Finite element discretization of Digital Material Representation models

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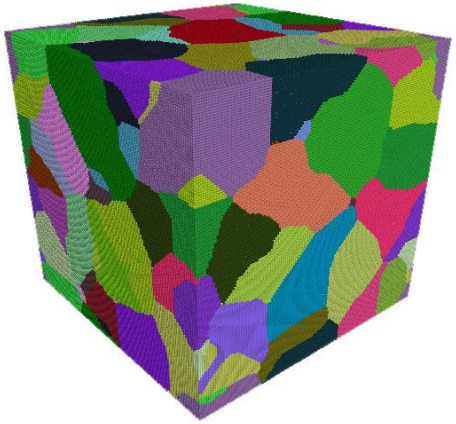

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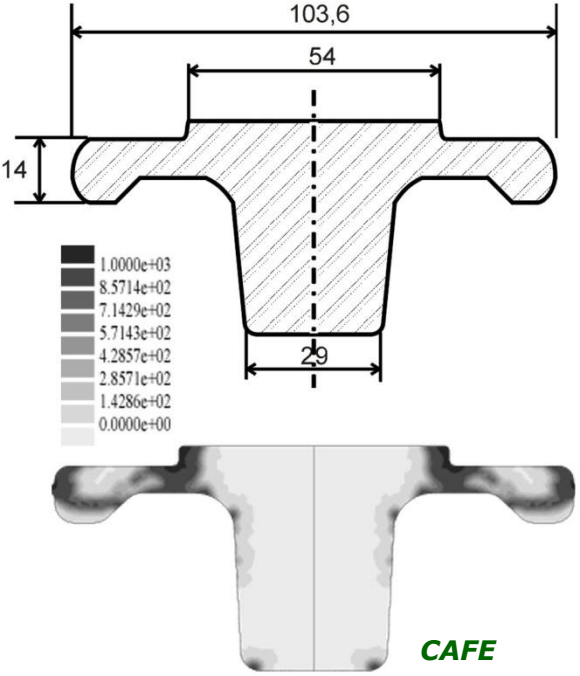
Outline

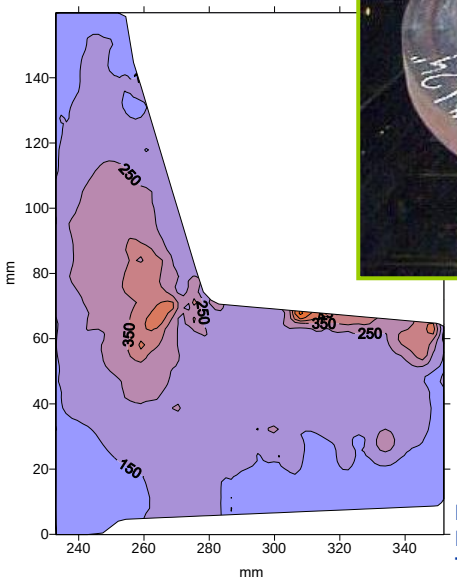
- Introduction - motivation
- Digital Material Representation in 2D and 3D
  - Experimentally/Statistically based DMR
  - Material properties
  - Incorporation into FEM models
    - Heterogeneous FE meshes in 2D and 3D
    - Adaptation techniques in 2D and 3D
  - Micro and multi scale simulations
- Conclusions and plans for future work

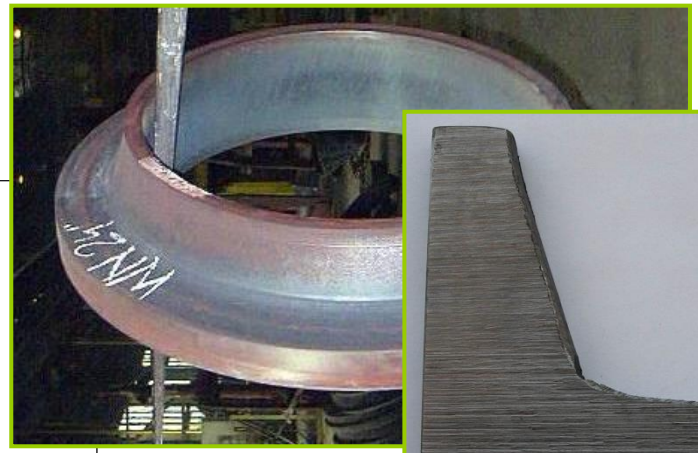
Introduction

Conventional modelling methods describe material as a continuum and provide the general information about e.g. phase distibution within the sample.



CAFE

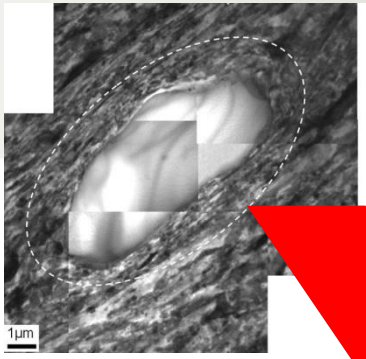


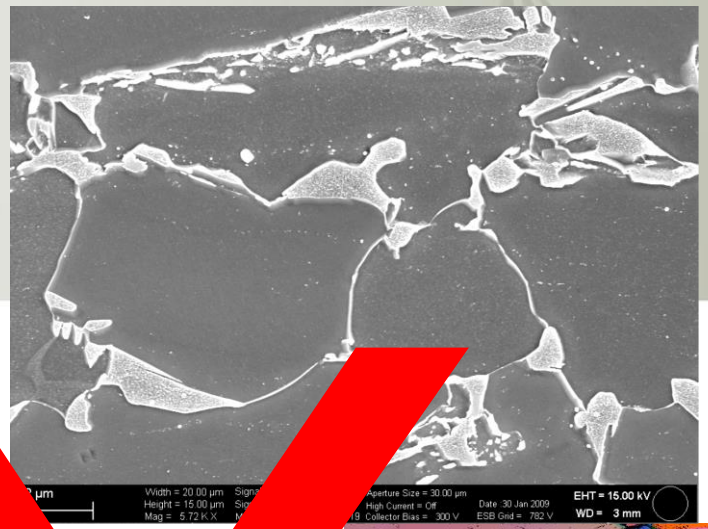


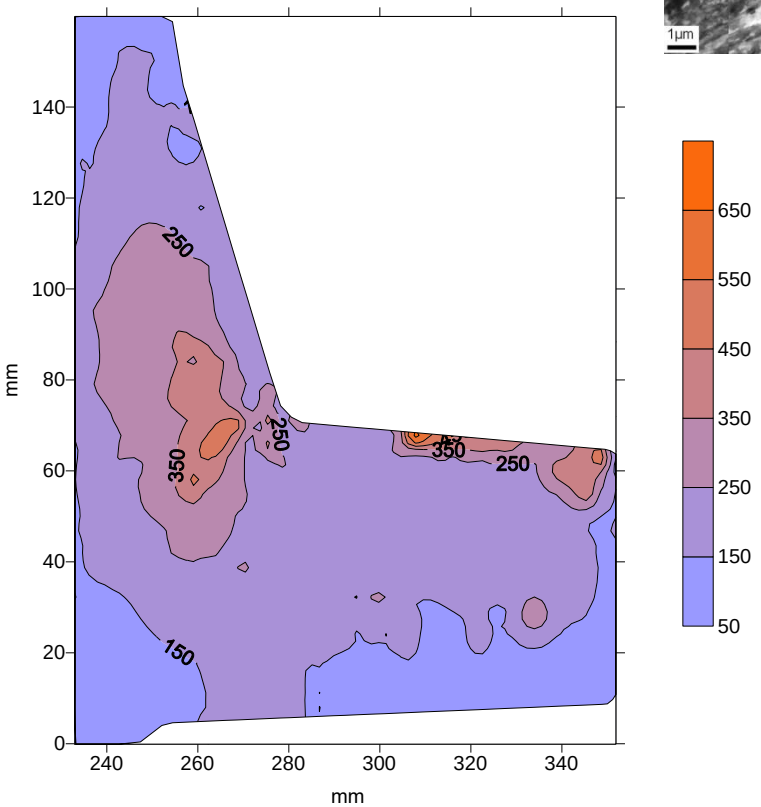
FE

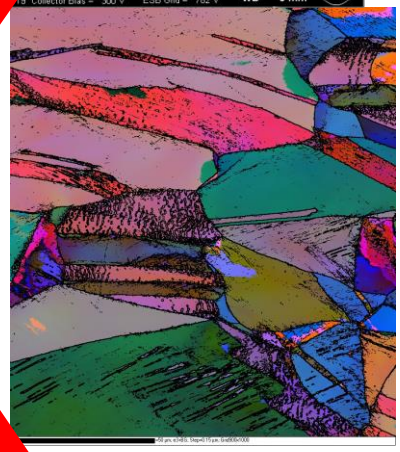
Malinowski Z., Głowacki M., Pietrzyk M., Madej W., „Finite Element Model for Efficient Simulation of Ring Rolling", Mat Konf. Pt. Materials Science & Technology 2004 Conference Proceedings, New Orleans, Louisiana USA, 26-29.09.2004r., s.397-401

Inclusion in aluminium alloy **DP**



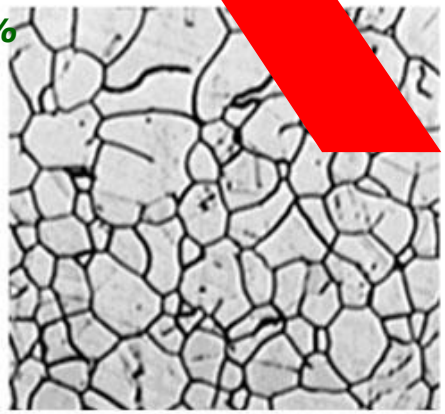






OFHC Copp *%*

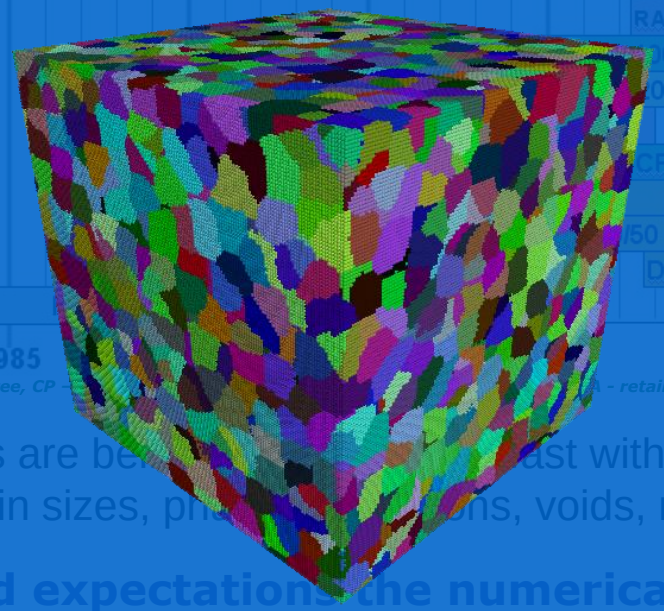
CuZn30 30%



Fe30Ni

Jaroni U., Imlaau K.P., Osburg B.: Neue Losungsansatze fur innovative produkte und umformtechnologien im automobilbau, Proc. ASK25, Aachen, 2010, pp. 3-14.

Numerical models based on the Digital Material Representation idea



This days new materials are be[illegible] ast with microstructures composed of different grain sizes, ph[illegible]ns, voids, nano particles etc.

