Virtual microstructure generation using Voronoi tessellation

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WF Institute Seminar

19 September, 2016

Motivation

- Microstructure modelling are required for a quantitative understanding of microstructure-property correlation

- To achieve this goal, one requires digital microstructures as an input for computational analysis (for example, for FE analysis)

- Digital microstructure can be obtained
  - From 3D computed tomography:
    - (+) meets the reality, captures the microstructural complexity
    - (-) deterministic, not always representative to the macroscopic samples
    - (-) costly and time consuming

Motivation

- An equivalent (or approximated) virtual microstructure from mathematical algorithms:
  - (+) approximated microstructure that meets the real statistics
  - (+) can be representative, flexible to generate, cost and time efficient
  - (-) not all microstructural complexity can be captured
  - (-) requires trials to get the real statistics
- A powerful mathematical tool for microstructure generation is VORONOI cells using those mathematical algorithms. Commonly used for polycrystalline alloys.
- In many cases, these mathematical tools can be used as an alternative to the 3D computed tomography approach

Voronoi based modelling - My history

From year 2007-2010:

Micromechanical Modelling of deformation for TiAl alloy (MTU Project)

- Using multiscale framework
- Crystal plasticity constitutive model

From year 2010 – 2015

Developing ideas and providing solutions for

- Size effect in CPFEM for different lamellar thickness
  - Use of strain gradient plasticity
- Simulation of Nanoindentation for grain scale property prediction
- Fracture of TiAl in multiscale framework
  - Using cohesive and XFEM
- <u>Microstructure modelling of TiAl to simulate CREEP (In MTU's interest)</u>

How to generate virtual microstructure for TiAl ??

Voronoi based modelling - My history

European Structural Integrity Society (ESIS) Joint Meeting of TC 1 and TC 8

Berlin 14-15 June 2012

11.30 Barbe, F. (INSA Univ. Rouen, Dept. Mécanique, France): Crystal plasticity based micromechanical local approach to cleavage fracture in bainite polycrystals.

Neper polycrystal generator

Open Source (https://sourceforge.net/projects/neper/)

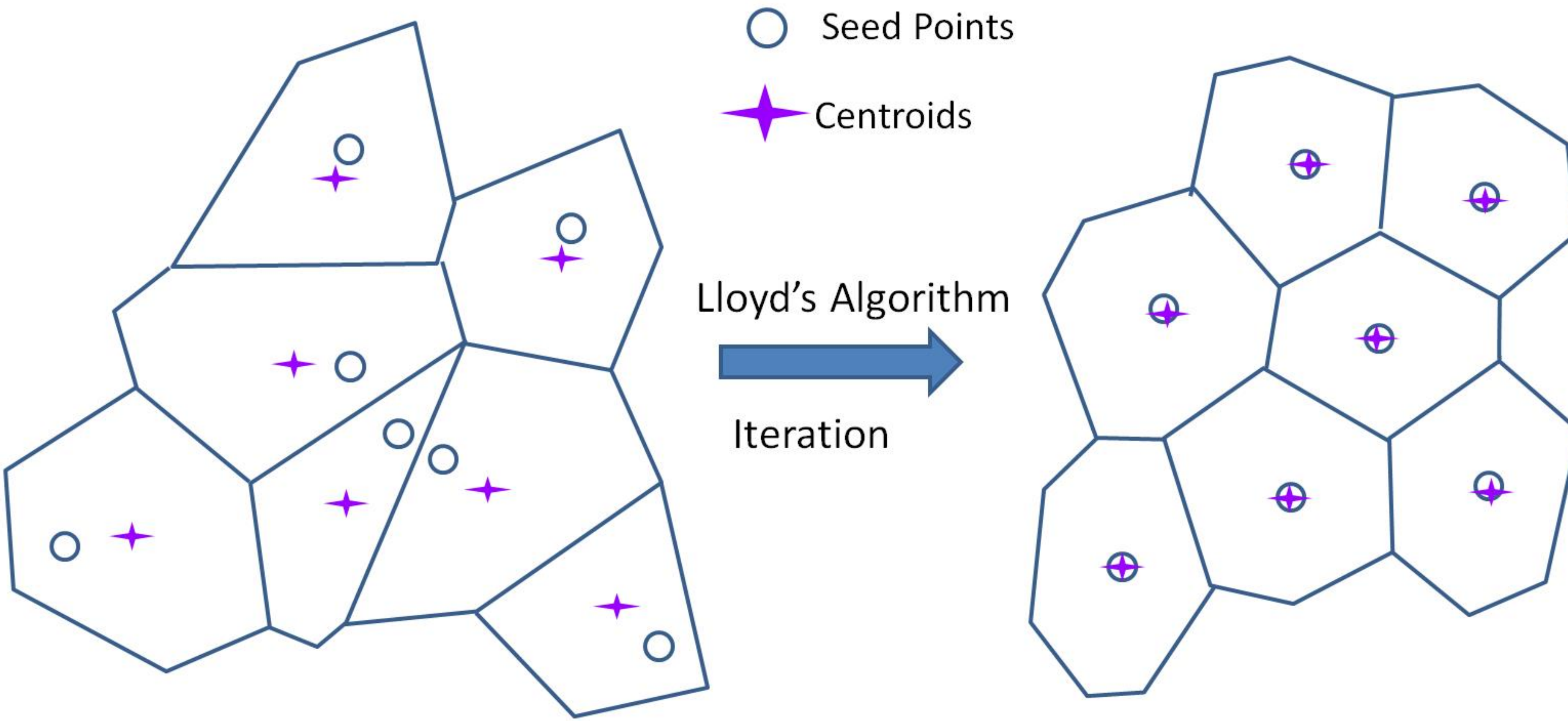
User Guidelines

If you use Neper for your own work, please,

- mention it explicitly in your reports (books, papers, talks, . . .).
- cite the following paper: *R. Quey, P.R. Dawson, F. Barbe. Large-scale 3D random polycrystals for the finite element method: Generation, meshing and remeshing. Computer Methods in Applied Mechanics and Engineering, vol. 200, pp. 1729–1745, 2011.*

Basics of Voronoi tessellations

Voronoi Tesselation – Centroidal Voronoi



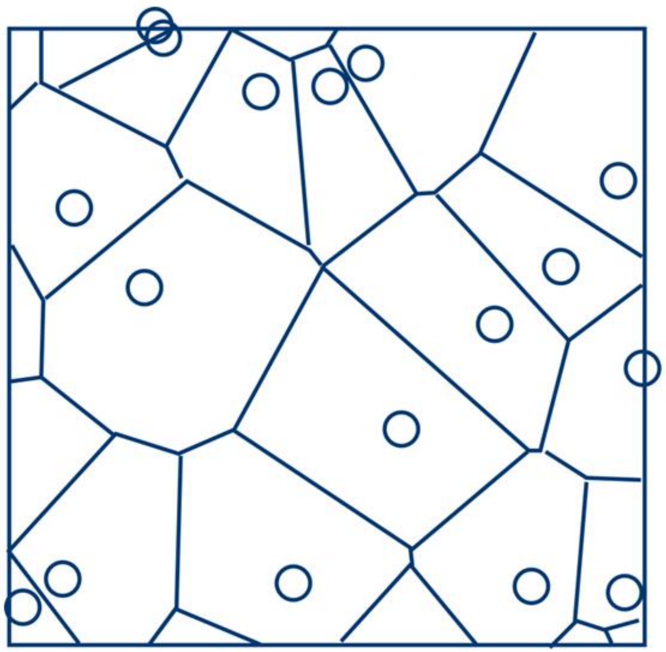
Voronoi

Centroidal voronoi

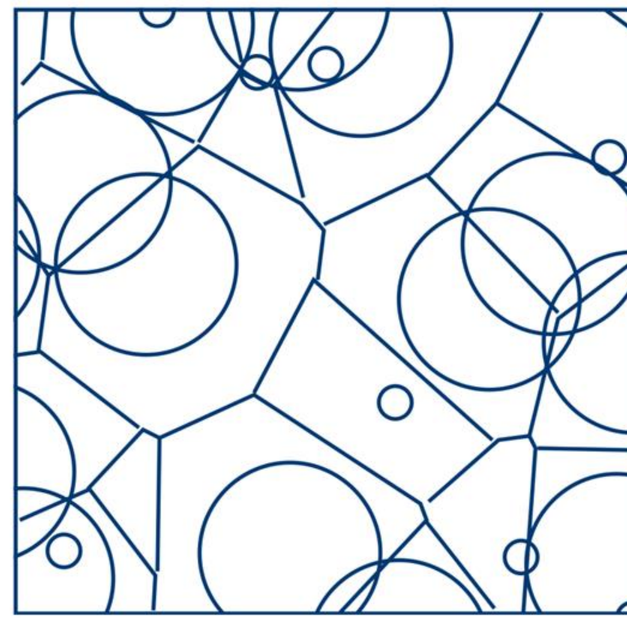
Voronoi Tessellation – Laguerre Tessellation

Seed Points

- Assign weight to the Seed
- Calculate power-distance of the seeds
  (Radius of circle at that seed)
- Cut through circle intersections

