Crosscutting Review Meeting, April 21st, 2016, Pittsburgh, PA

New Mechanistic Models of Long Term Evolution of Microstructure and Mechanical Properties of Nickel Based Alloys

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Acknowledgments

- Postdoctoral researchers:
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  - Dr. Agnieszka Truszkowska

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

This material is based upon work supported by the Department of Energy National Energy Technology Laboratory under Award Number(s) DE-FE0024065.

Background & Motivation

- Current approaches to predicting creep and creep-fatigue behavior are highly empirical
  - Power law creep constitutive laws
    - e.g., Norton Law
  - Linear creep-fatigue damage accumulation

ruptured steel boiler pipe
http://sirius.mtm.kuleuven.be/

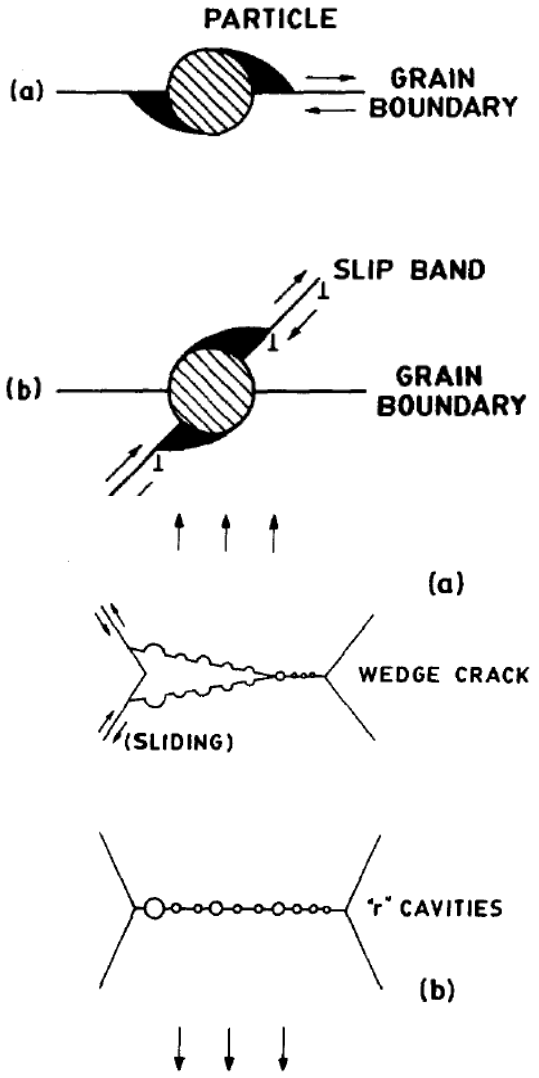
$$\varepsilon = At\sigma^n \exp\left(-Q/RT\right)$$

- Not easily extendible outside measured ranges
  - Longer lifetimes
  - Variable operating conditions

$$\underbrace{\sum_j \left(\frac{n}{N_d}\right)_j}_{\text{Cyclic Damage}} + \underbrace{\sum_k \left(\frac{\Delta t}{T_d}\right)_k}_{\text{Creep Damage}} \leq D$$

Background & Motivation

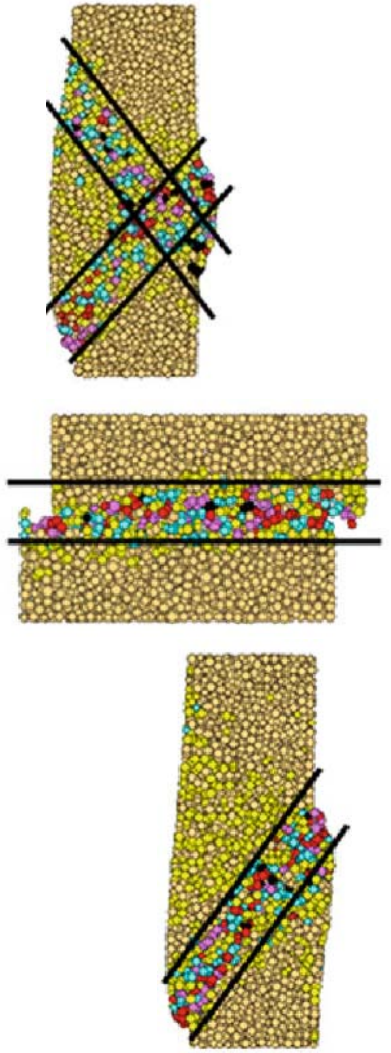
- Review article by Pineau and Antolovich (2009):
  - Generalized approaches to lifetime prediction likely not successful
  - Suggest inclusion of critical damage mechanisms into material and service condition specific models
- Challenge
  - Difficult to include stochastic damage mechanisms in current modeling methods (e.g., FEM) in predictive manner



