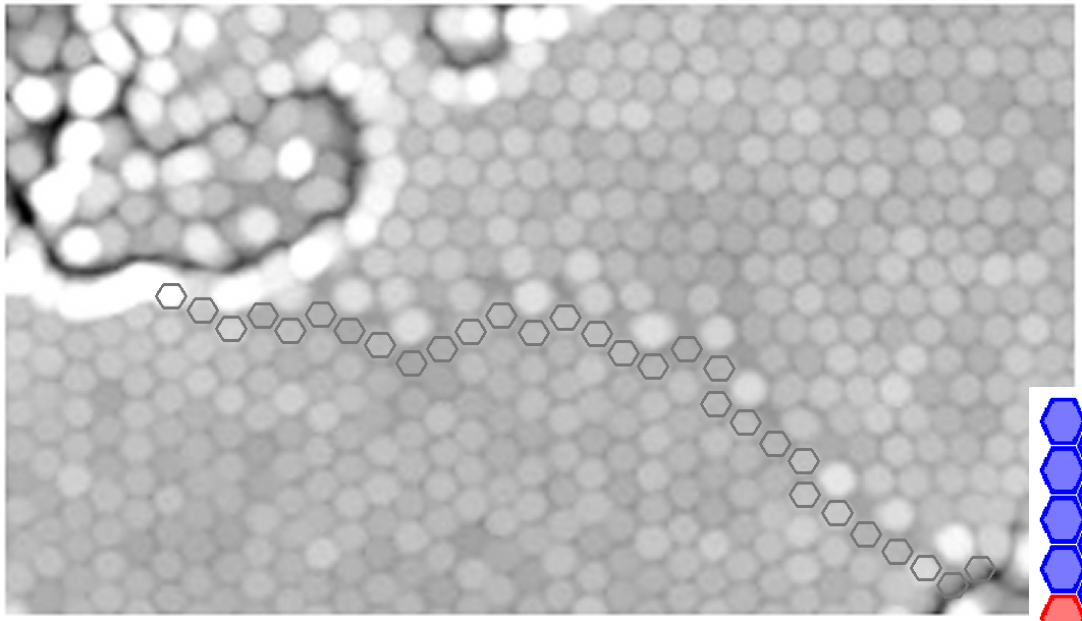
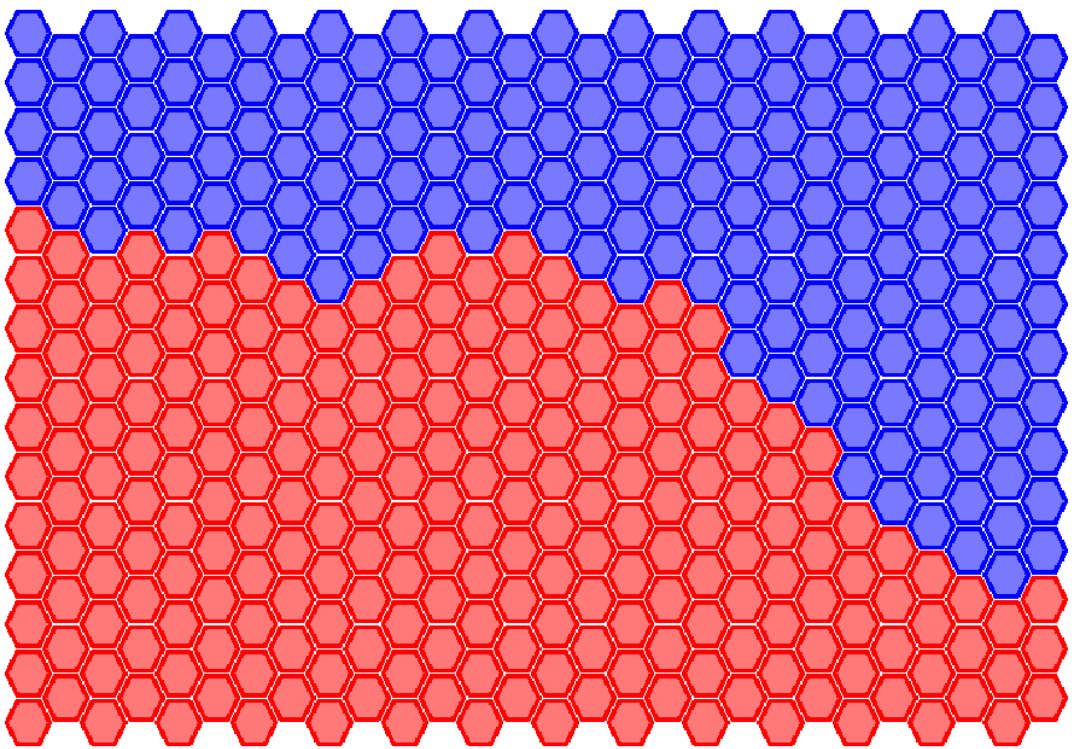
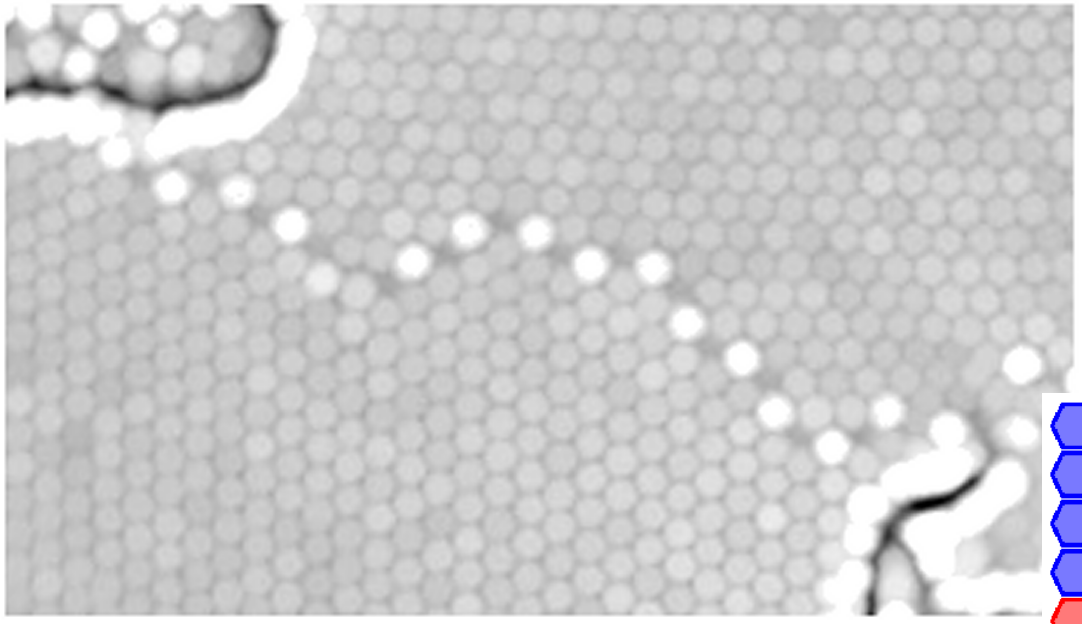


