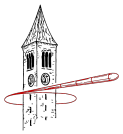
Mechanical Metrics (MechMet)



Overview

- **MechMet**: **MatLab** code for computing mechanical metrics of Virtual Polycrystals
- Utilizes Virtual Polycrystals created by **Neper**
- Solves field equations for elasticity using the finite element method
- From computed displacement fields, computes several mechanical metrics
- Generates a formatted output file for visualization with **Paraview** or **VisIt**

Mechanical metrics:

- Strain and stress tensors
- Embedded (apparent) directional stiffness
- Isolated (single-crystal) directional stiffness
- Normalized Schmid Factor
- Directional strength-to-stiffness ratio
- Eigenmodes of deformation (in-development)

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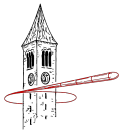

MechMet origins and intent:

- Draws on codes/scripts/functions developed at Cornell over the years in:

  MAE courses, **ODFPF** package, **FEpX** pre- and post-processing scripts
- Intended as a relatively 'quick-and-easy' tool for investigating mechanical behaviors of polycrystals, especially in conjunction with *in-situ* loading diffraction experiments
- Not intended for more complex elastoplastic simulations (such as possible with **FEpX**).

MechMet code and interfaces:

- Code runs on laptops (mesh size limited by computer memory)
- 10-node tetrahedral elements w/15 point quadrature rule (same as **FEpX**).
- Code utilizes **MatLab** in-line sparse solver (facilitating meshes with 100-200K elements)

MechMet itself is a stand-alone **MatLab** FE package that works with two other resources:

1. *Input from:* Virtual polycrystal instantiation tools for microstructure and mesh (**Neper)**
2. *Output to:* Visualization/interpretation tools **(Paraview** or **VisIt)**

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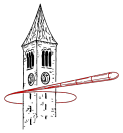

Running MechMet:

- Generate/obtain **Neper** files for the virtual polycrystal. Necessary files are: *filename*.grain, *filename*.ori, and *filename*.mesh
- *filename*.ori specifies the lattice orientations of each grain. Angles should be in Kocks convention and the file suffix should be 'kocks'. The basename for the orientations should be the same as that for the grains.
- The single crystal properties are specified in *filename*.matl files. Line 1 is the crystal type (3 for cubic-fcc; 4 for cubic-bcc; 6 for hex); Line 2 lists the elastic moduli; Line 3 lists the slip system strengths. The **Neper** files and the .matl file need not have the same basename. **MechMet** handles multi-phase polycrystals as defined by **Neper.**
- **MechMet** is executed by running MechMet and providing the filename and loading information requested (.m files and data files all in the same directory).
- *filename*.vtk file is then imported into either **Paraview** of **VisIt** for visualization

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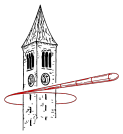

Mechanical response:

- Linear elasticity w/anisotropic Hooke's Law (for cubic and hexagonal symmetries)
- Loading modes: uniaxial extension in x, y or z and biaxial extension in x-y, y-z, or z-x planes. Imposed boundary displacements set to produce nominal strain of 0.001.
- Solves for displacement field, then computes strain (from grad **u**)
- Computes stress from strain field, together with Hooke's law.

Mechanical metrics:

- Single crystal directional stiffness: reciprocal (diagonal of compliance matrix).
- Embedded (apparent) stiffness: ratio of average stress to local (fem) strain.
- Schmid Factor: ratio of resolved shear stress to applied stress (assumes nominal stress).
- Strength-to-Stiffness: critical resolved shear stress / embedded stiffness (Poshadel&Dawson (MMTA,2019))