Developing a Crystal Plasticity Model for Nickel Based Turbine Alloys Based on the Discrete Element Method

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Acknowledgments

- Collaborators
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  - Dr. Kyle Rozman (NETL, Albany)

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Background & Motivation

- Predicting creep and creep-fatigue behavior is highly empirical
  - Power law creep constitutive laws
    - e.g., Norton Law

$$\dot{\varepsilon} = A t \sigma^{n} \exp\left(-Q/\ \right)$$

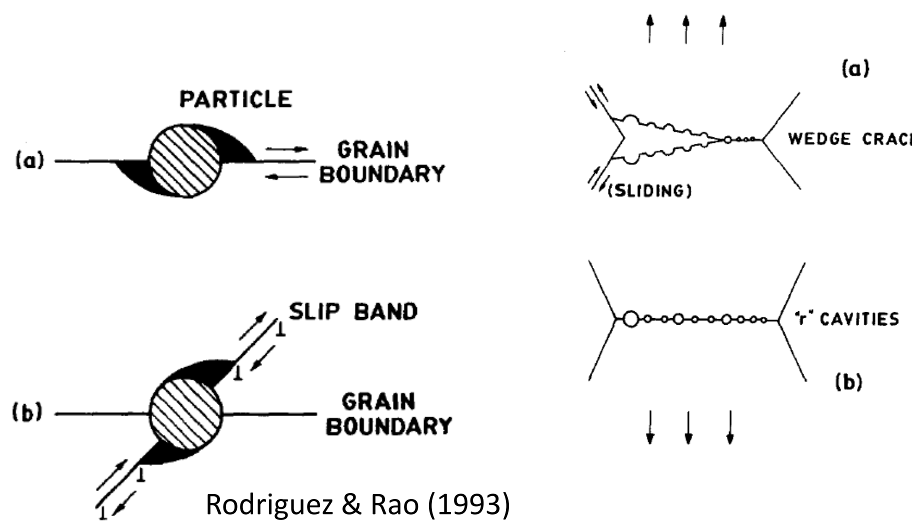
  - Linear cre… accumula…

- Not easily ex… measured ranges
  - Longer lifetimes
  - Variable operating conditions

- Including stochastic damage mechanisms in current modeling methods (e.g., FEM) in predictive manner is a challenge

We need a modeling platform with inherent stochastic features

…e blades
Australian Transport Safety Bureau (2011)



Rodriguez & Rao (1993)

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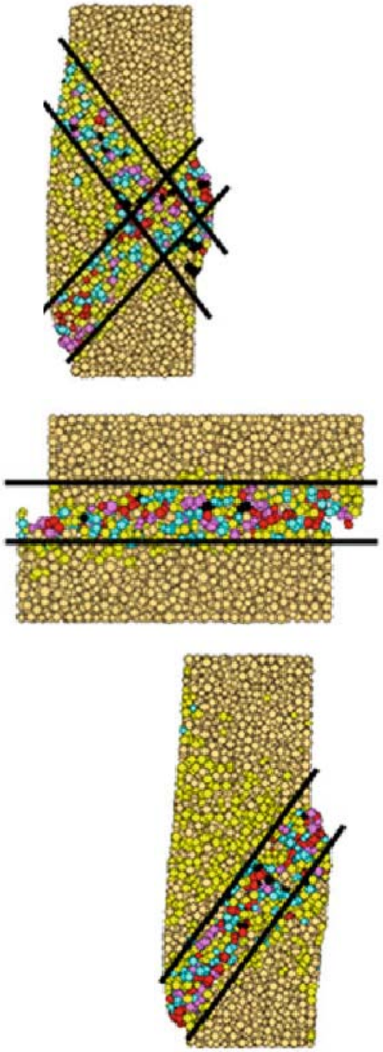
Discrete Element Method (DEM)

- Discrete element method widely used for granular media
  - Each particle is modeled as a discrete element
  - One-to-one correlation between element and particle
  - Sands, mined materials, and powders are commonly modeled
- Properties modeled include:
  - Granular body deformation
  - Granular body creep
  - Granular sintering and microstructure evolution
- Stochastic phenomena naturally emerge in DEM
  - Shear bands
  - Fracture nucleation and propagation
  - Void formation and growth



Zhao & Evans (2011)

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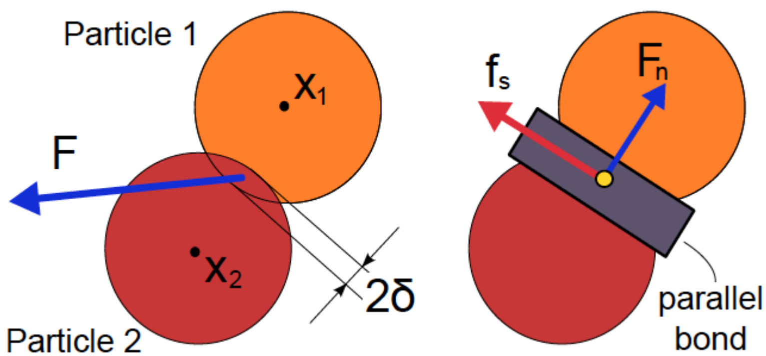
Adapting DEM for modeling solids

- Traditional DEM
  - Granular materials
  - Significant motion of discrete elements
  - Compression loading is straightforward

Oregon sand dunes

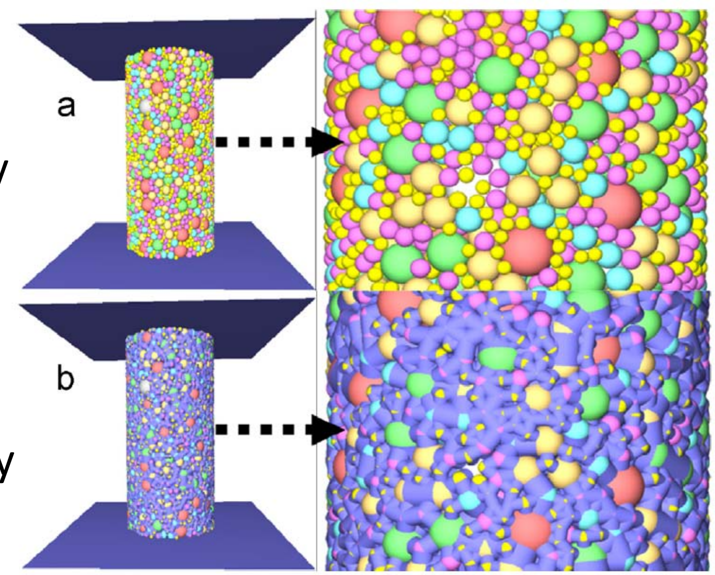
- Solid material DEM
  - Bond elements using parallel solid bonds
  - Full range of loading configurations can be simulated (tension, bending, etc.)

Now an element is meso-scale domain



unbound assembly

bonded assembly



Cai et al. (2014)

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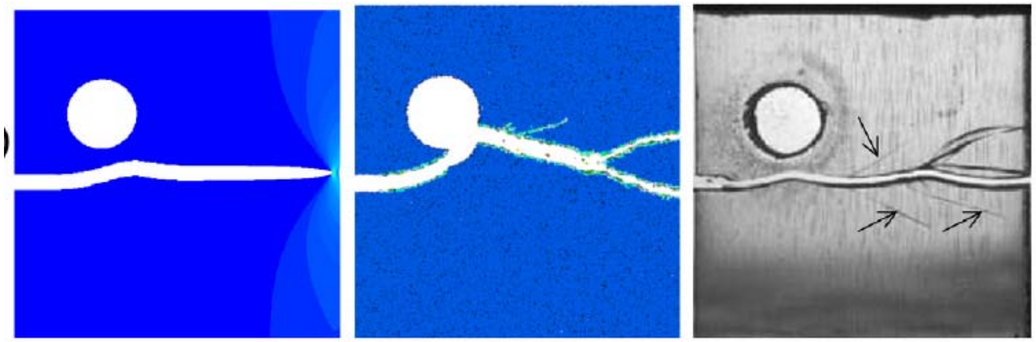
Adapting DEM for modeling solids

- Solid materials DEM has been used for:
  - Amorphous materials (silica glass, polymers)
  - Particle reinforced composites
- No need to predefine crack location/path
  - Emerge naturally from DEM model

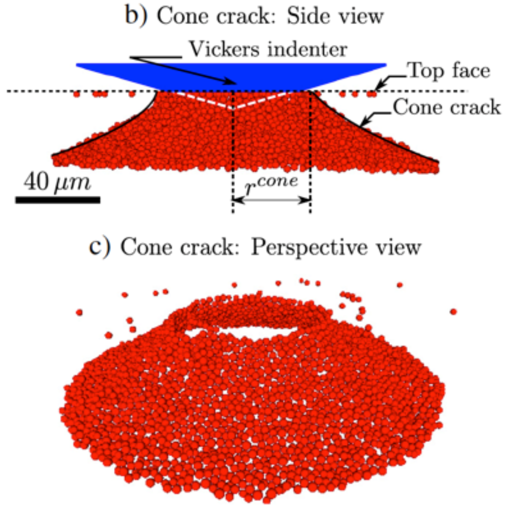
<u>FEM Model:</u>
No crack branching predicted

<u>DEM Model:</u>
Crack branching matches experiment



Hedjazi et al. (2012)

<u>DEM Model:</u>
Cone crack emerges under indent in silica glass



Jebahi et al. (2013)

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Adapting DEM for modeling solids

DEM started like this:

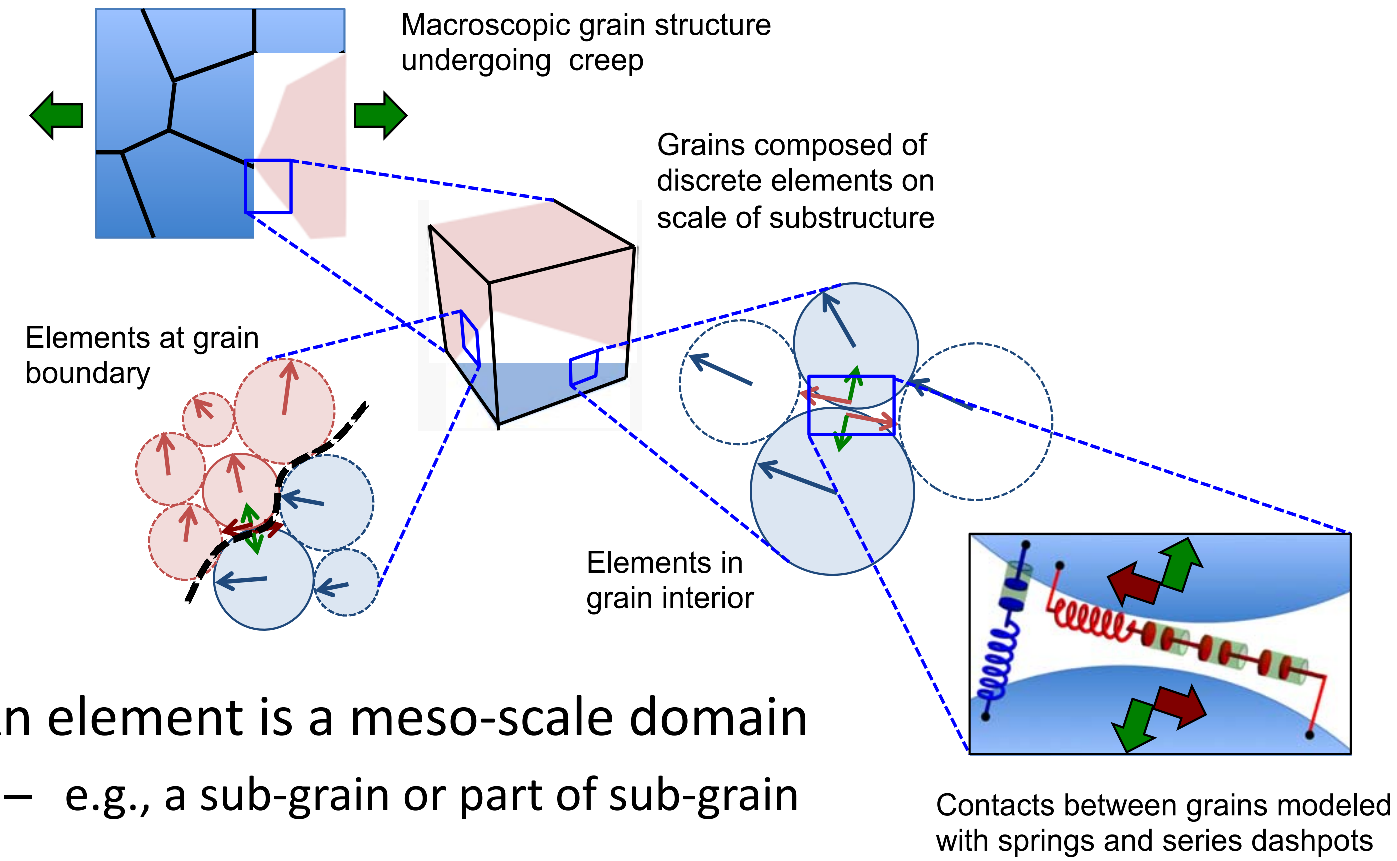
Oregon sand dunes

Next we want to model this:

Turbine blisk

Our approach

- DEM crystal plasticity model for predicting creep and creep-fatigue of nickel based alloys



- An element is a meso-scale domain
  - e.g., a sub-grain or part of sub-grain

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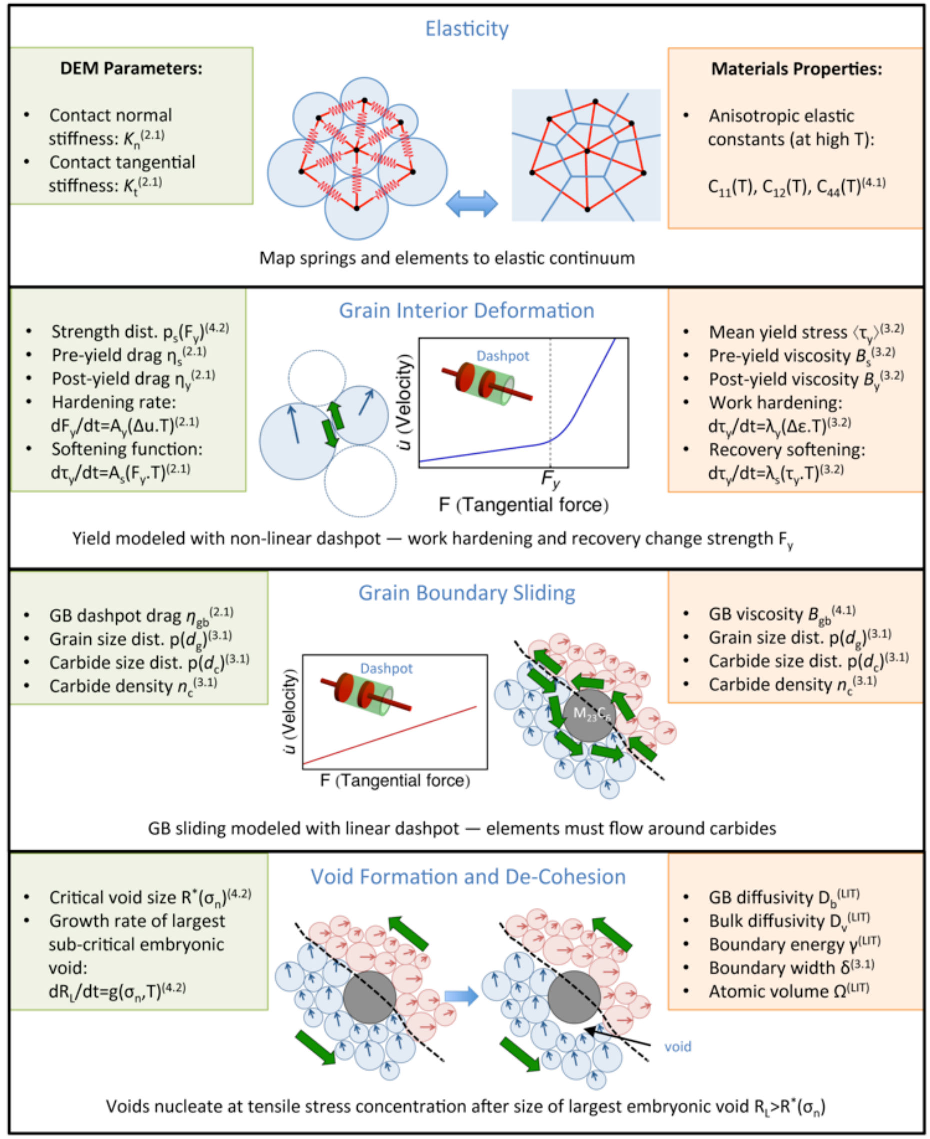
What are we working towards?

- We propose to adapt DEM to correctly capture:
  - Polycrystal deformation (plasticity, creep)
  - Microstructure evolution
  - Stochastic damage evolution (voids, cracking)



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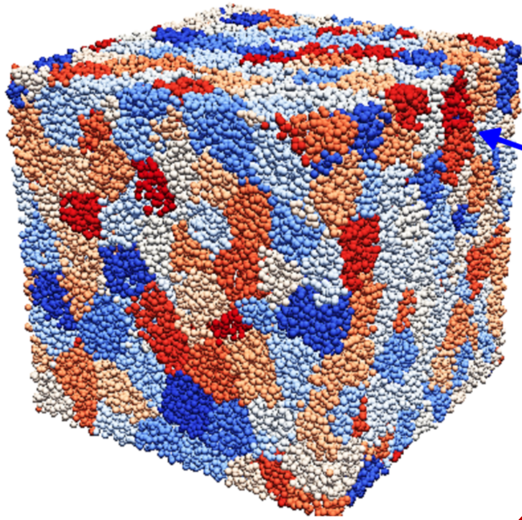
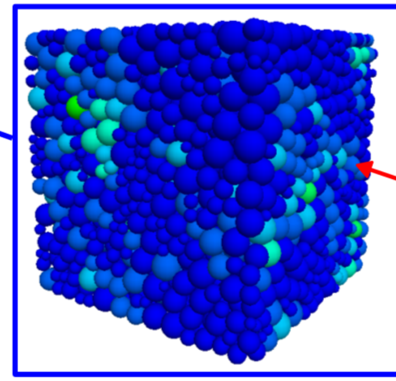
Developing the DEM model

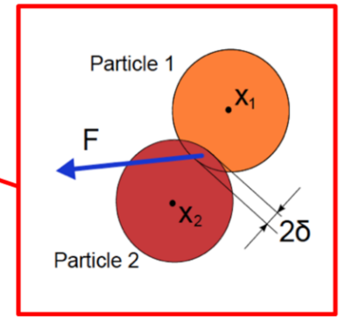
Collection of grains

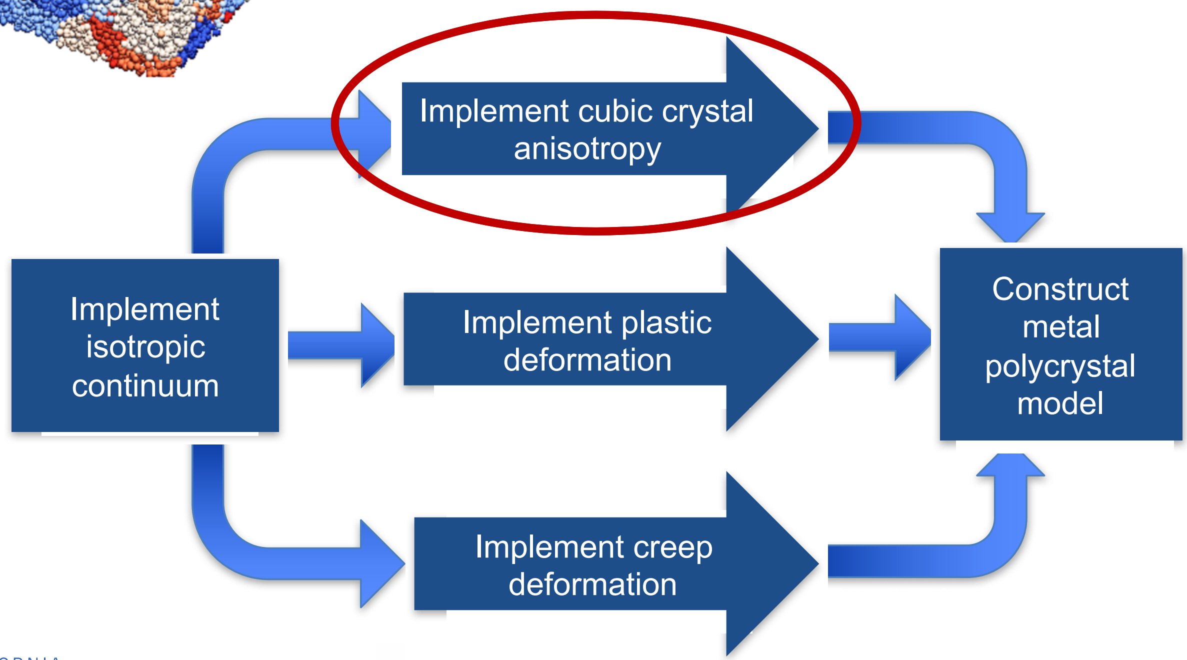


Single grain



Single elements - sub-grains



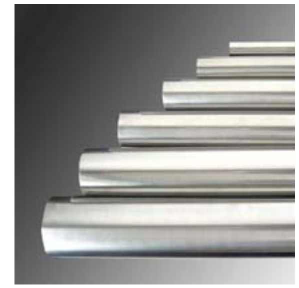


Material Selection

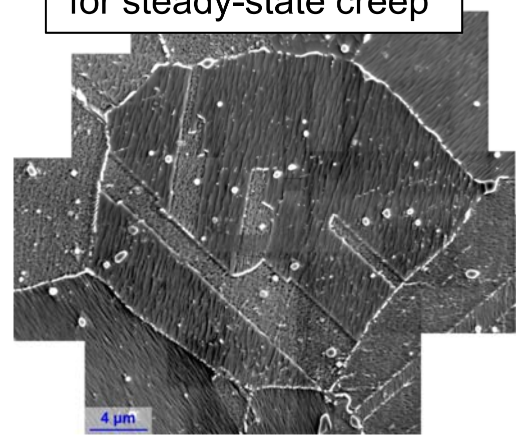
- <u>Nimonic 75 chosen as model alloy</u>
  - Simple Ni-20Cr solid solution microstructure represents many superalloys
    - Austenitic, solid solution grains
    - Chromium rich, globular grain-boundary carbides normally of the type $M_{23}C_6$
  - Certified tensile and creep reference material
    - We purchased a standardized microstructure certified to have specific tensile and creep properties
  - Model will be developed for 600°C deformation
    - Creep behavior certified at 600°C

JRC
EUROPEAN COMMISSION

irmm
Institute for Reference Materials and Measurements



typical microstructure for steady-state creep



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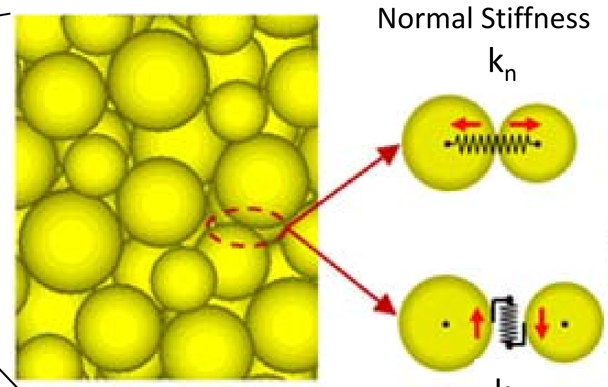
Adapting DEM for elastic anisotropy

Oregon sand dunes

Particle Assembly



http://www.ngi.no/

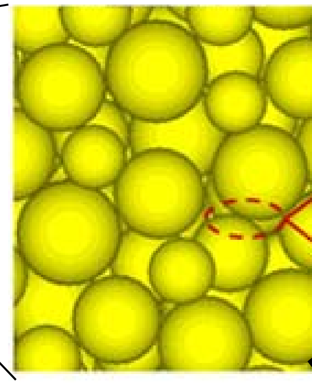
We must develop contact behaviors to make sand elastic

Homogeneous and isotropic in elastic response

Adapting DEM for elastic anisotropy

Oregon sand dunes

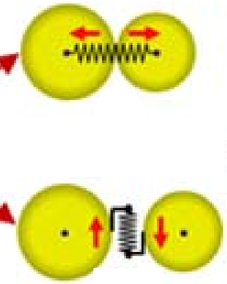
Particle Assembly



http://www.ngi.no/

Normal Stiffness

k_n



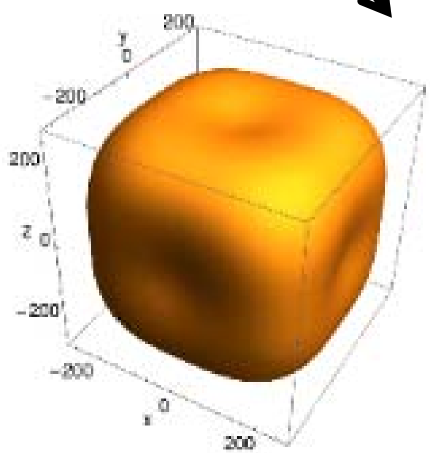
k_s

Shear Stiffness

We must define particle interactions k_n and k_s to produce full stiffness tensor

More than that we must make sand anisotropic elastic!