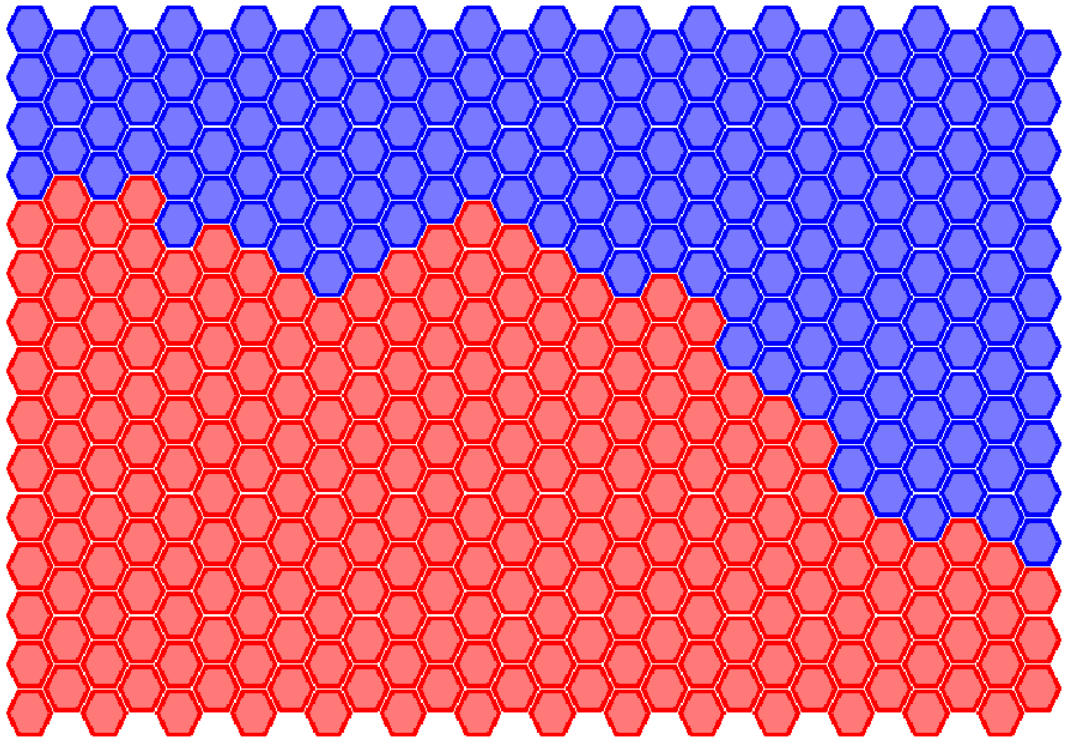


t = 0.0 min

Going back to 2D Grain Growth

2D Potts model simulation:

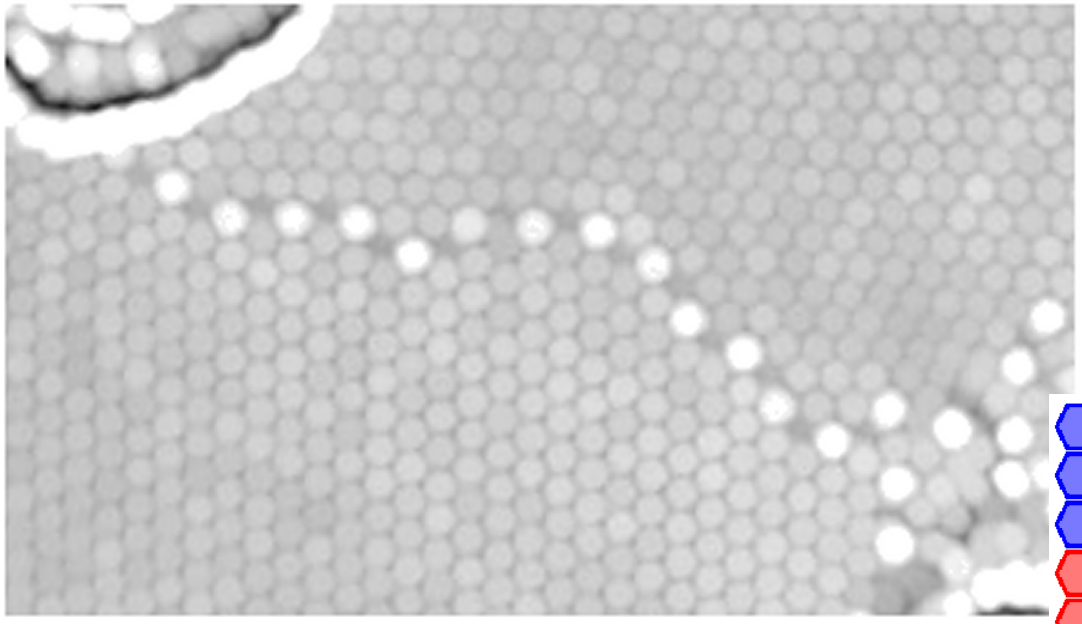


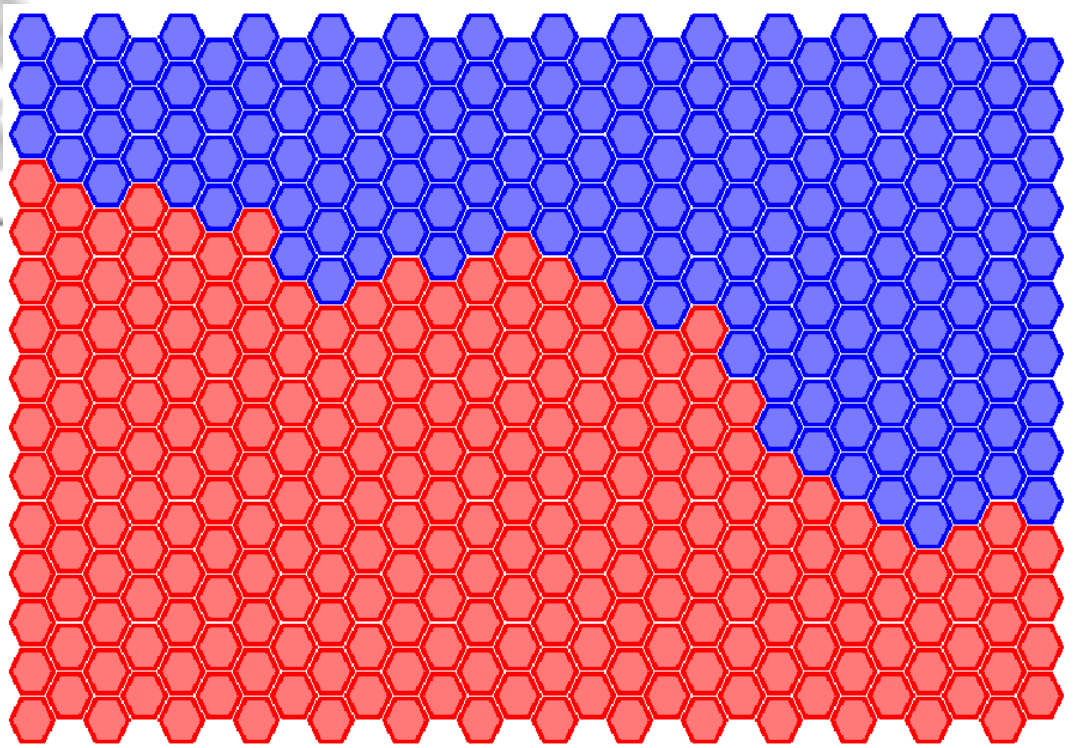


t = 2.5 min

Going back to 2D Grain Growth

2D Potts model simulation:

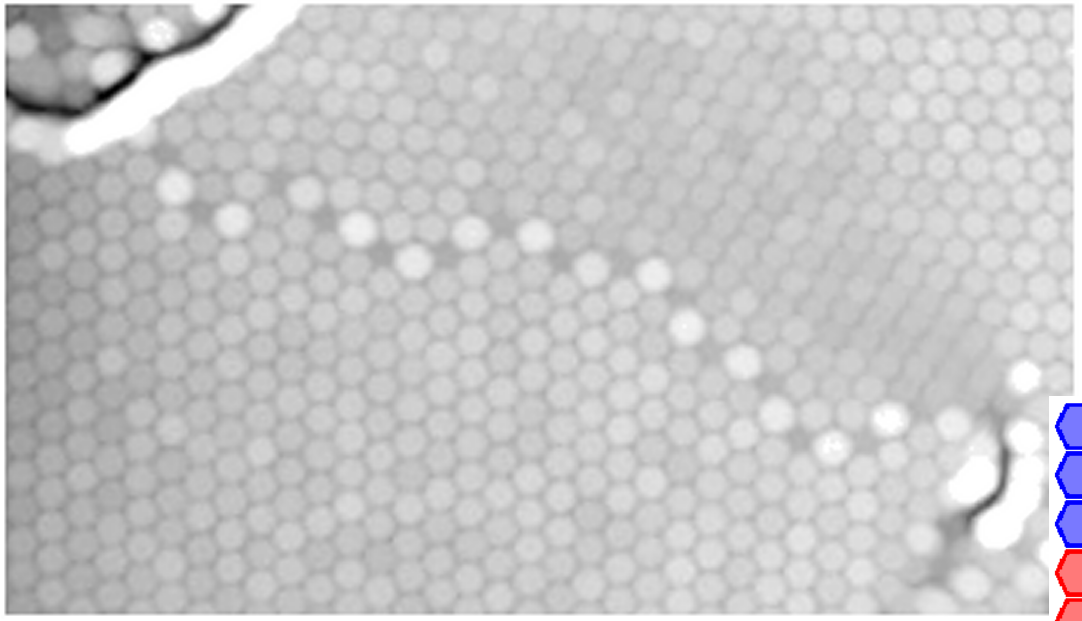


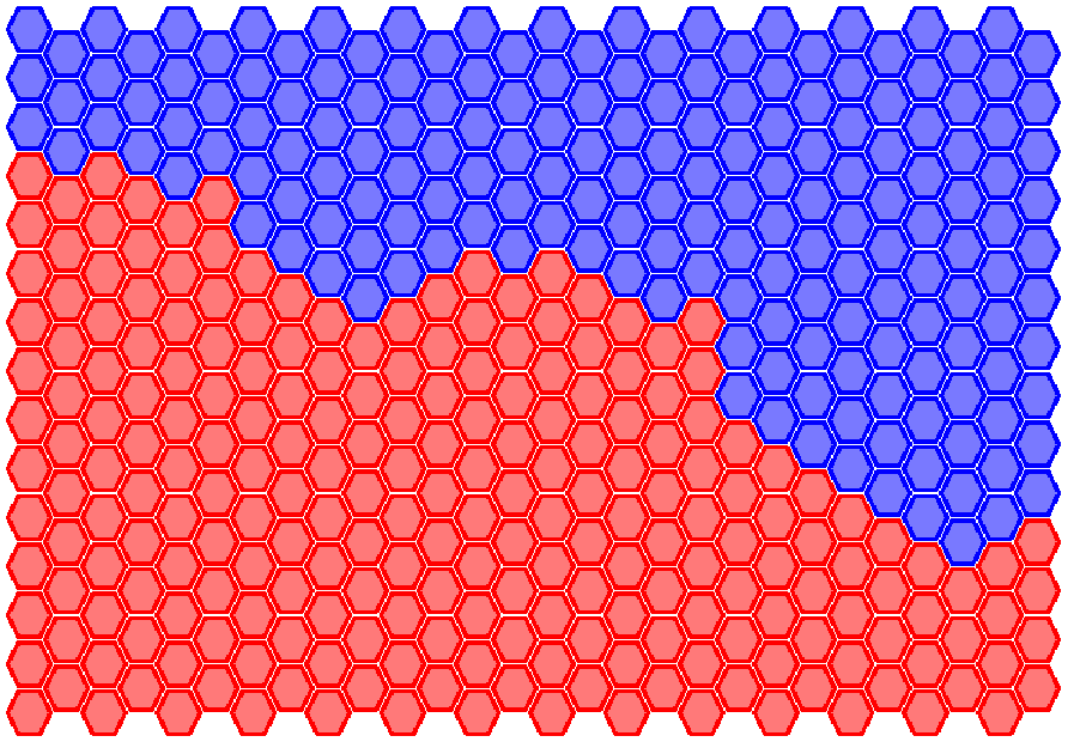


t = 5.0 min

Going back to 2D Grain Growth

2D Potts model simulation:

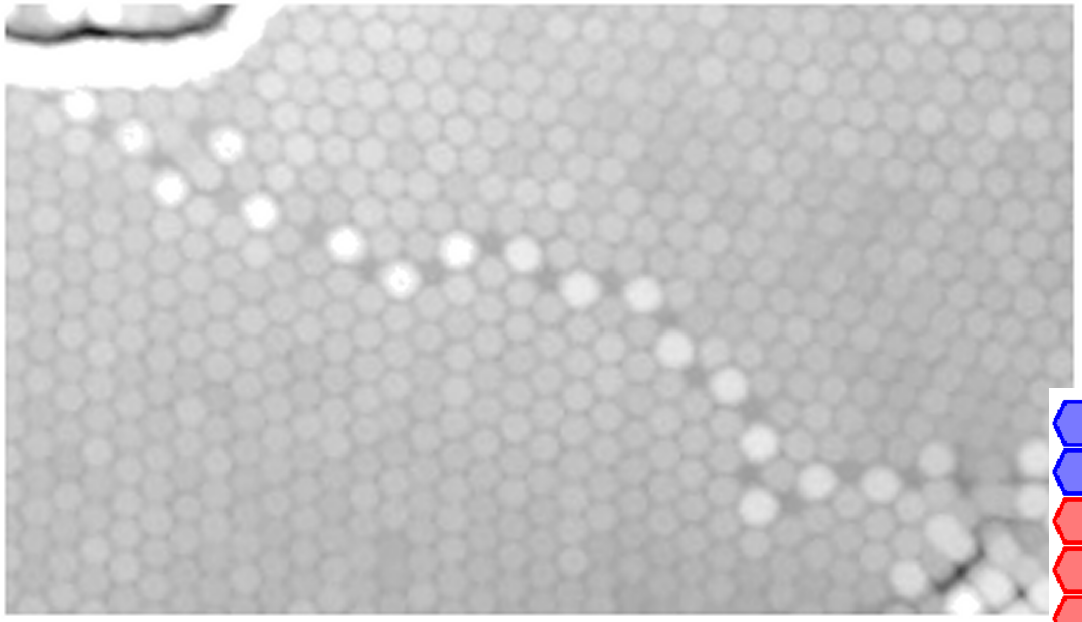


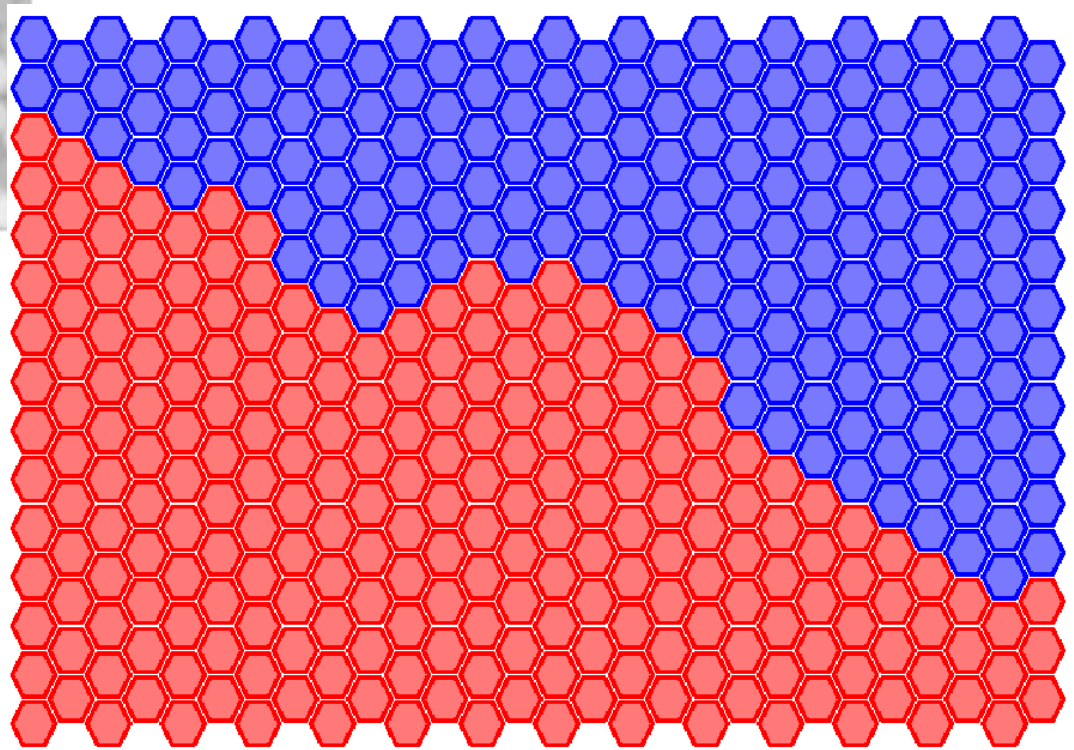


t = 7.5 min

Going back to 2D Grain Growth

2D Potts model simulation:

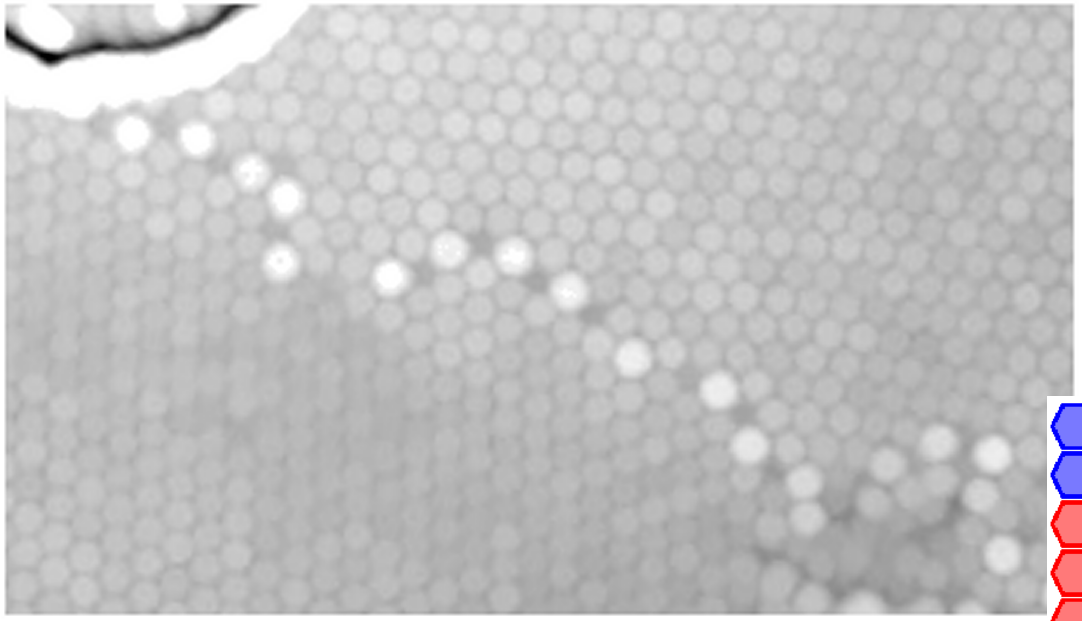




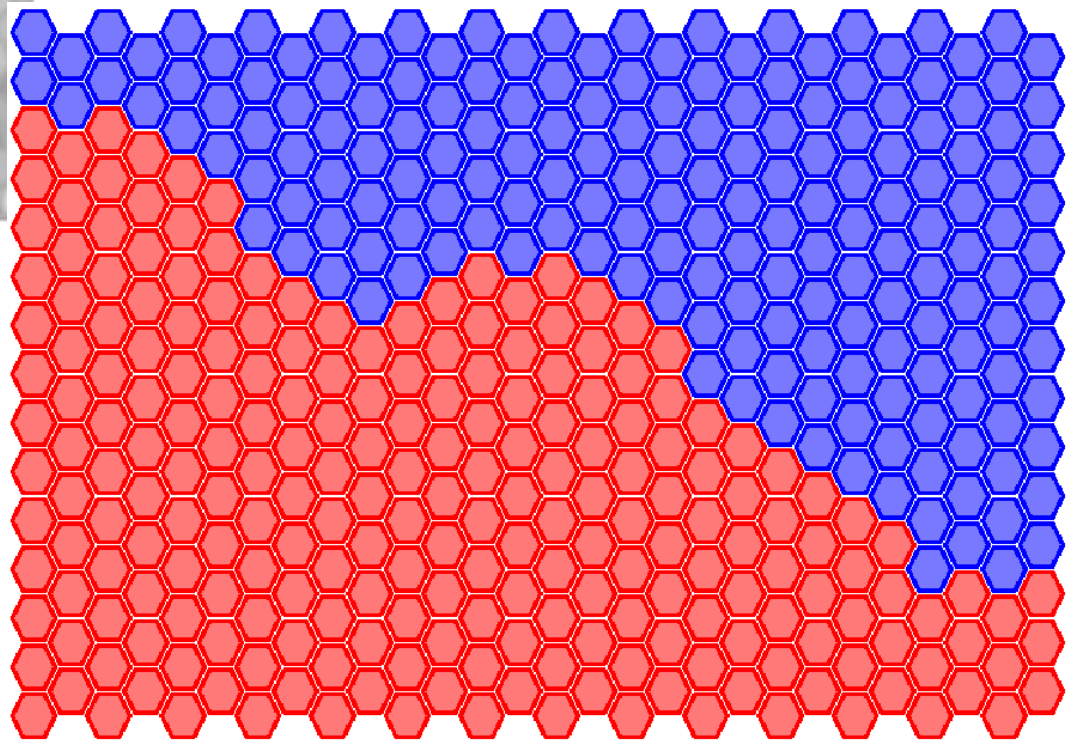
t = 10.0 min

Going back to 2D Grain Growth

2D Potts model simulation:

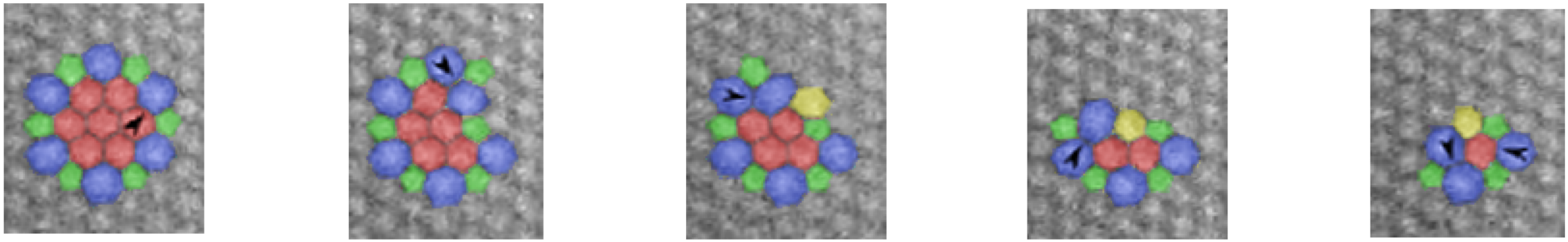


t = 12.5 min



Going back to 2D Grain Growth

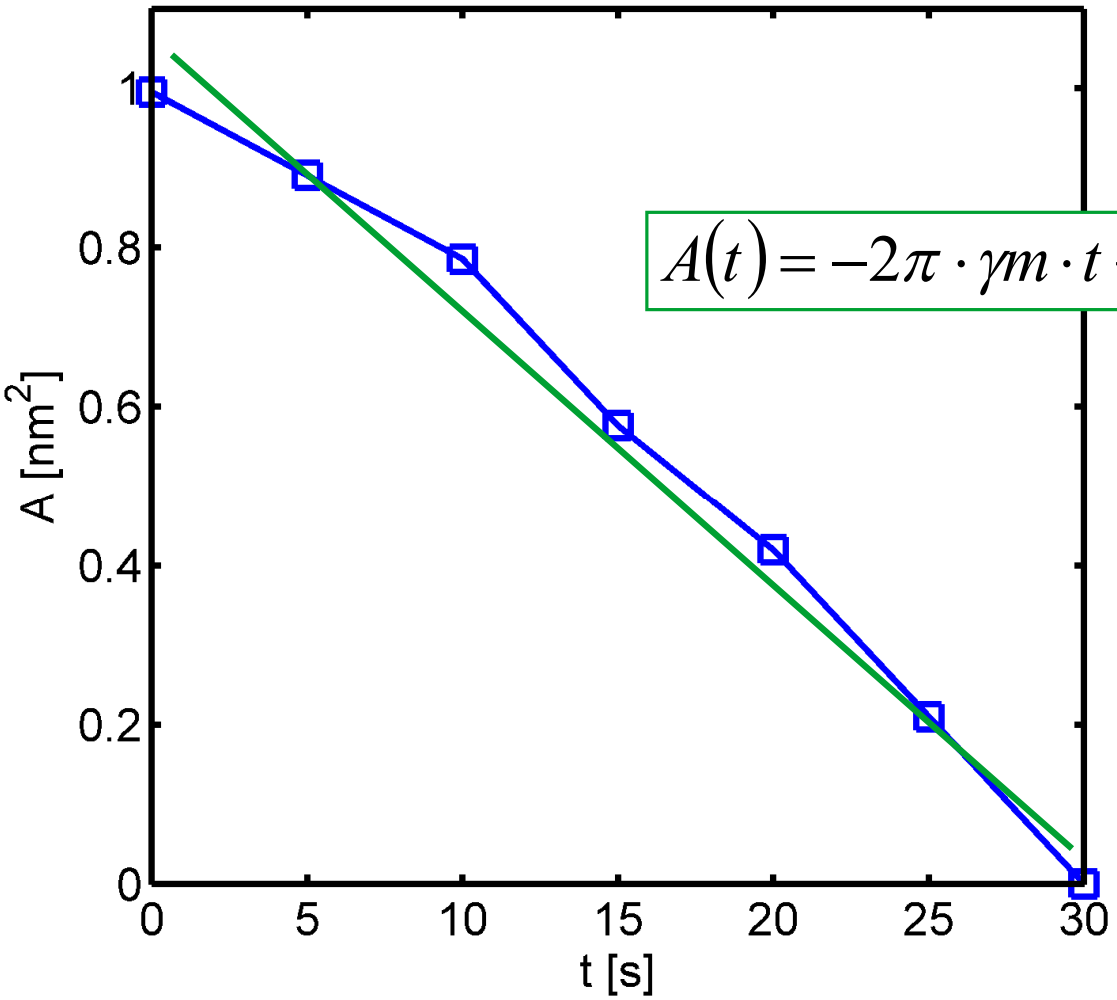
2D Potts model simulation: flower defect