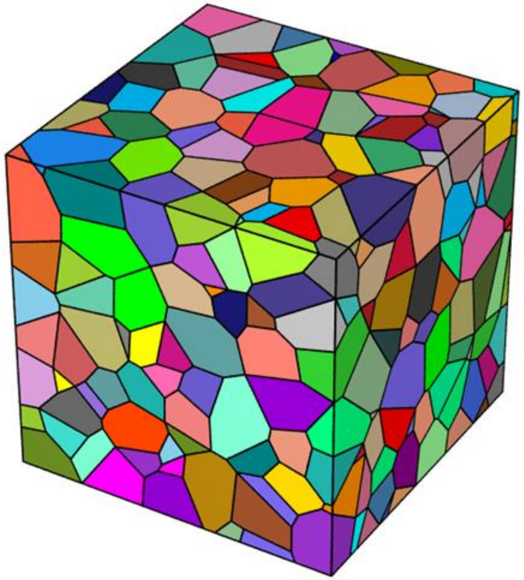


Voronoi



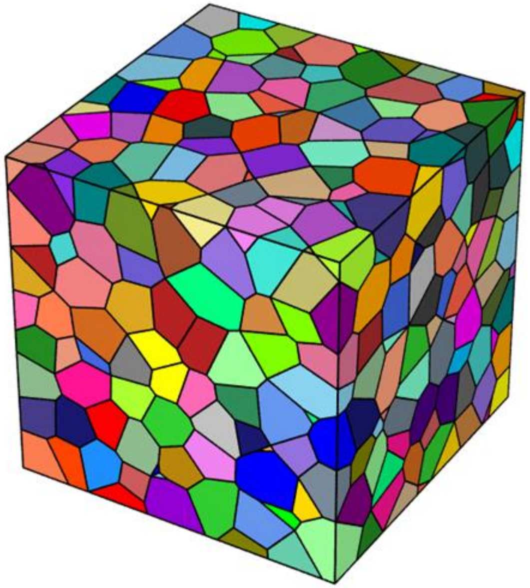
Laguerre

Neper polycrystal examples



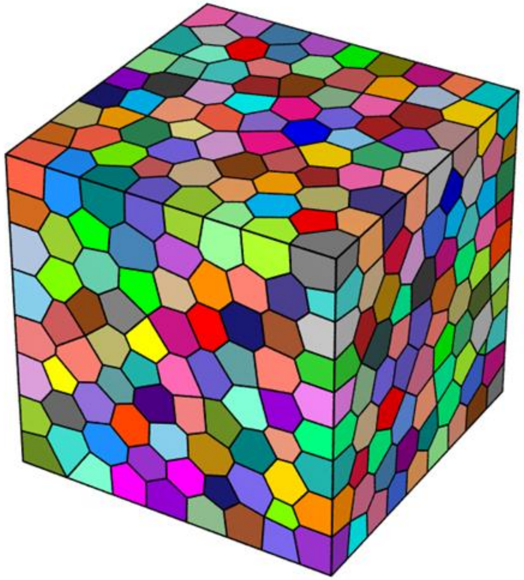
Poisson Voronoi

Seed positions are random



Hardcore Voronoi

Exists a non-zero minimum distance between the seeds.

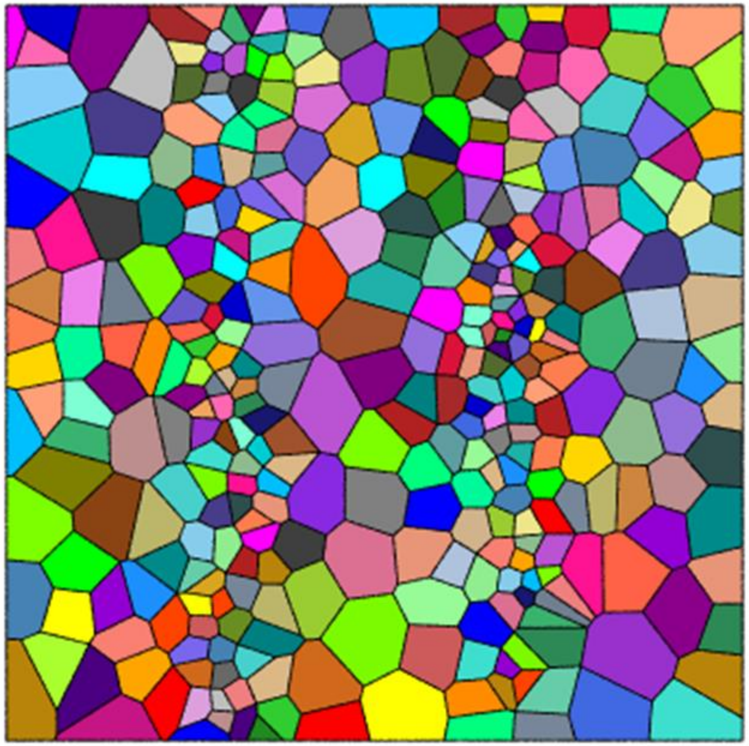


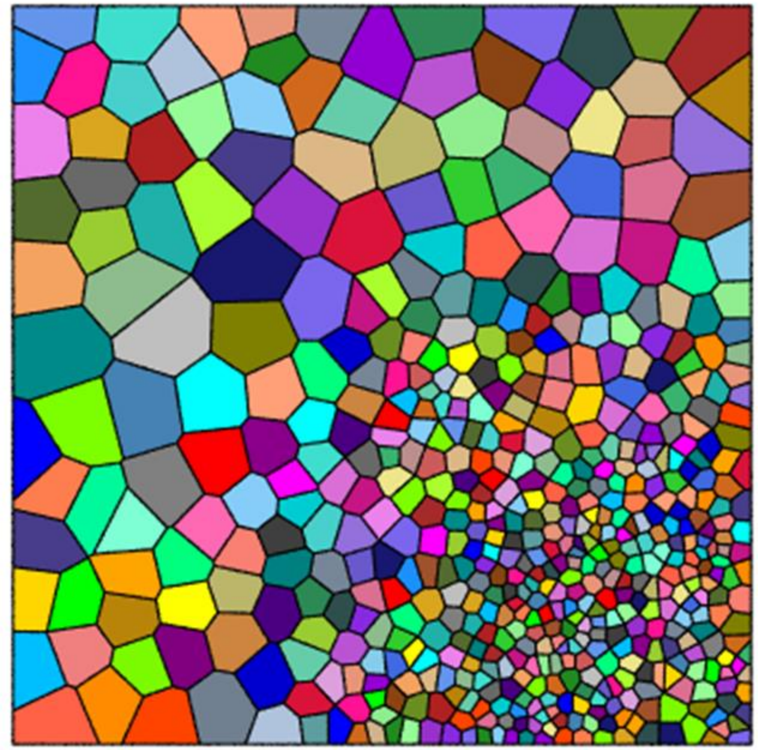
Centroidal Voronoi

Seeds and centroids coincide

Target microstructure using Neper

Grain Cluster (domain based seeds)



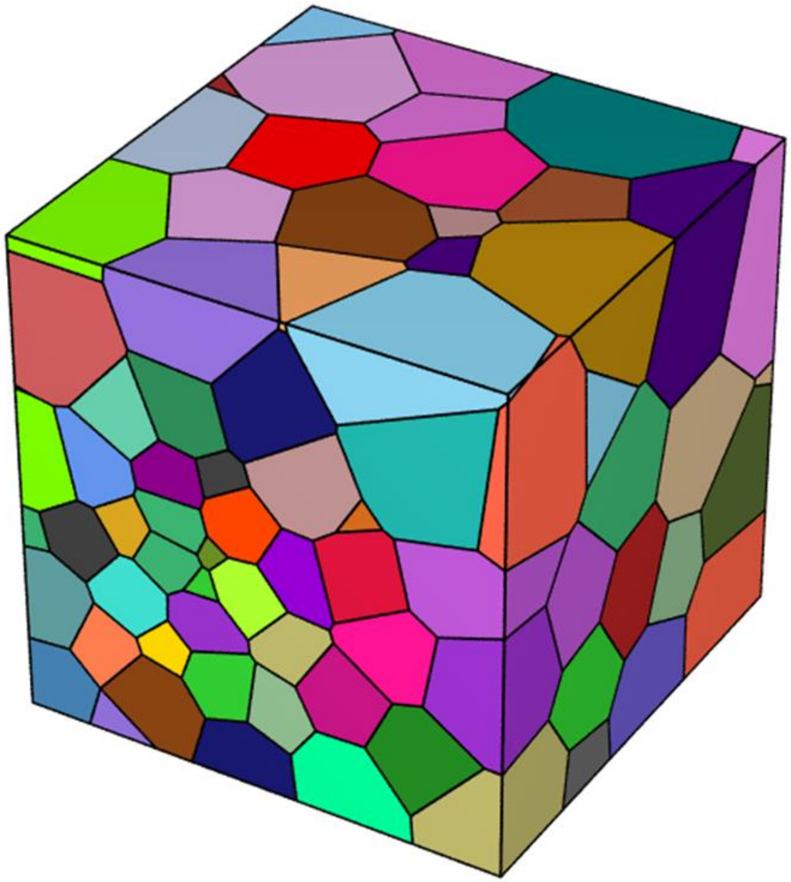


Procedure followed:

- Manipulate seed density
- Mix hardcore and centroidal voronoi

Grain cluster (Bi-modal seed distribution)

