Basic Approaches to the Simulation of Recrystallization and Grain Growth

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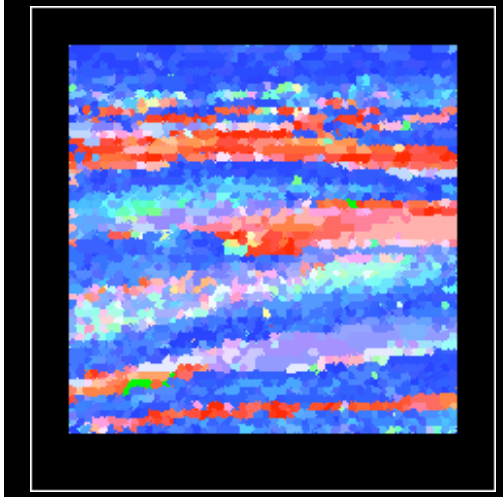

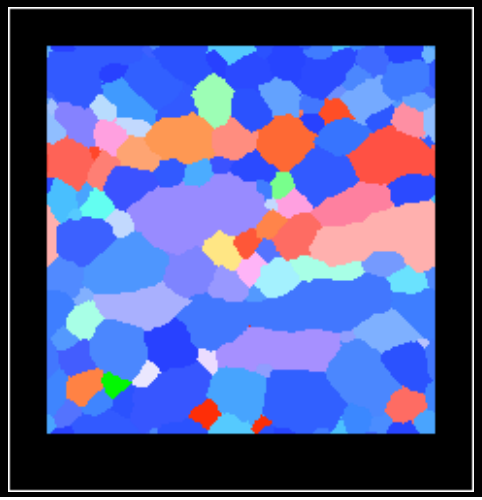

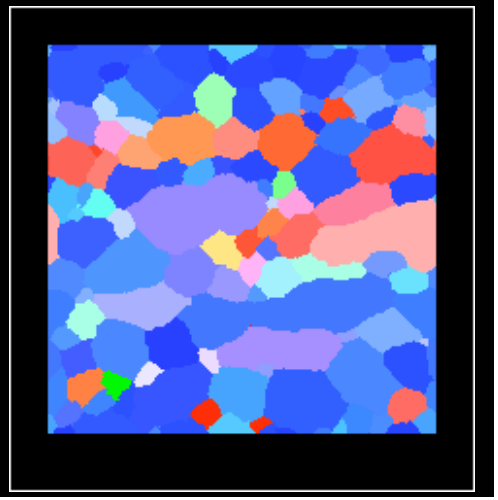

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*http://*www.mpg.de *http://*www.mpie.de *http://*edoc.mpg.de/

Max-Planck Project Report

Project Partners

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Outline *)

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- **Simulations: why ? how?**
- **Discrete simulation methods**
- **Examples**