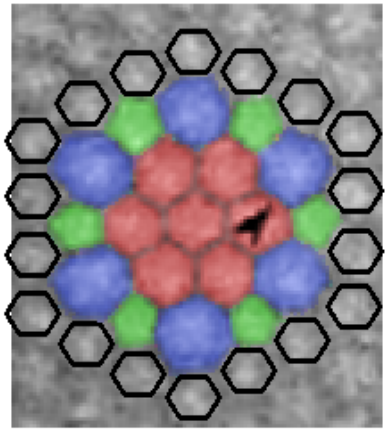
[S. Kurasch, J. Kotakoski, O. Lehtinen, V. Skákalová, J. Smet, C.E. Krill III, A.V. Krasheninnikov, U. Kaiser: Nano Letters 12 (2012) 3168]

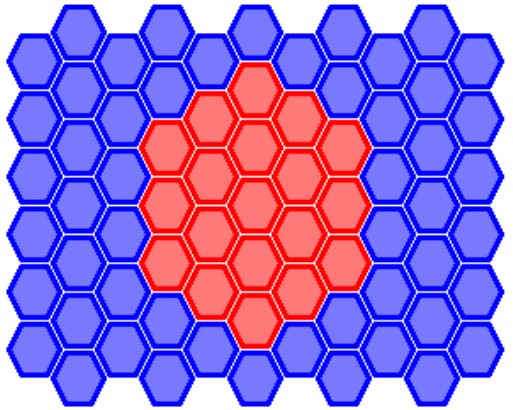
Going back to 2D Grain Growth

2D Potts model simulation: flower defect



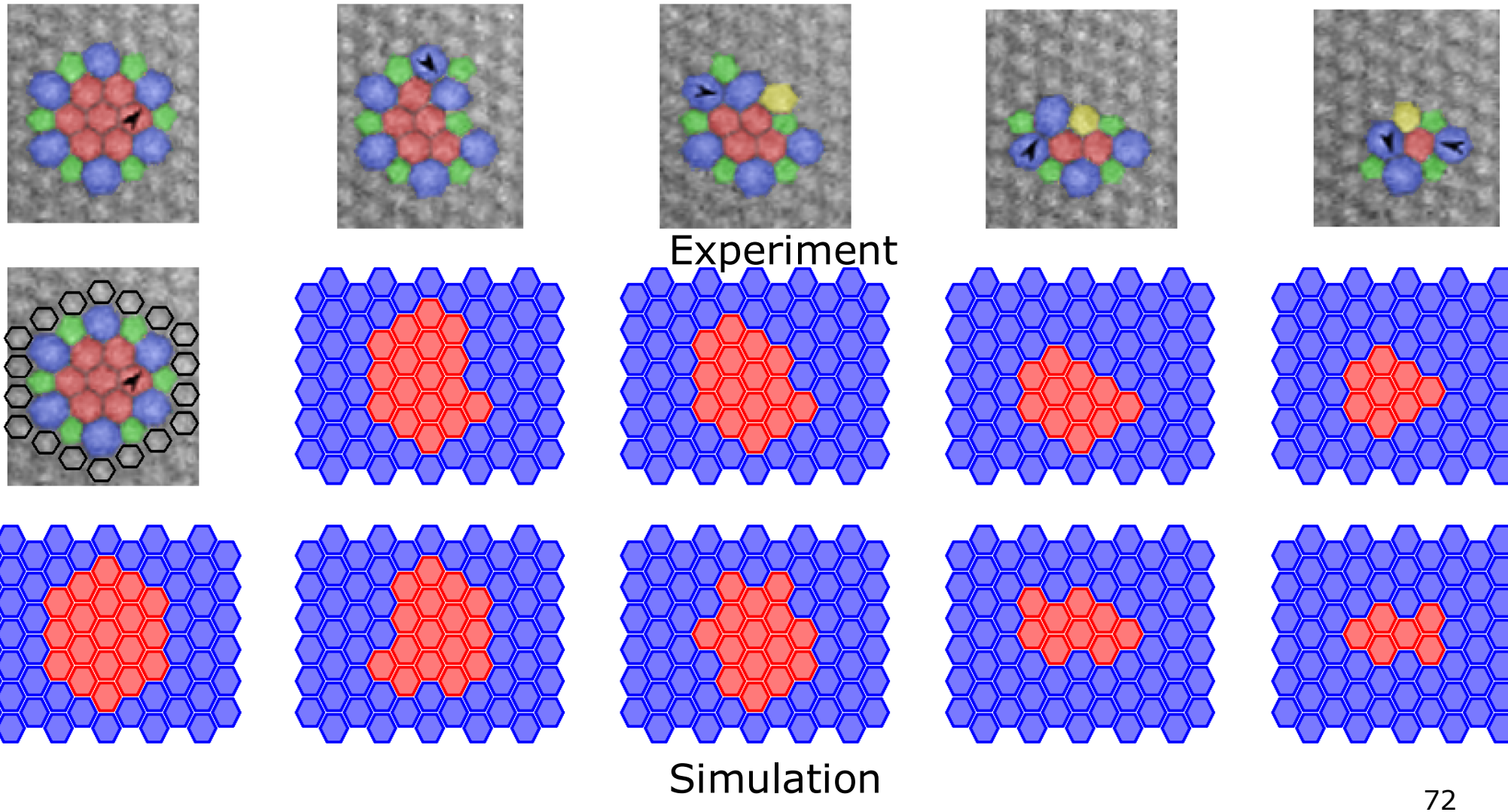
$$A(t) = -2\pi \cdot \gamma m \cdot t + A(t=0)$$