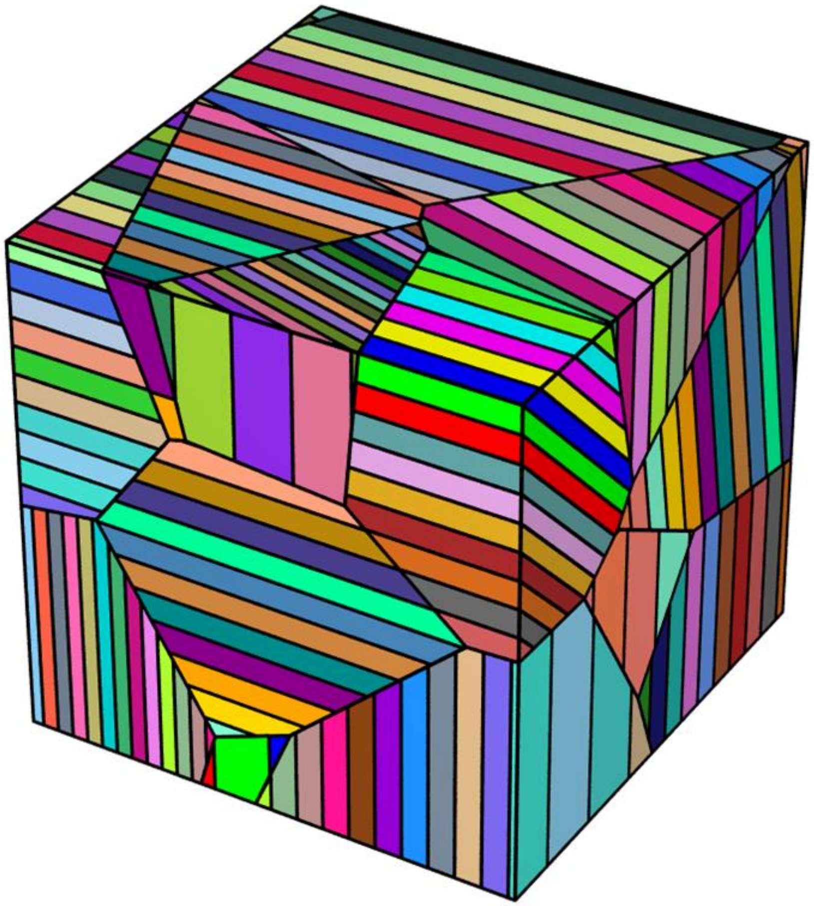
Seeds generated using MATLAB by Henning Richter



Procedure followed:

- Replace original seeds by external seeds
- Use Lloyd algorithm to control the distance between seeds and centroids

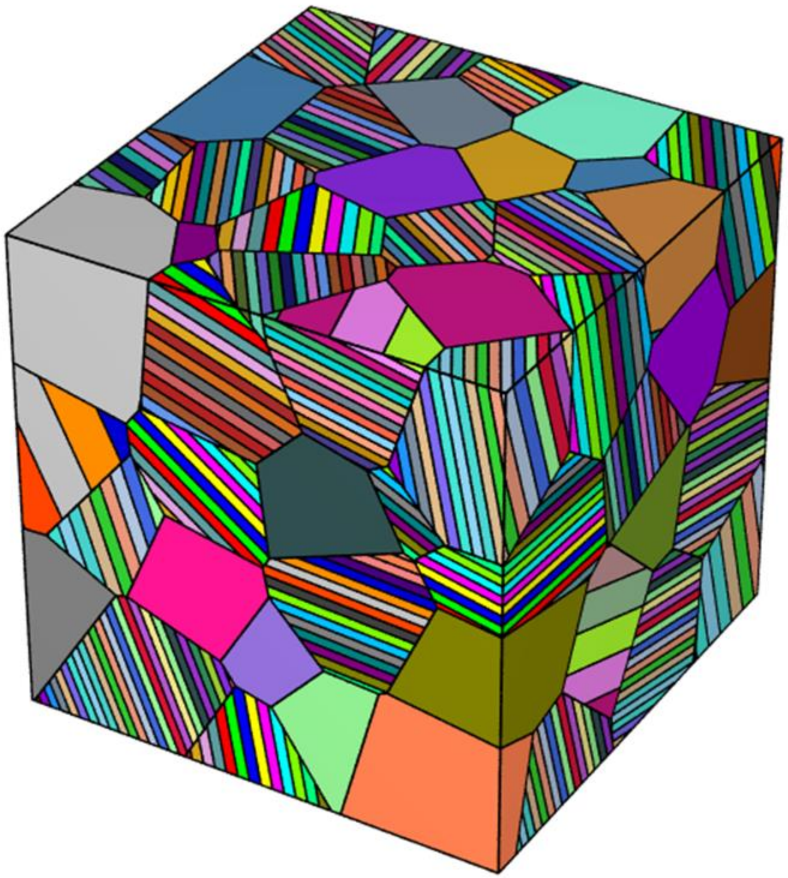
Lamellar microstructure



Procedure followed:

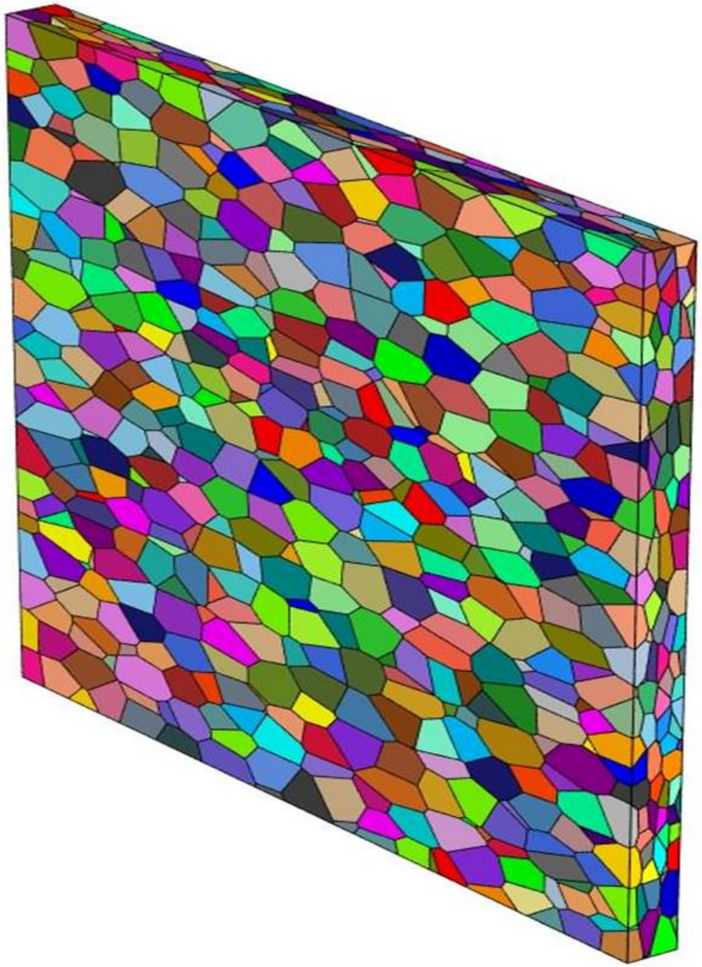
- Generate cells with random seeds
- For each cell define lamellar thickness and lamellar normal

Duplex microstructure



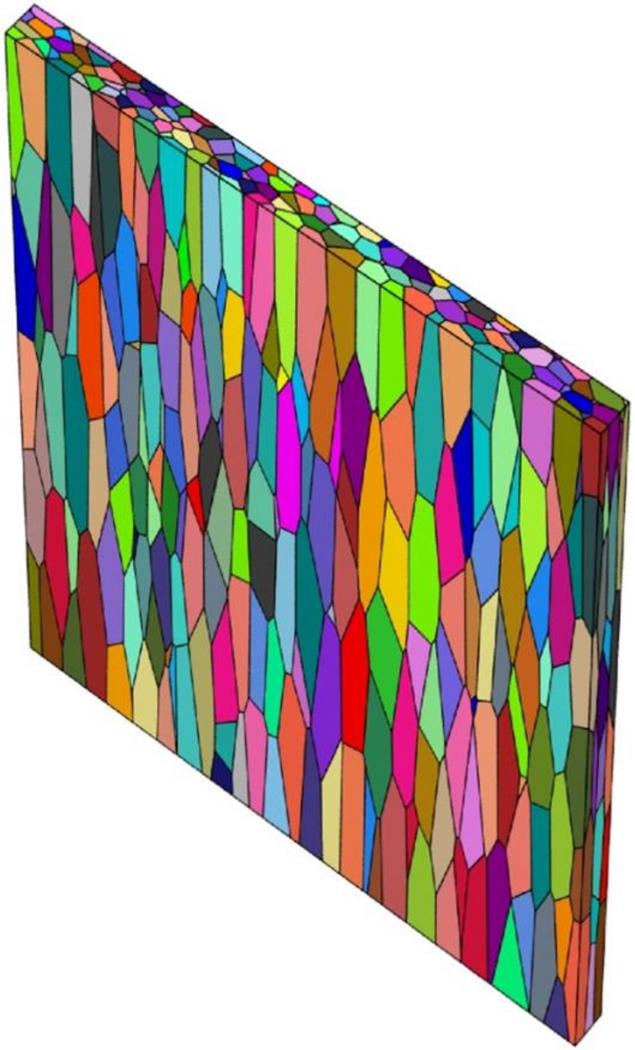
Procedure followed:
- Generate cells with random seeds
- Only for selected cells define lamellar thickness and lamellar normal

Equiaxed grains (cast/forged microstructure)