- **Conclusions**

*) *soft magnetic steels*

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Outline

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Simulations: why ?

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- Understanding (prerequisite to optimization)
- Models available
- (Some) material data available

- Investment ratio: experiments/computers: factor 100

  (Cost reduction via computational materials design)

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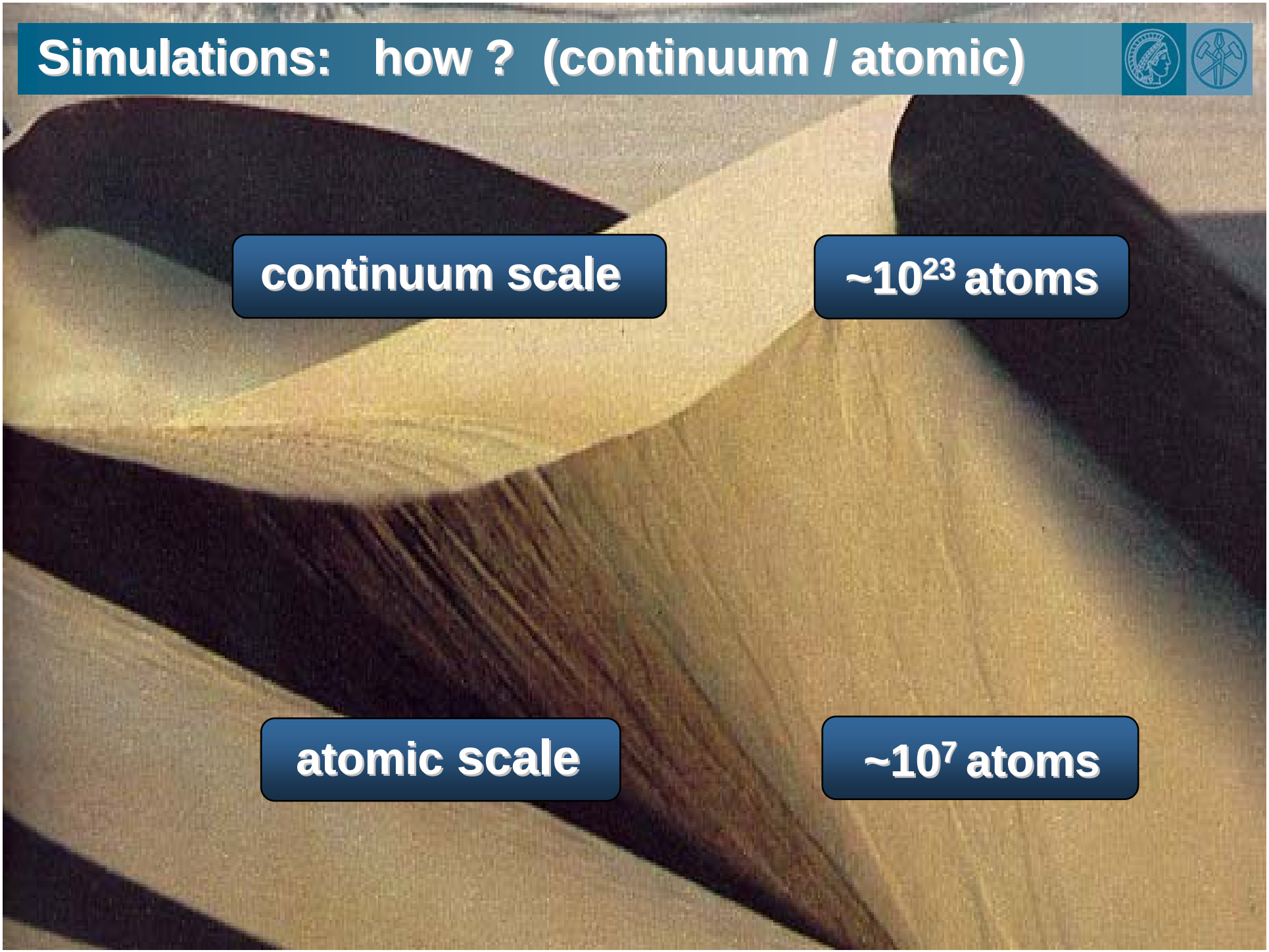
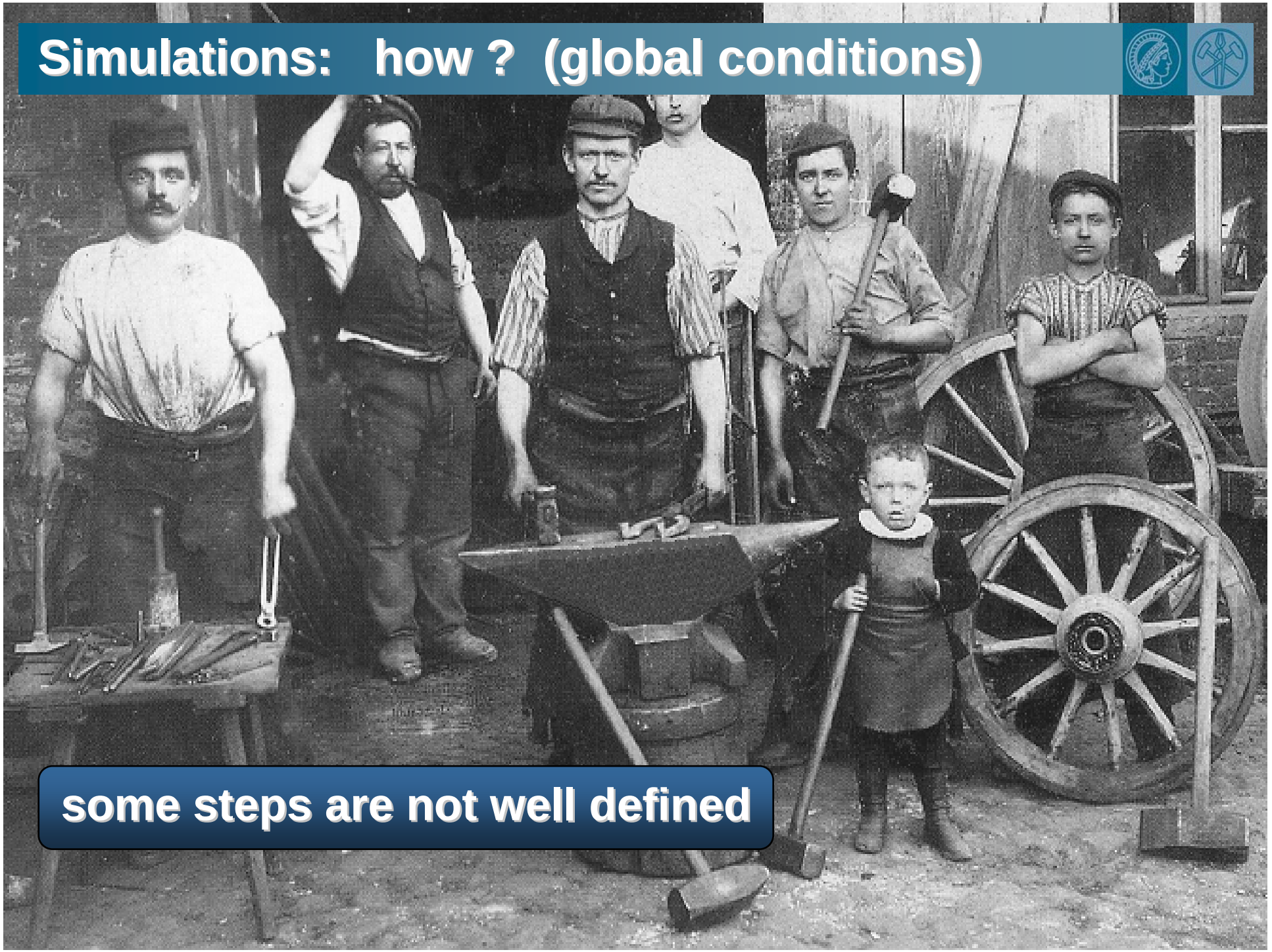
Simulations: how ? (continuum / atomic)