Rodriguez & Rao (1993)

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)

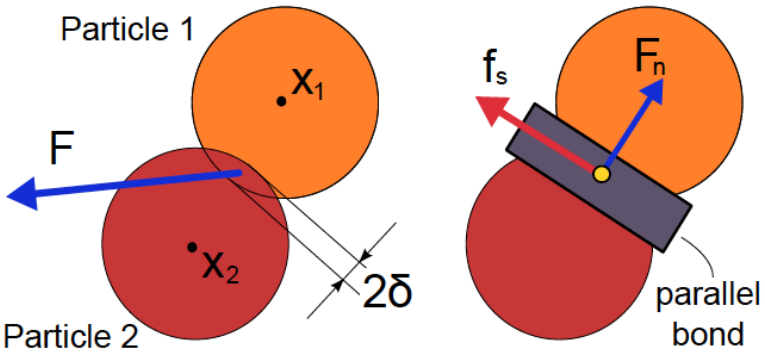
Adapting DEM for modeling solids

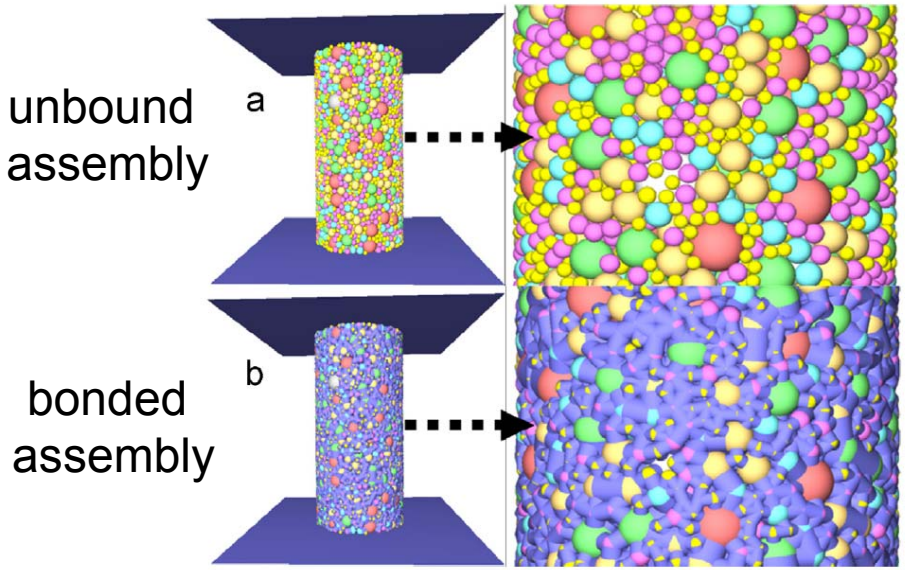
- Traditional DEM
  - Granular materials
  - Significant motion of discrete elements
  - Compression loading is straightforward

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





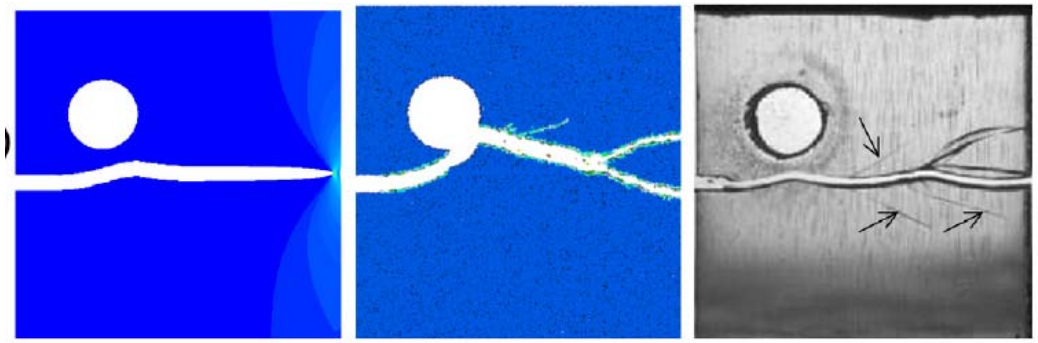
Cai et al. (2014)