Ni-Cr: homogeneously elastic, but anisotropically elastic

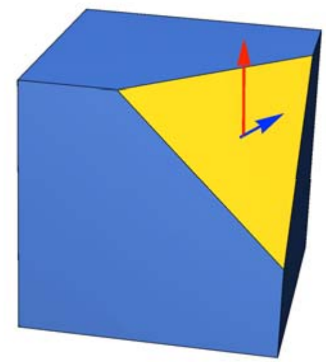


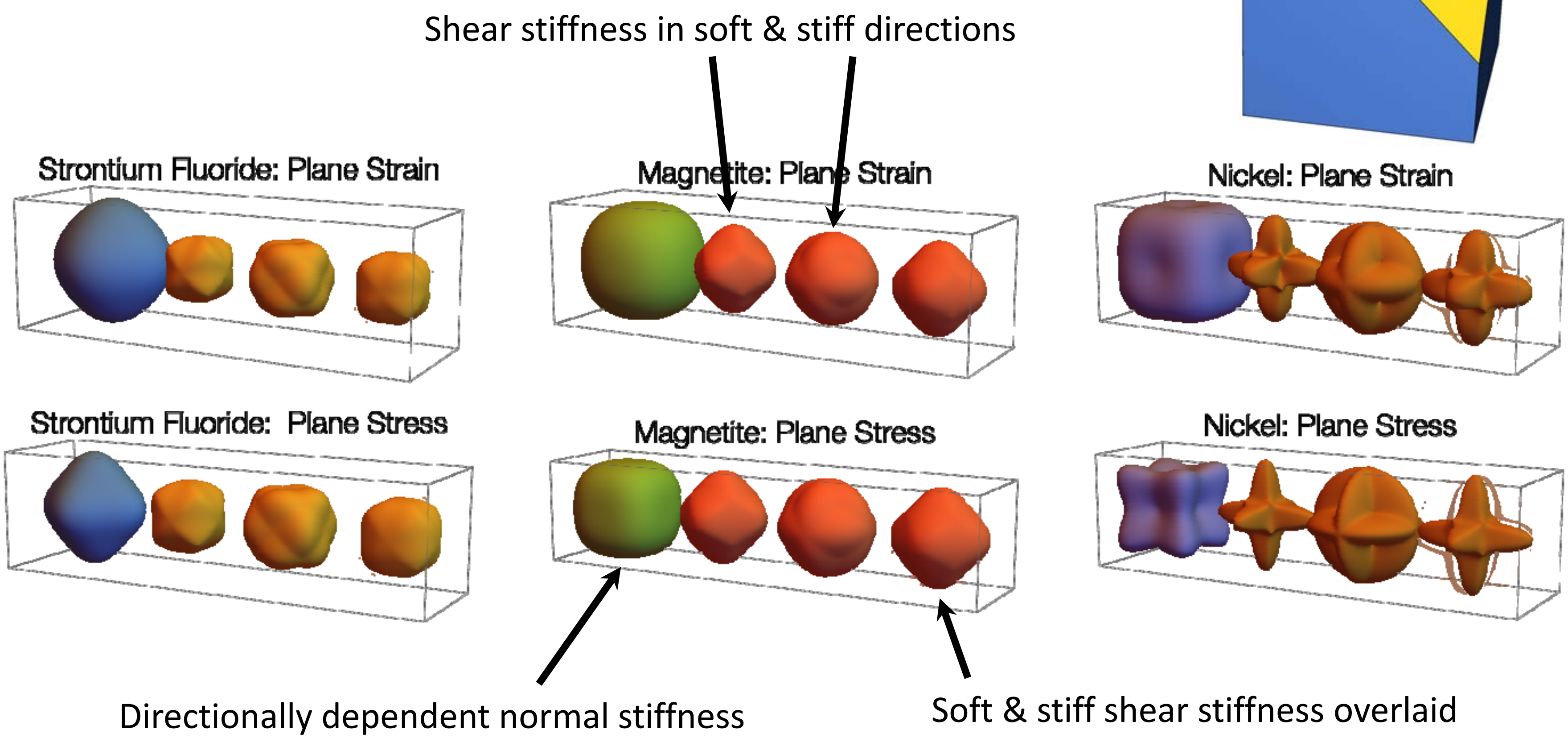
$$C_{ij} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

Adapting DEM for elastic anisotropy

The subtleties of anisotropic elasticity...

- Directionally dependent elastic response of cubic single crystals





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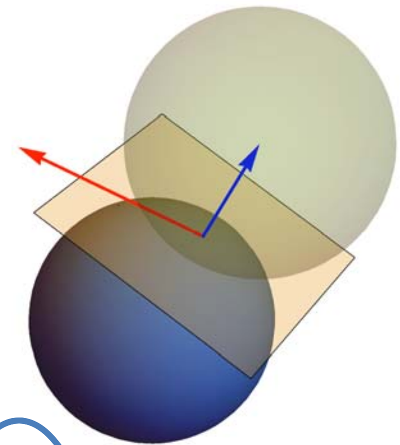
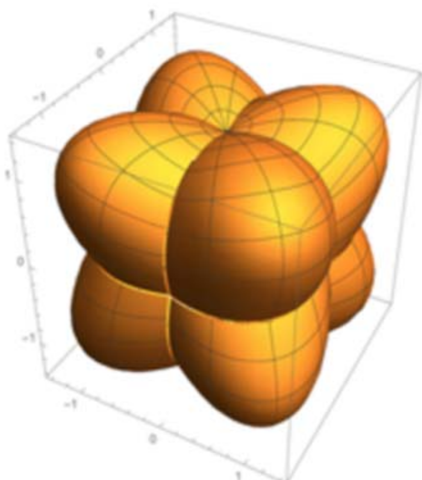
Adapting DEM for elastic anisotropy

Define angularly dependent contact stiffness $k_n(\theta,\Phi)$ and $k_s(\theta,\Phi)$ with cubic symmetry



Define $k_n(\theta,\Phi)$ as 4 spheroids aligned along <111> directions



$$r_{j1} = \frac{a_j^{\frac{2}{3}}}{\sqrt{\frac{1}{3}(n_x - n_y + n_z)^2 + 2.0(n_x^2 + n_x n_y + n_y^2 - n_x n_z + n_y n_z + n_z^2)a_j^2}}$$

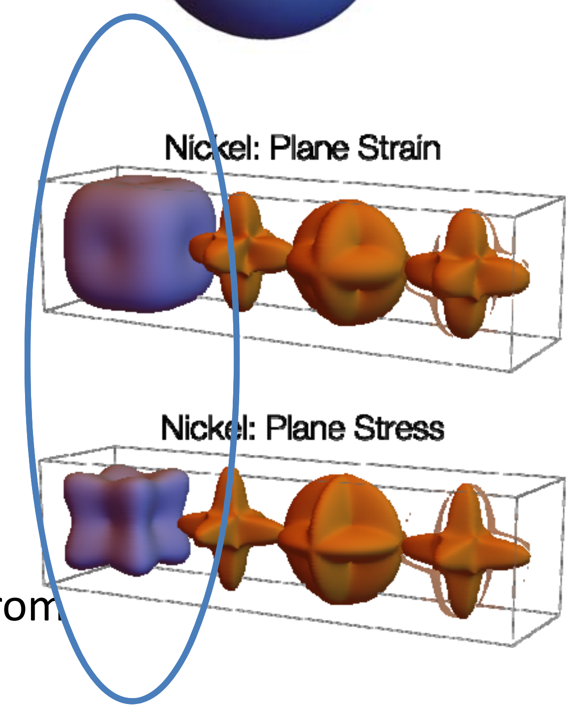
$$r_{j2} = \frac{a_j^{\frac{2}{3}}}{\sqrt{\frac{1}{3}(n_x + n_y - n_z)^2 + 2.0(n_x^2 - n_x n_y + n_y^2 - n_x n_z + n_y n_z + n_z^2)a_j^2}}$$

$$r_{j3} = \frac{a_j^{\frac{2}{3}}}{\sqrt{\frac{1}{3}(-n_x + n_y + n_z)^2 + 2.0(n_x^2 + n_x n_y + n_y^2 - n_x n_z - n_y n_z + n_z^2)a_j^2}}$$

$$r_{j4} = \frac{a_j^{\frac{2}{3}}}{\sqrt{\frac{1}{3}(n_x + n_y + n_z)^2 + 2.0(n_x^2 - n_x n_y + n_y^2 - n_x n_z - n_y n_z + n_z^2)a_j^2}}$$

$$r_j = \max(r_{j1}, r_{j2}, r_{j3}, r_{j4})$$

$$k_l = \frac{A_b}{L_b} r_l \bar{k}_l$$



Cubic elasticity will emerge from collection of particles

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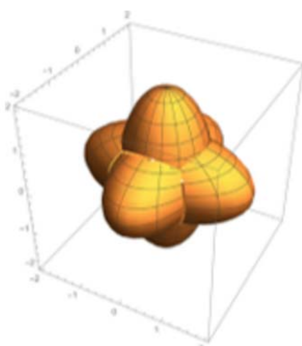
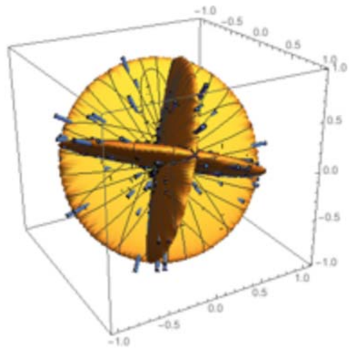
Adapting DEM for elastic anisotropy

Define angularly dependent contact stiffness $k_n(\theta,\Phi)$ and $k_s(\theta,\Phi)$ with cubic symmetry