Procedure followed:
- Use hardcore voronoi
- Control edge length size
- Define grain aspect ratio

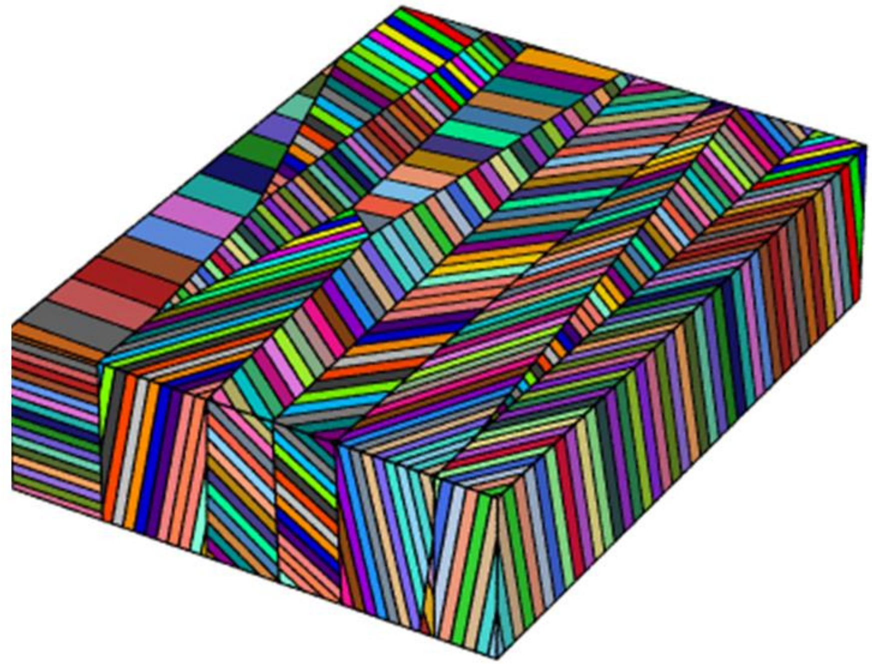
Elongated grains (Extruded Microstructure)



Procedure followed:
- Use hardcore voronoi
- Define grain aspect ratio
- Translate coordinates along x/y/z direction

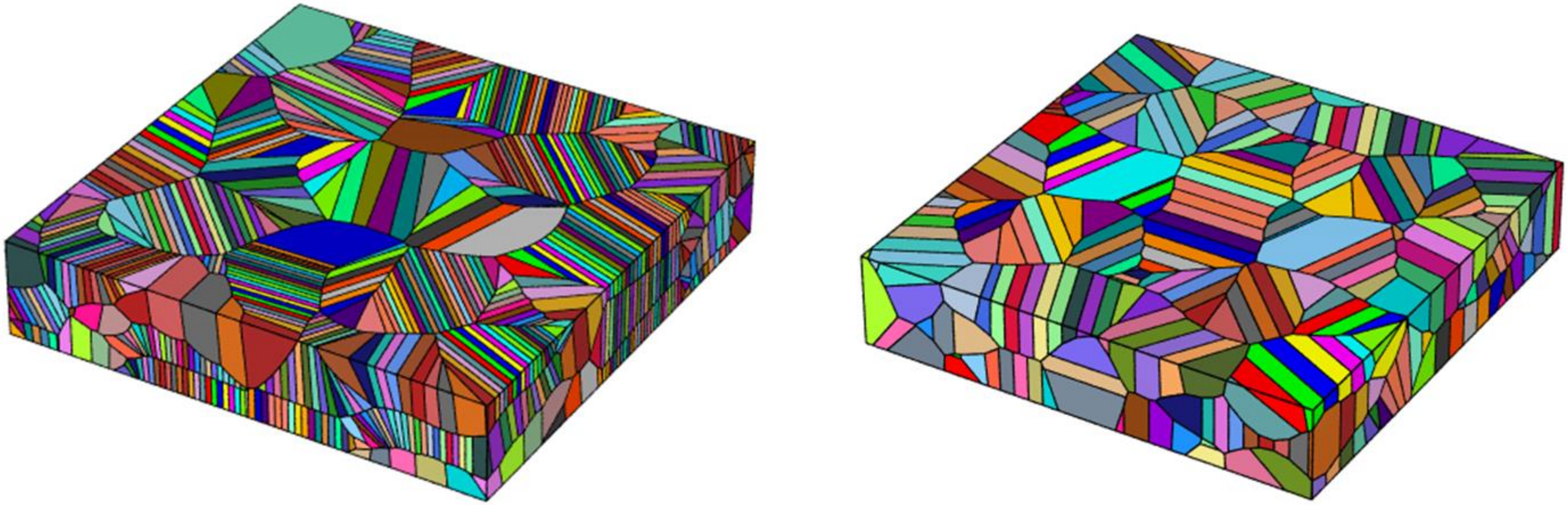
Martensite approximation with lamellar microstructure-1

SLM Microstructure Ti6Al4V
Fig 4b from
Kasperovich et al.
Materials and Design 105 (2016) 160–170



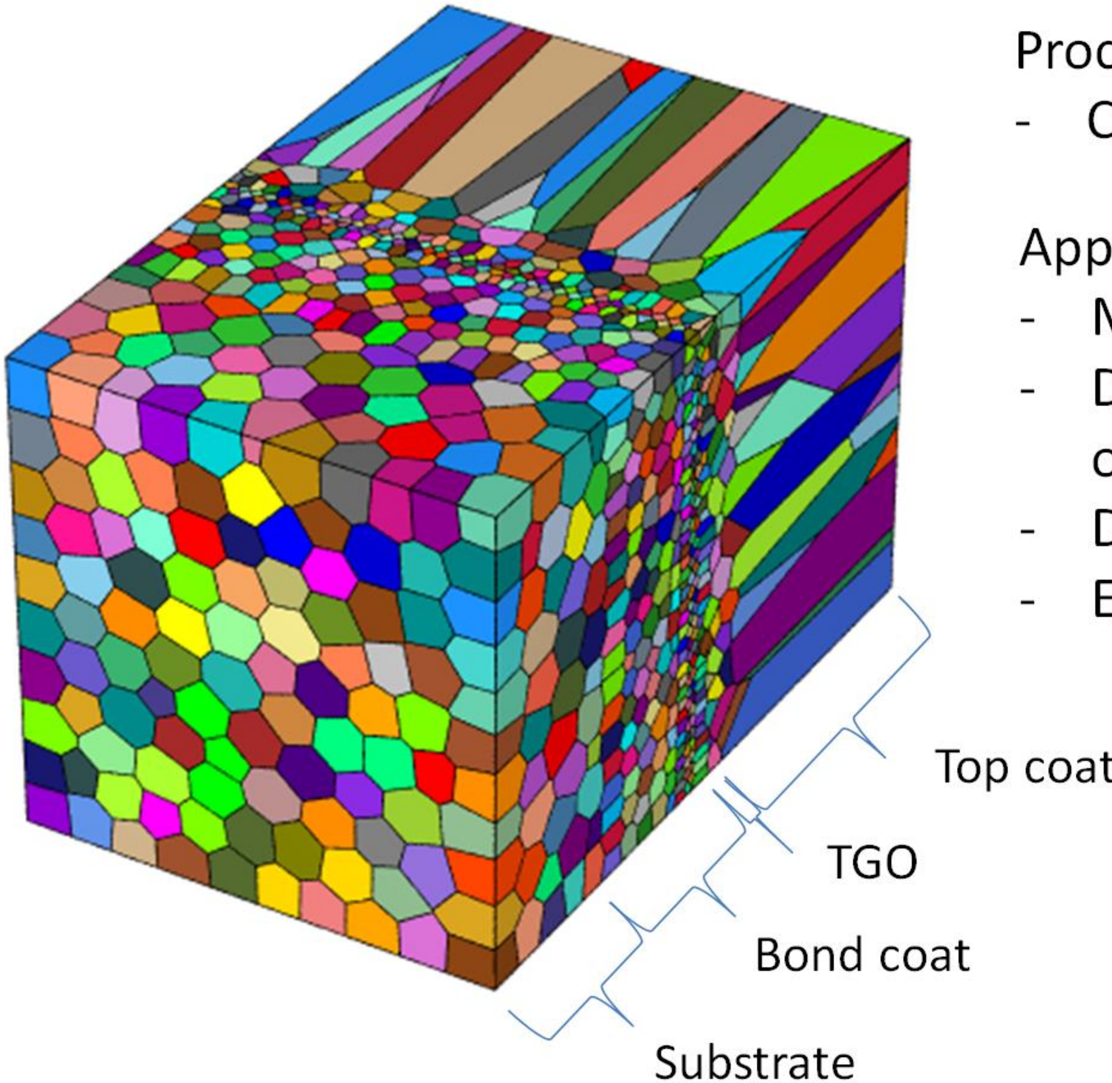
- Needlelike structure is approximated as fine lamellae
- Pores are not modelled