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

2D microstructure

Optical microscopy

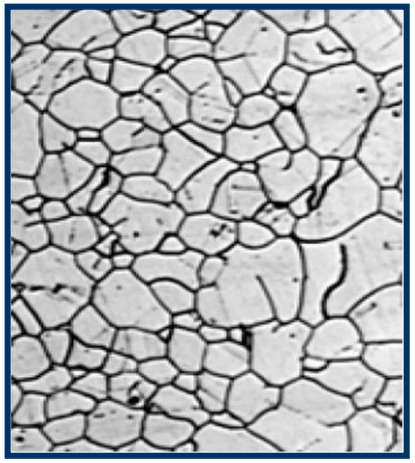
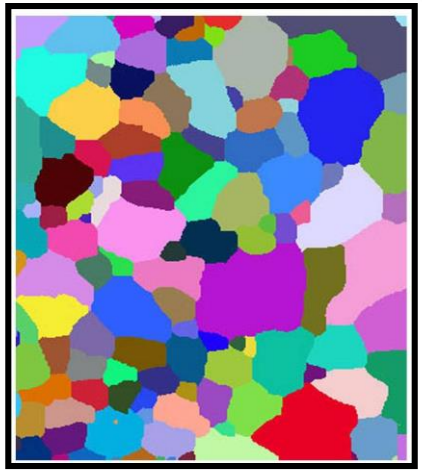
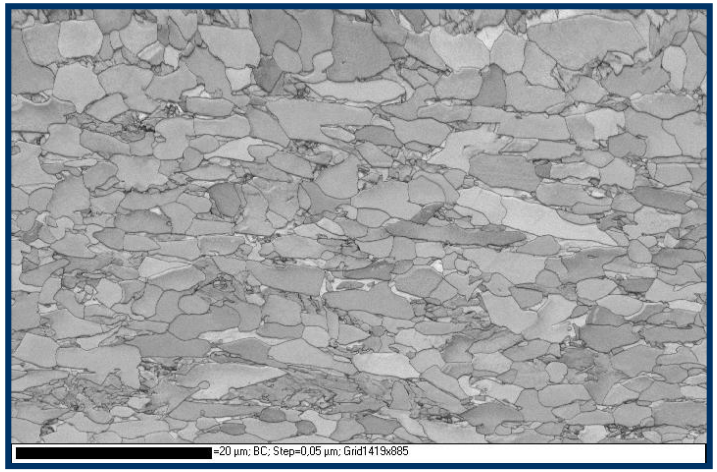


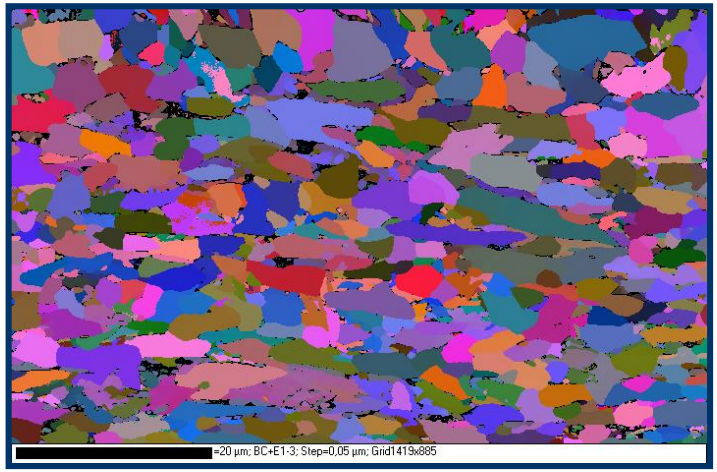
Image processing



SEM



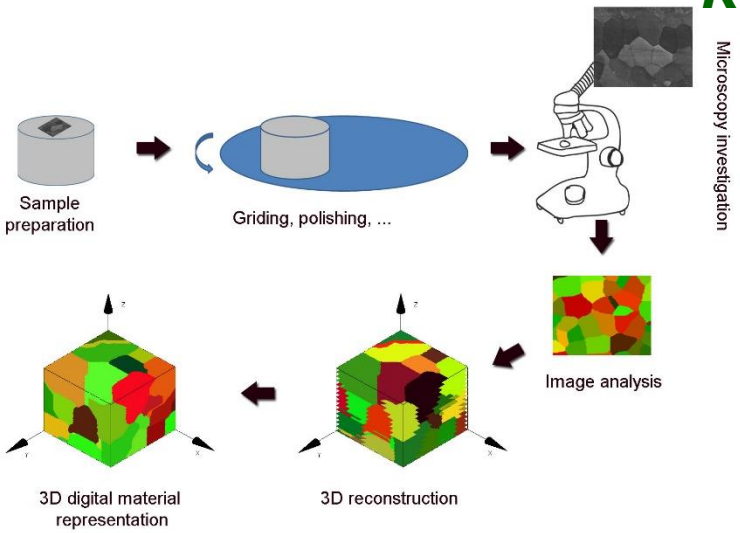
EBSD



3D microstructure

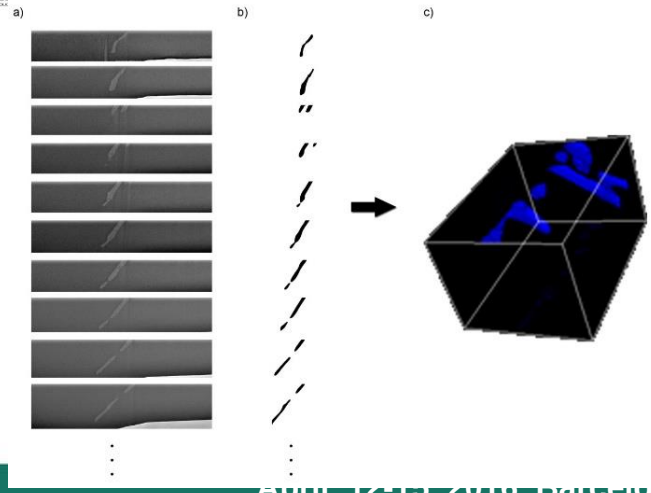
Undergrad students
PhD students
Postdocs

Serial sectioning

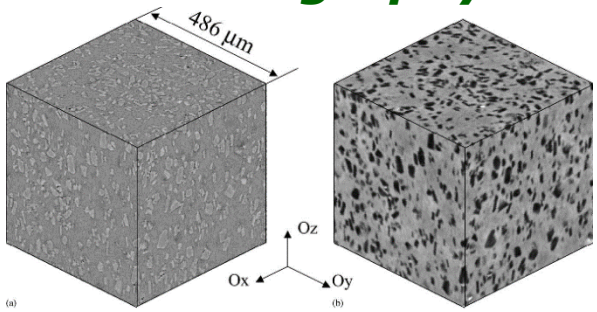


RoboMet

FIB



Tomography

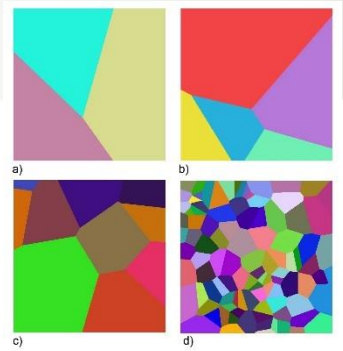


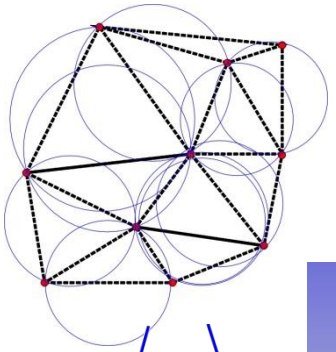
A Borbély - 2004

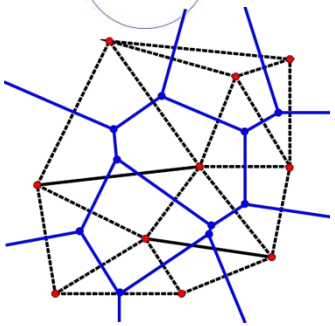
Pietrzyk M., Madej L., Rauch L., Szeliga D., Computational Materials Engineering: achieving high accuracy and efficiency in metals processing simulations, Butterworth-Heinemann Elsevier, 2015.