Define $k_s(\theta,\Phi)$ as 3 spheroids aligned along <100> directions





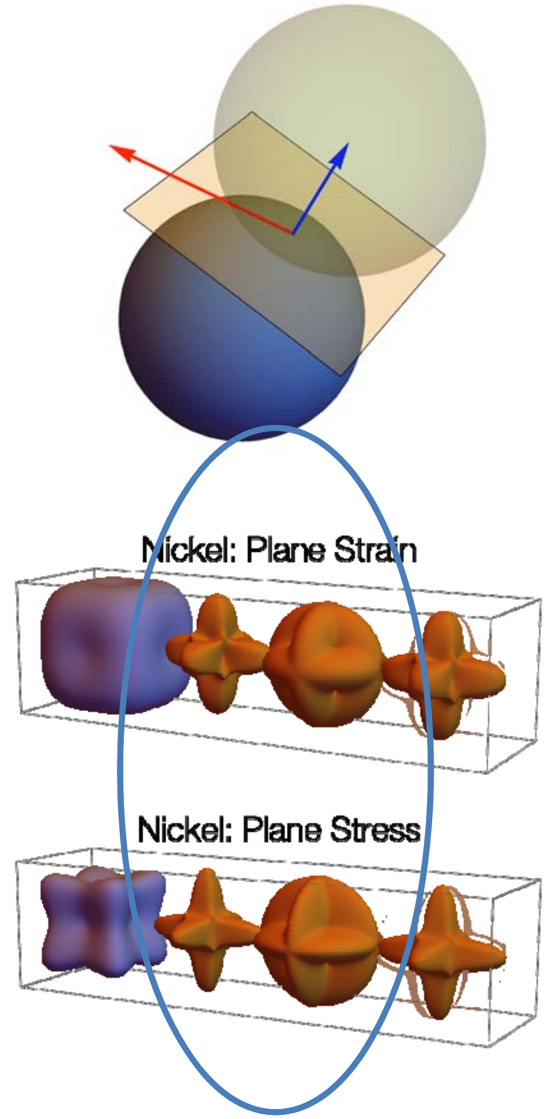
$$r_{i1} = \sqrt{\frac{a_i^{\frac{2}{3}}}{n_x^2 + (n_y^2 + n_z^2)a_i^2}}$$

$$r_{i2} = \sqrt{\frac{a_i^{\frac{2}{3}}}{n_y^2 + (n_x^2 + n_z^2)a_i^2}}$$

$$r_{i3} = \sqrt{\frac{a_i^{\frac{2}{3}}}{n_z^2 + (n_y^2 + n_x^2)a_i^2}}$$

$$r_i = \max(r_{i1}, r_{i2}, r_{i3})$$

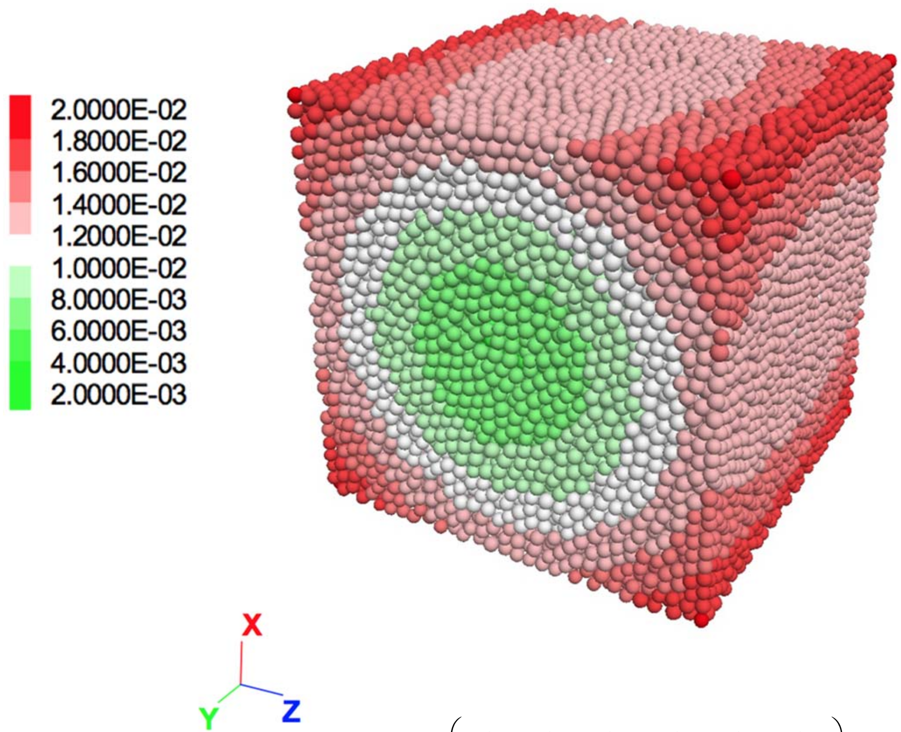
$$k_l = \frac{A_b}{L_b} r_i \bar{k_l}$$



Cubic elasticity will emer
collection of particles

Elasticity simulations

- Representative volume of 30,700 elements and 118,008 bonds
- Simultaneous compression and shear forces applies
- Elastic response used to calculate C_{11}, C_{12}, C_{44} of stiffness tensor



$$C_{ij} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

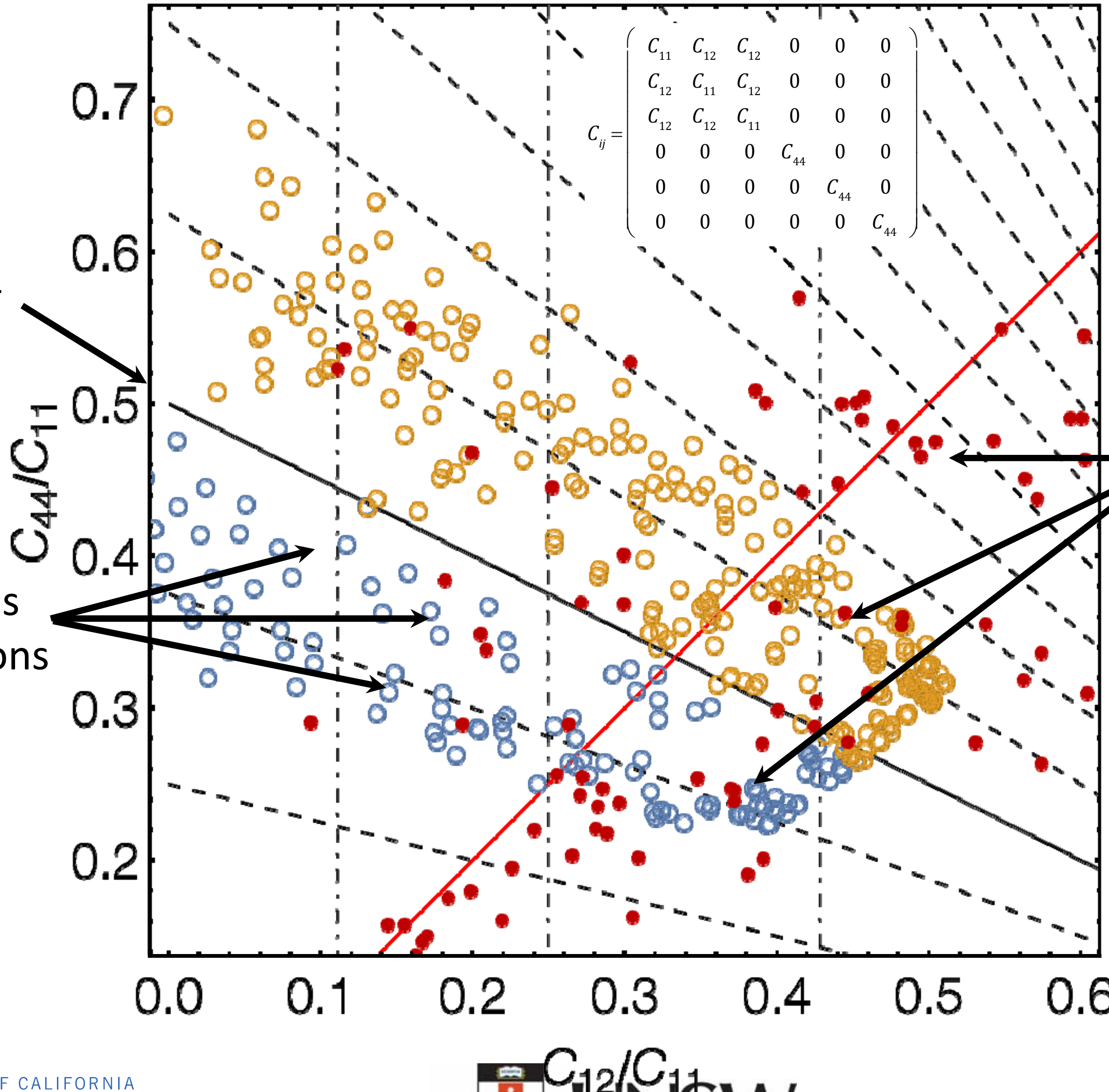
Results of Elasticity Simulations

$$Z = \frac{2C_{44}}{C_{11} - C_{12}}$$

Zener ratio = 1
isotropic

Open symbols
DEM simulations

Solid symbols
Real cubic
crystals



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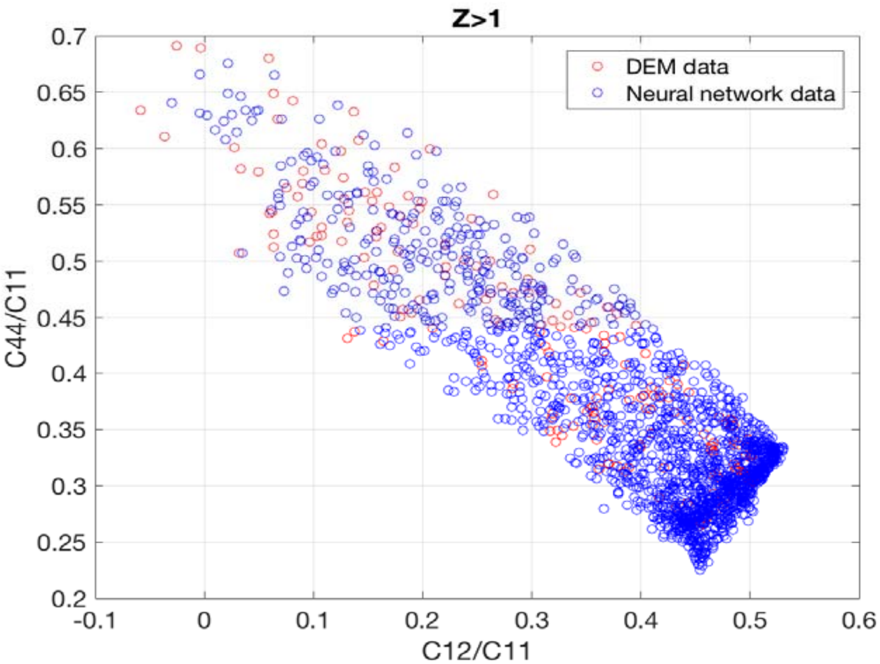
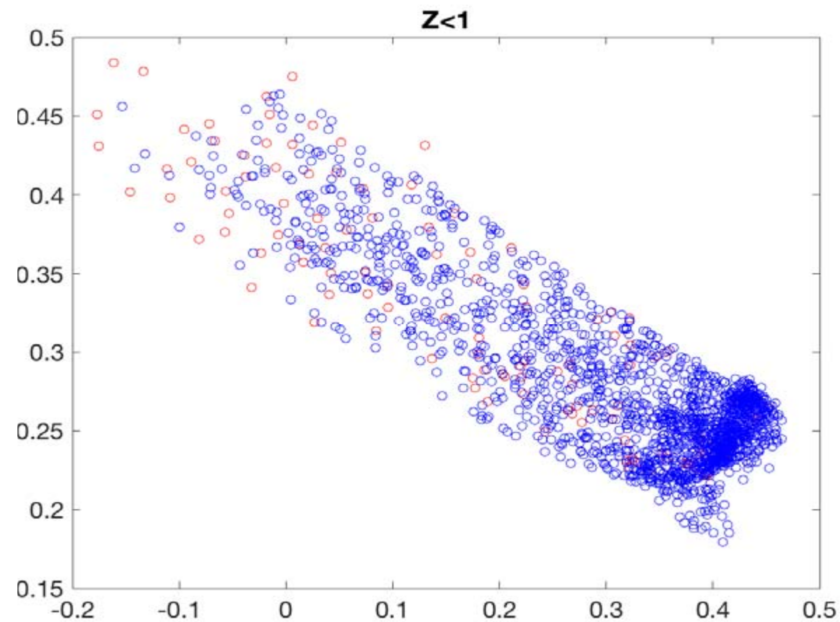
Accessible anisotropic properties

- Neural network approach was used to interpolate the DEM model results
- Range of cubic crystals accessible by our approach is represented