Martensite approximation with lamellar microstructure-2



Martensite lamellae in regular grains

Graded Microstructure: Example TBC



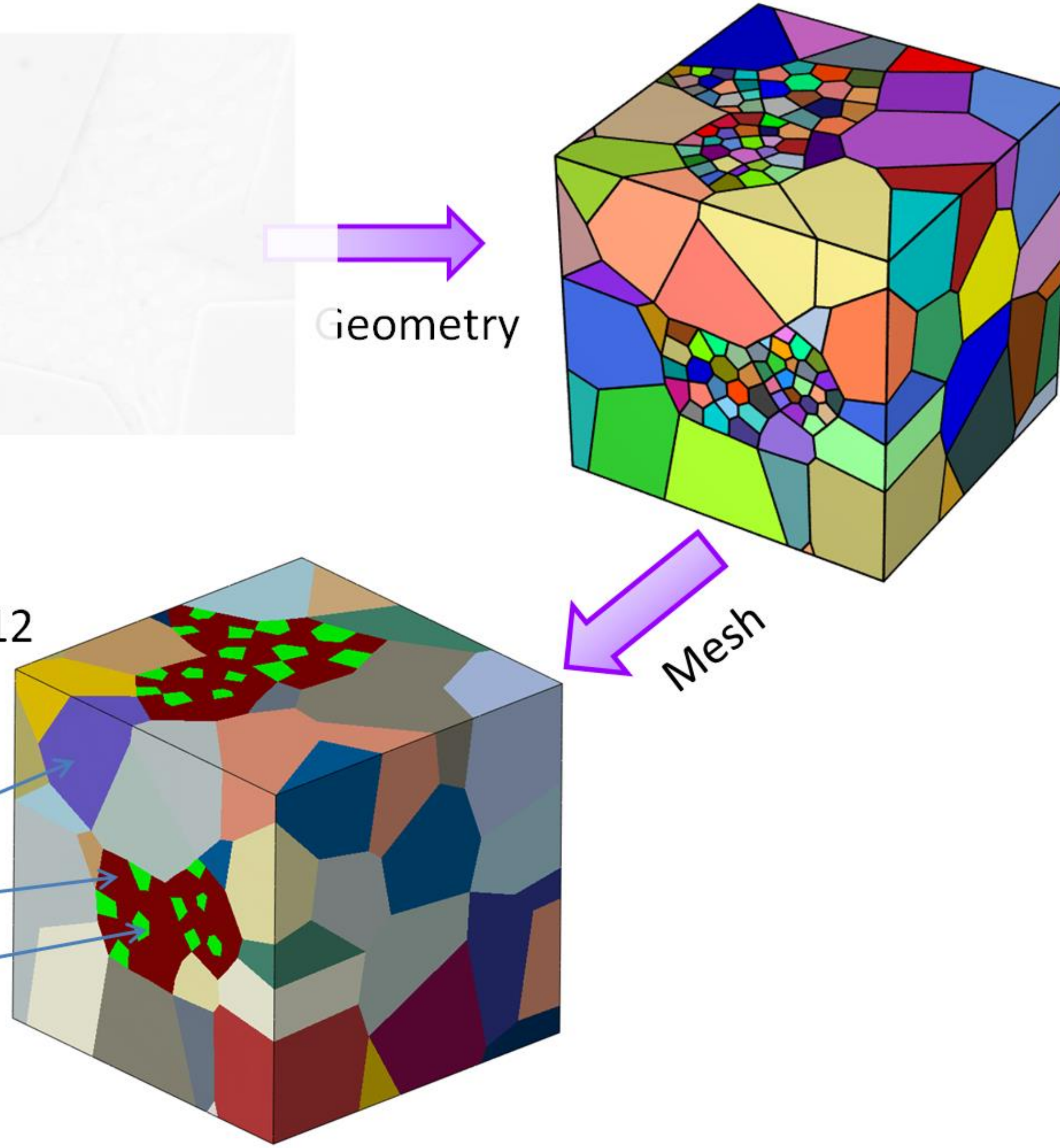
Procedure followed:

- Clustered voronoi tessellation

Application: Modelling of

- Mechanical properties of TBC
- Damage and fracture modelling of TBC
- Determination of permeability
- Etc.

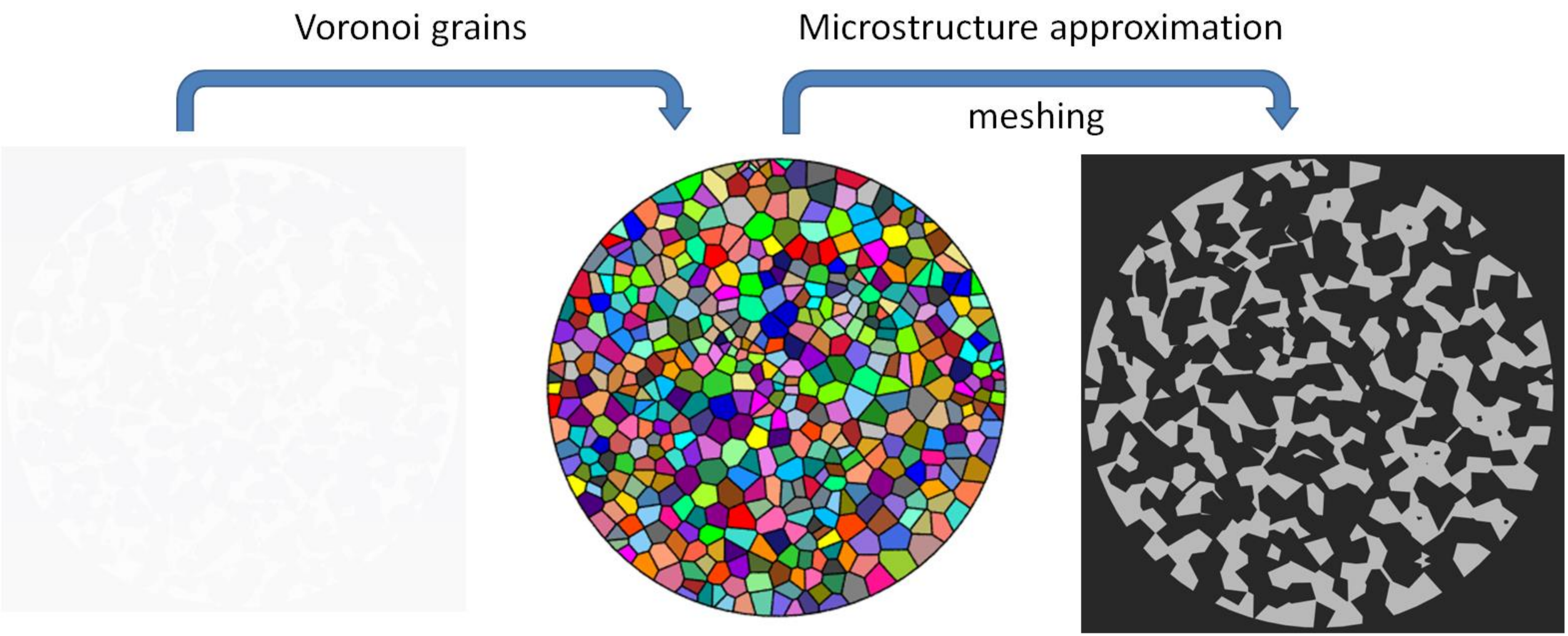
Primary and secondary microstructure



Skutterudite Material
Fig 4.3 (a)(b)
Andreas Sesselmann, Thesis 2012

Primary Phase
Secondary Phase
Precipitates

Two-phase microstructure



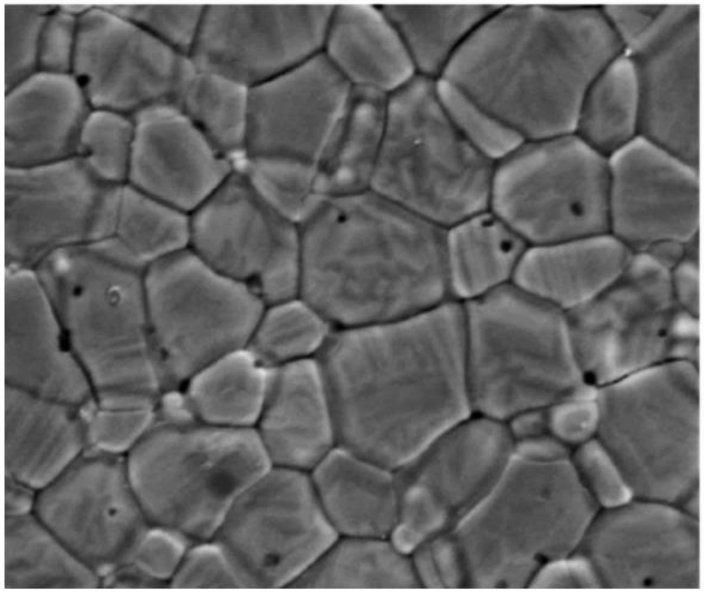
Metal-Aerogel composite

Virtual Microstructure

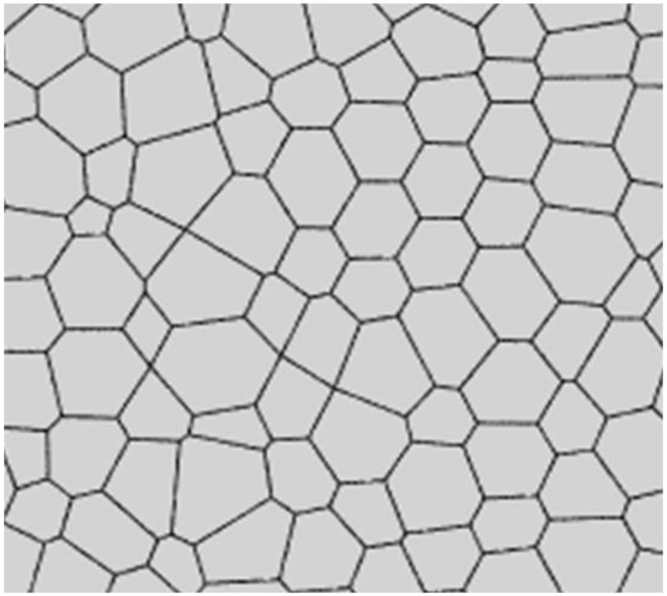
Fig. 12
Orth et al., Mat Sci and Tech, 2016, p 1-8