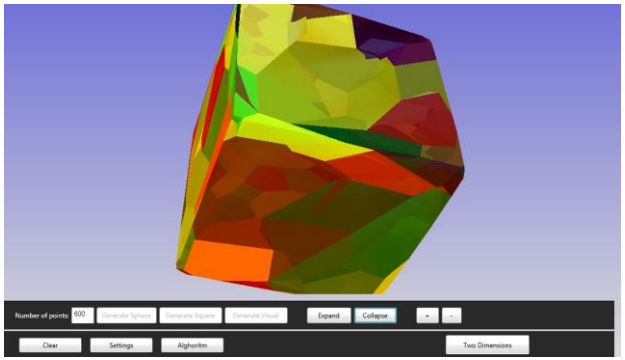
Cellular Automata

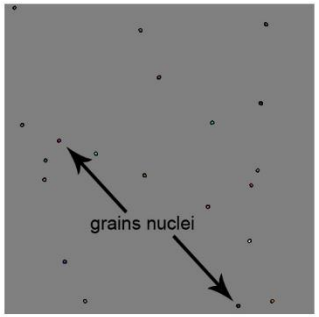
Voronoi

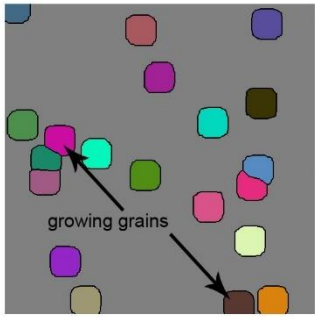


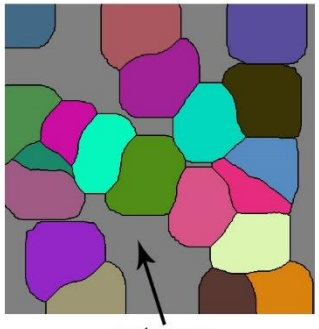


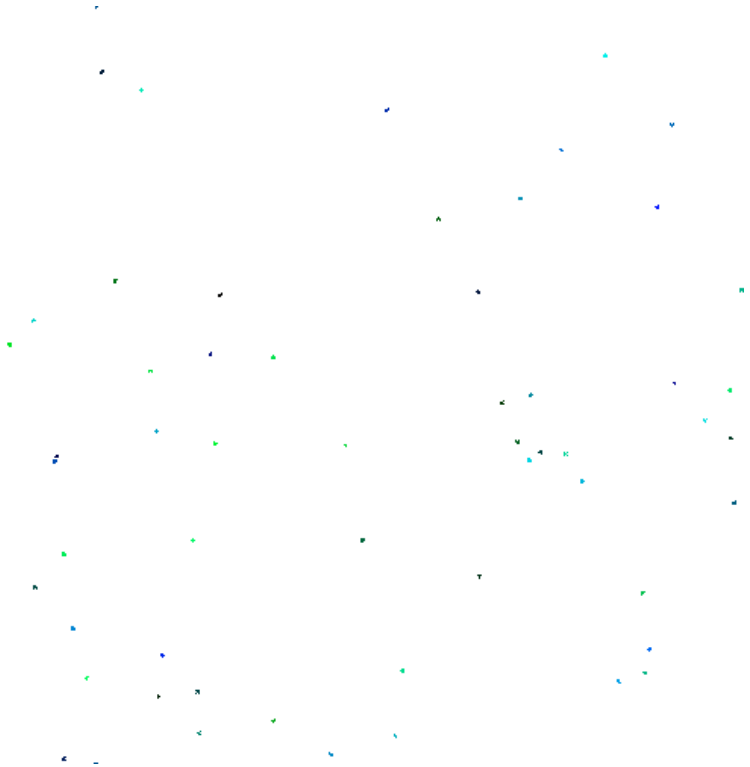




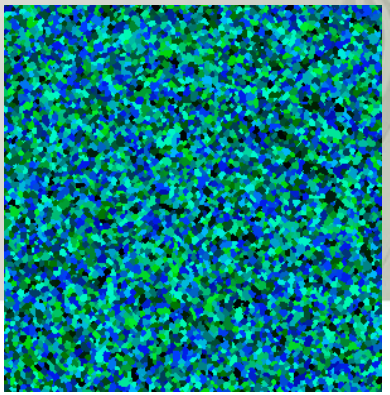


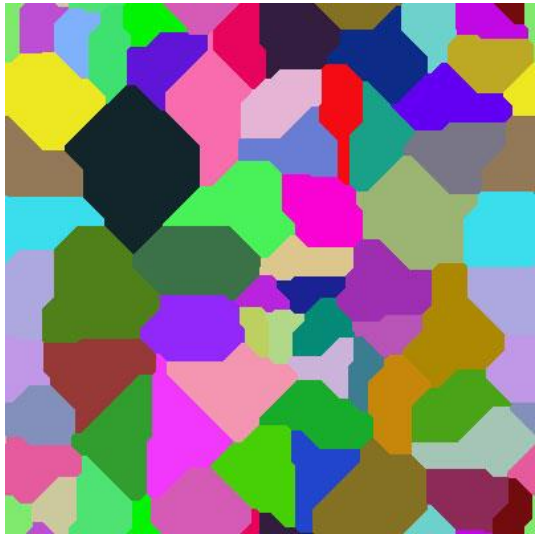




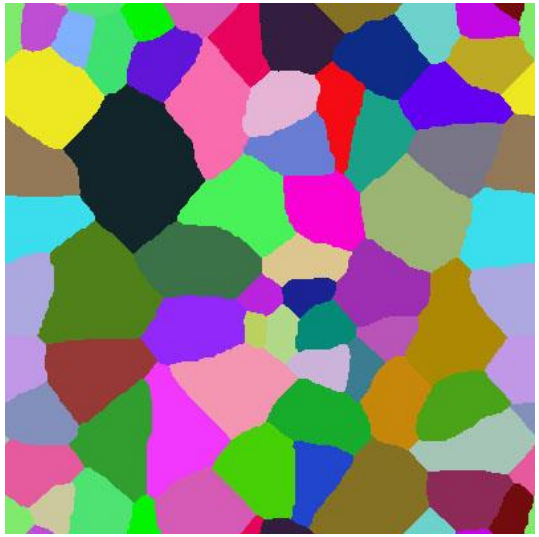


Cellular Automata + Monte Carlo

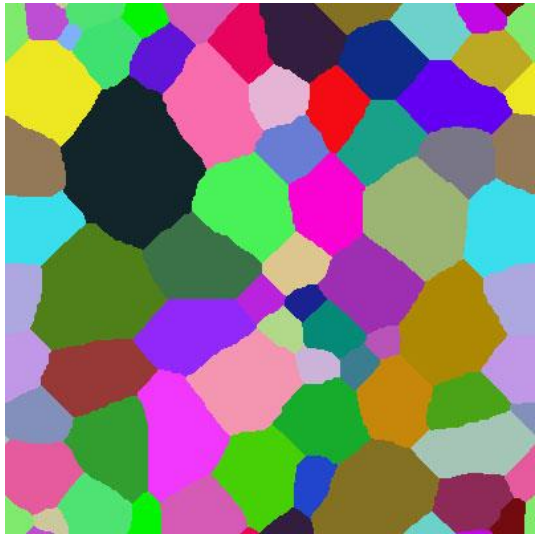




initial



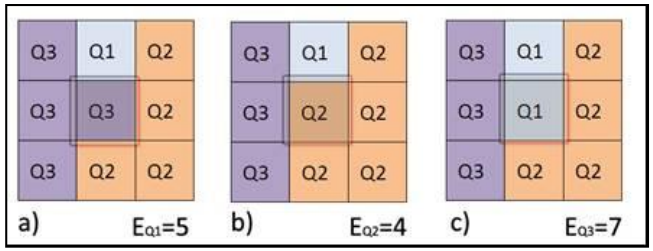
middle



final

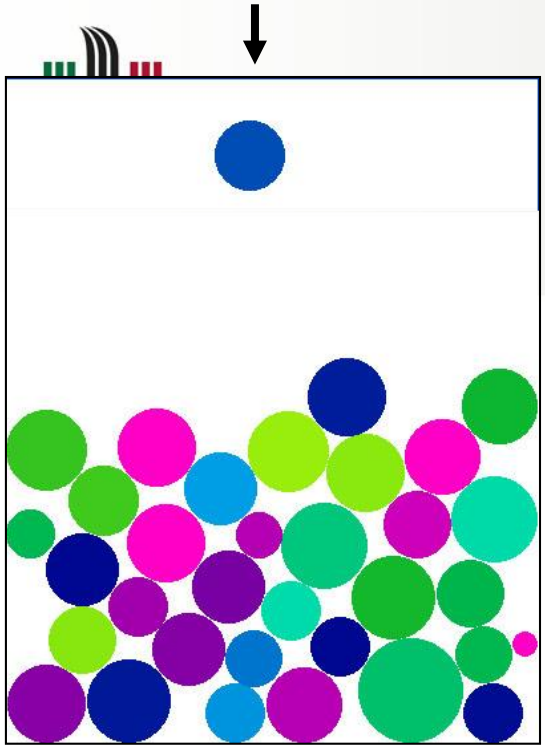
Potts Model

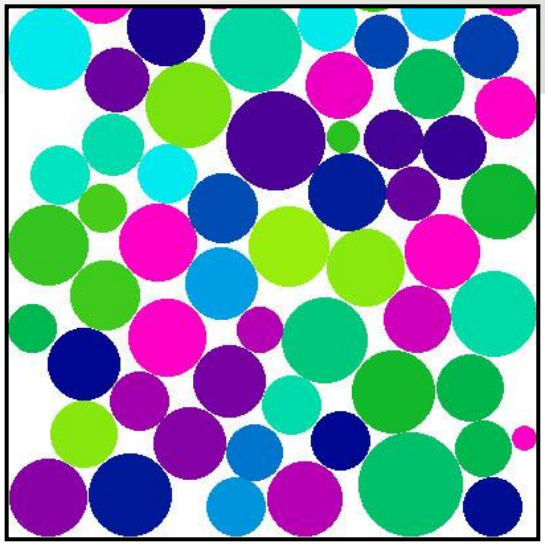
$$p(\Delta E) = \begin{cases} 1 & \Delta E \le 0 \\ \exp\left(-\dfrac{\Delta E}{kT}\right) & \Delta E > 0 \end{cases}$$

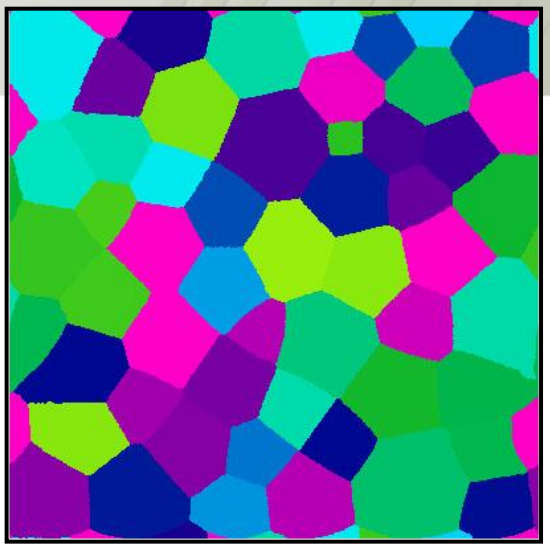


$$E = J_{gb} \sum_{<i,j>} \left(1 - \delta_{S_i S_j}\right)$$

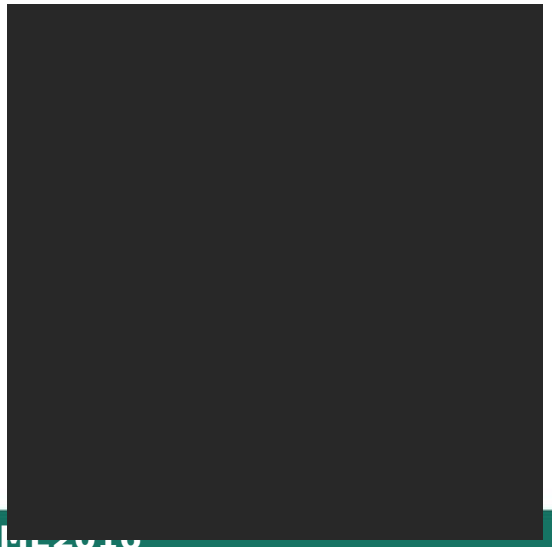
Cellular Automata + Sphere Growth



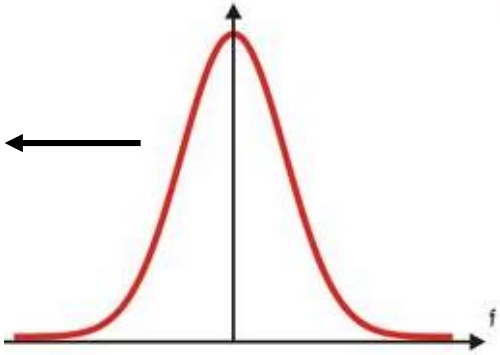




Sphere generation

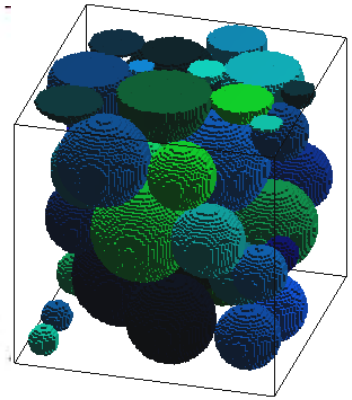


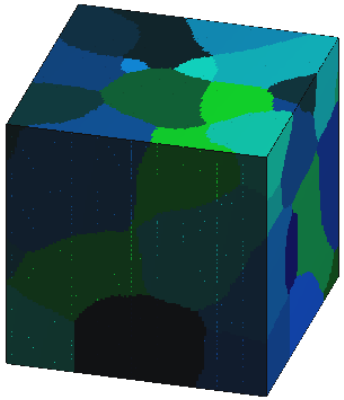
Spheres



R expected

CA sphere growth

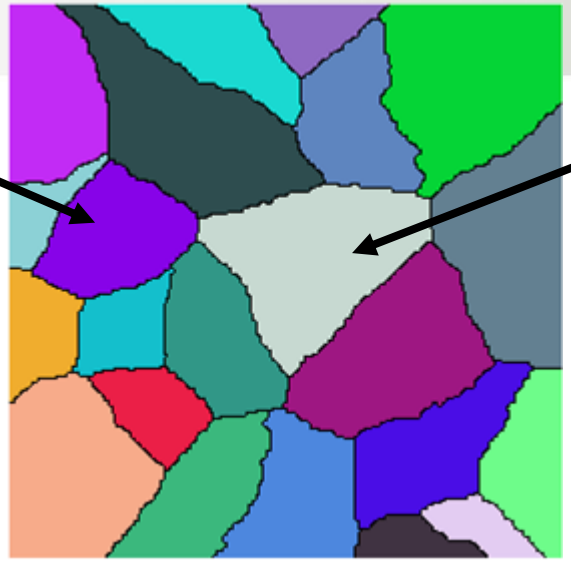




Properties

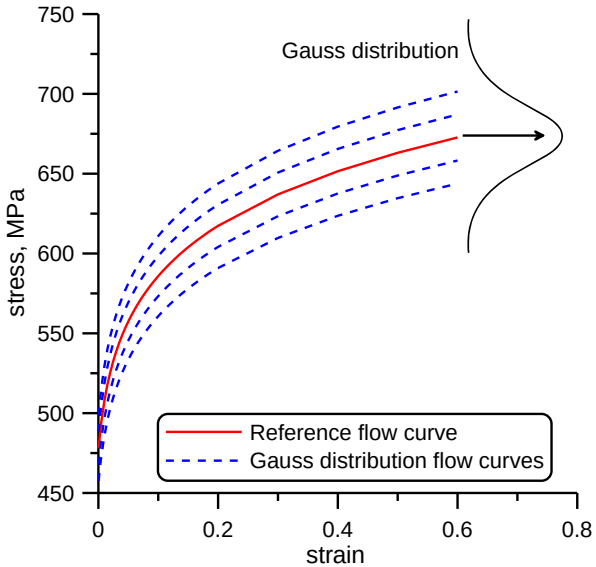
scalar
K

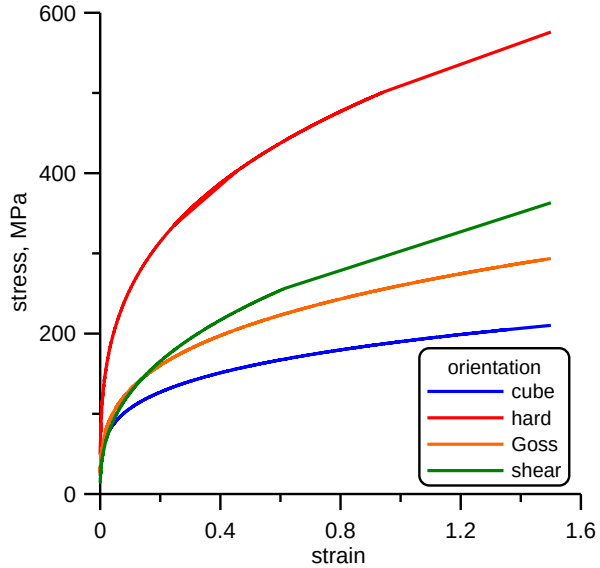
vector
– ϕ, θ, ψ
– K, n, m

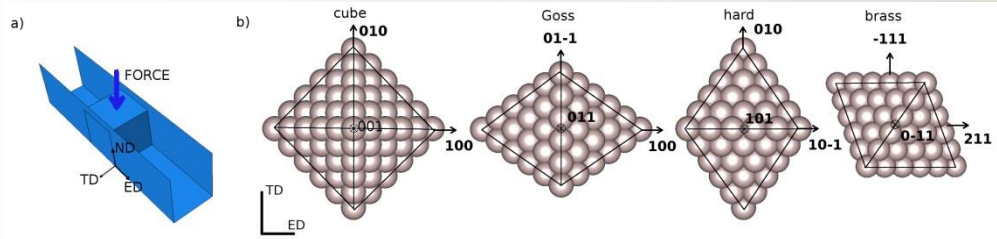


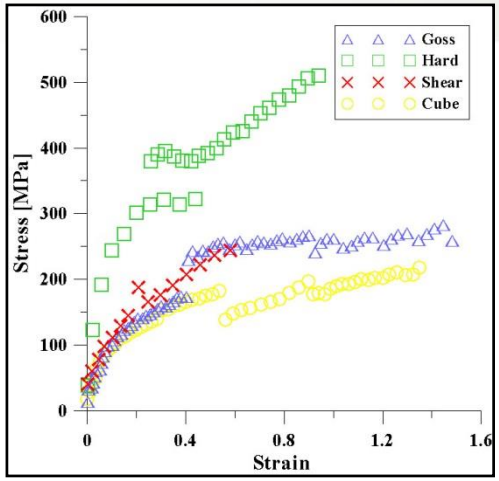
$$\sigma = K\varepsilon^n$$

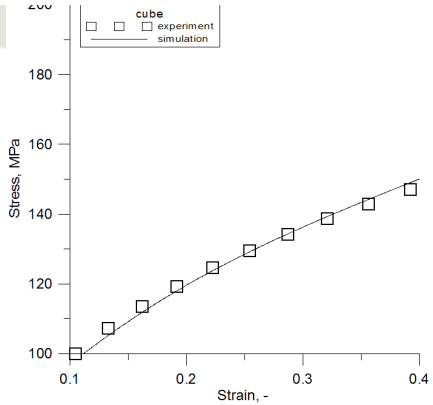
$$\sigma = K\varepsilon^n \dot{\varepsilon}^m$$