Stiffer along <111> cubic directions



Stiffer along <100> cubic directions

$$Z = \frac{2C_{44}}{C_{11} - C_{12}}$$

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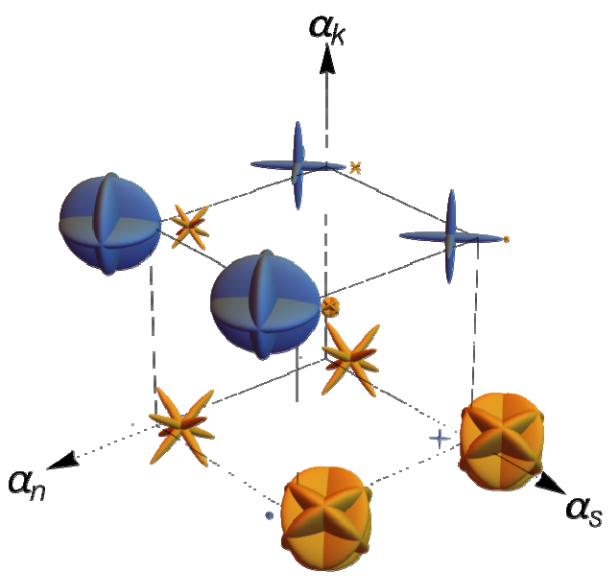
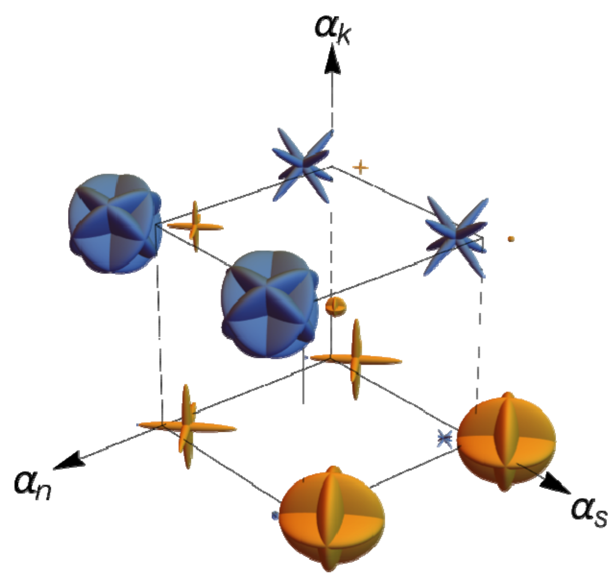
Limitations and potential solutions

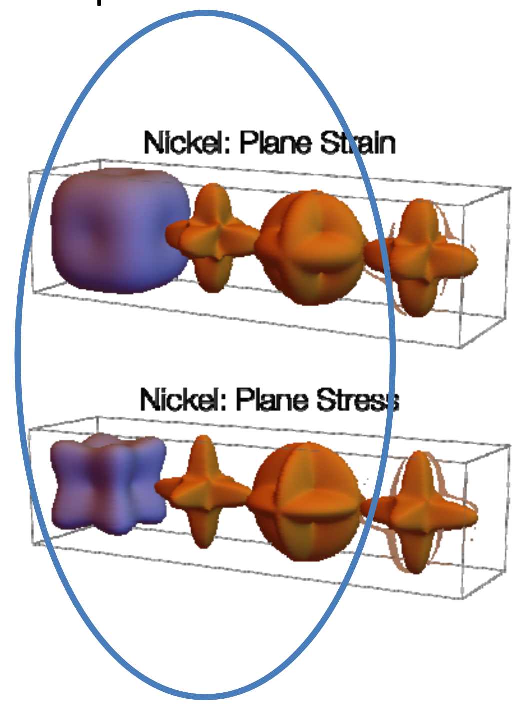
- Standard PFC software does not allow soft and stiff shear direction
  - We only define a single shear stiffness
  - Anisotropy becomes limited by extreme spheroid shapes
    - Small contact rotations give big changes in stiffness
- Move to an open source platform (LAMMPS, Yade, Esys-Particle) or develop new contact model for PFC



Zener ratio < 1; stiffest along ⟨100⟩



Zener ratio > 1; stiffest along ⟨111⟩



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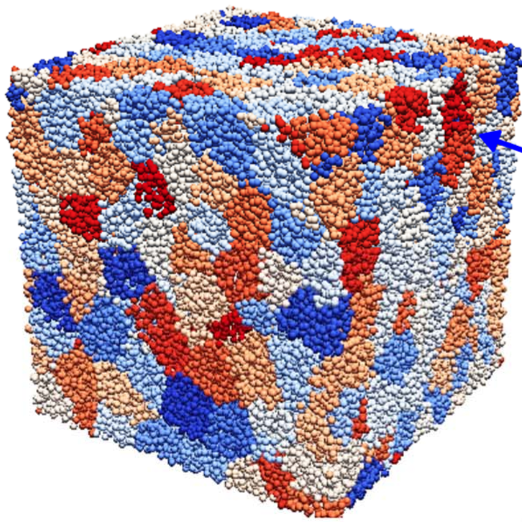
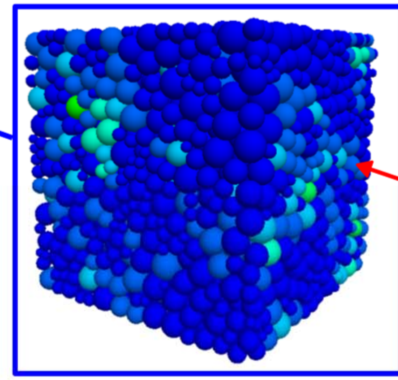
Developing the DEM model

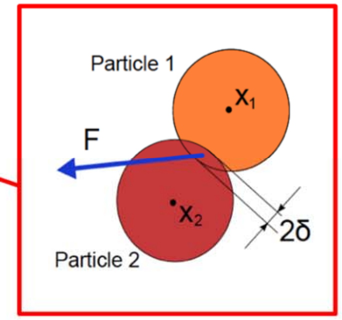
Collection of grains

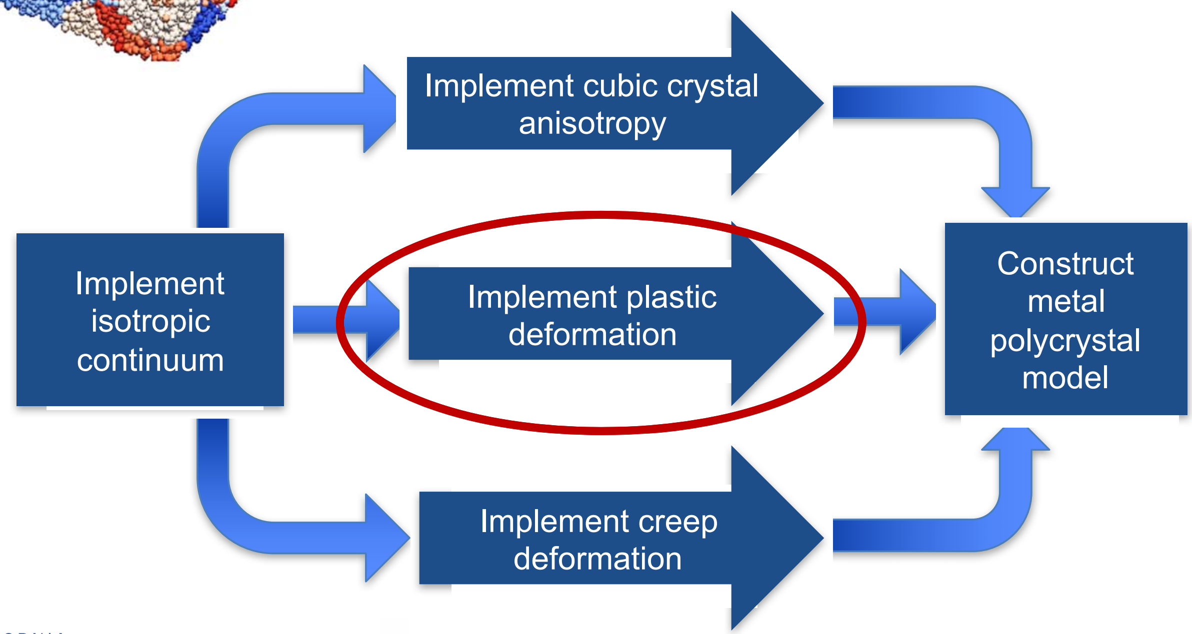


Single grain

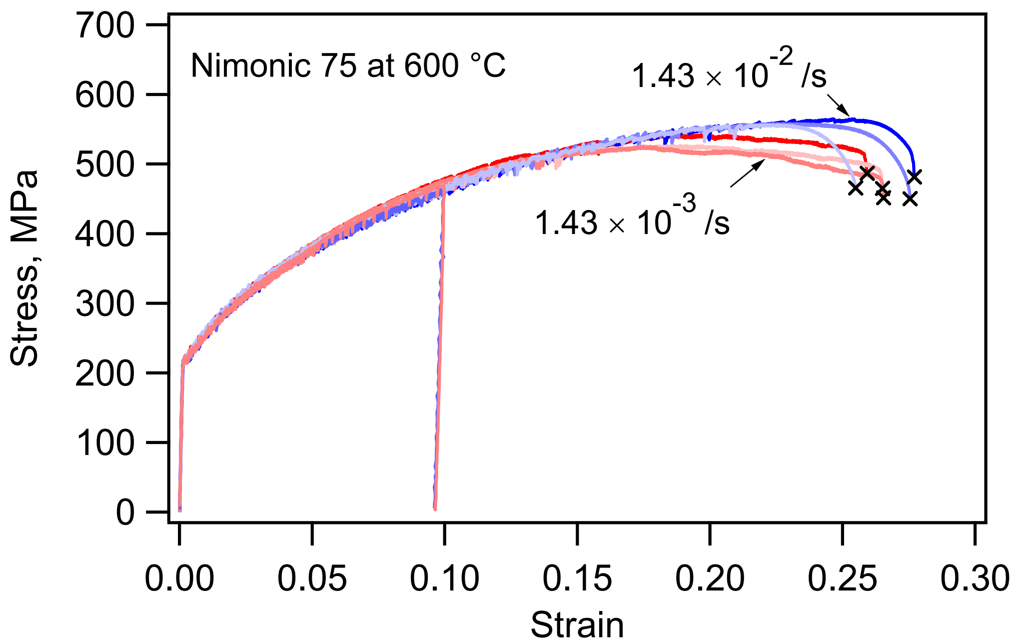


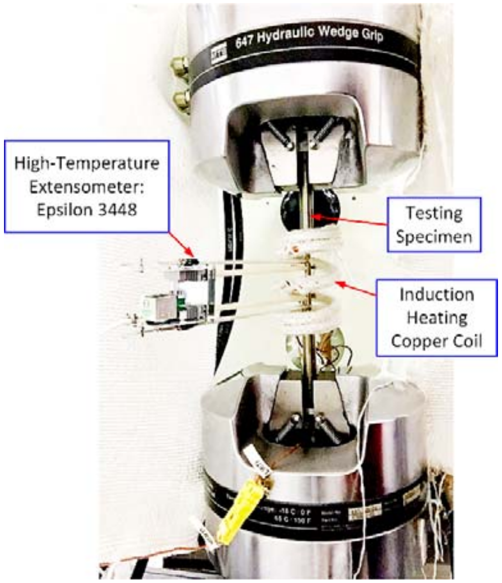
Single elements - sub-grains

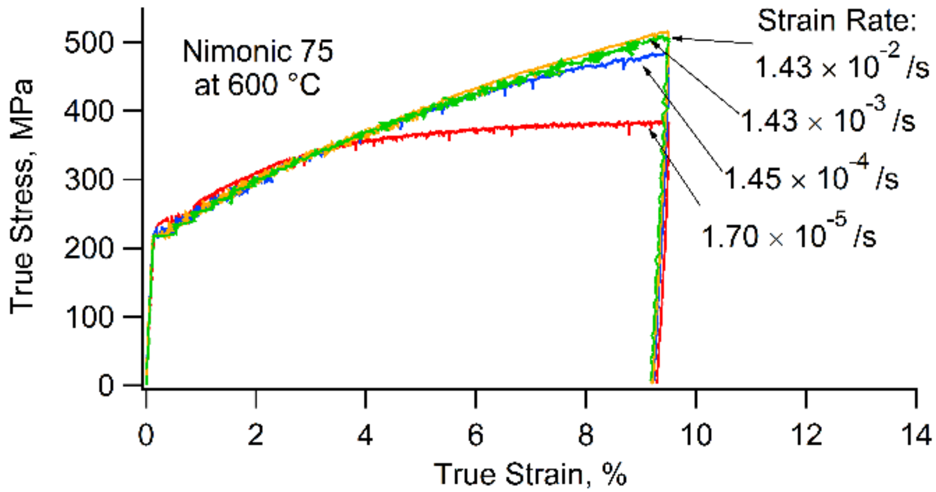




Stress-strain behavior of Nimonic 75 (600°C)







