SAND2006-4678P

Microstructure Construction of Polycrystal Materials for Crystal Plasticity Simulations

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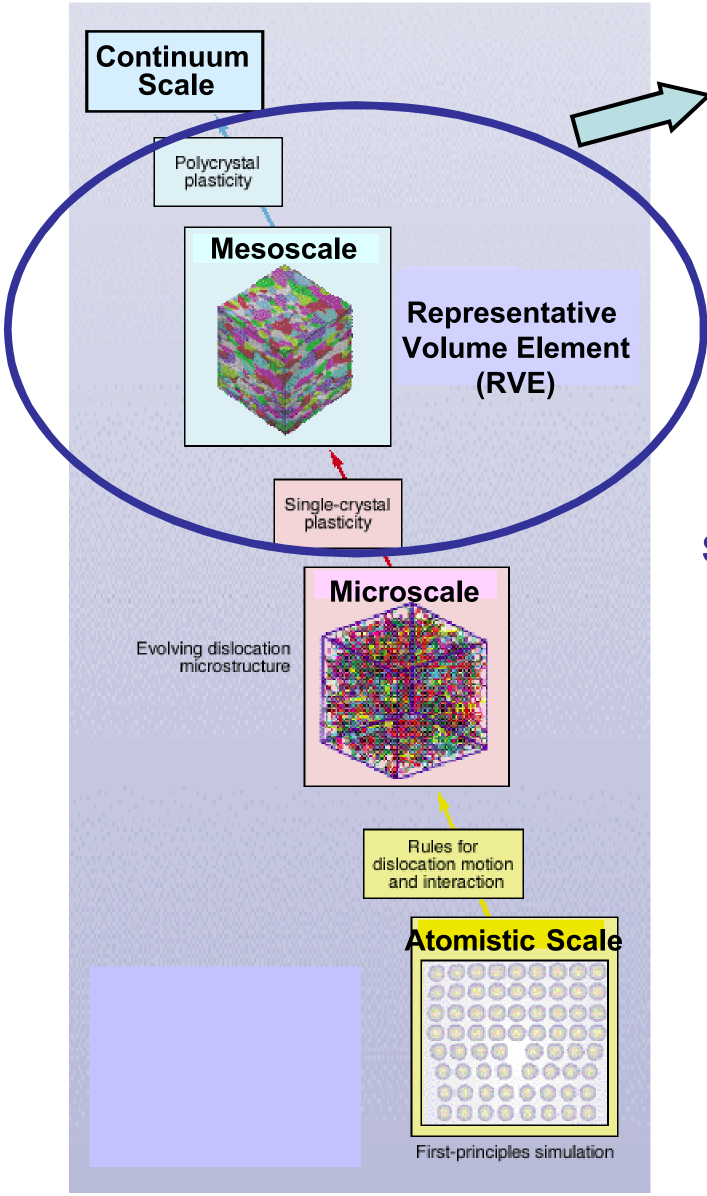
Outline

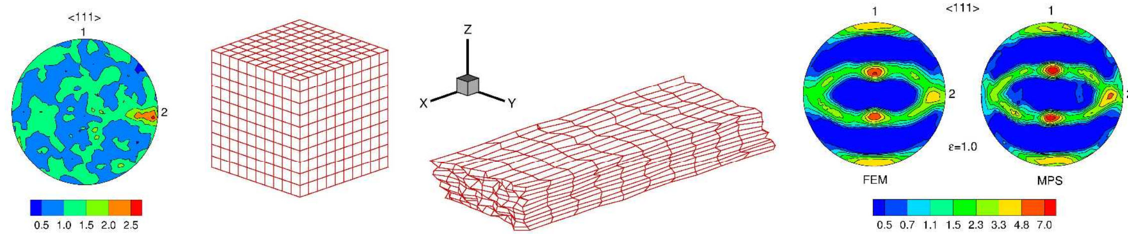
- Motivation
- Methods to construct digital microstructures
- Crystal plasticity model
- Some simulation results using digital microstructures
- Summary

The Multiscale Approach to Materials Modeling



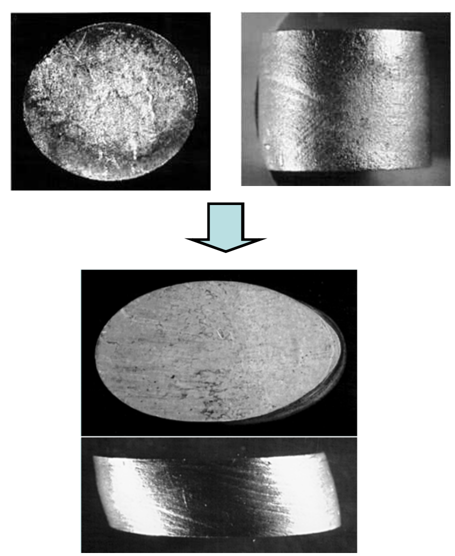
Some mesoscale simulations using Crystal Plasticity Theory

Plane Strain Compression of RVE:

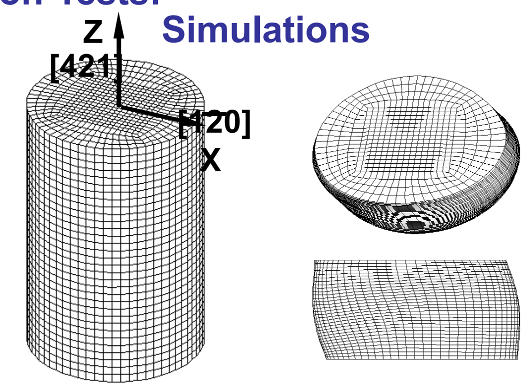


Single Crystal Uniaxial Compression Tests:

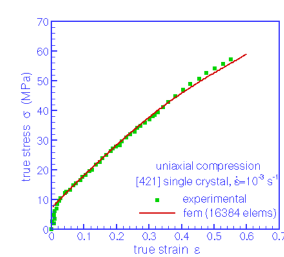
Experiments



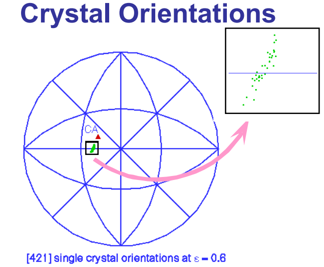
Simulations



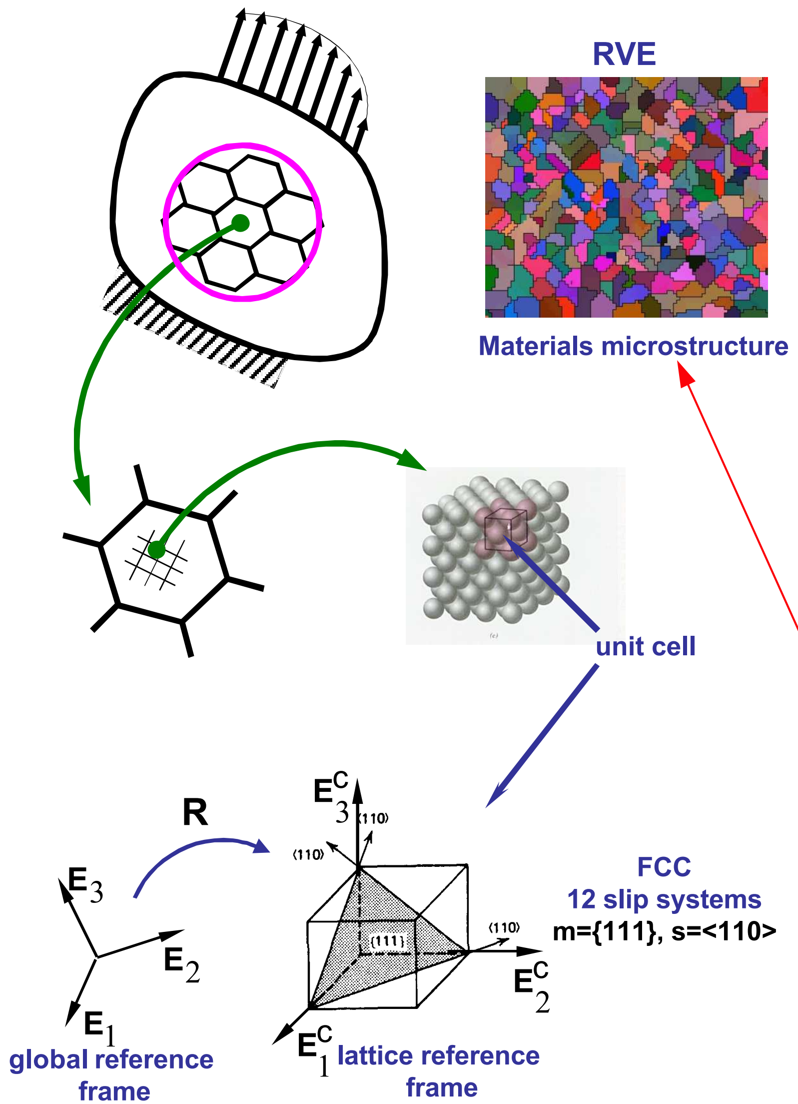
Stress Response



Crystal Orientations



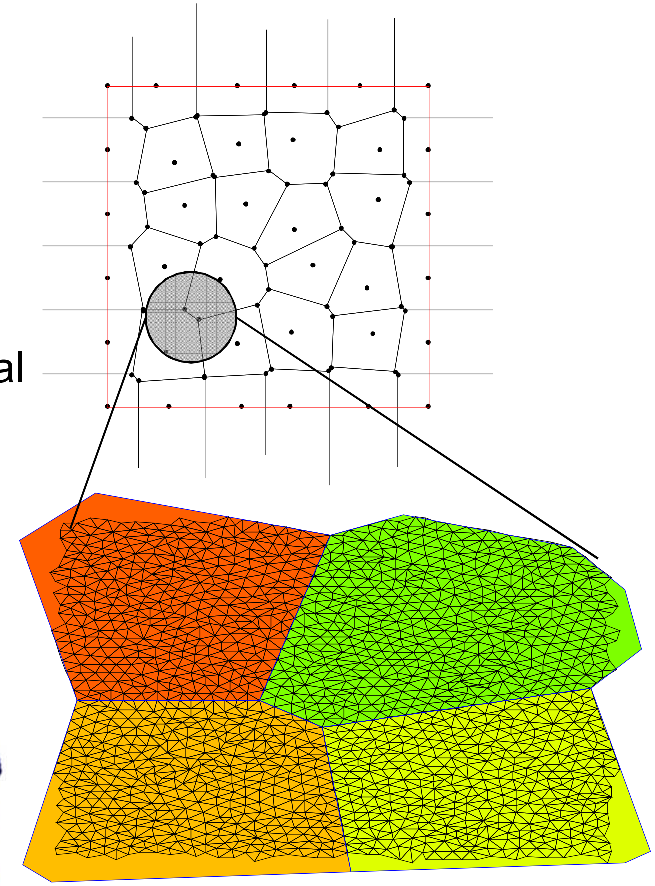
Main Features of Crystal Plasticity as a Mesoscale Approach to Materials Modeling