Simulations: how ? (global conditions)



some steps are not well defined

Simulations: how ? (local conditions)

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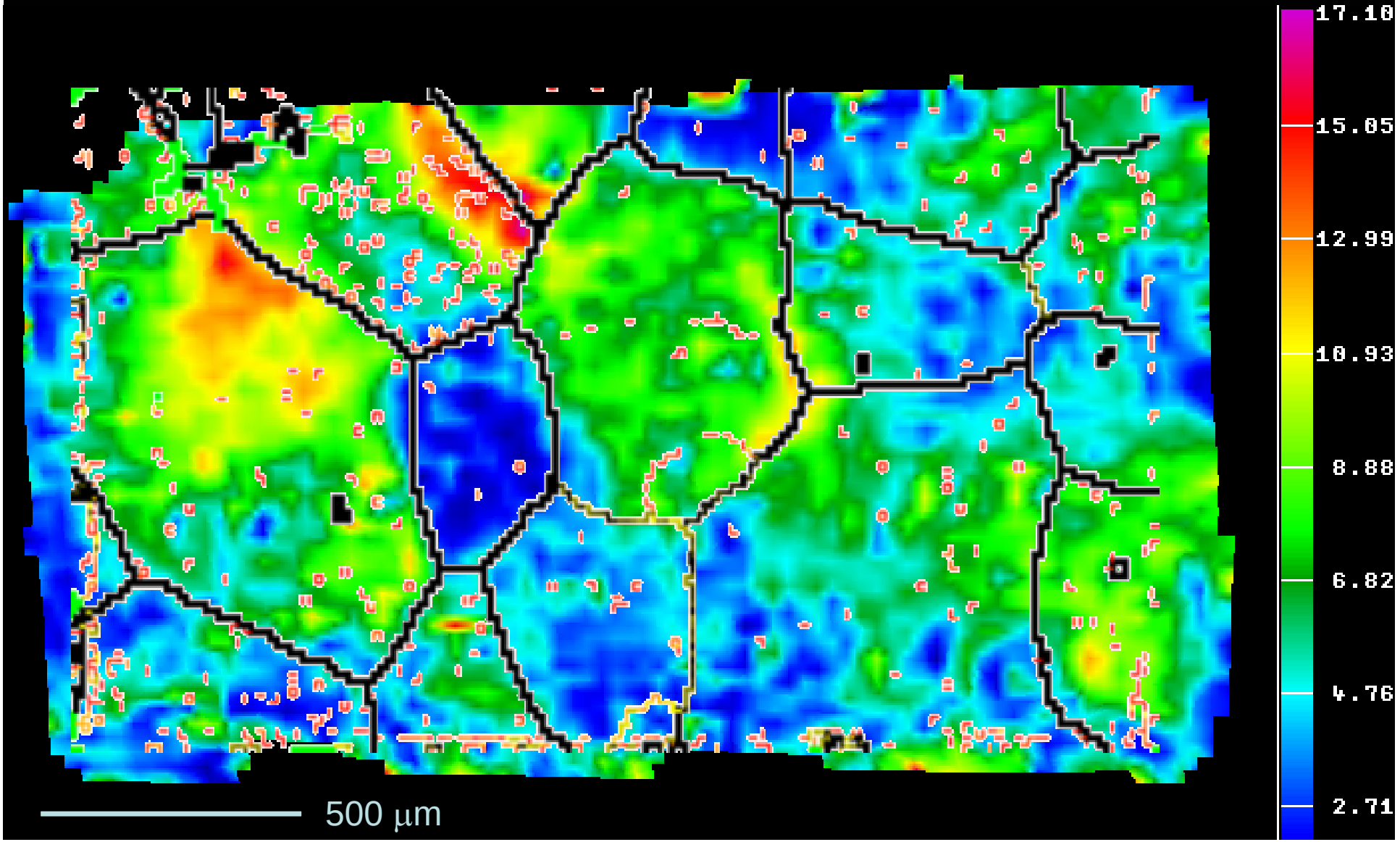
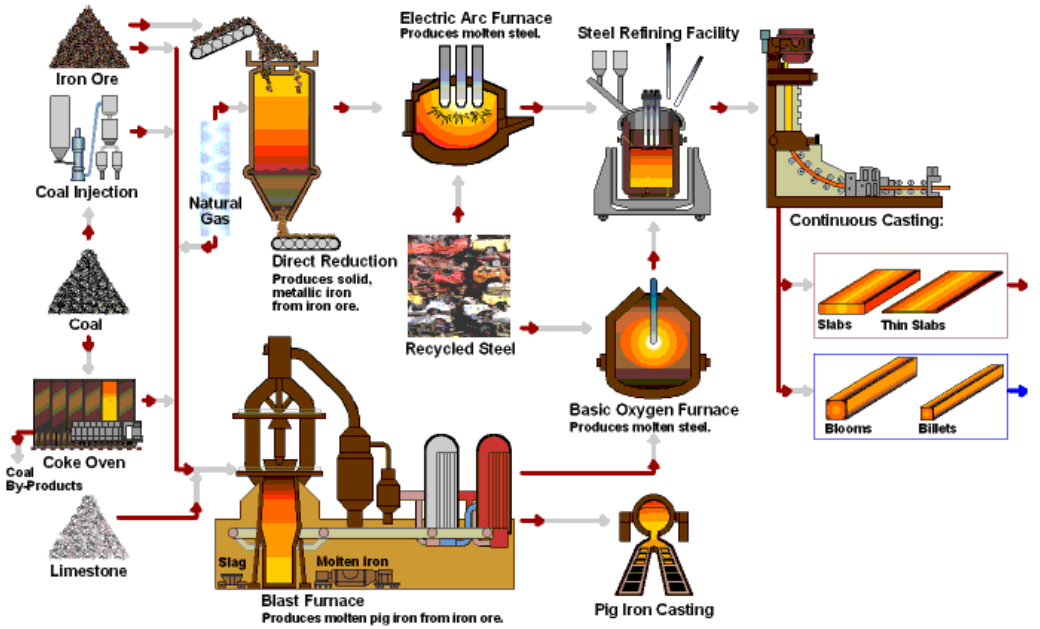
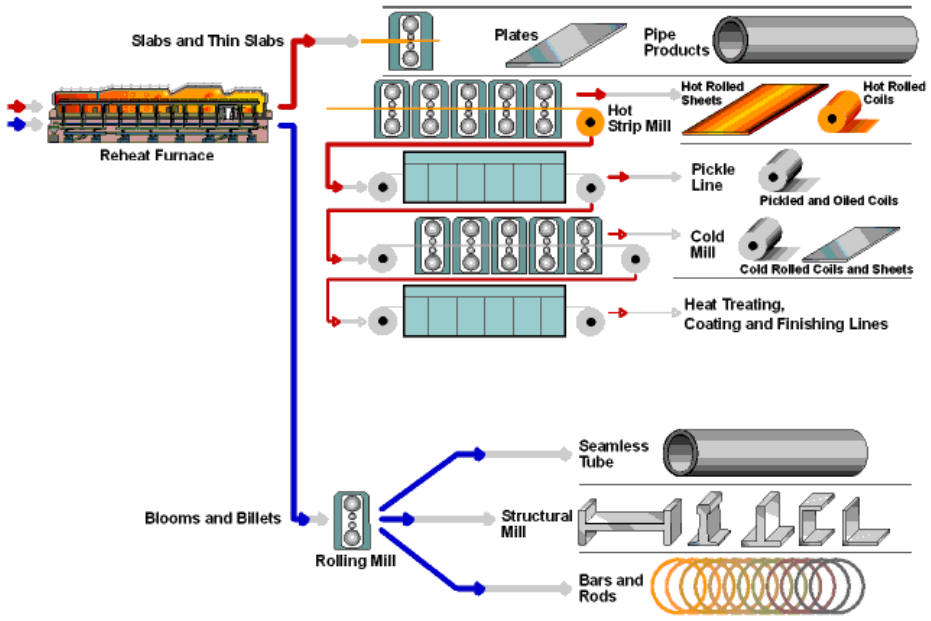
color code: total v. Mises strain



Simulations: how ? (inheritance)