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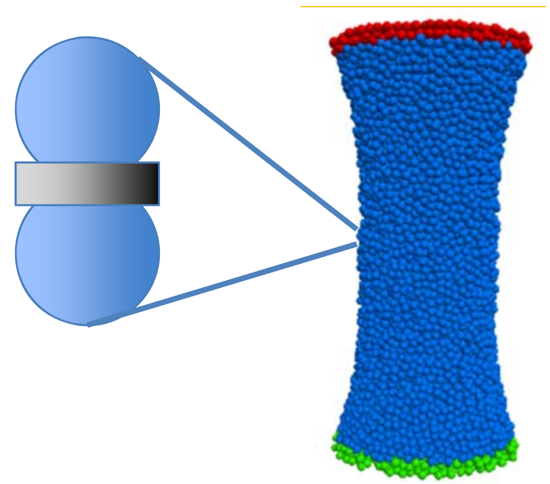
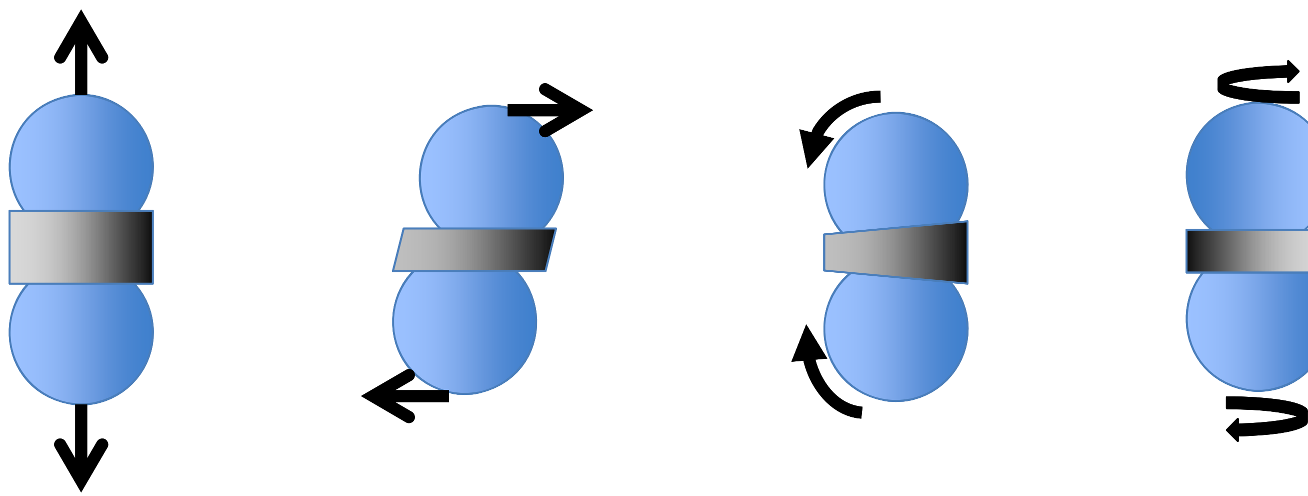
Adapting DEM for plasticity

- Parallel bonded discrete elements:
  - Consider as meso-scale domains
  - Potential sub-grains



Potential Bond Breaking Phenomena

Normal stretch | Shear stretch | Tilt stretch | Twist stretch



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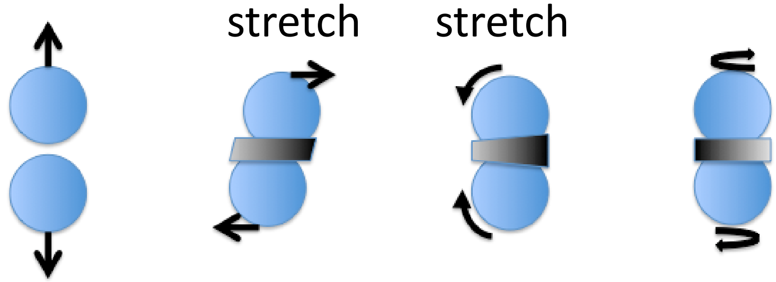
Adapting DEM for plasticity

Shear stretch

Tilt stretch

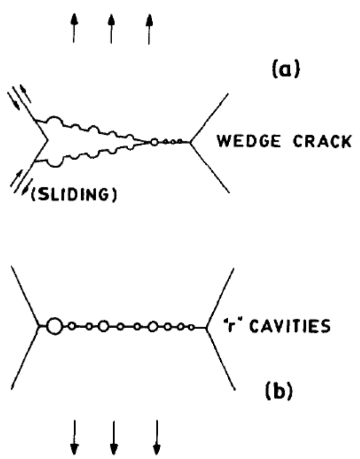
Normal stretch



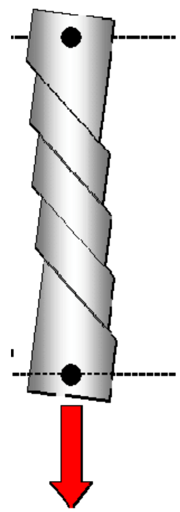
Twist stretch

Corresponding Physical Phenomena

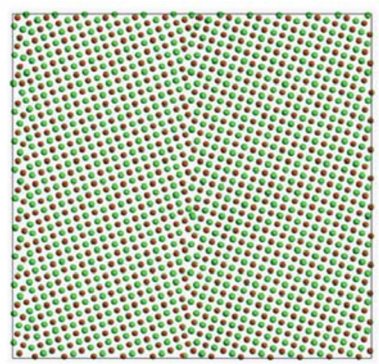
Crack or Void Formation



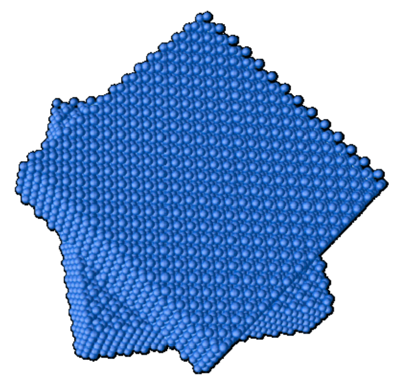
Plastic slip



Tilt Boundary Formation



Twist Boundary Formation



sub-grain evolution

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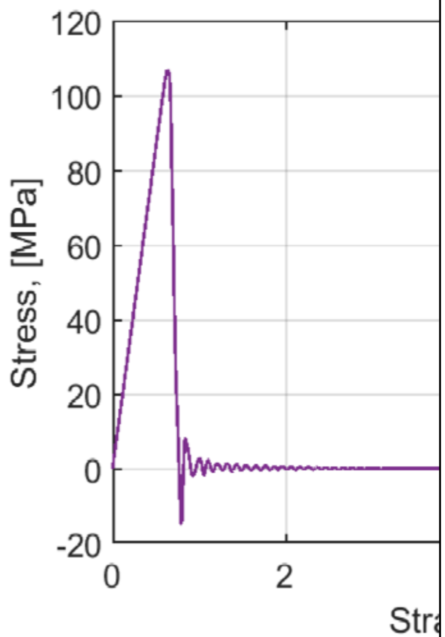
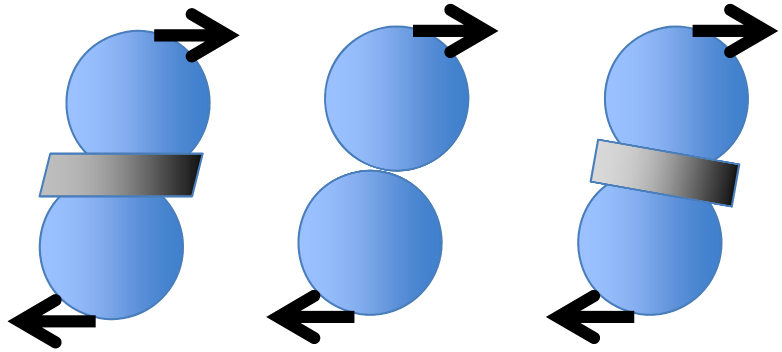
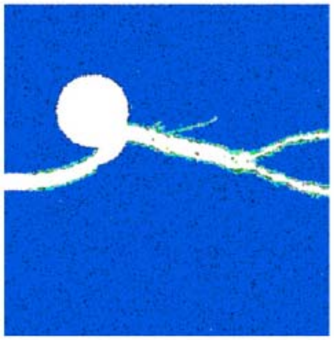
Brittle response in DEM

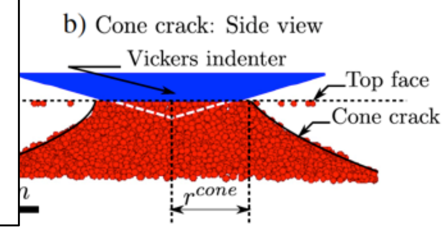


We must introduce bond reforming to get slip-like plasticity





Hedjazi et al. (2012)



Jebahi et al. (2013)

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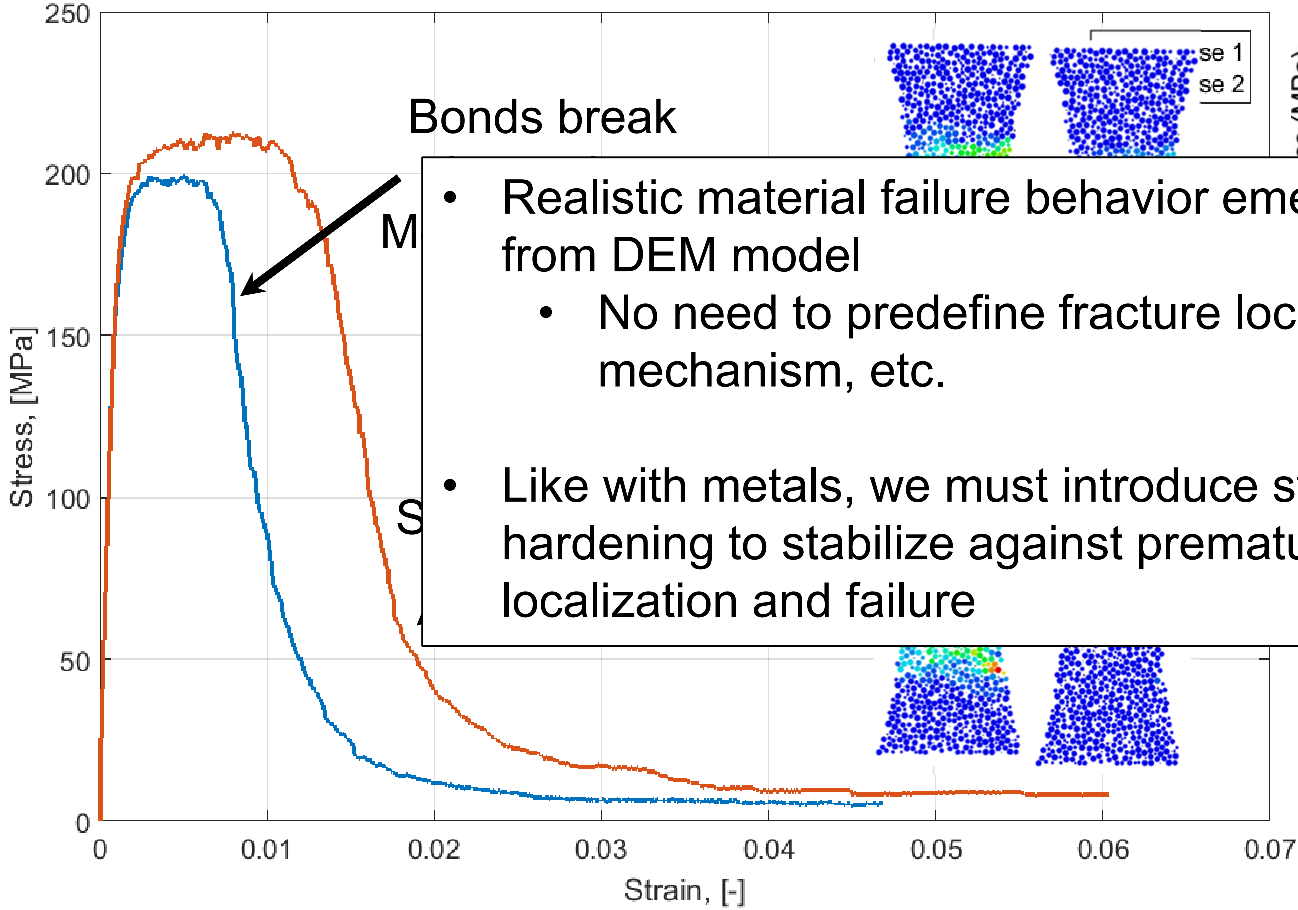
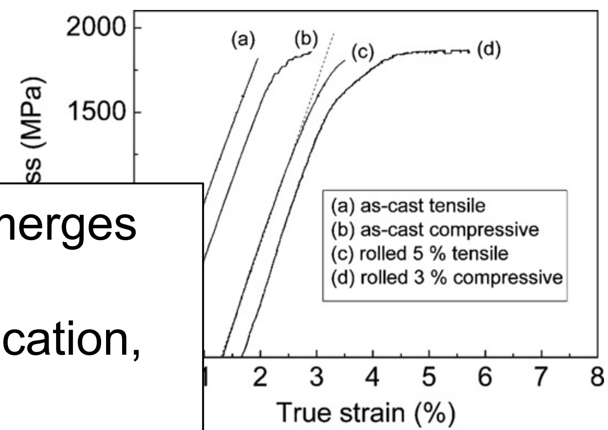
Non-hardening plasticity