- Explicitly models discrete grains and slip systems, accounting then for the anisotropy of single crystal properties and crystallographic texture.
- Slip system level constitutive equations for dislocation glide kinetics and work hardening are based on phenomenological models.
- More predictive and robust than macroscopic plasticity since it explicitly addresses evolution of crystallographic texture and models both anisotropic elasticity and plasticity. However, the approach is computationally expensive.
- Predictive capability can be improved by having Initial microstructure configurations (RVEs) as close as possible to real grain structures ➡ construction of digital microstructures.
- Approach used to study aggregate of crystals to obtain a better understanding of polycrystal behavior ➡ improved continuum plasticity models.

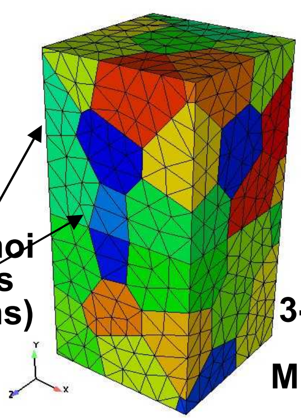
Some Methods To Create Digital Microstructures with Embedded Mesh

Voronoi Tessellation



- Point set + boundary = grain structure

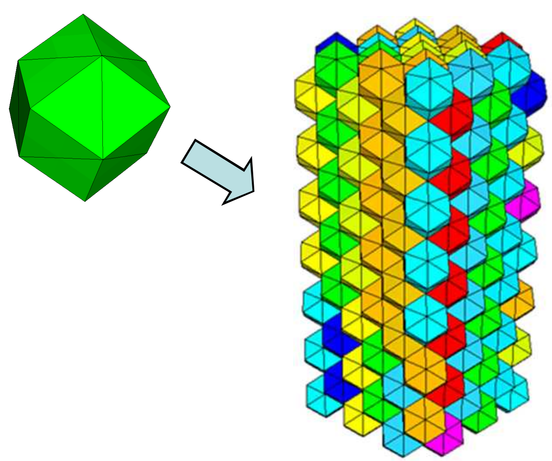
- Point set may be modified to produce microstructures with desired grain size and/or orientation distribution
- Each point produces a grain that can be assigned material properties and meshed to the desired resolution using existing meshing tools (e.g. Cubit)
- Robust enough for 2-D and 3-D microstructures



Voronoi cells (grains)

3-D RVE with Synthetic Microstructure

Dodecahedra (48 tetrahedral)



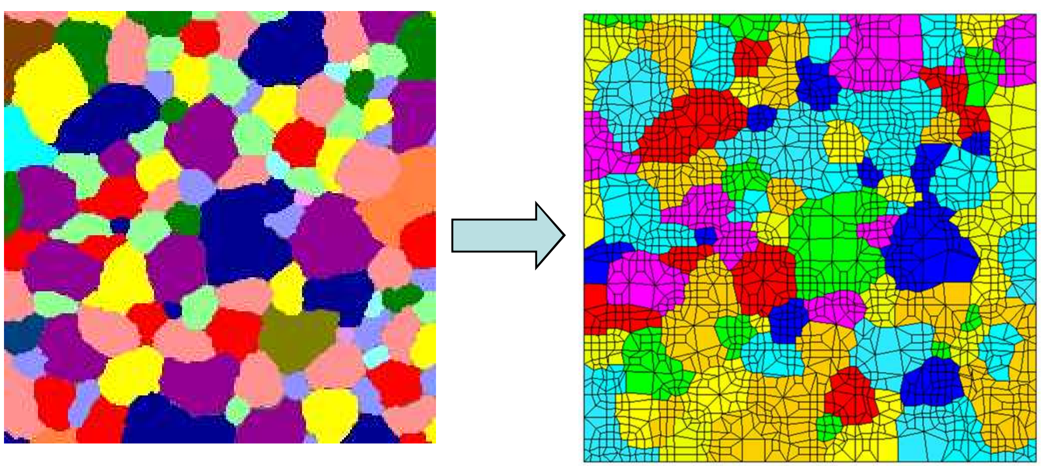
(Jobie Gerken, Cornell Univ.)

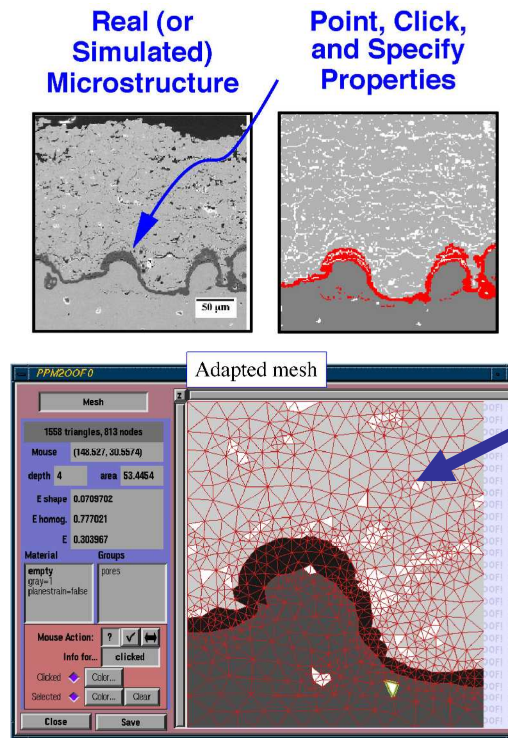
Some Methods To Create Digital Microstructures with Embedded Mesh

Digitizing Real Microstructures

- Realistic microstructures can be produced using digitized images of the micrographs of real poly-crystalline materials.
- **OOF2** : Object-Oriented Finite element analysis of real material microstructures:

  Converts an image of a heterogeneous material into a 2-D finite element mesh with constitutive properties specified by the user (2-D RVE).