materials have a history





Neuronal simulation methods

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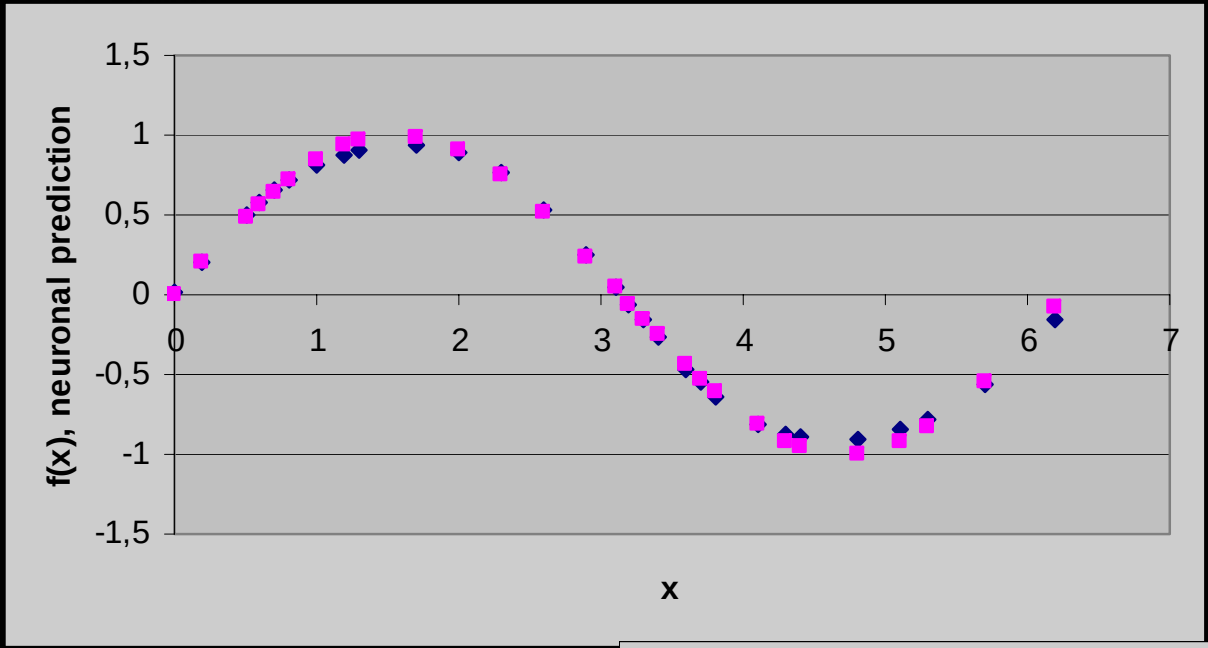
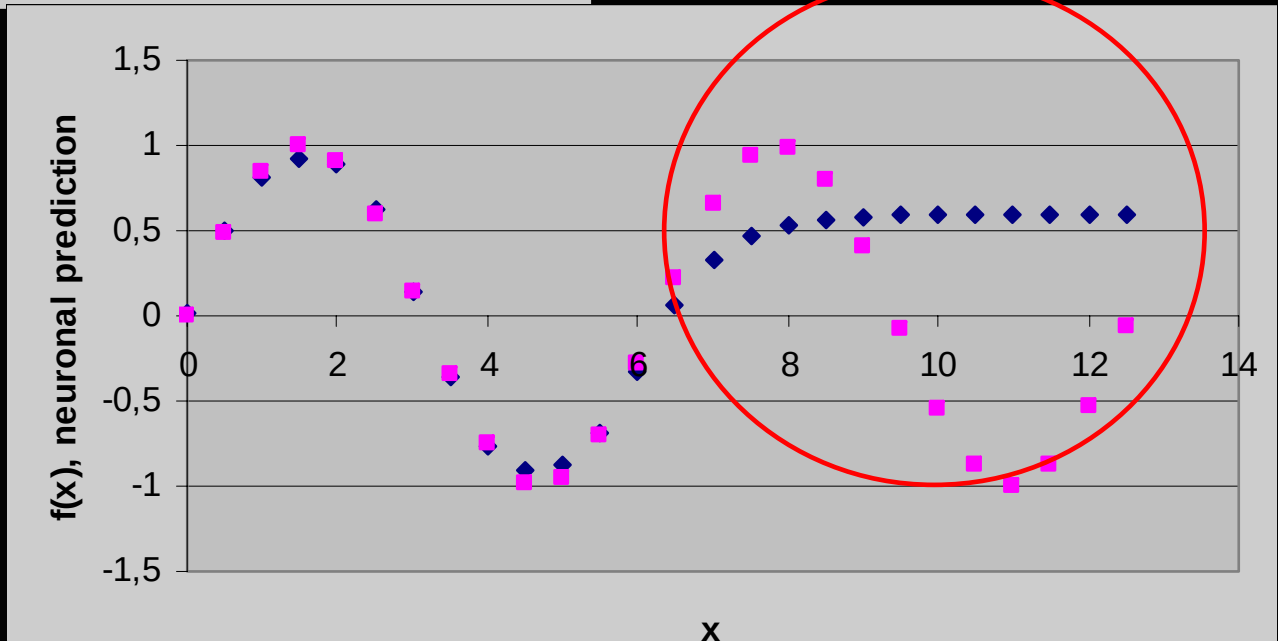


Training up to 2π
data fit: OK

Application beyond 2π
prediction: not OK



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Simulations: how ? (mechanisms)

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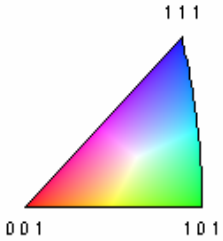
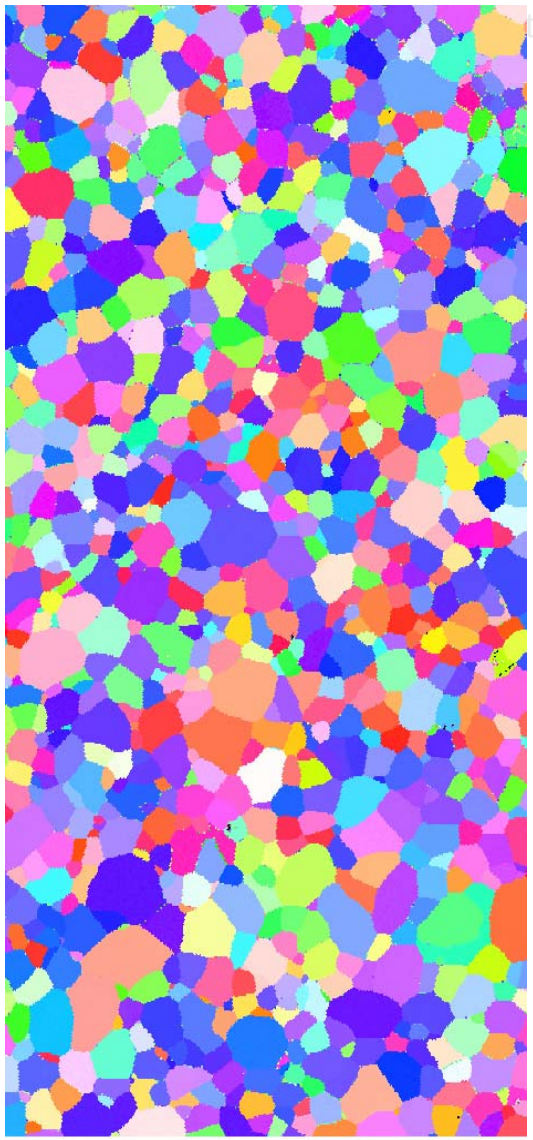
large data sets

(10^4 • 10^3)





70.00 µm = 70 steps

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Simulations: how ? (summary)

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- **Continuum scale**
- **Large data sets**
- **Complex boundary conditions**
- **Integrated modeling (microstructure inheritance)**
- **Input data available?**
- **Quantitative?**

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Outline , MPG edoc report

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- **Simulations: why ? how?**
- **Discrete simulation methods**
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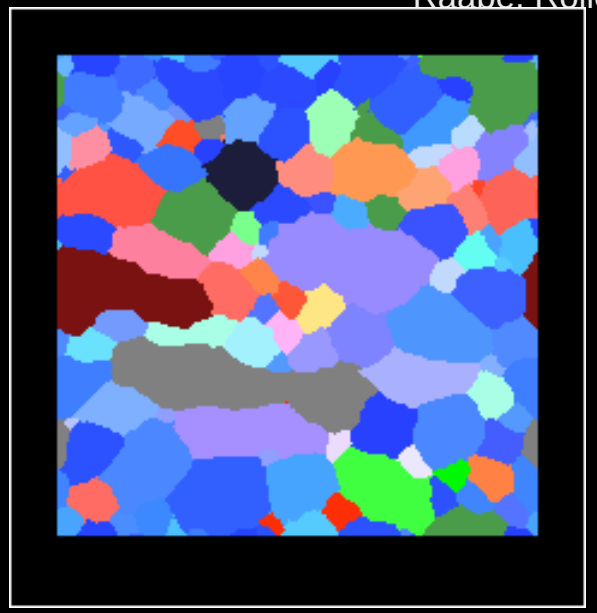
Discrete simulation methods