- Realistic material failure behavior emerges from DEM model
  - No need to predefine fracture location, mechanism, etc.
- Like with metals, we must introduce strain hardening to stabilize against premature localization and failure

Metallic Glass Behavior



dino et al., Scr. Mater. (2011)

Hofmann *et al. Nature* (2008)

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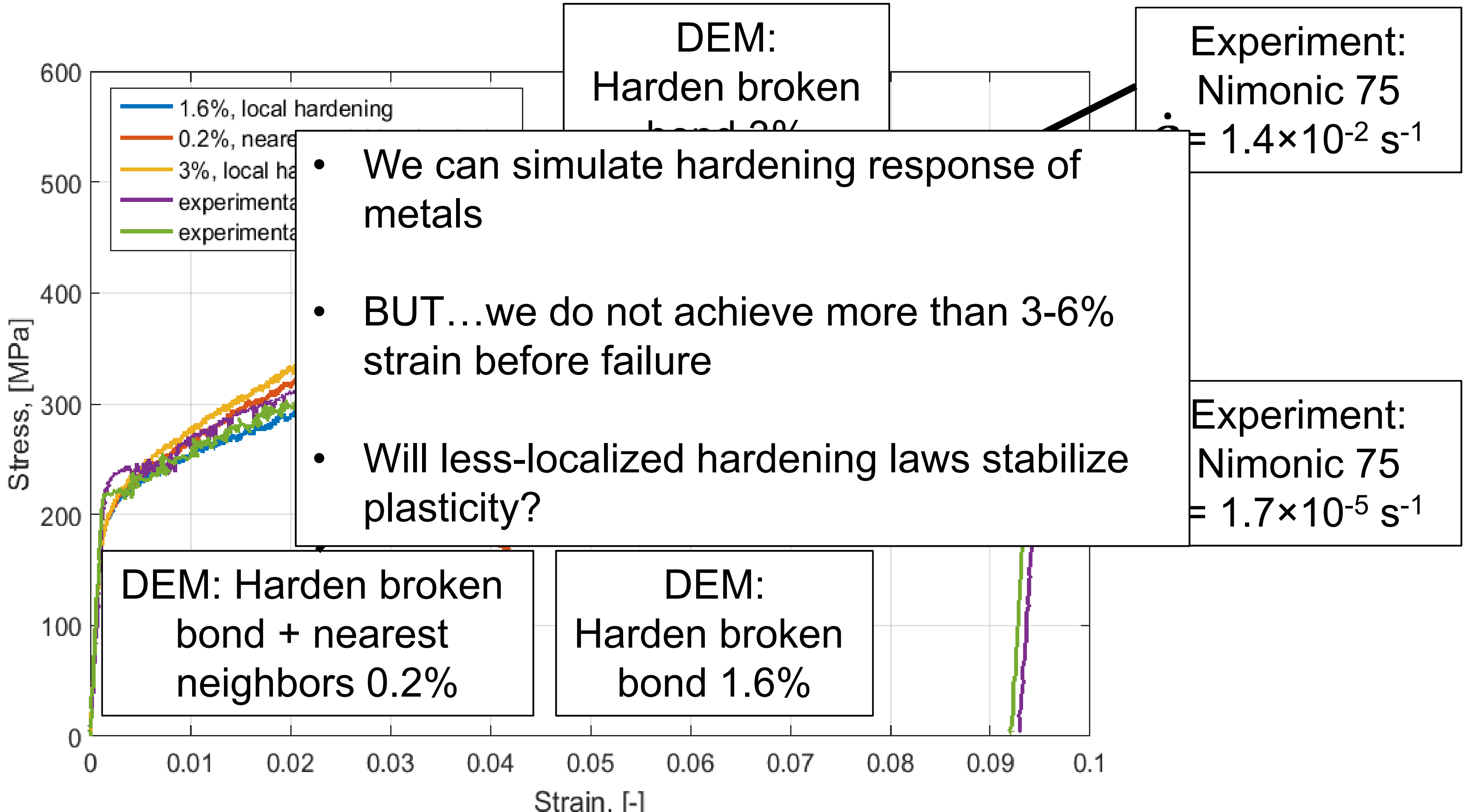
Strain hardening plasticity

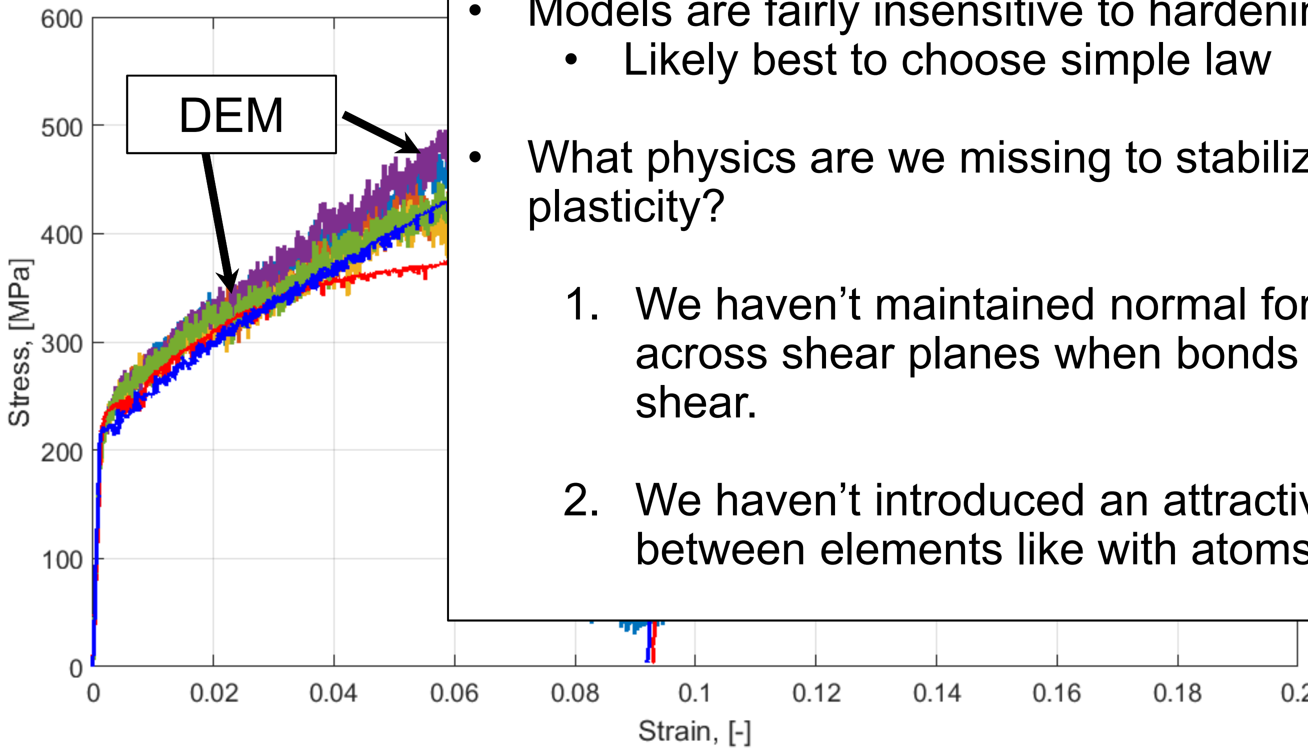
All bonds are failing in shear to simulate slip



- We can simulate hardening response of metals
- BUT…we do not achieve more than 3-6% strain before failure
- Will less-localized hardening laws stabilize plasticity?

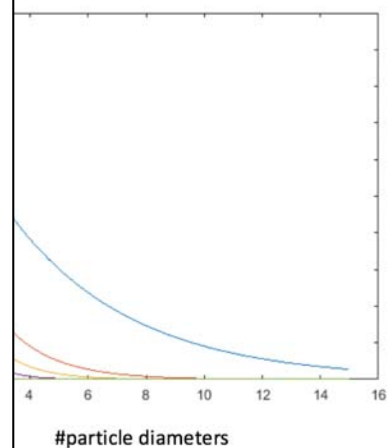
Insensitivity to hardening laws

All bonds are failing in shear to simulate slip



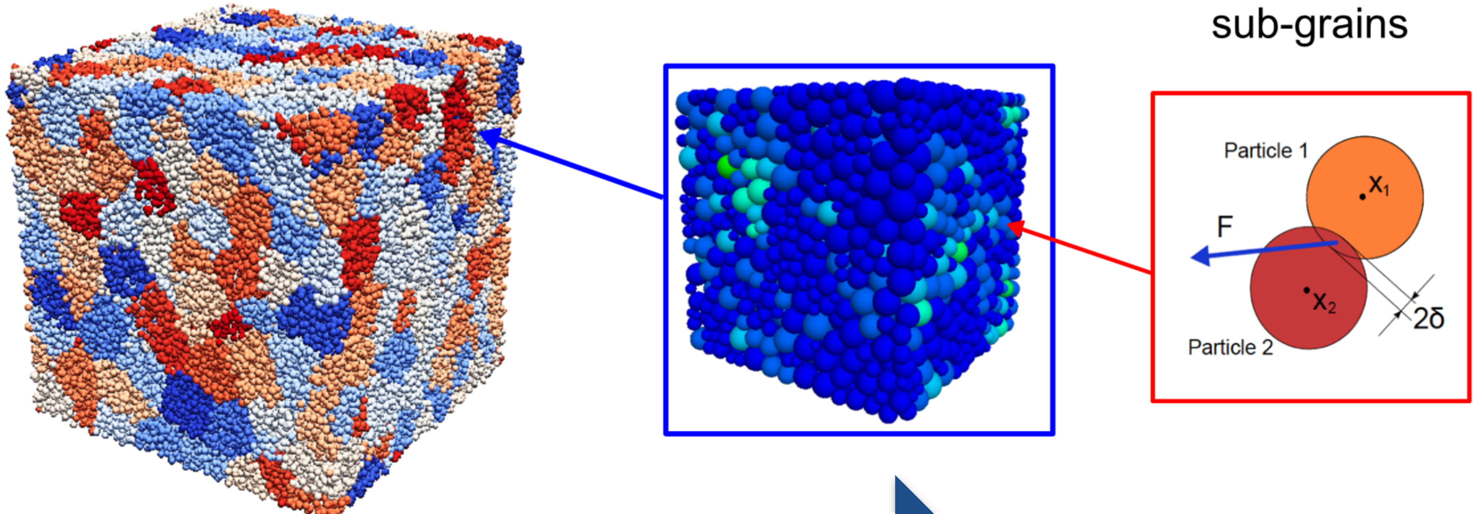
- Models are fairly insensitive to hardening law.
  - Likely best to choose simple law
- What physics are we missing to stabilize plasticity?