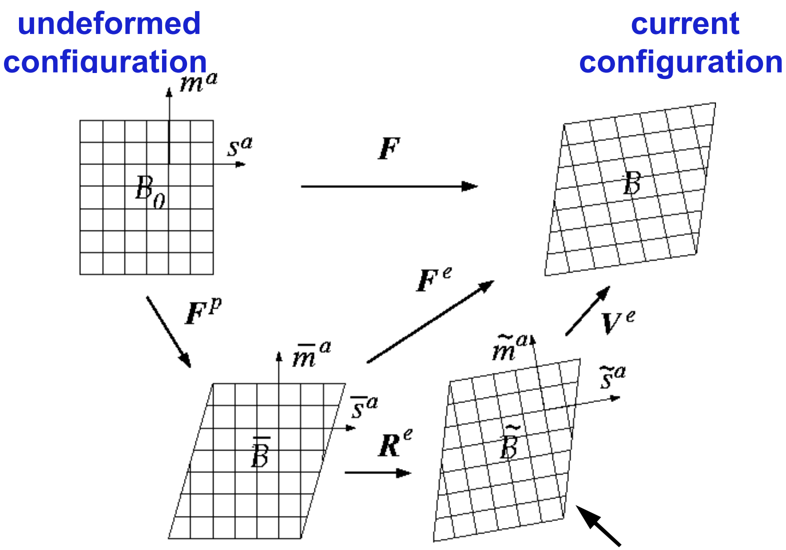


Mesh can be Translated to Input file for 2-D FEA (Abaqus)

Could be used to construct 3-D RVE

(*http://www.ctcms.nist.gov/oof/*)

Crystal Plasticity Model



$$F = V^e R^e F^p$$

Small elastic strains:

$$\tilde{E}^e = \frac{1}{2}(V^{eT}V^e - I), \quad V^e = I + \varepsilon^e, \quad \| \varepsilon^e \| << 1$$

Free Energy:

$$\tilde{\Psi} = \hat{\tilde{\Psi}}(\tilde{E}^e, \varepsilon_s^\alpha) = \frac{1}{2}\tilde{E}^e : \tilde{C}^e : \tilde{E}^e + \frac{1}{2}\sum_1^M \mu_{ef}\, c_\kappa \varepsilon_s^\alpha \varepsilon_s^\alpha$$

Kinematics:

$$d = \overset{\nabla}{\varepsilon}{}^e + \tilde{D}^p, \quad \overset{\nabla}{\varepsilon}{}^e = \dot{\varepsilon}^e + \varepsilon^e \tilde{\Omega}^e - \tilde{\Omega}^e \varepsilon^e$$

$$w = -\mathrm{skw}(\dot{\varepsilon}^e \varepsilon^e) + \tilde{\Omega}^e + \tilde{W}^p$$

Elasticity:

$$\tau = \tilde{C}^e : \varepsilon^e \Rightarrow \begin{cases} \mathrm{dev}\tau = \tilde{C}^e_d : \mathrm{dev}\varepsilon^e + \tilde{H}^e_{dv}\varepsilon^e_{kk} \\ p_\tau = \tilde{H}^e_{dv} : \mathrm{dev}\varepsilon^e + M^e_v \varepsilon^e_{kk} \end{cases}$$

Plasticity:

$$\tilde{D}^p = \sum_{\alpha=1}^{M} \dot{\gamma}^\alpha \mathrm{sym}(\tilde{Z}^\alpha)$$

$$\tilde{W}^p = \sum_{\alpha=1}^{M} \dot{\gamma}^\alpha \mathrm{skw}(\tilde{Z}^\alpha)$$

$$\dot{\gamma}^\alpha = \Phi(\tau^\alpha, \kappa_s^\alpha)$$

$$\tau^\alpha = \tau : \mathrm{sym}(\tilde{Z}^\alpha) = \tau : \tilde{Z}^\alpha$$

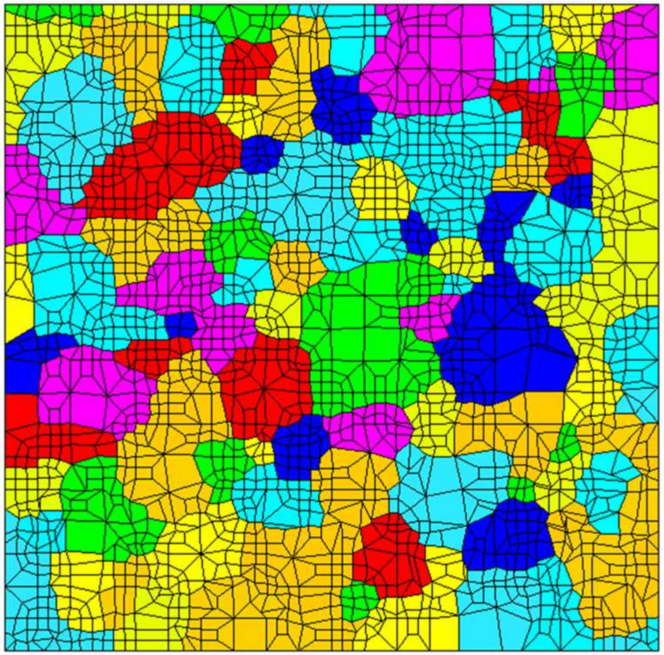
$$\dot{\varepsilon}_s^\alpha = \Theta(\dot{\gamma}^\alpha, \varepsilon_s^\alpha), \qquad \kappa_s^\alpha = \mu_{ef} c_\kappa \varepsilon_s^\alpha$$

