Finite element discretization of Digital Material Representation models

Lukasz Madej,
Aleksander Fular, Krzysztof Banas, Filip Kruzel, Pawel Cybulka, Konrad Perzynski

AGH University of Science and Technology, Kraków, Poland,

lmadej@agh.edu.pl
home.agh.edu.pl/lmadej
Outline

• Introduction - motivation
• Digital Material Representation in 2D and 3D
  • Experimentally/Statistically based DMR
  • Material properties
  • Incorporation into FEM models
    • Heterogeneous FE meshes in 2D and 3D
    • Adaptation techniques in 2D and 3D
  • Micro and multi scale simulations
• Conclusions and plans for future work
Conventional modelling methods describe material as a continuum and provide the general information about e.g. phase distribution within the sample.

Inclusion in aluminium alloy

OFHC Copper 20%
CuZn30 30%
Fe30Ni

DP
This days new materials are being developed very fast with microstructures composed of different grain sizes, phases, inclusions, voids, nano particles etc.

To meet elevated expectations the numerical simulations have to take these features explicitly into account.
2D microstructure

Optical microscopy

SEM

Image processing

EBSD
3D microstructure

Serial sectioning

A Borbély - 2004

RoboMet

A Fully Automated, Serial Sectioning System for Three-Dimensional Microstructural Investigations

B. A. RoboMet 3D

FIB
Cellular Automata + Monte Carlo

\[ p(\Delta E) = \begin{cases} 
1 & \Delta E \leq 0 \\
\exp\left(-\frac{\Delta E}{kT}\right) & \Delta E > 0 
\end{cases} \]

Potts Model

\[ E = J_{gb} \sum (1 - \delta_{S_i, S_j}) \]

a) \( E_{Q1}=5 \)  

b) \( E_{Q2}=4 \)  

c) \( E_{Q3}=7 \)
Cellular Automata + Sphere Growth

Sphere generation

Spheres

CA sphere growth

$R$ expected
Properties

\[ \sigma = K \varepsilon^n \]

- scalar \( K \)
- vector \( \phi, \theta, \psi \)
- \( K, n, m \)

\[ \sigma = K \varepsilon^n \dot{\varepsilon}^m \]

Gauss distribution flow curves

Reference flow curve

stress, MPa

strain

orientation
- cube
- hard
- Goss
- shear

stress, MPa

strain
\[ \text{Err} = \frac{1}{n} \sum_{i=1}^{n} \sqrt{\left( \frac{\sigma_{\text{exp}} - \sigma_{\text{sim}}}{\sigma_{\text{exp}}} \right)^2} \]

Goal function

| Parameter | \( a \) \( \text{s}^{-1} \) | \( n_r \) | \( h_0 \) \( \text{MPa} \) | \( \tau_0 \) \( \text{MPa} \) | \( q_s \) | 
|-----------|-----------------|-------|-----------------|-----------------|-----|-------|
| cube      | 3.52E-05        | 1.88  | 114.11          | 59.94           | 5.15| 0.0   |
| Goss      | 1.41E-04        | 1.19  | 127.07          | 49.65           | 5.57| 0.0   |
| shear     | 1.78E-04        | 1.03  | 117.52          | 49.22           | 6.04| 0.0   |
| average   | 1.18E-04        | 1.37  | 119.57          | 52.94           | 5.58| 0.0   |
| std. Dev. | 7.45E-05        | 0.45  | 6.72            | 6.07            | 0.44| -     |
Focused Ion Beam

Step 1
Ga⁺ (30 kV 5 nA)

Step 2
Ga⁺ (30 kV 0.3 nA)

Step 3
Ga⁺ (30 kV 50 pA)

Uniform mesh generation for the DMR

Forge2,3
1. **Import of the grain boundary geometry.**

Points located along the grain boundaries are further used during the Delaunay triangulation. This assures generation of the conforming FE mesh.

2. **Generation of additional points located inside the grain area.**
3. Delaunay triangulation on the basis of the available points.

4. Mesh correction
   - the Laplace smoothing algorithm is applied in order to obtain finite elements with regular shapes.
   - edge swapping algorithm
Non-uniform mesh generation for the DMR

1. Non-uniform mesh generation for the DMR
2. Assignment of the finite elements to particular grains.
Local mesh refinement and adaptation

Zienkiewicz-Zhu error indicator

\[ e^*_{\sigma} = \sigma^* - \sigma_h \]

\[ \|e\| = \sqrt{\int_{\Omega} e^T_{\sigma} D^{-1} e_{\sigma} d\Omega} \]

- \( e^*_{\sigma} \): recovered stress tensor
- \( \sigma_h \): standard stress tensor computed using derivatives of shape functions
- \( D \): elasticity matrix with material constants

Refinement with geometrical similarity - Child elements are similar to parent element
Local mesh refinement and adaptation

The key aspect in this approach is to ensure that an accurate partitioning strategy is used in the global model for extracting the steady state boundary conditions to be imposed to the sub-model.

Transfer of the displacement boundary conditions taken from the global simulation into the submodel.
Numerical simulation of drawing process

Hole Expansion Test
Brittle-ductile fracture modelling

Brittle fractures

Ductile fractures

Brittle fractures

Ductile fractures
Microstructure generation

FE mesh generator

CA model:
- DRX
- Phase transformation
- Fracture
- Strain localization
- etc.

Crystal plasticity

Micro scale modeling

Multi scale modeling

CA model:
- DRX
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Crystal plasticity

Micro scale modeling

Multi scale modeling
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