Potts

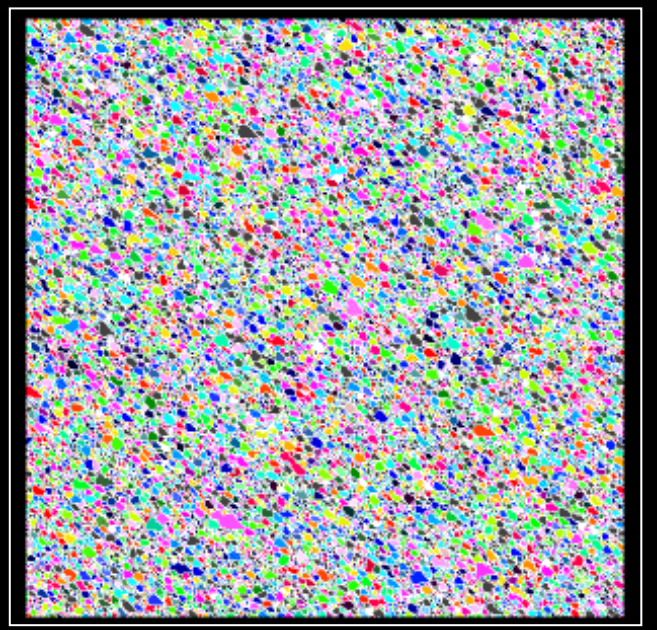
- o Monte Carlo (probabilistic), local thermodynamics, kinetics of transients
- \+ simple codes (available), flexible, data input simple
- \- no real kinetics, lattice based



N. Chen (Max-Planck-Institut für Eisenforschung)

Discrete simulation methods

D. Raabe (Max-Planck-Institut für Eisenforschung)



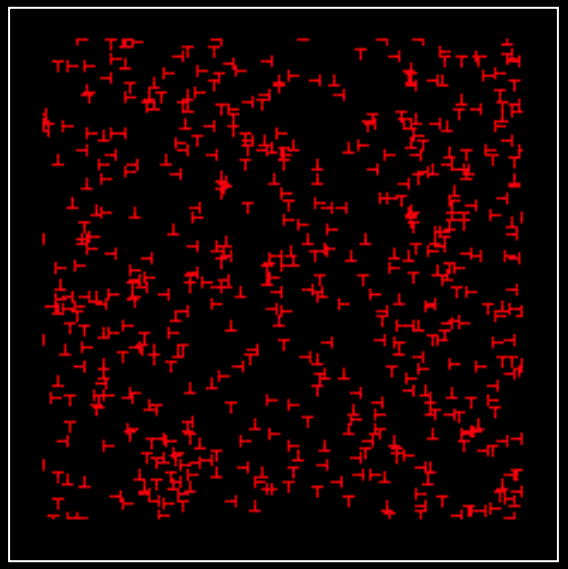
Cellular automata

- o deterministic, synchronous update
- \+ simple codes (available), flexible, real kinetics, data input simple
- \- lattice based

Discrete simulation methods

Dislocation dynamics

- o deterministic, synchronous update
- \+ dynamics of small angle boundaries
- \- difficult codes (3D), slow, small scale



F. Roters (Max-Planck-Institut für Eisenforschung)

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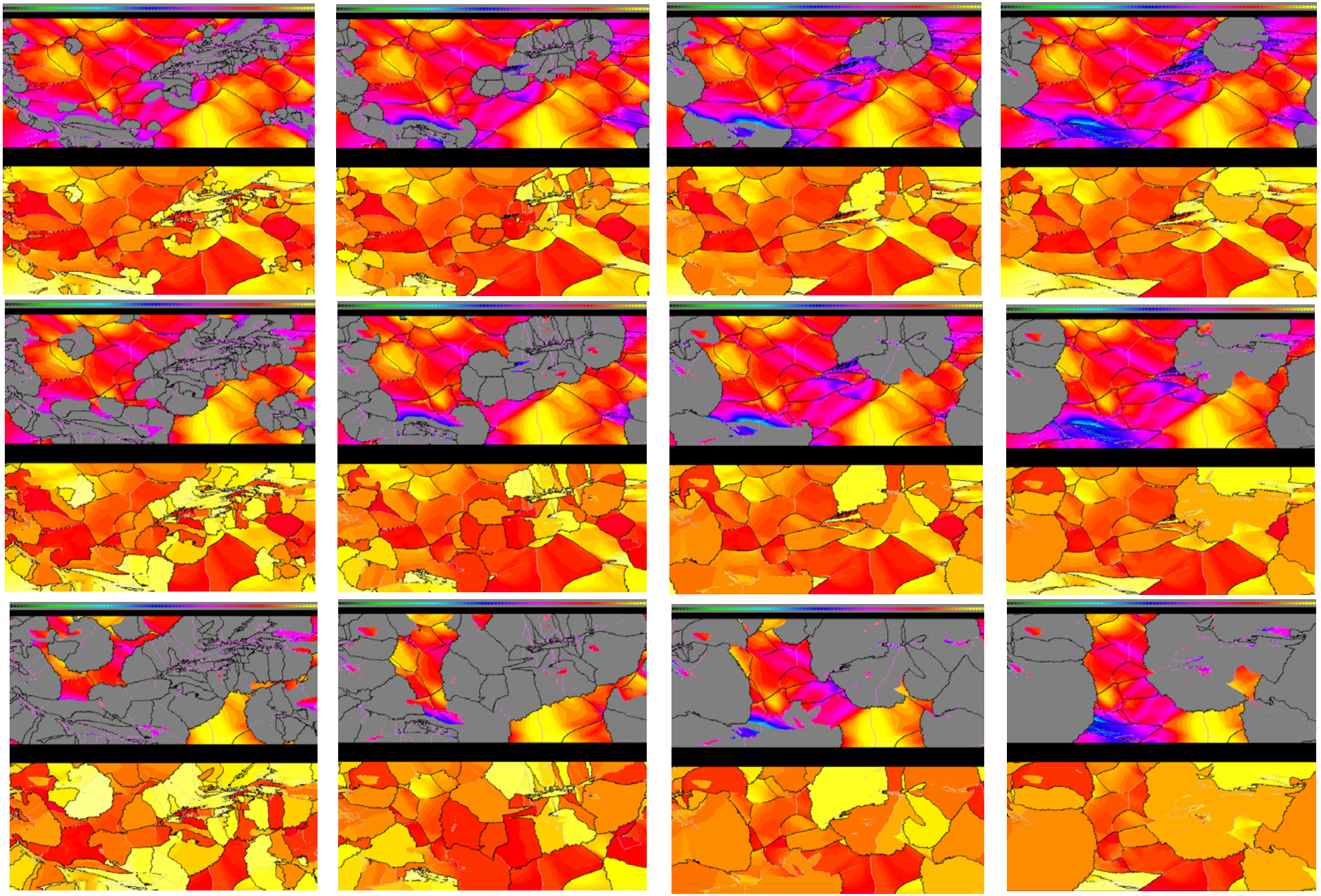
Example #1: FEM + CA