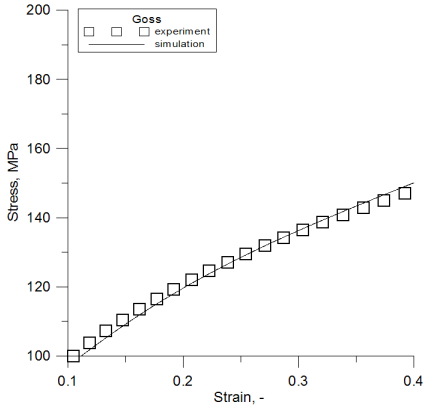


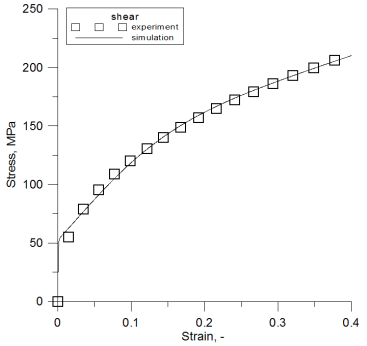


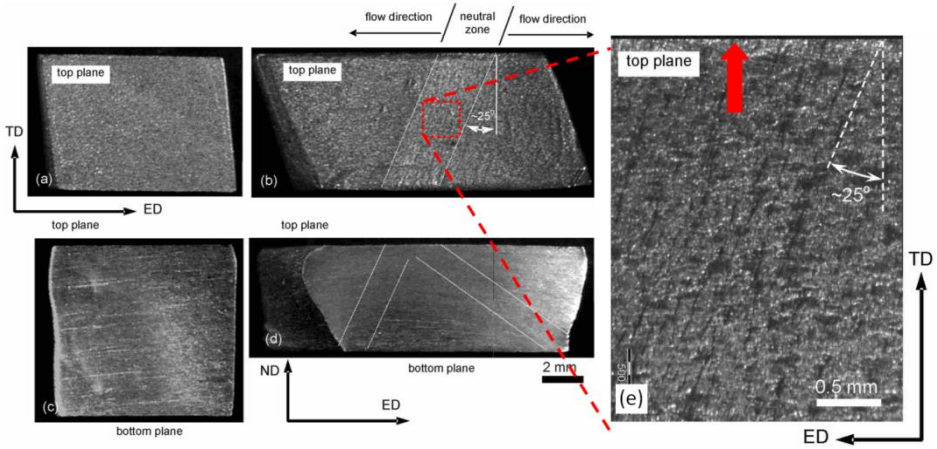










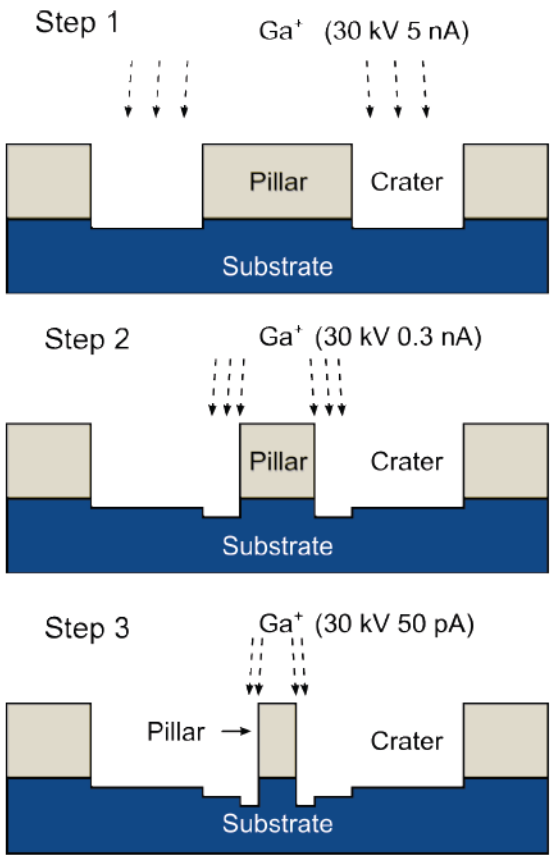


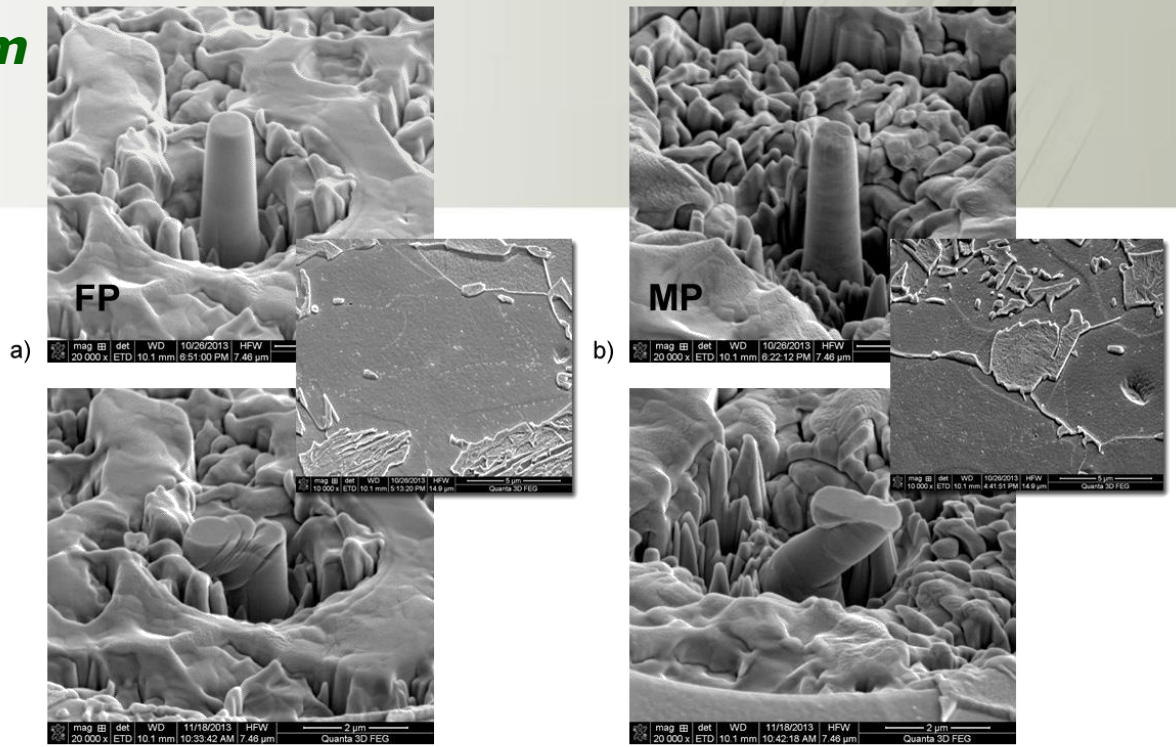
Goal function

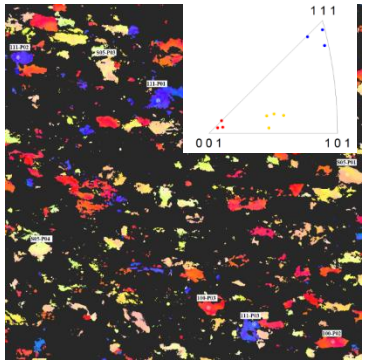
$$Err = \frac{1}{n}\sum_{i=1}^{n}\sqrt{\left(\frac{\sigma_{exp} - \sigma_{sim}}{\sigma_{exp}}\right)^2}$$

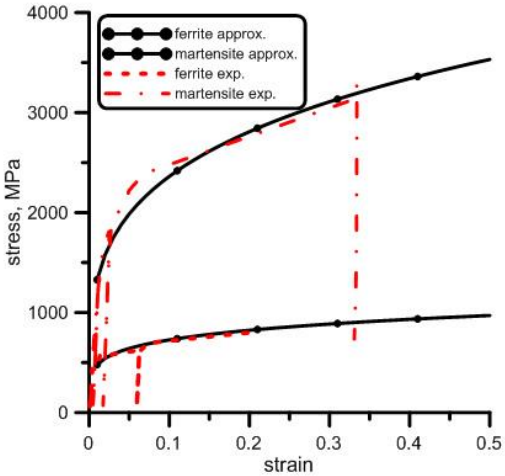
parameter / orientation	$\dot{a}$, s^{-1}	n, -	h_o, MPa	τ_s, MPa	τ_0, MPa	q, -
cube	3.524E-05	1.88	114.11	59.94	5.15	0.0
Goss	1.419E-04	1.19	127.07	49.65	5.57	0.0
shear	1.787E-04	1.03	117.52	49.22	6.04	0.0
average	**1.186E-04**	**1.37**	**119.57**	**52.94**	**5.58**	0.0
std. Dev.	7.450E-05	0.45	6.72	6.07	0.44	-

Focused Ion Beam





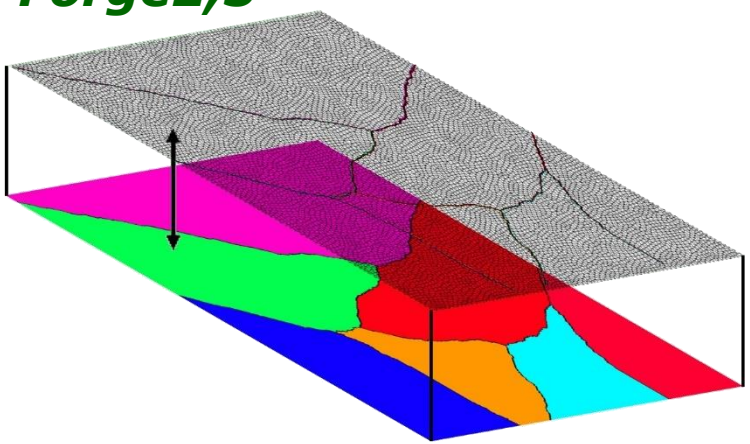


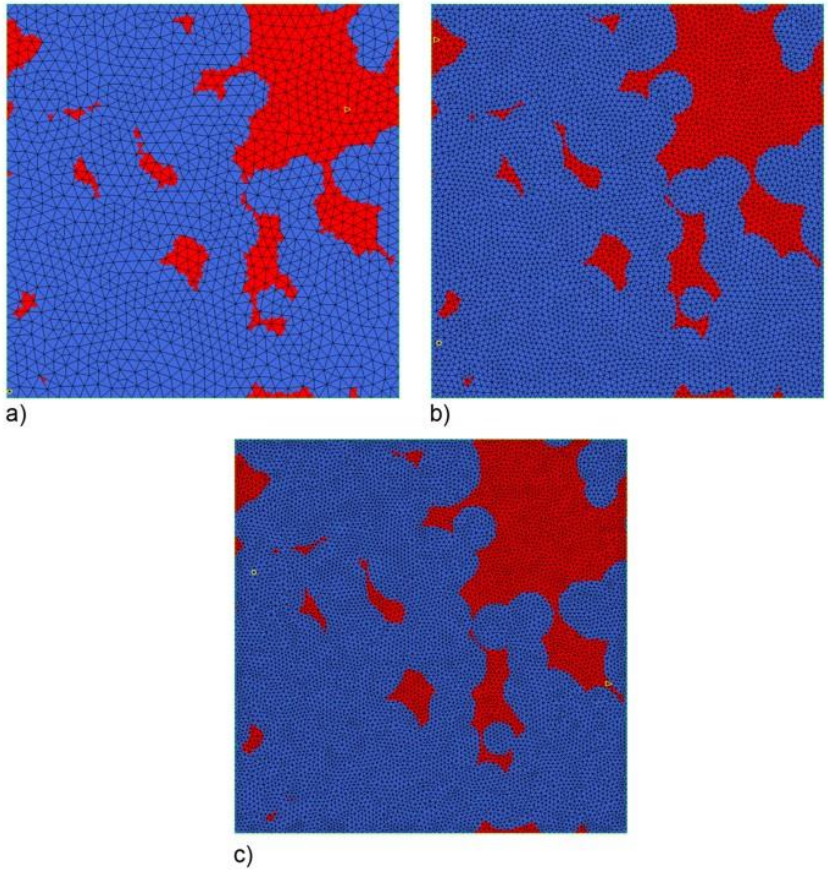


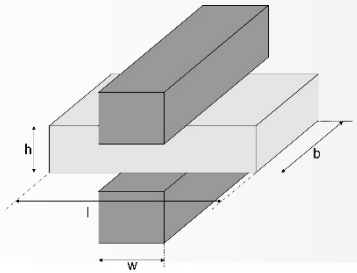
Madej L., Wang J., Perzynski K., Hodgson P.D., Numerical modelling of dual phase microstructure behavior under deformation conditions on the basis of digital material representation, Computational Material Science, 95, 2014, 651–662.