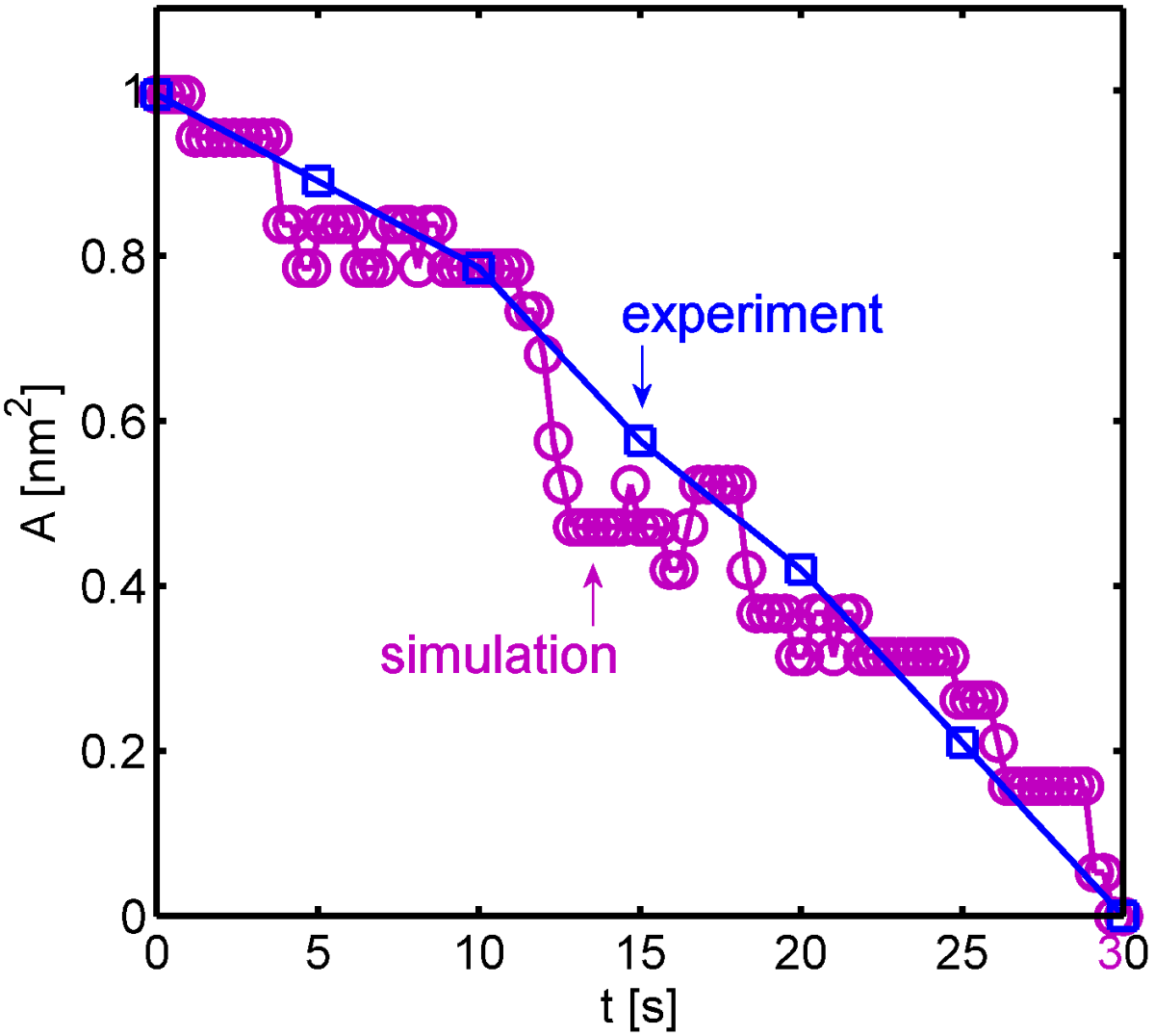
Going back to 2D Grain Growth

2D Potts model simulation: flower defect



Going back to 2D Grain Growth

2D Potts model simulation: flower defect



Summary and Outlook

Summary:

- simulation of grain boundary migration and normal as well as nanocrystalline grain growth by Monte Carlo Potts model
- expectations (e.g. parabolic growth law, self-similarity) are fulfilled
- individual growth kinetics allows prediction of average growth law solely from kinetics of quadruple points
- mesoscopic 2D Potts model represents grain boundary migration in graphene quite well

Summary and Outlook

Outlook:

- anomalous growth kinetics in nanocrystalline materials explained by junction control or abnormal grain growth?
- experimental determination of grain size distribution and topology in nanocrystalline materials
- junction drag in nanocrystalline thin films
- grain boundary migration in polycrystalline graphene

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