Example #2: EBSD + Potts - start data

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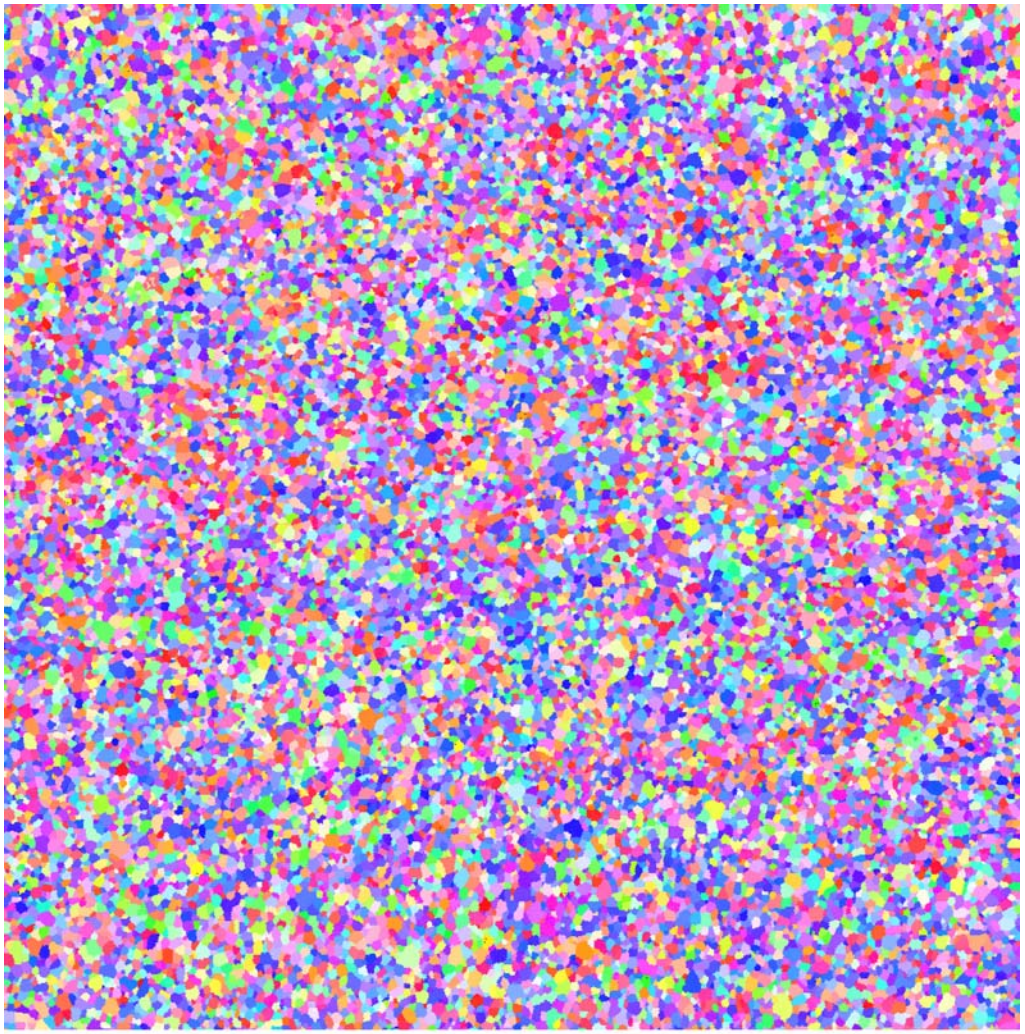
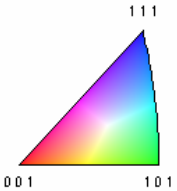
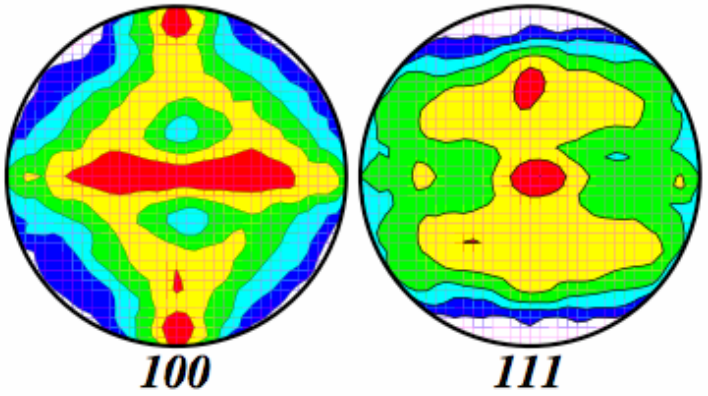


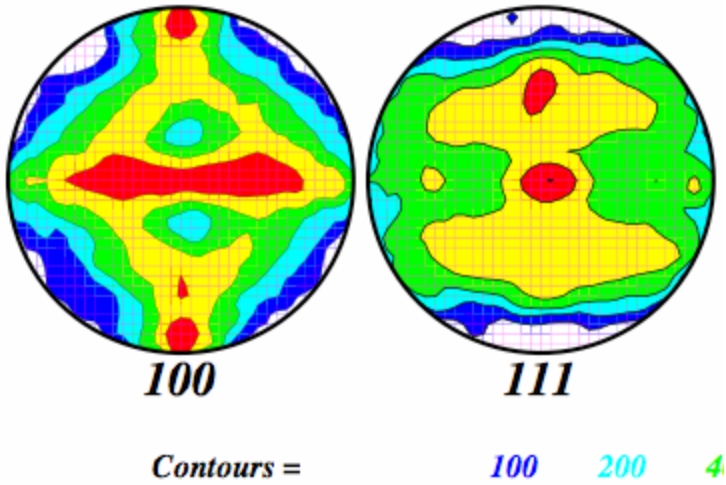
200.0 µm = 100 steps IPF [001]



experimental map (after RX)



experimental



result of texture fit

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Example #2: EBSD + Potts - basics

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System Energy :

$$E = \frac{1}{2}\sum_{j}^{N}\sum_{i}^{n}\gamma(S_i,S_j)\left(1-\delta_{S_iS_j}\right)$$

Reorientation Probability :

$$P = \begin{cases} \dfrac{\gamma(S_i,S_j)}{J_{\max.}}\dfrac{M(S_i,S_j)}{M_{\max.}}\times 1 & \Delta E \le 0 \\ \dfrac{\gamma(S_i,S_j)}{J_{\max.}}\dfrac{M(S_i,S_j)}{M_{\max.}}\times \exp\left(\dfrac{-\Delta E}{JT}\right) & \Delta E > 0 \end{cases}$$

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Example #2: EBSD + Potts - parameters