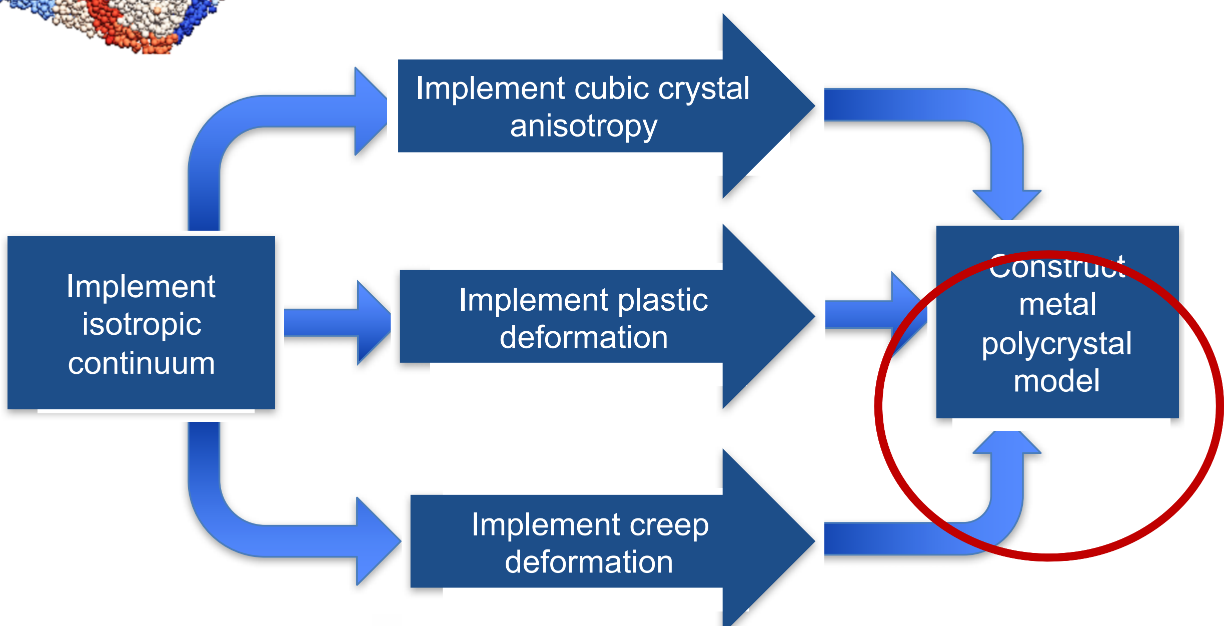
  1. We haven't maintained normal forces across shear planes when bonds break in shear.
  2. We haven't introduced an attractive force between elements like with atoms.



Developing the DEM model

Collection of grains | Single grain | Single elements - sub-grains





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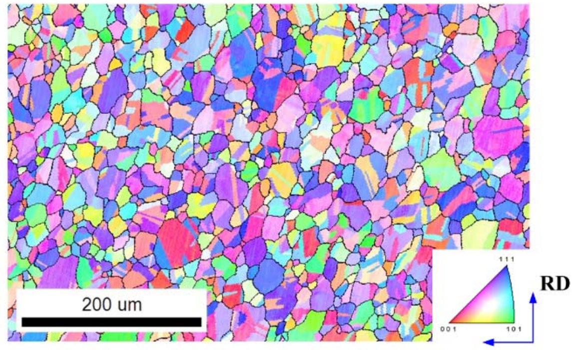
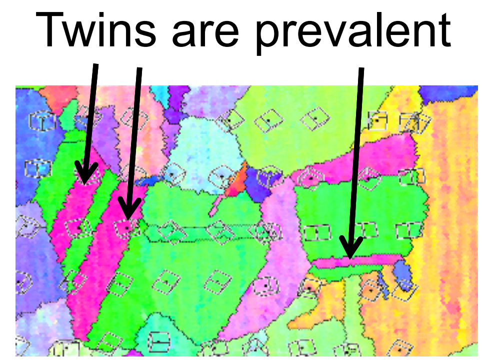
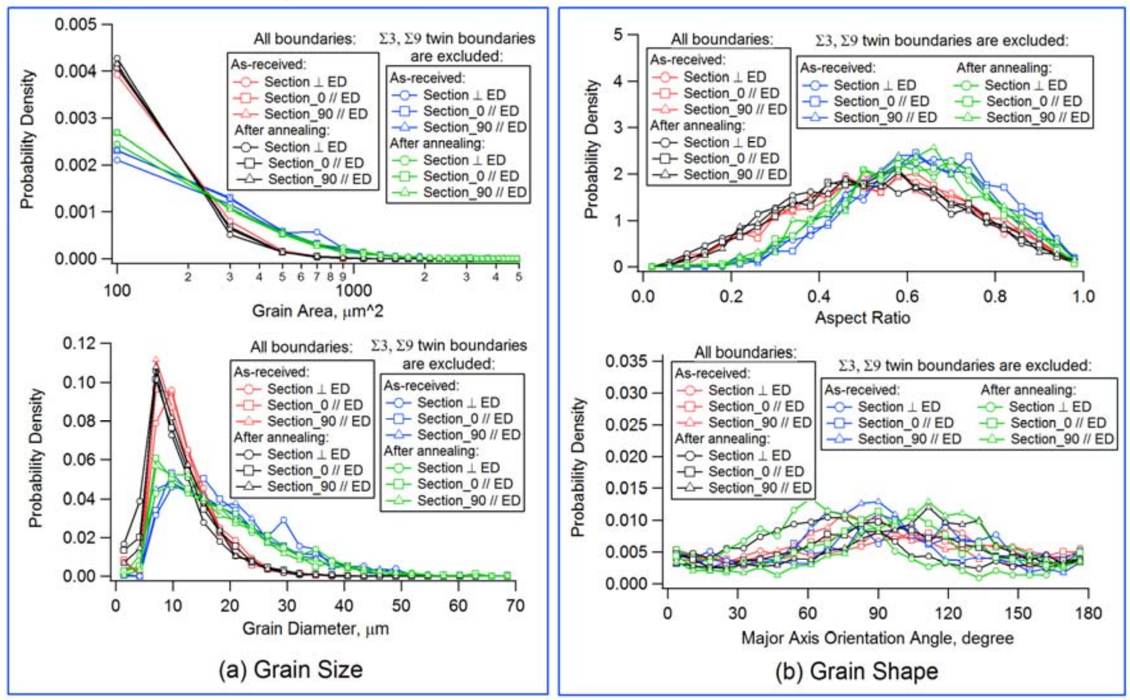
Creating a DEM Polycrystal

- EBSD used to quantify grain structure
  - Presence of twins skews apparent distributions
  - Σ3 and Σ9 annealing twin boundaries are unlikely damage sites (Zhang & Field, 2013)
  - Twin-free microstructure will be used for our DEM model



(b) As Annealed (400 hr 600 ºC)



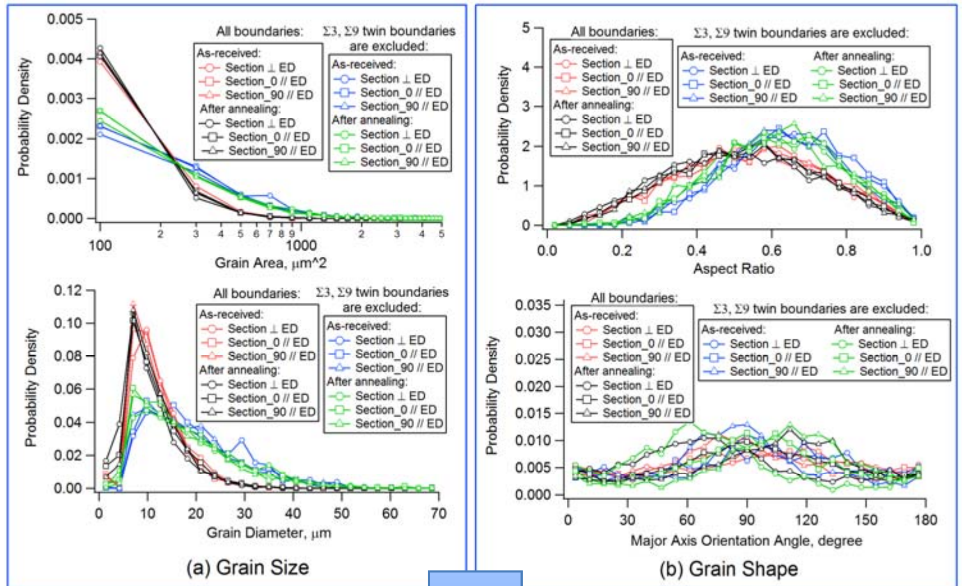


(a) Grain Size

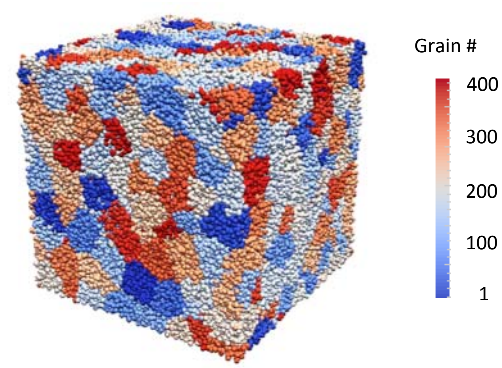
(b) Grain Shape

Creating a DEM Polycrystal

- A 3-D Voronoi algorithm for crystal plasticity has been adapted for making a ploycrystalline DEM assembly
- Assembly captures essential grain size/shape statistics
- Microstructure also being measured in steady state creep regime
  - Steady state microstructure will be used for model



(a) Grain Size
(b) Grain Shape



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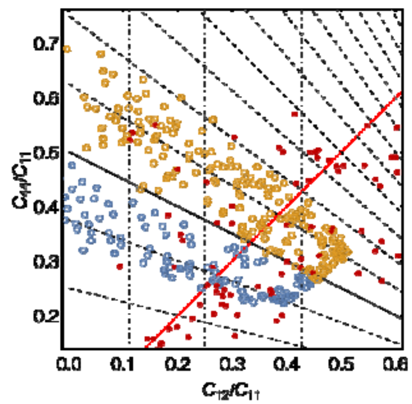
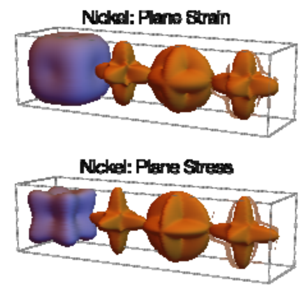
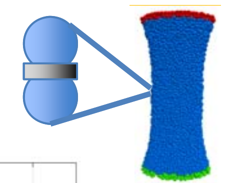
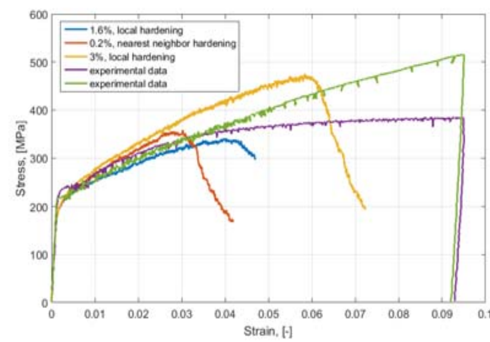
Conclusions

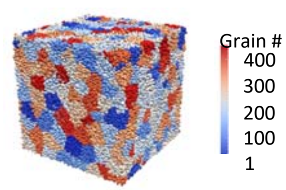
- Developed an anisotropic elasticity DEM formulation to simulate cubic anisotropy
  - Next step is to correctly capture soft and stiff shear directions
- Developed bond breaking and reforming scheme to simulate metal plasticity
  - Currently working to maintain correct forces between slipping elements to avoid premature failure
  - Next step will be adding time dependence (creep)
- Developed a meshing of DEM for metal polycrystals
  - Final step will be correctly developing the grain boundary element interactions











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Questions?