- Open channels by selecting grains
- Fine details by selecting mesh at GB
- Pores by deleting elements

Sintered ceramic microstructure



Palmero, Nanomaterials 5, 656



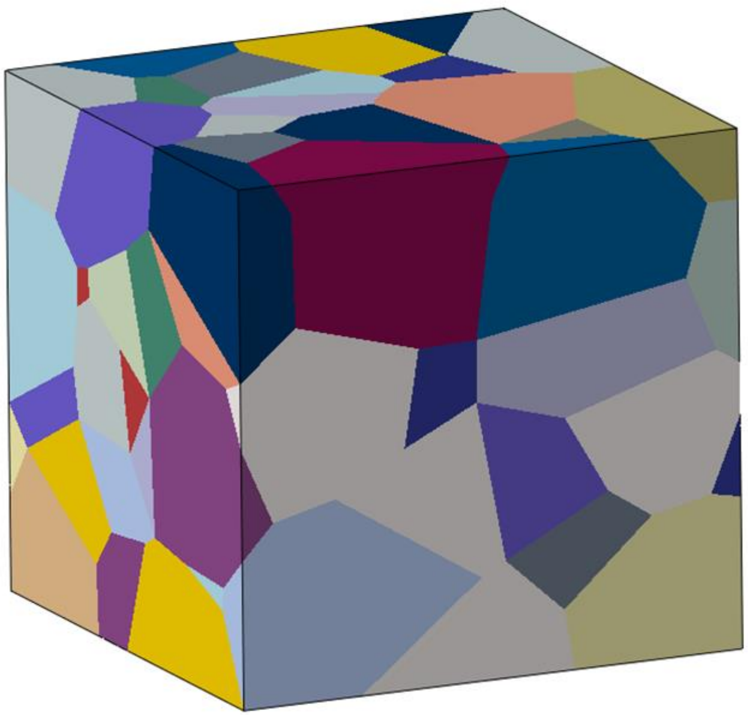
Procedure followed:

- Seed distribution using Dirac distribution
- Use weighted voronoi

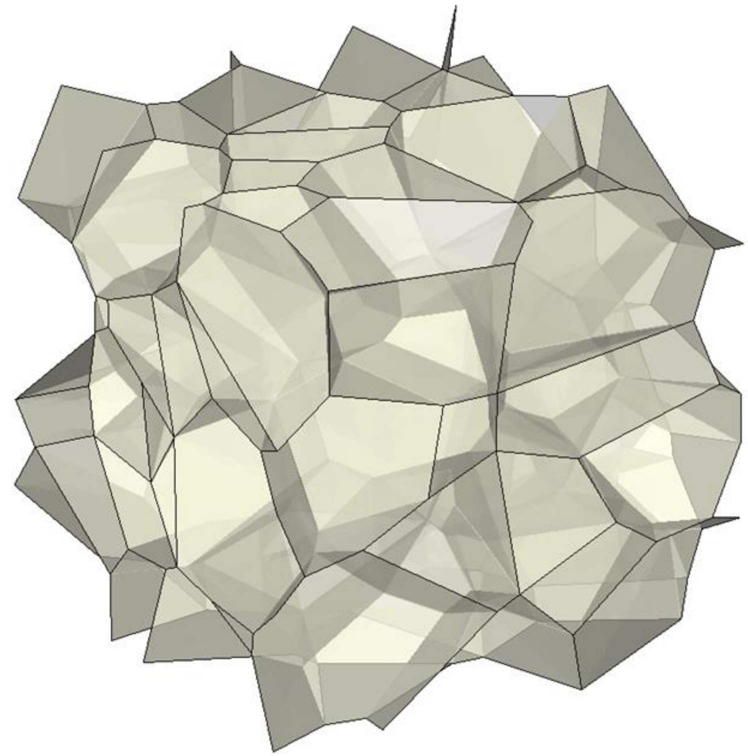
Grain boundary modelling (Explicit description of GB)

- GB influenced material behavior:
  - damage and fracture
  - stress corrosion cracking
  - creep behavior
  - Secondary phases
  - transport properties
    - diffusion
    - conductivity etc

Zero-thickness grain boundary



Random Grains



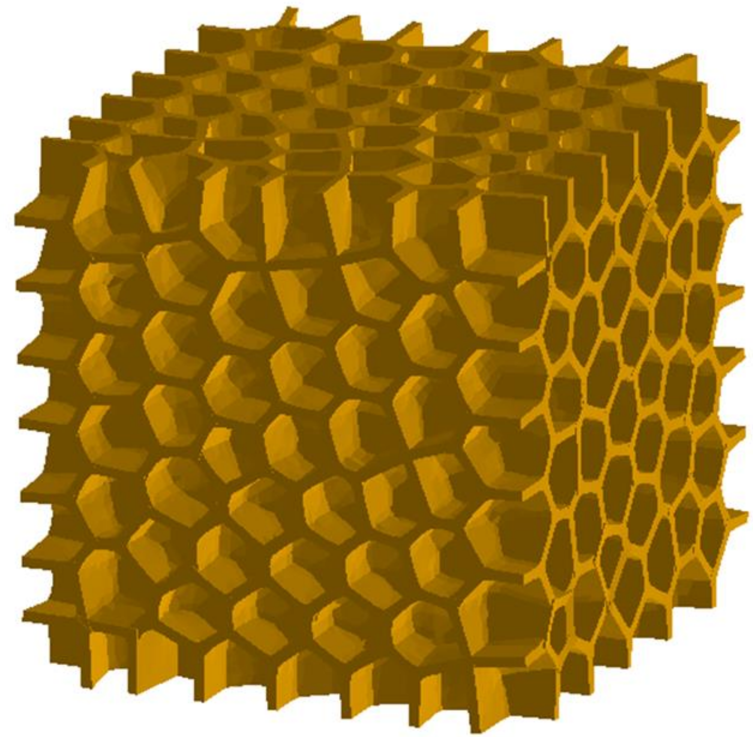
Grain boundaries using zero-thickness element

Grain boundary assisted virtual microstructure

Closed cell foam

μCT of closed cell
Polymer foam

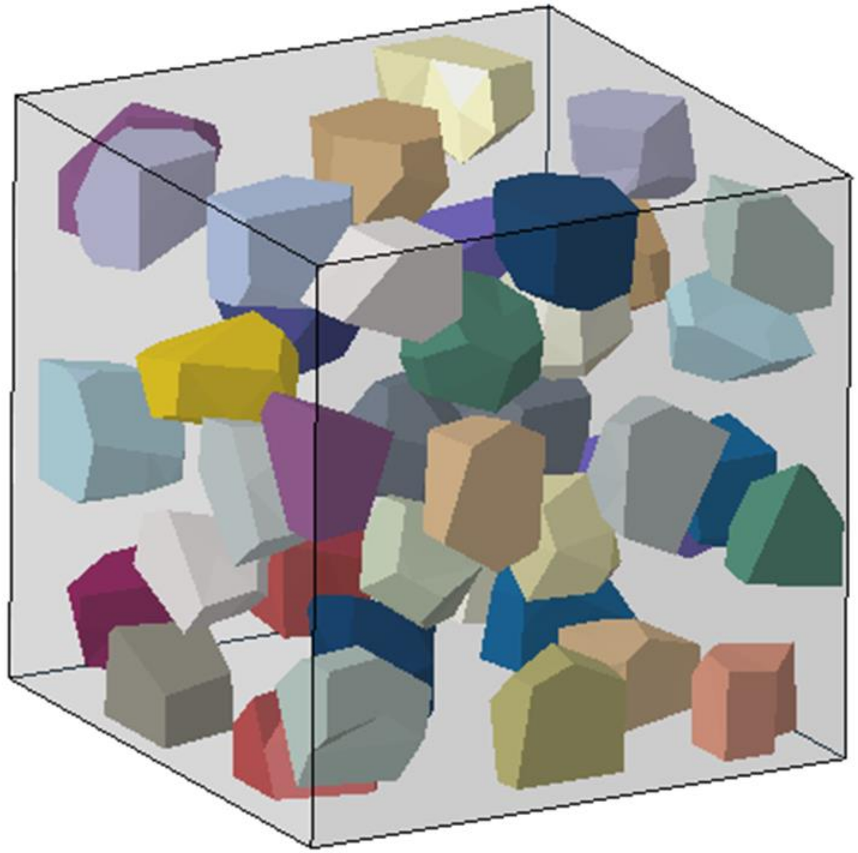
http://engineering.jhu.edu/drlab/publications/