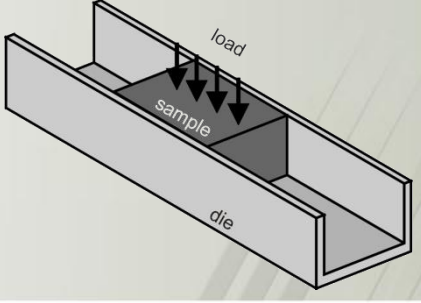
Uniform mesh generation for the DMR

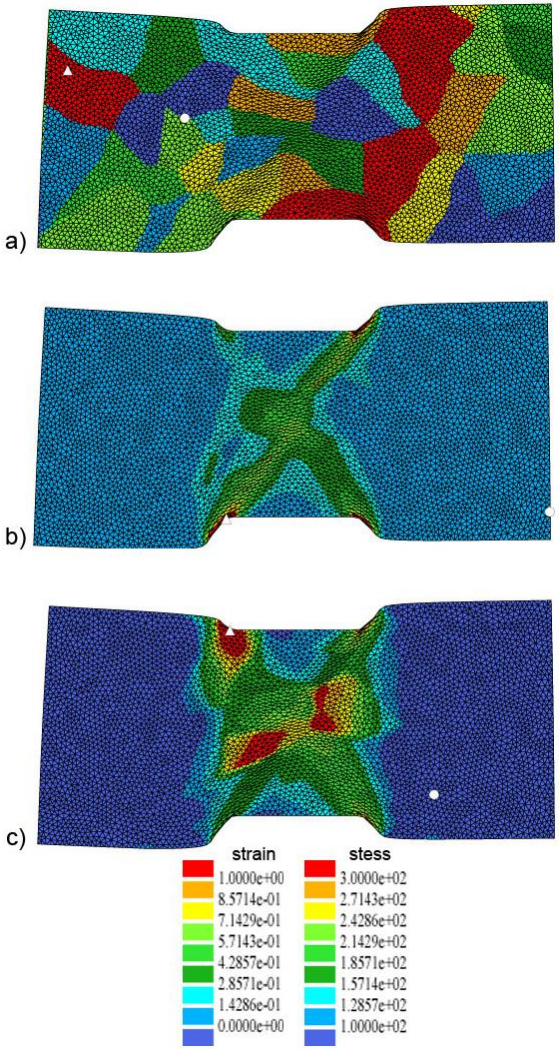
Forge2,3

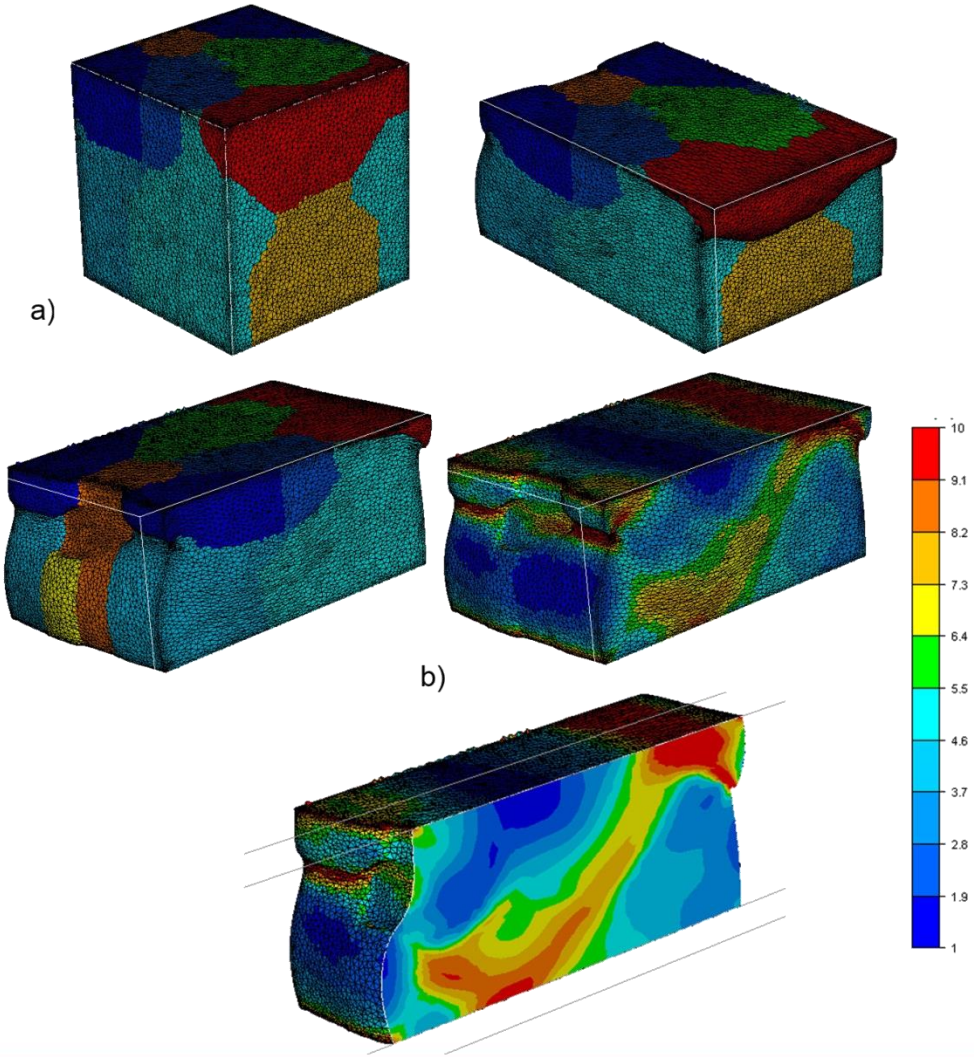





h
b
l
w


load
sample
die

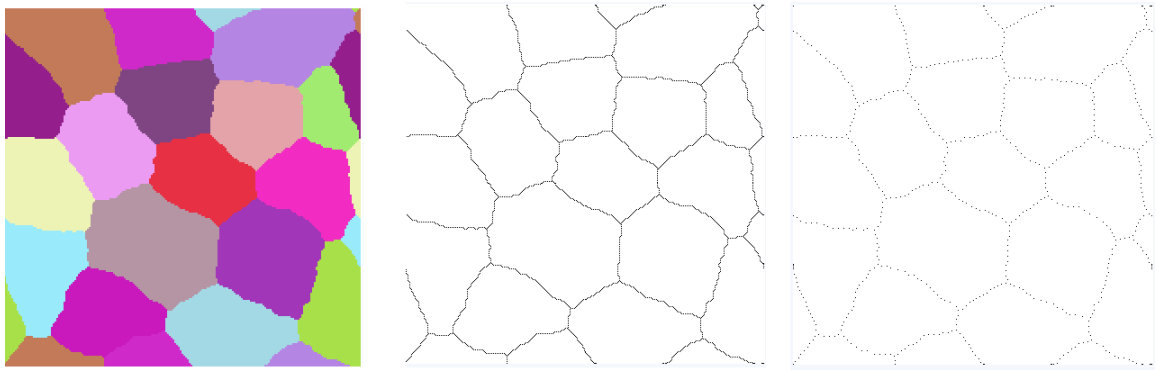

a)
b)
c)
strain
1.0000e+00
8.5714e-01
7.1429e-01
5.7143e-01
4.2857e-01
2.8571e-01
1.4286e-01
0.0000e+00
stess
3.0000e+02
2.7143e+02
2.4286e+02
2.1429e+02
1.8571e+02
1.5714e+02
1.2857e+02
1.0000e+02


a)
b)
10
9.1
8.2
7.3
6.4
5.5
4.6
3.7
2.8
1.9
1

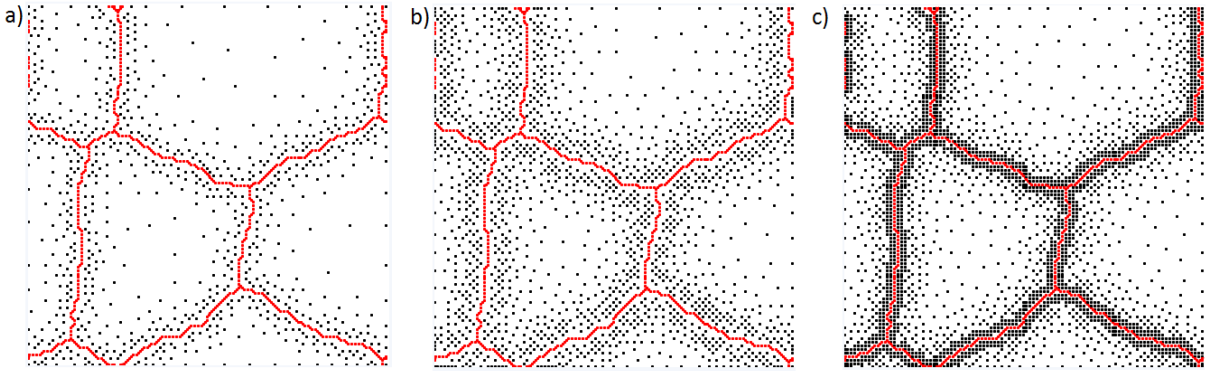
Non-uniform mesh generation for the DMR

1. *Import of the grain boundary geometry.*

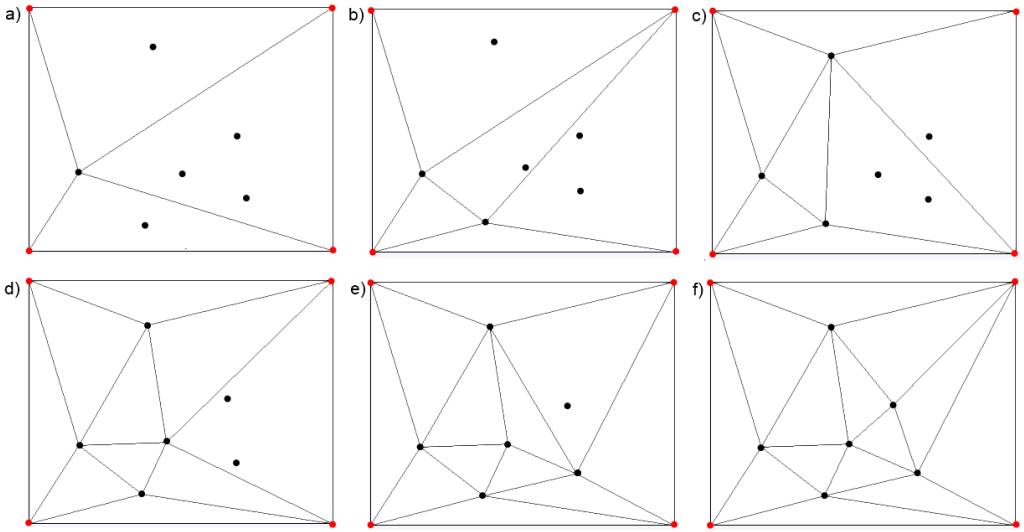
Points located along the grain boundaries are further used during the Delaunay triangulation. This assures generation of the conforming FE mesh.



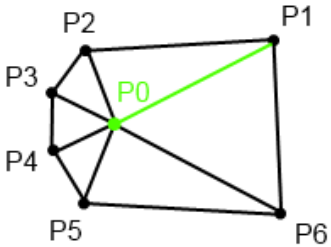
2. Generation of additional points located inside the grain area.