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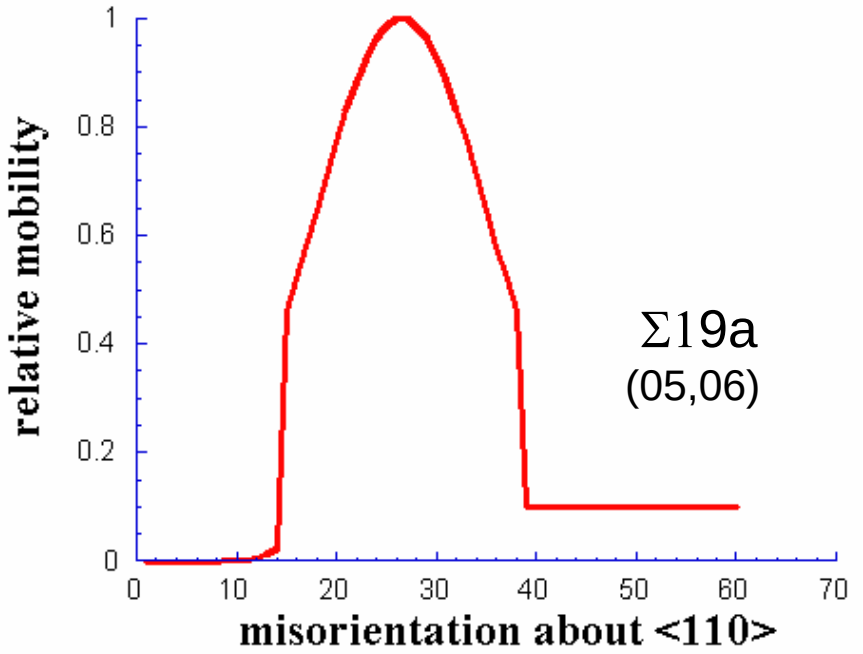

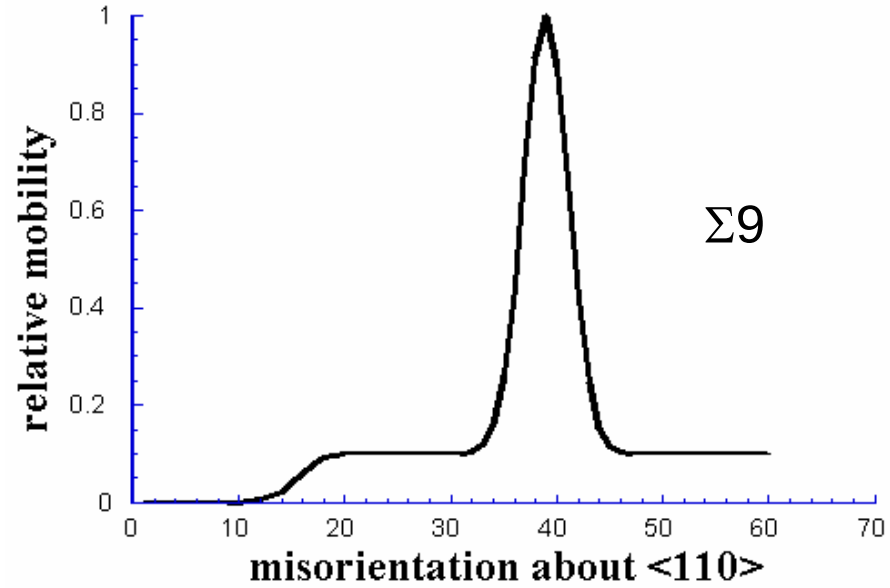

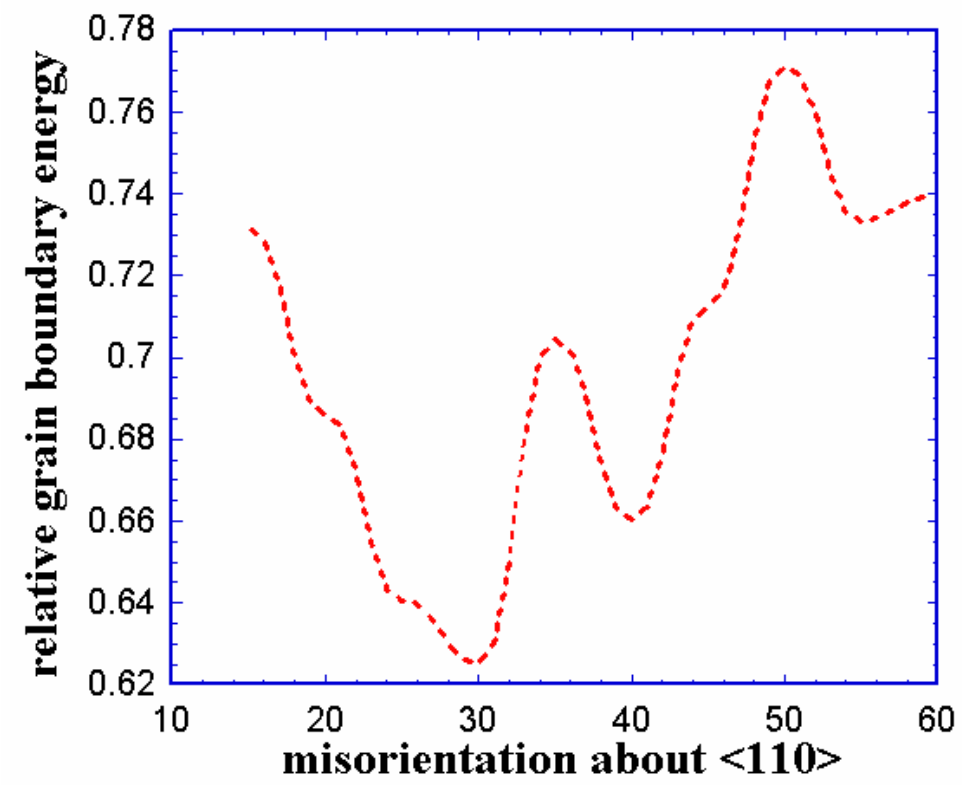

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Example #2: EBSD + Potts - results grains