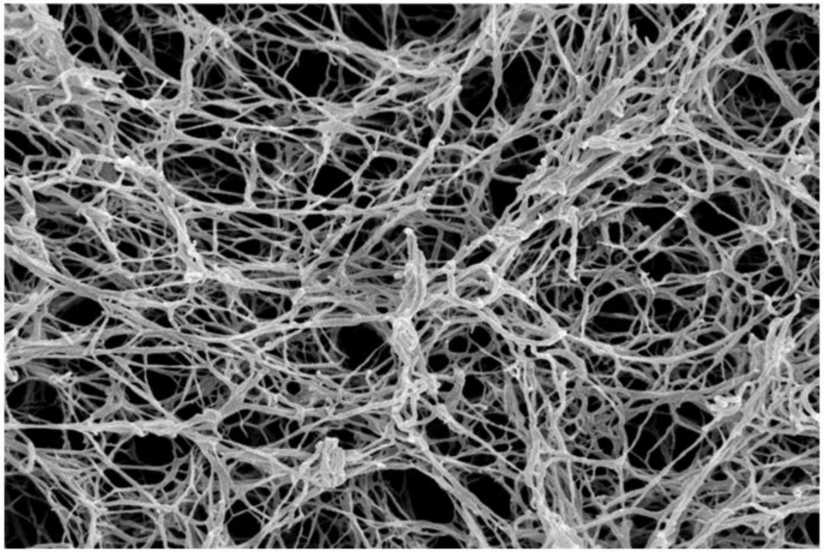
Virtual microstructure

Metal matrix composite

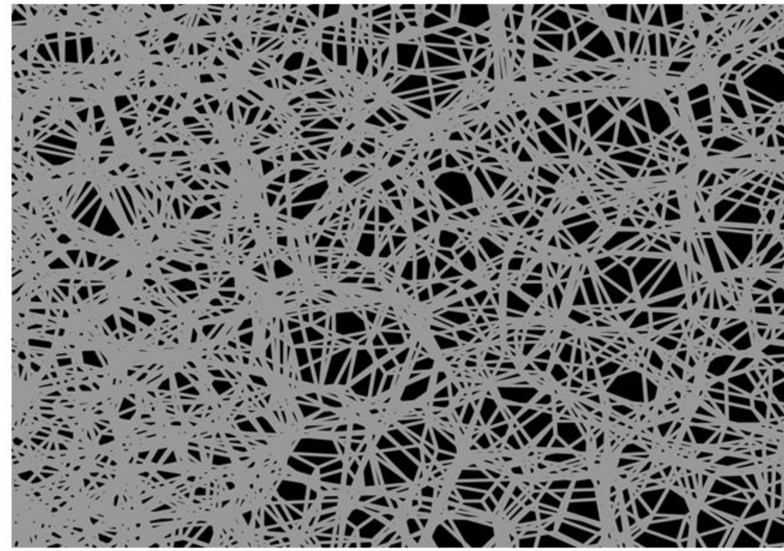
Input from Henning Richter



Cellulose microstructure



Cellulose Aerogel
Fig courtesy: Prof. L Ratke
http://www.dlr.de/wf/en/desktopdefault.aspx/tabid-9795/16796_read-40751/



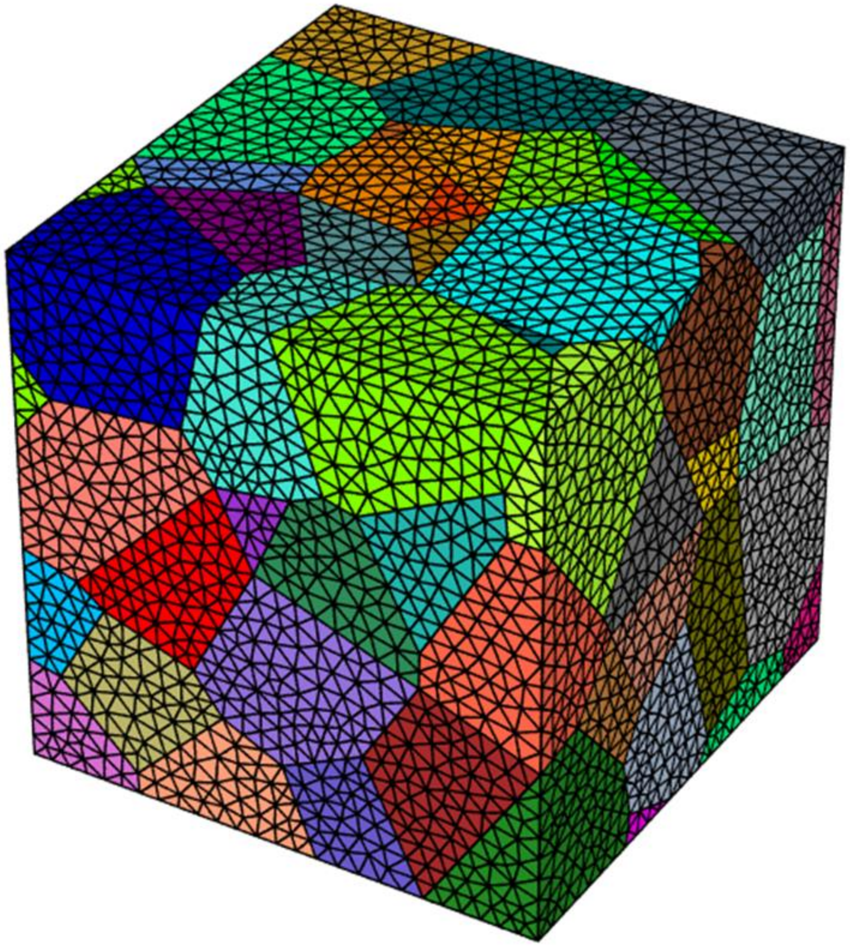
Microfibrils are generated using line elements at the grain boundaries (3D)

Mesh generation

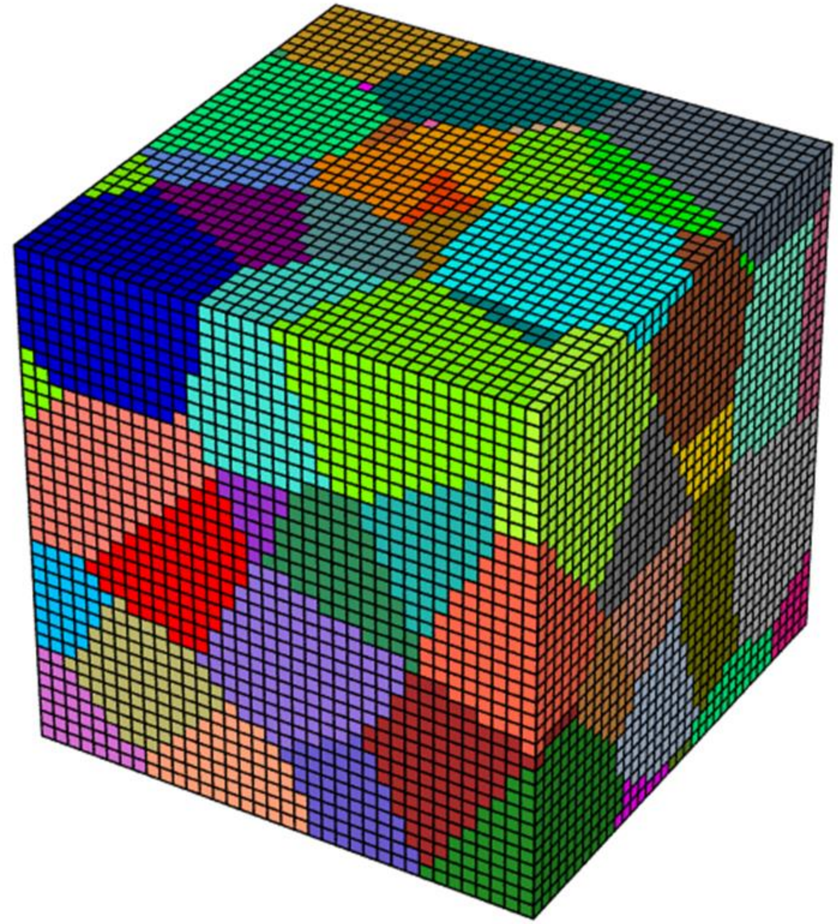
for

FE analysis

Mesh generation (Using GMESH)



Tetrahedral mesh



Voxel mesh

Graded microstructure with graded mesh

My Script

Mesh size

↓

Ƒ (Grain Volume)

Application in FE model:

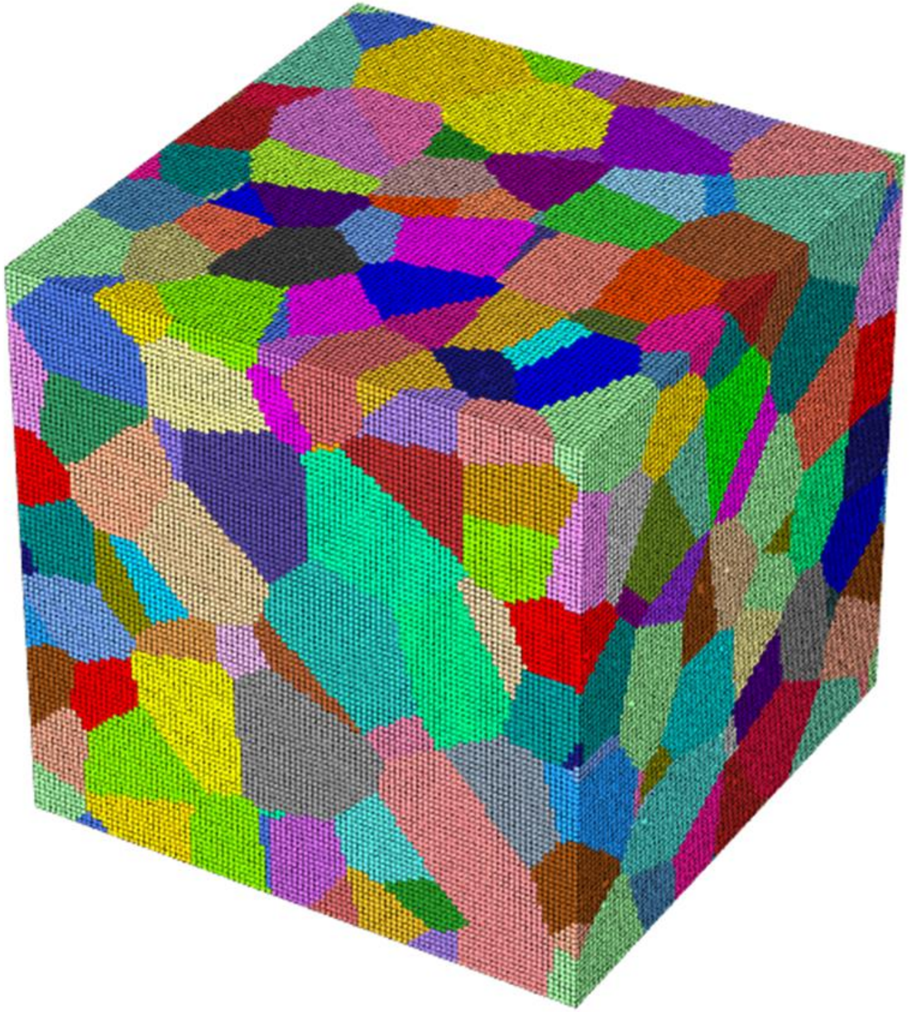
- Useful for submodelling at problem zone
- Reduce model size by focusing on the localized area
- Minimize errors at domain boundary strain transfer

Periodic microstructure

and

periodic mesh

Periodic Microstructure



Features:

- Microstructure is periodic
- Mesh is periodic
- Only voxel mesh
- Periodicity is not guaranteed for tetrahedral mesh

Can be used for homogenization of local properties

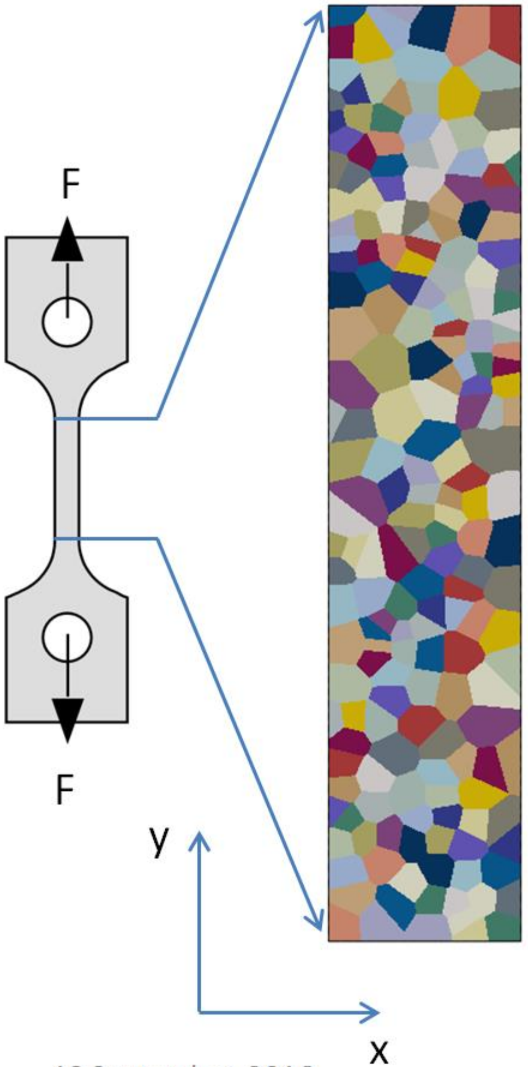
- Elastic / Elasto-plastic
- Transport properties etc.

Numerical example

Tensile failure
Using Voronoi grains

2D case

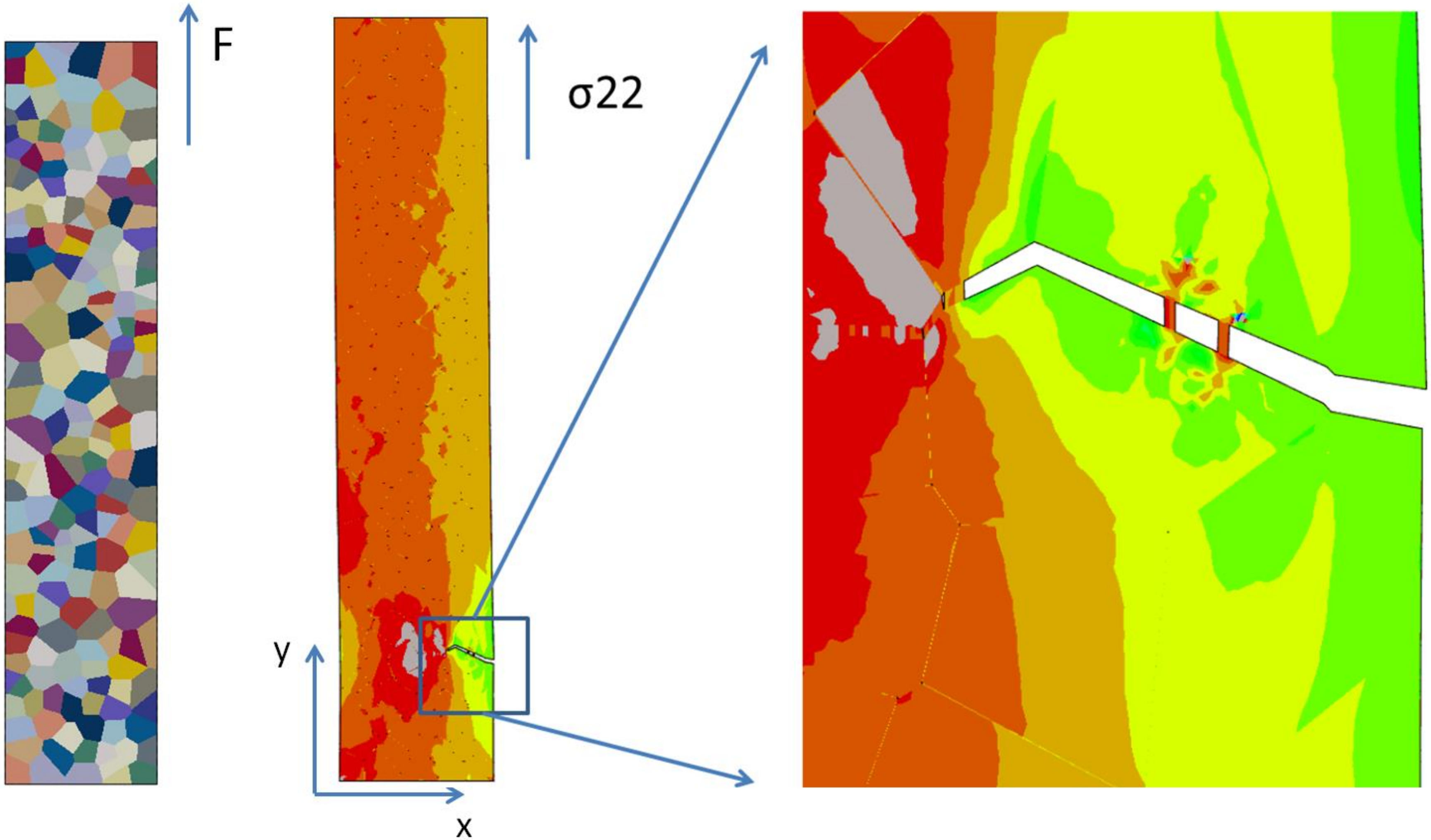
Application: Zero-thickness Grain Boundary for modelling of damage and fracture



Suggested Application areas:

- Influence of grain boundary morphology on fracture and damage behavior
- Strength degradation due to aging
- Mass-diffusion through grain boundaries
- Many more……

Grain Boundary fracture (Model demonstration)



Modelling of microstructure sensitive damage and fracture

2D case: Estimation of damage parameters by comparing strain profile with the DIC images

3D case: Estimation of damage parameters by comparing in-Situ synchrotron tomography experiment for crack initiation and propagation

Summary

Virtual microstructure generation using voronoi tessellation is demonstrated.

The presented approach is:

- **Adaptable**: It can be adapted (approximated) for real microstructures with a degree of complexity
- **Robust and flexible**: Model generation is flexible to the variations of microstructural parameters (obtained from experiments)
- **Transferable**: The geometries are meshable and therefore, can be exported to FE tools for micromechanical analysis.

Summary

Application areas:

- **Microstructure-Property correlations:** Analysis type can be micromechanical, thermo-mechanical, thermo-electrical , etc.
- **Effective properties**: Via homogenization theories using periodic unit cell
- **Damage and fracture**: Grain morphology and grain boundary influences on damage and fracture, interface strength, ageing, etc.
- **Multi-physics**: Gas absorption through grain boundary

The presented approach shows a way to **overcome some bottlenecks** in microstructure modelling.

Thank you for your attention

For further details please contact:

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