Non-uniform mesh generation for the DMR

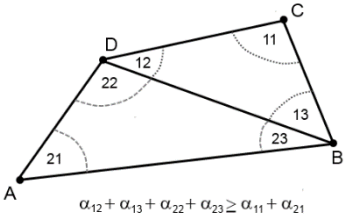


3. Delaunay triangulation on the basis of the available points.

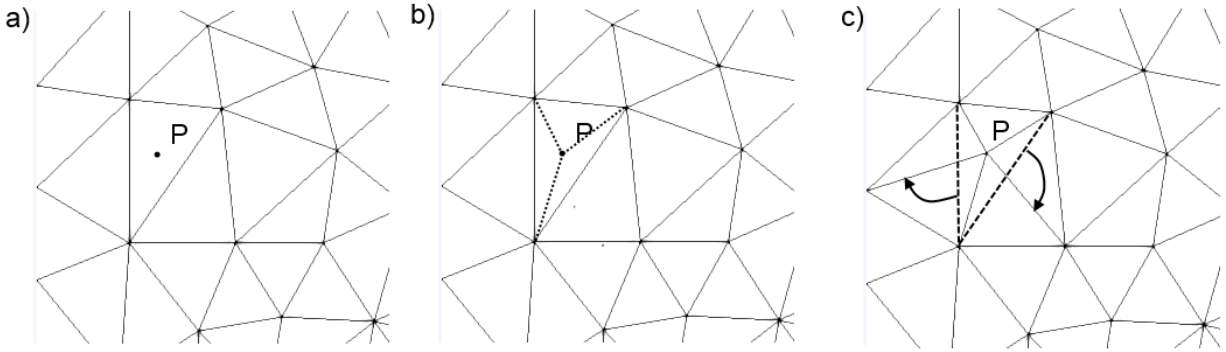


4. Mesh correction

- ***the Laplace smoothing algorithm is applied in order to obtain finite elements with regular shapes.***
- ***edge swaping algorithm***

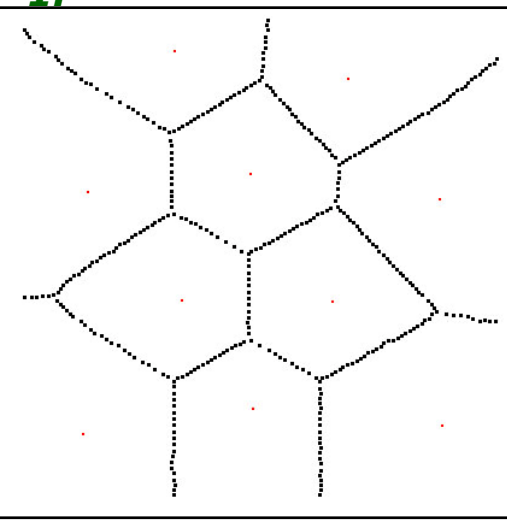


$$\alpha_{12}+\alpha_{13}+\alpha_{22}+\alpha_{23} \geq \alpha_{11}+\alpha_{21}$$

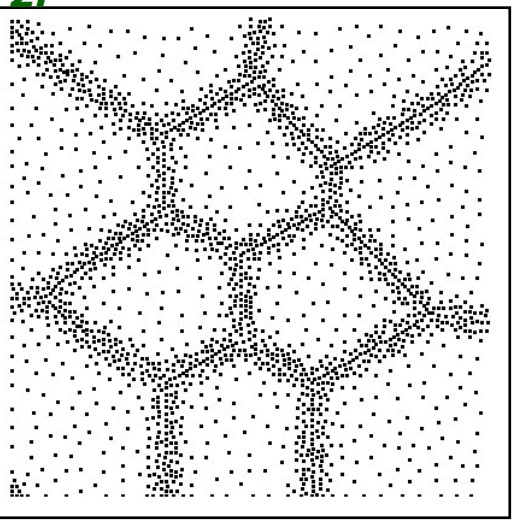


Non-uniform mesh generation for the DMR

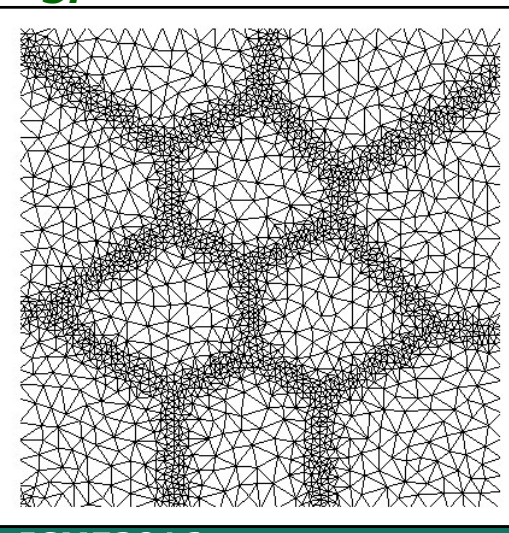
1.



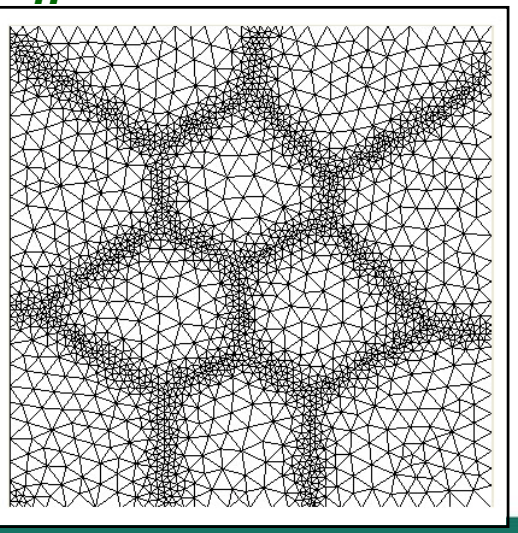
2.



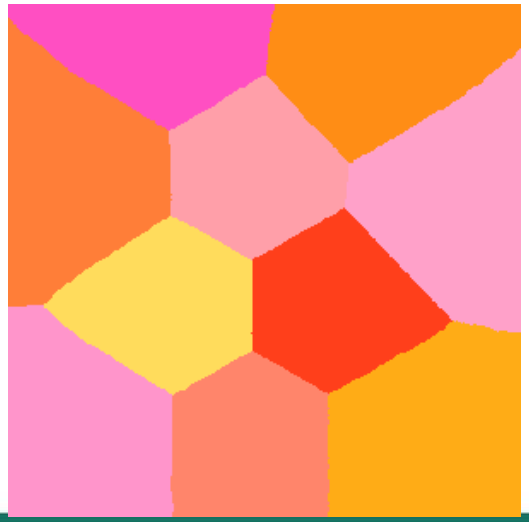
3.



4.



5. Assignment of the finite elements to particular grains.



Plik Edytuj Opcje Kodowanie Pomoc

```
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0 0 1 49
0 0 2 49
0 0 3 49
0 0 4 49
0 0 5 49
0 0 6 49
0 0 7 49
0 0 8 49
0 0 9 49
0 0 10 49
0 0 11 49
0 0 12 49
0 0 13 49
0 0 14 49
0 0 15 49
0 0 16 49
0 0 17 49
0 0 18 49
0 0 19 49
0 0 20 49
0 0 21 49
0 0 22 49
0 0 23 49
0 0 24 49
0 0 25 49
0 0 26 49
0 0 27 49
0 0 28 38
0 0 29 38
0 0 30 38
0 0 31 38
0 0 32 38
```
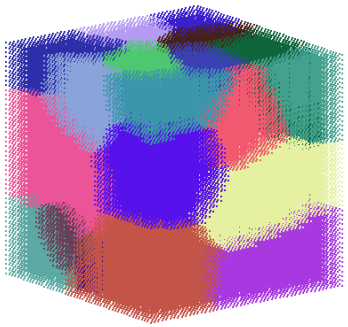

txt

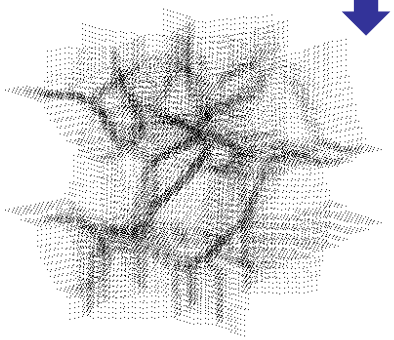
Plik Edytuj Opcje Kodowanie Pomoc

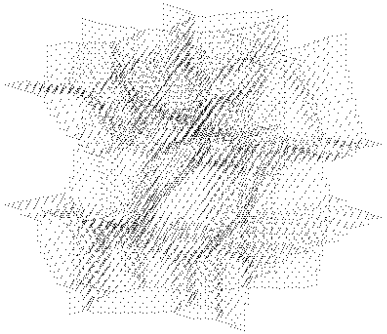
```
# vtk DataFile Version 3.0
t = 36 s
ASCII

DATASET STRUCTURED_POINTS
DIMENSIONS 111 71 71
ORIGIN 0 0 0
SPACING 0.5 0.5 0.5

CELL_DATA 539000

SCALARS korn int
LOOKUP_TABLE default
 2 2 2 2
 2 2 2 2
 2 2 2 2
 2 2 2 6
 6 6 14 14
 14 14 14 14
 14 14 14 14
 25 25 25 25
 25 25 25 25
 25 25 25 25
 25 40 40 40
 40 56 56 56
 56 56 56 56
 56 56 56 56
 56 56 56 56
 56 56 56 56
 56 56 80 80
```