where:

$$\tilde{\Omega}^e = \dot{R}^e R^{eT} \quad \tilde{D}^p = R^e \bar{D}^p R^{eT} \quad \tilde{W}^p = R^e \bar{W}^p R^{eT}$$

(E. Marin, SAND2006-XXXX.)

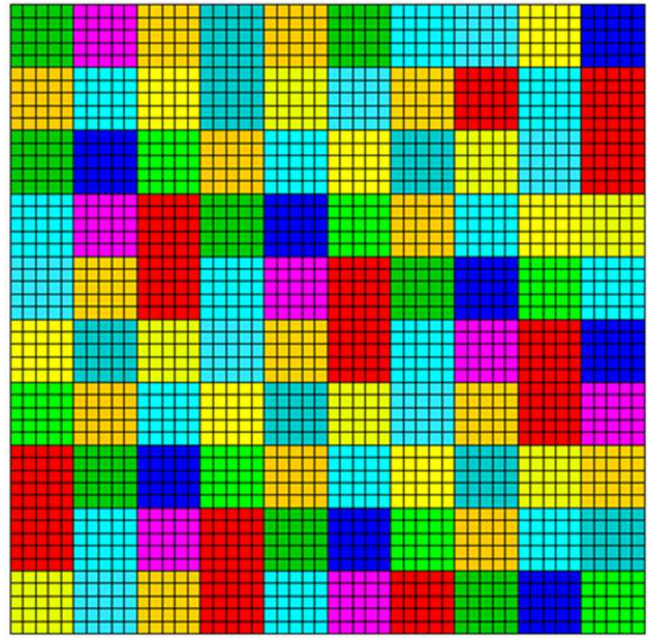
2-D Microstructures



115 grains

2486 mesh elements

Constructed from an actual microstructure using OOF2 software



100 grains

2500 mesh elements

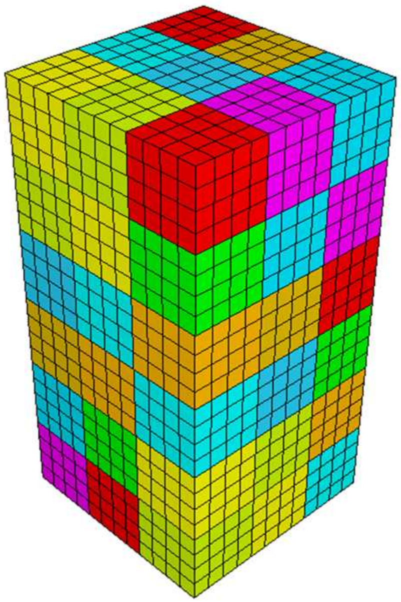
Constructed using Abaqus CAE

2-D Microstructures - Comparison

This slide will contain deformed meshes and stress strain curves (similar to slides 10-12) for the 2-D meshes if these results are obtained.