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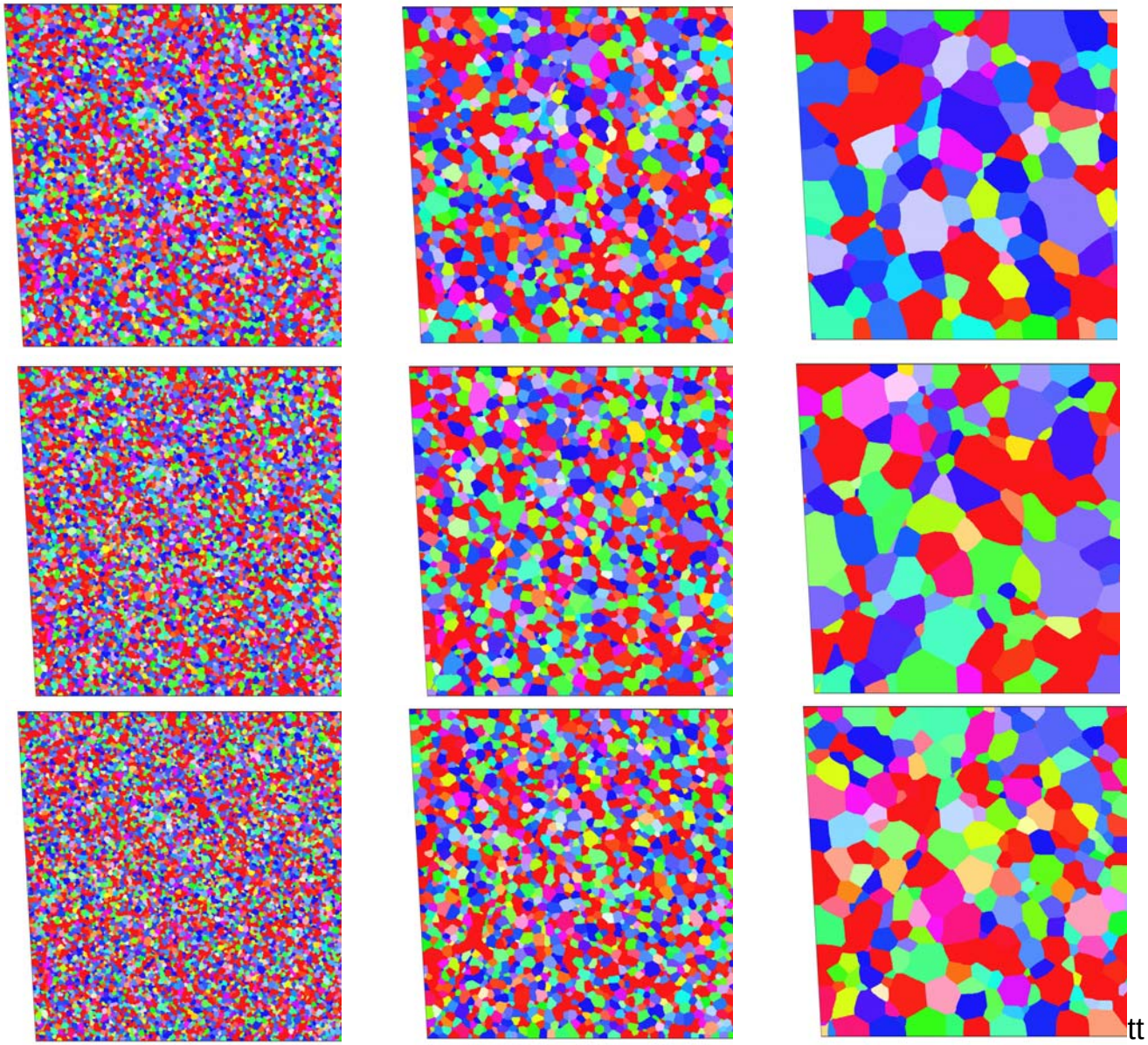
10^7 MCS | 10^8 MCS | 10^9 MCS

Broad mobility peak at 27°<110>

27°<110> with energy anisotropy

Sharp Σ9 mobility peak, with energy anisotropy



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Example #2: EBSD + Potts - results texture

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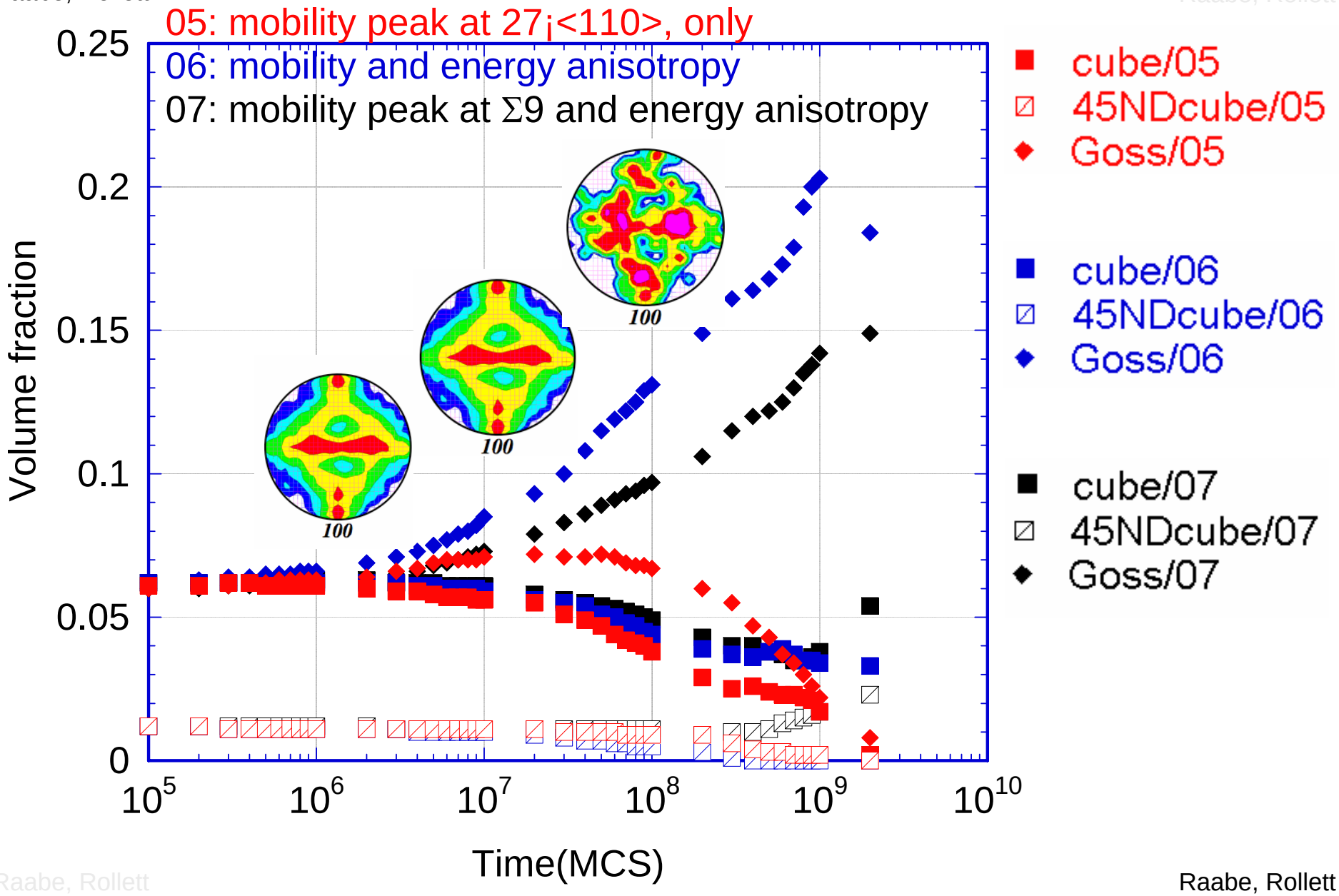

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Conclusions, MPG edoc report

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Simulation methods (general thoughts)

- Potts / CA: robust, flexible, 3D, codes available
- Vertex: pure front tracking, difficult for 3D
- phase field: 2nd phase, impurities, 3D

Examples

- Potts: Goss growths for mobility+energy effect
  what about particles ?
  not abnormal
- CA+FEM: example for integrated modeling

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