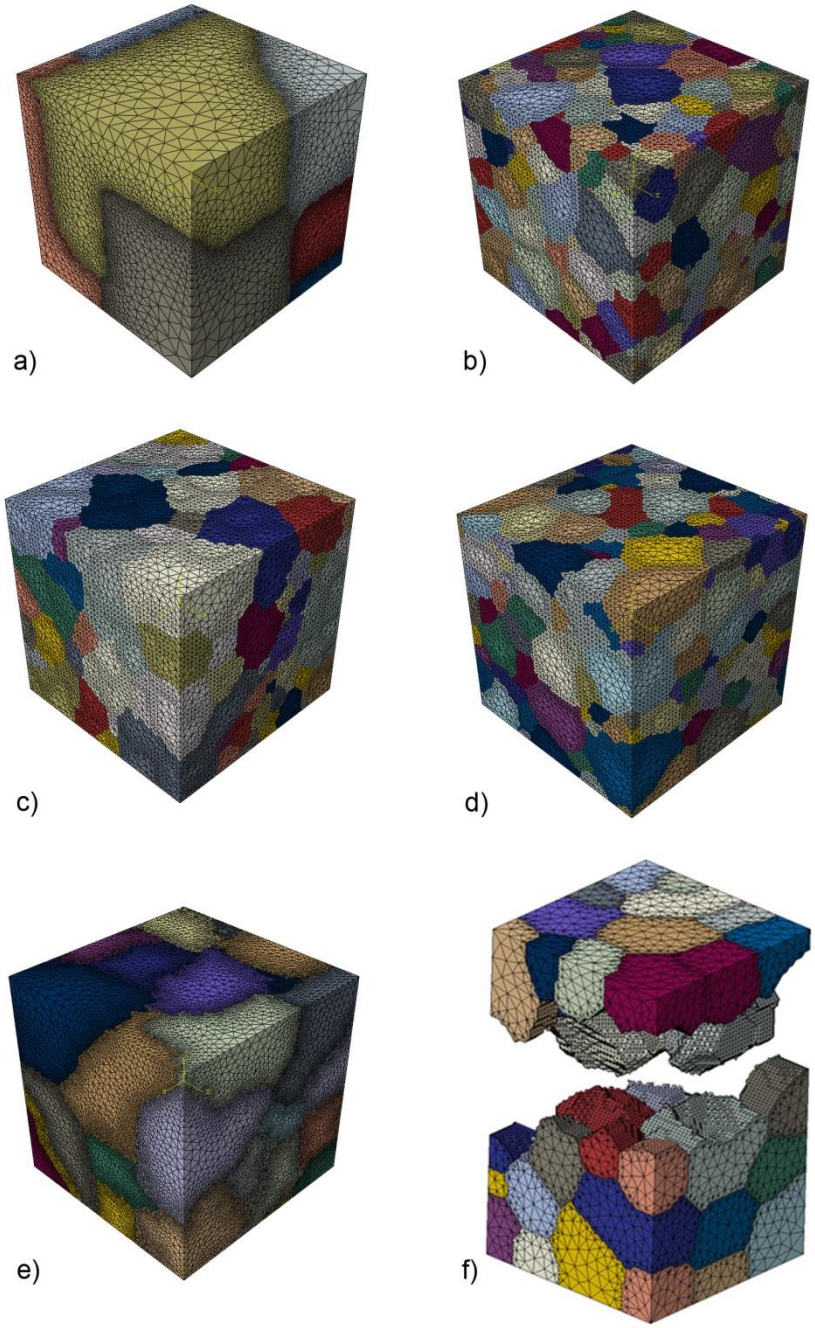
vtk

micress®







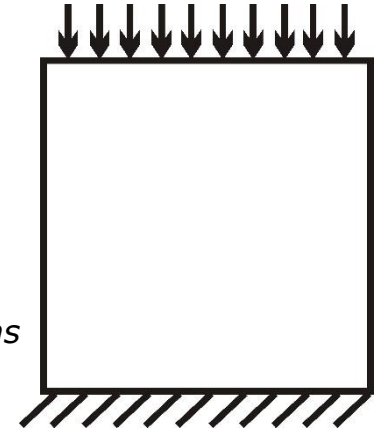


Local mesh refinement and adaptation

Zienkiewicz-Zhu error indicator

$$e_\sigma^* = \sigma^* - \sigma_h$$

$$\|e\| = \sqrt{\int_\Omega e_\sigma^T D^{-1} e_\sigma \, d\Omega}$$

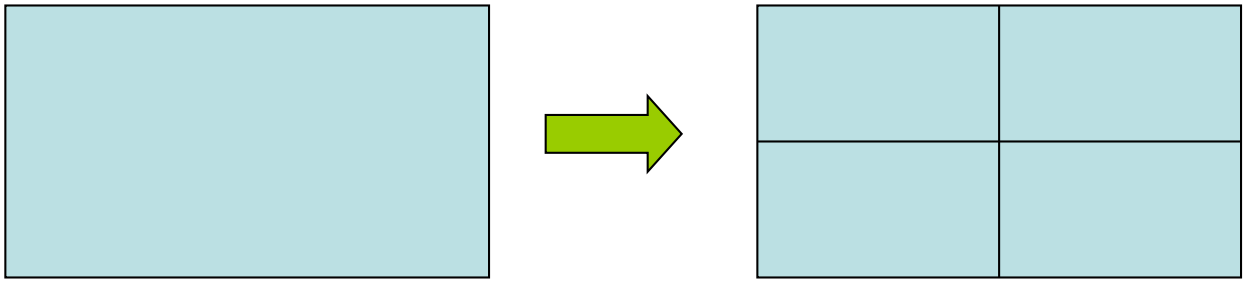


σ^* *recovered stress tensor*

σ_h *standard stress tensor computed using derivatives of shape functions*

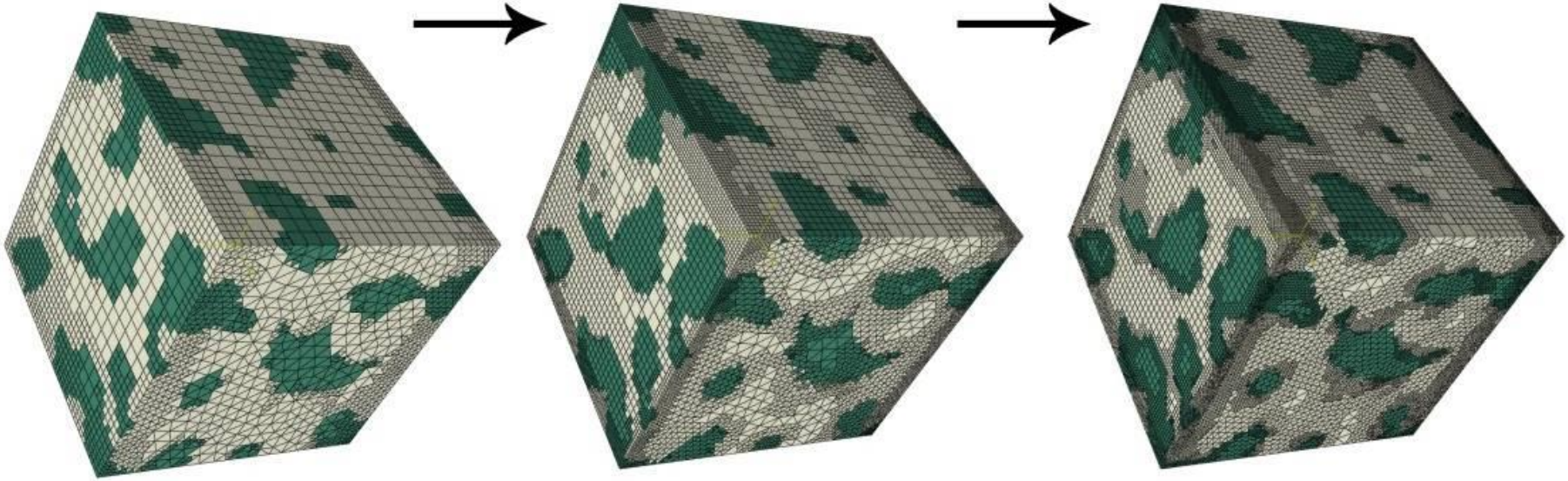
$\boldsymbol{D}$ *elasticity matrix with material constants*

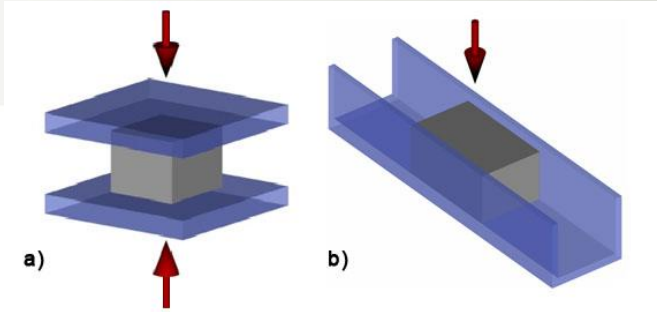
Refinement with geometrical similarity - Child elements are similar to parent element

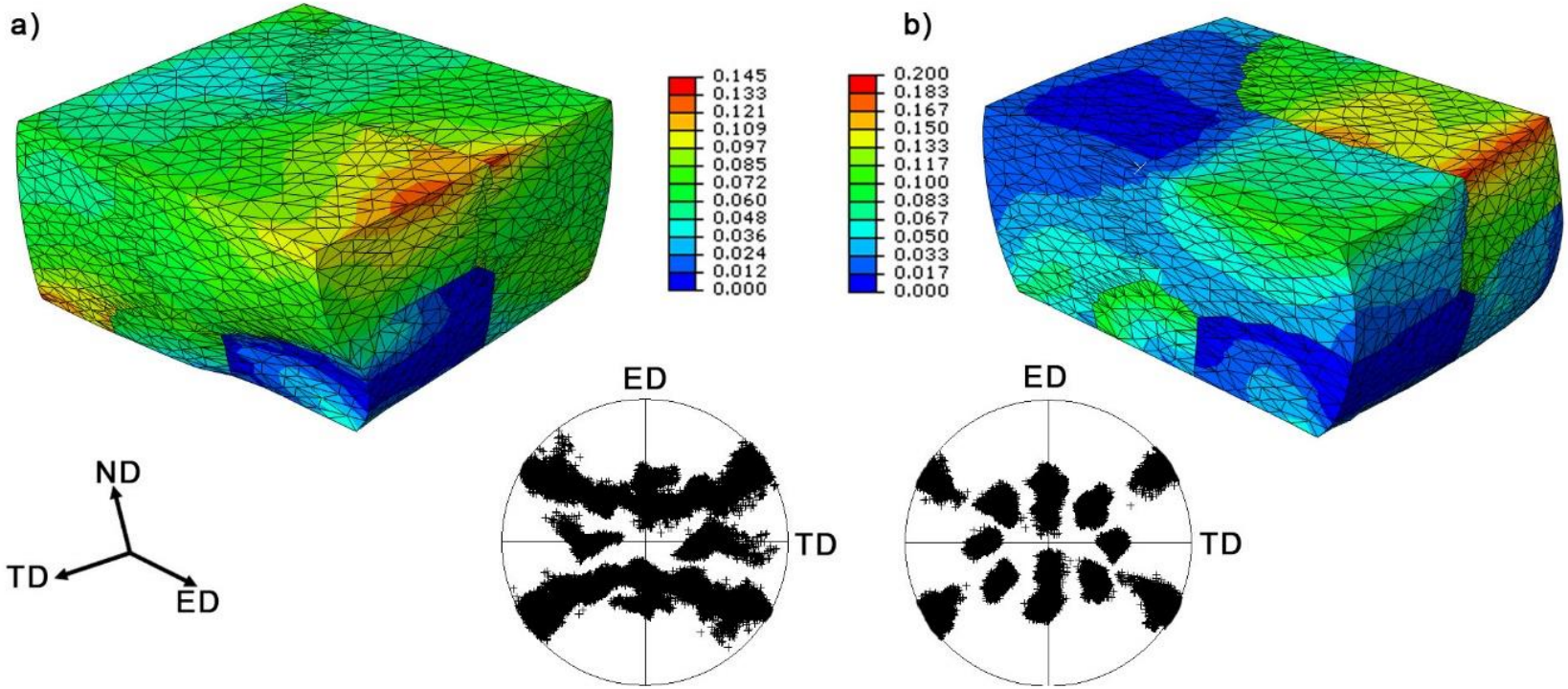


Local mesh refinement and adaptation

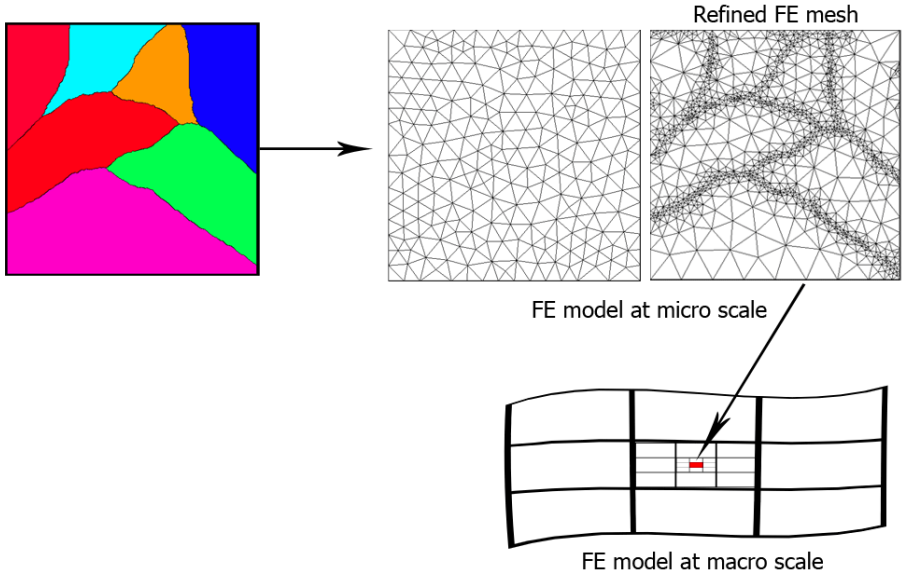
Kruzel F., Madej L., Perzynski K., Banas K., Development of 3D adaptive mesh generation for multi scale applications, International Journal for Multiscale Computational Engineering.




a)
b)

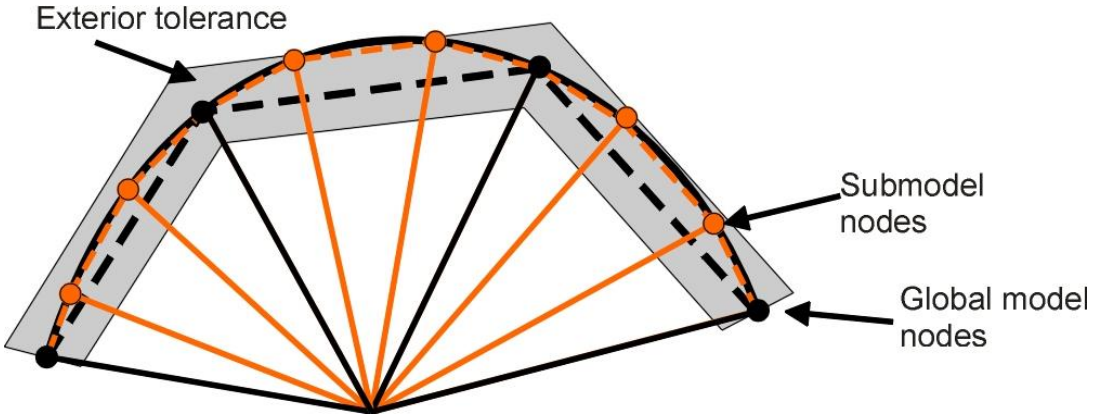

a)
b)
0.145
0.133
0.121
0.109
0.097
0.085
0.072
0.060
0.048
0.036
0.024
0.012
0.000
0.200
0.183
0.167
0.150
0.133
0.117
0.100
0.083
0.067
0.050
0.033
0.017
0.000
ND
TD
ED
ED
TD
ED
TD