3-D Microstructures

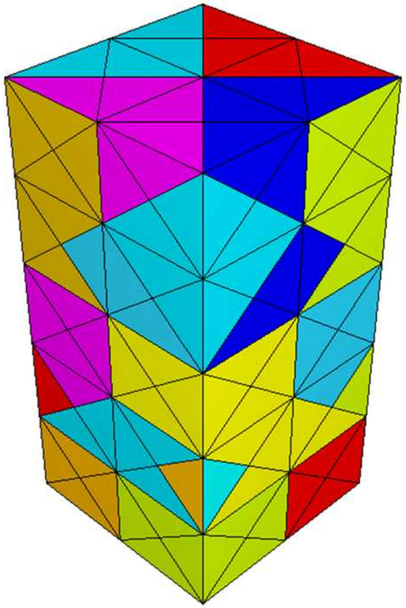
Brick Mesh



54 grains

3456 mesh elements

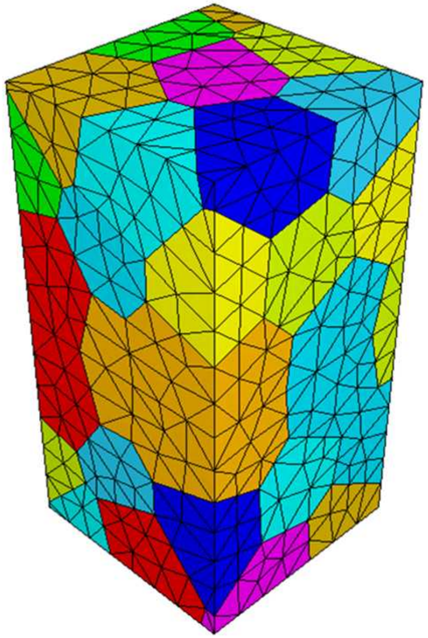
Dodecahedra Mesh



47 grains

480 mesh elements

Voronoi Mesh



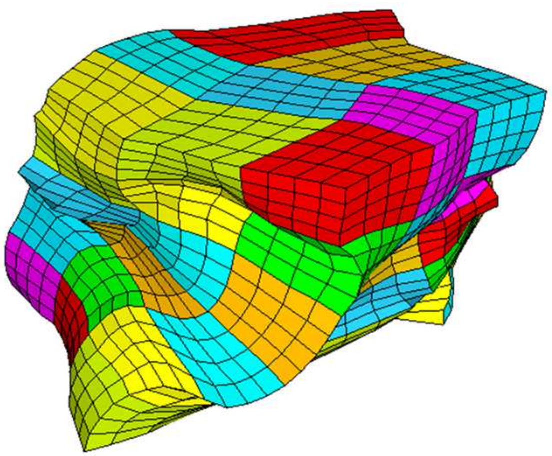
44 grains

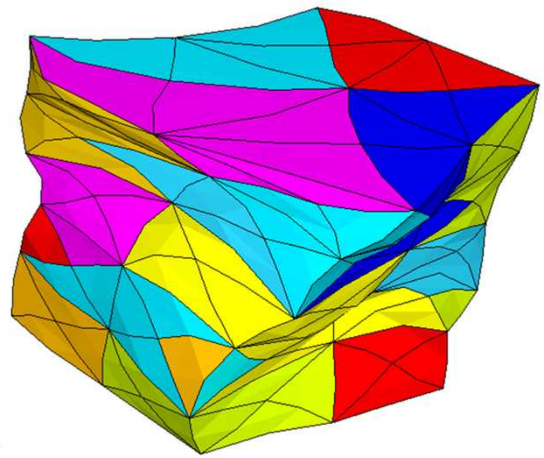
4500 mesh elements

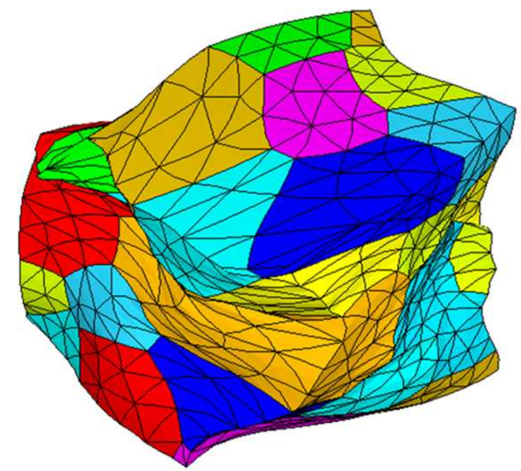
- All meshes simulate materials with FCC crystal structure
- Brick mesh constructed in Abaqus CAE. Dodecahedra and Voronoi meshes were constructed using software from Cornell University.

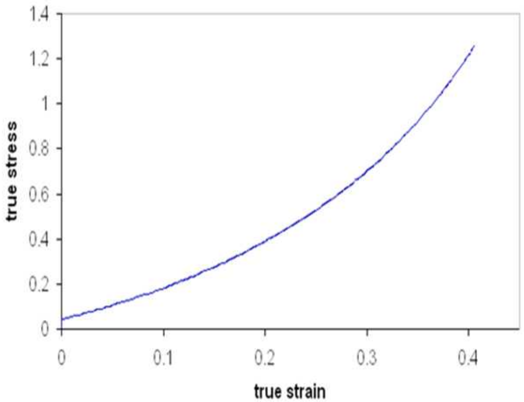
3-D Microstructures - Comparison

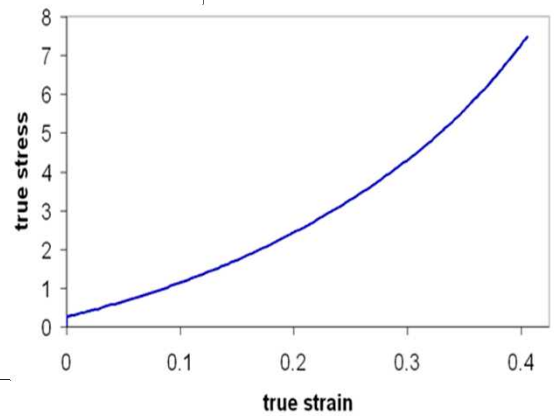
Compression Test at constant strain rate = -1