Heterogeneous FE mesh – multi scale model

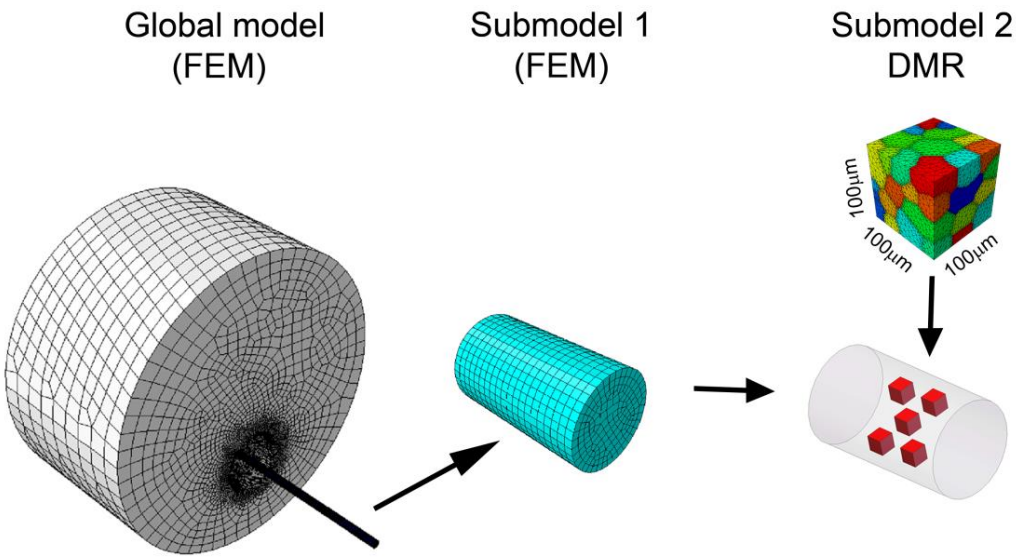


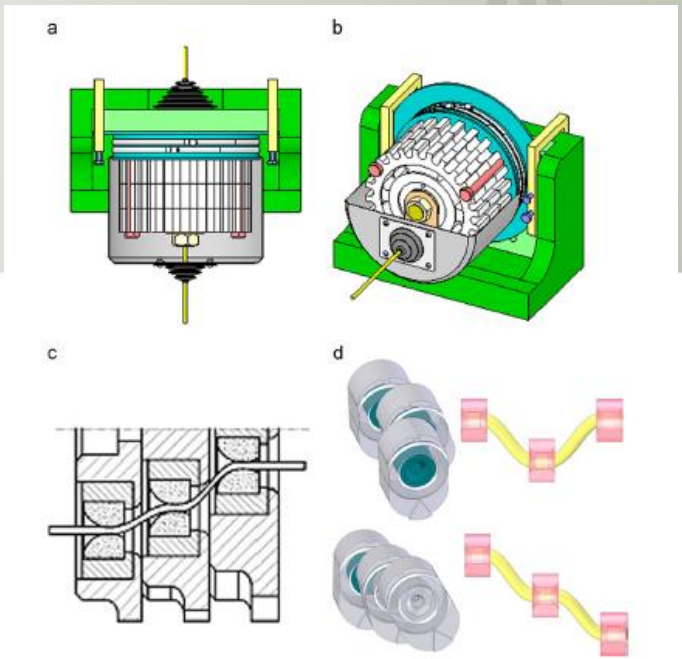
The key aspect in this approach is to ensure that an accurate partitioning strategy is used in the global model for extracting the steady state boundary conditions to be imposed to the sub-model

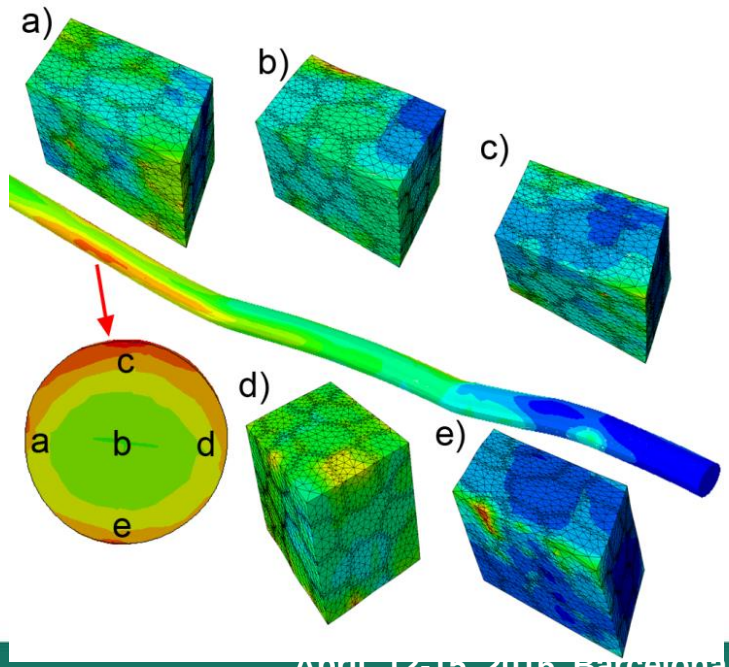
Transfer of the displacement boundary conditions taken from the global simulation into the submodel



Numerical simulation of drawing process

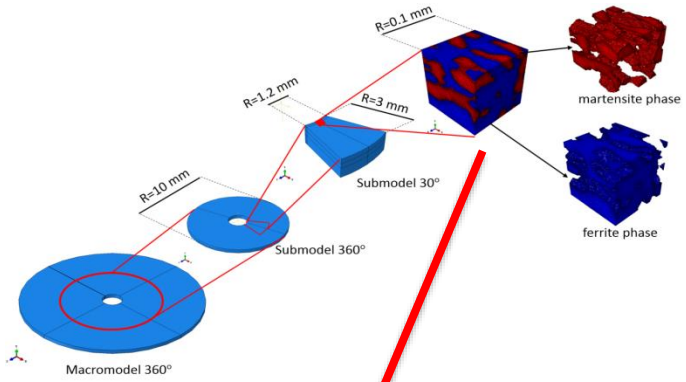


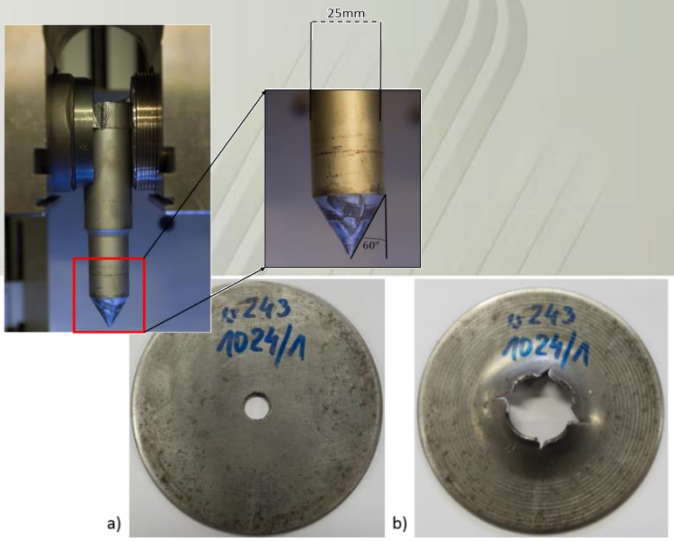




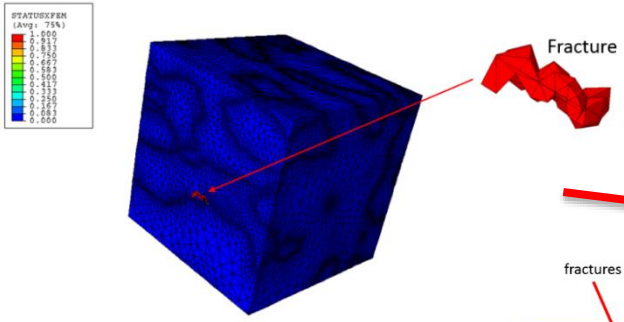
Muszka K., Madej L., Majta J., The effects of deformation and microstructure inhomogeneities in the Accumulative Angular Drawing (AAD), Materials Science and Engineering A, 574 , 2013, 68–74.

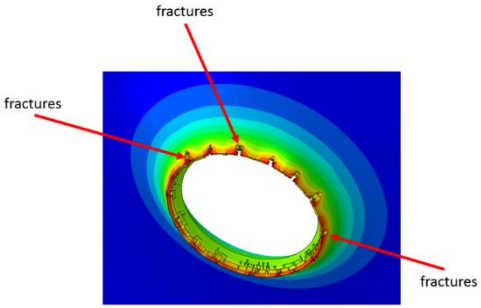
Hole Expansion Test
Brittle-ductile fracture modelling



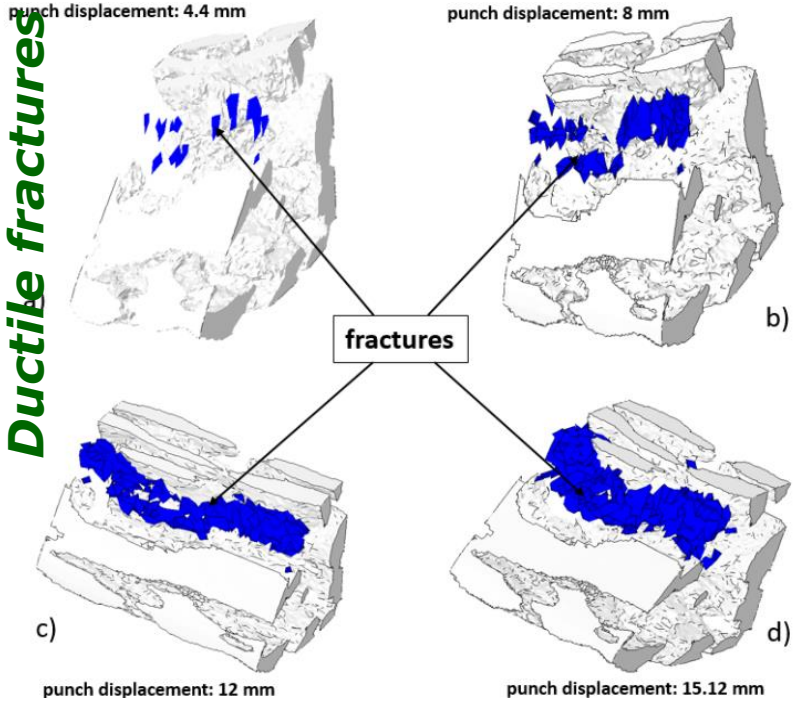


Brittle fractures



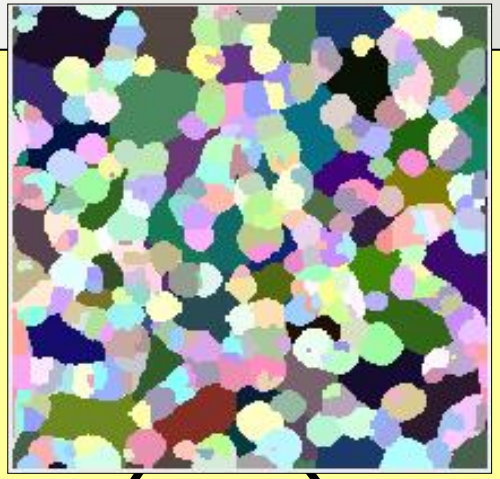


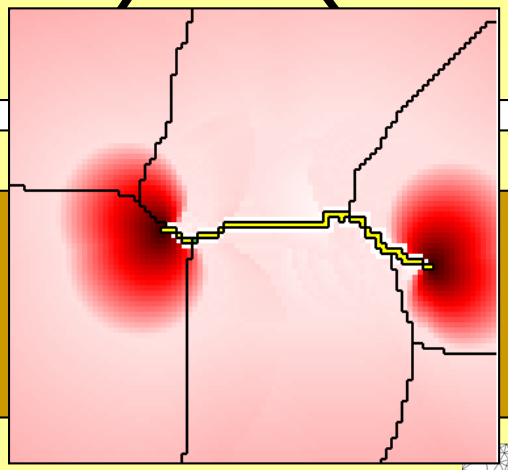
Ductile fractures



Microstructure generation

FE mesh generator

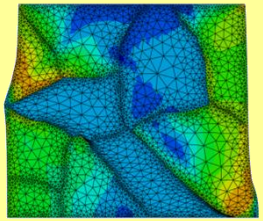




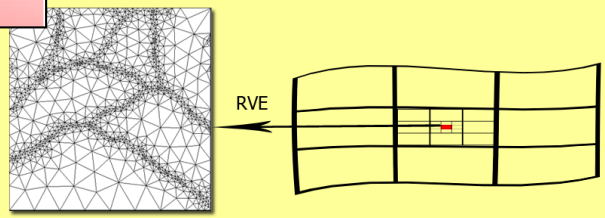
CA model:
-DRX
-Phase transformation
-Fracture
-Strain localization
-etc.

Crystal plasticity

Micro scale modeling



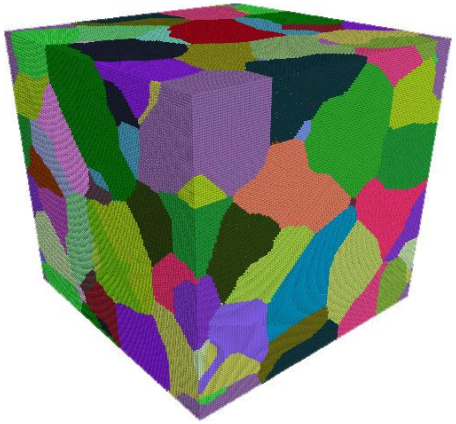
Multi scale modeling



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,



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home.agh.edu.pl/lmadej