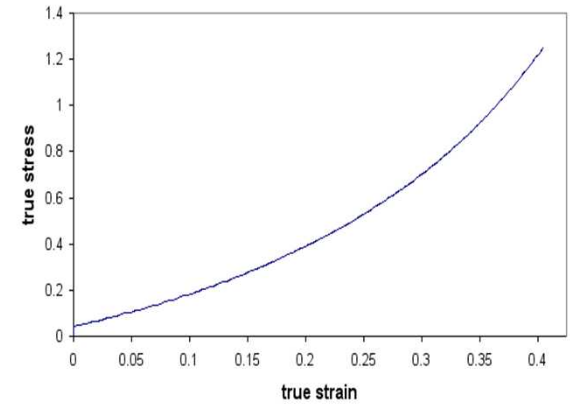






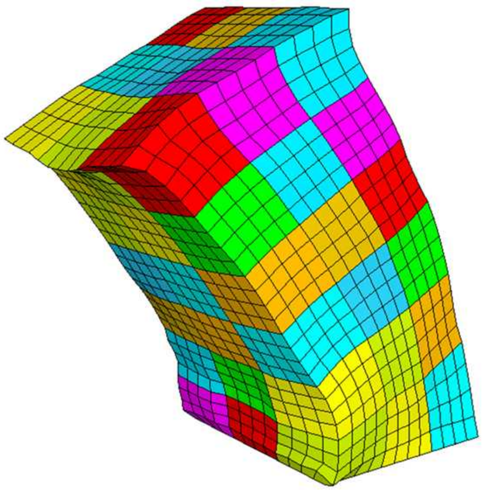


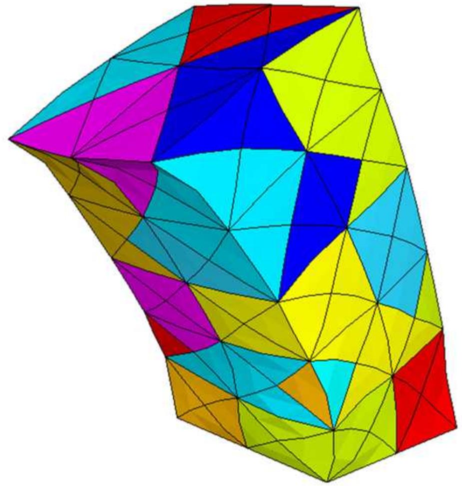


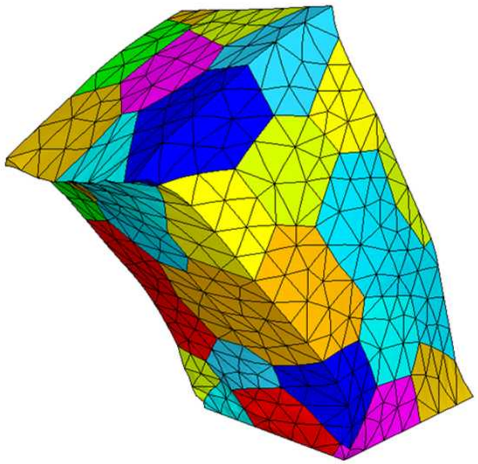


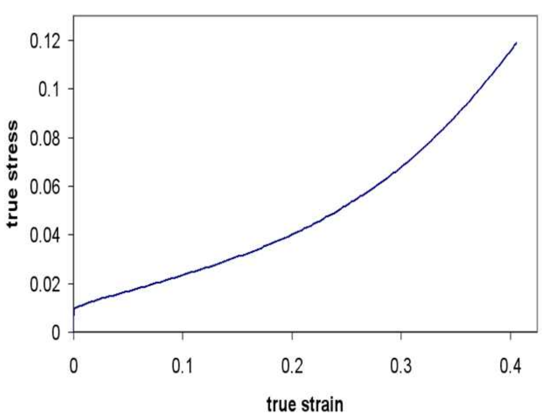
3-D Microstructures - Comparison

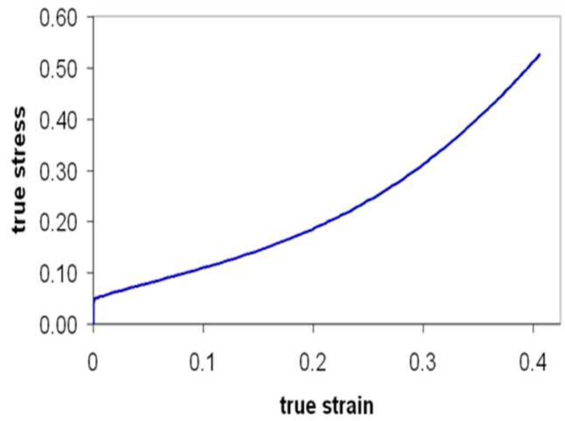
Shear loading test

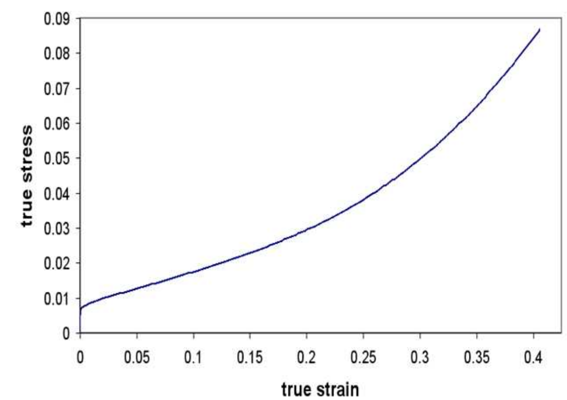






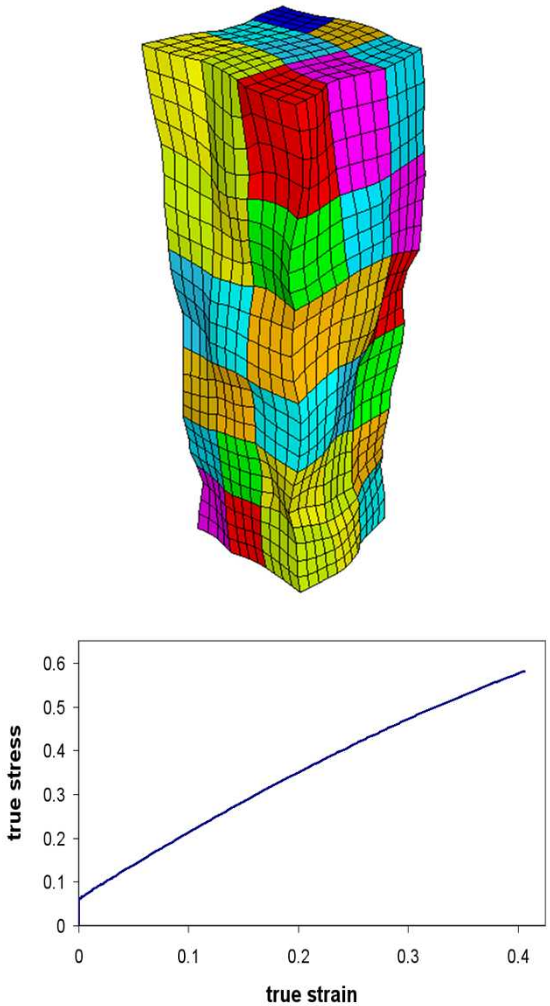


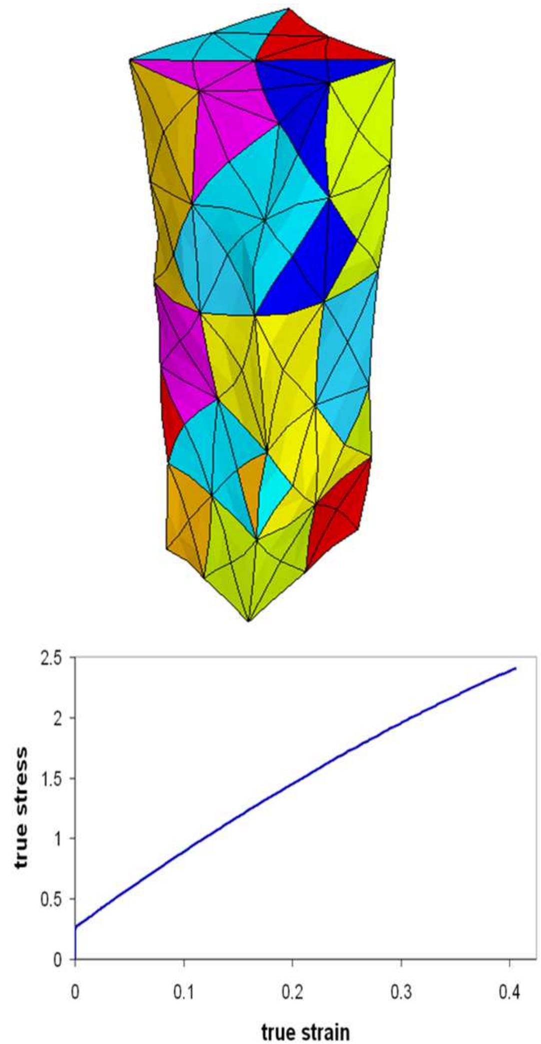


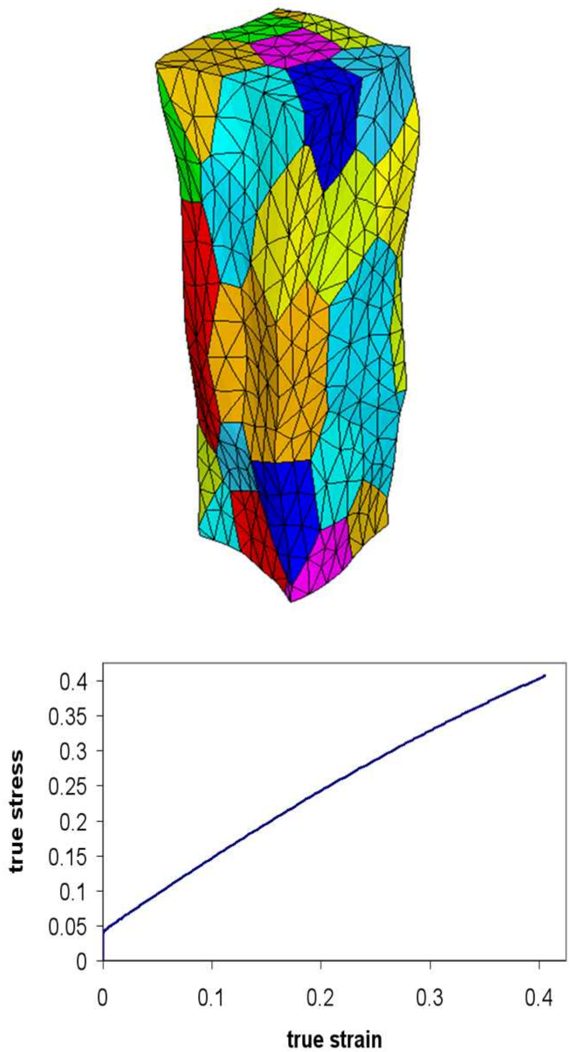


3-D Microstructures - Comparison

Tensile load at constant strain rate = 1







3-D Microstructures - Results

This slide will contain a basic analysis of the deformed meshes and the stress strain curves presented in the previous slides.

Summary

- Microstructure plays an important role in determining various properties in materials made of aggregates of crystalline grains. In particular, materials are intrinsically inhomogeneous on mesoscopic and microscopic scales due to the presence of grain boundaries.
- Crystal plasticity theories form the basis of grain-level (mesoscale) approaches to materials modeling using multi-scale strategies.
- The numerical simulation and modeling of polycrystalline materials using these theories will be more predictive if the initial microstructure configuration used resembles realistic grain structures.
- This work is the initial step towards the use of available geometric tools to generate and use digital microstructures in our crystal plasticity simulations.