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

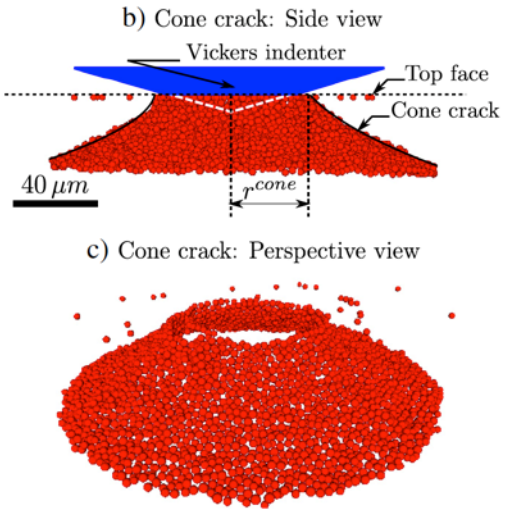
FEM Model:
No crack branching predicted

DEM Model:
Crack branching matches experiment



Hedjazi et al. (2012)

DEM Model:
Cone crack emerges under indent in silica glass



Jebahi et al. (2013)

Adapting DEM for modeling solids

DEM started like this:

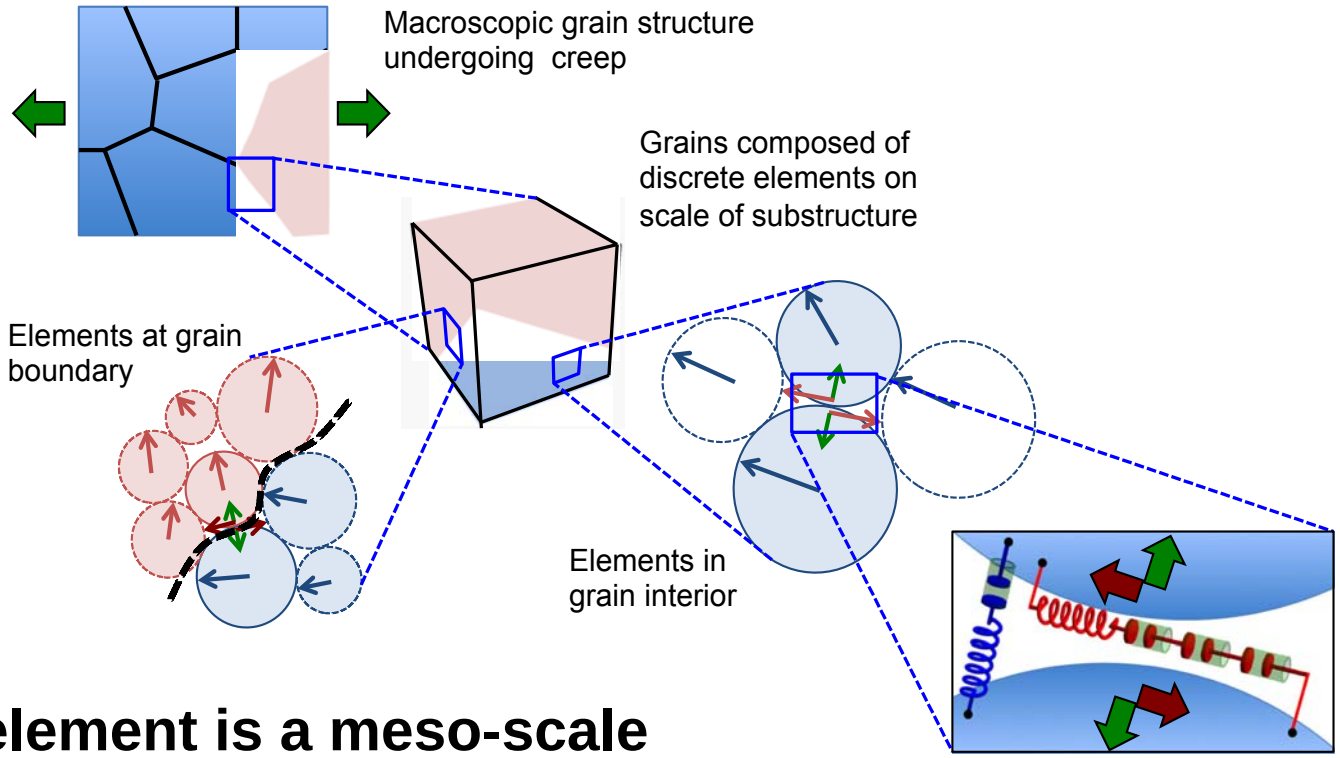
Oregon sand dunes

Next we want to model this:

Turbine blisk

Our approach

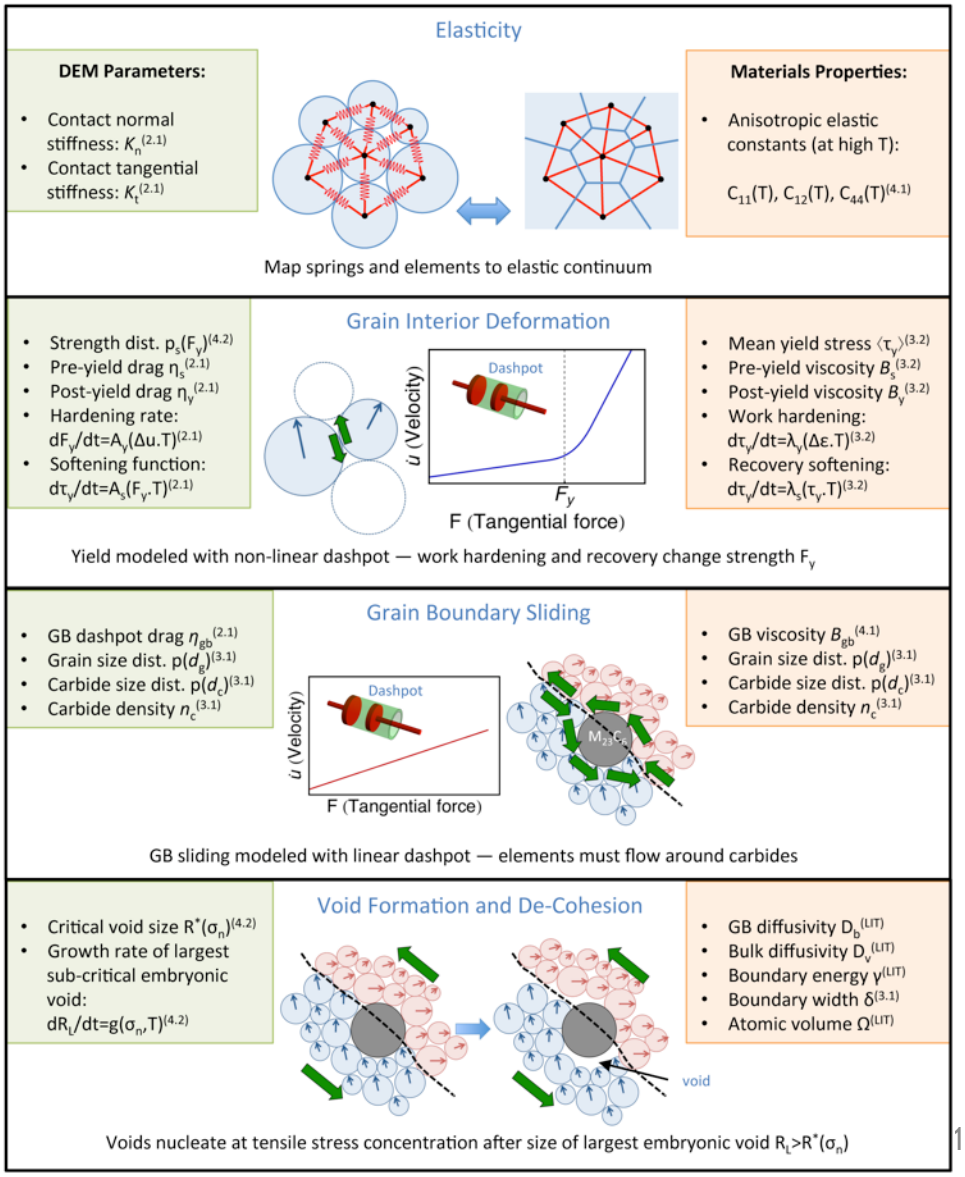
- DEM crystal plasticity model for predicting creep and creep-fatigue of nickel based alloys



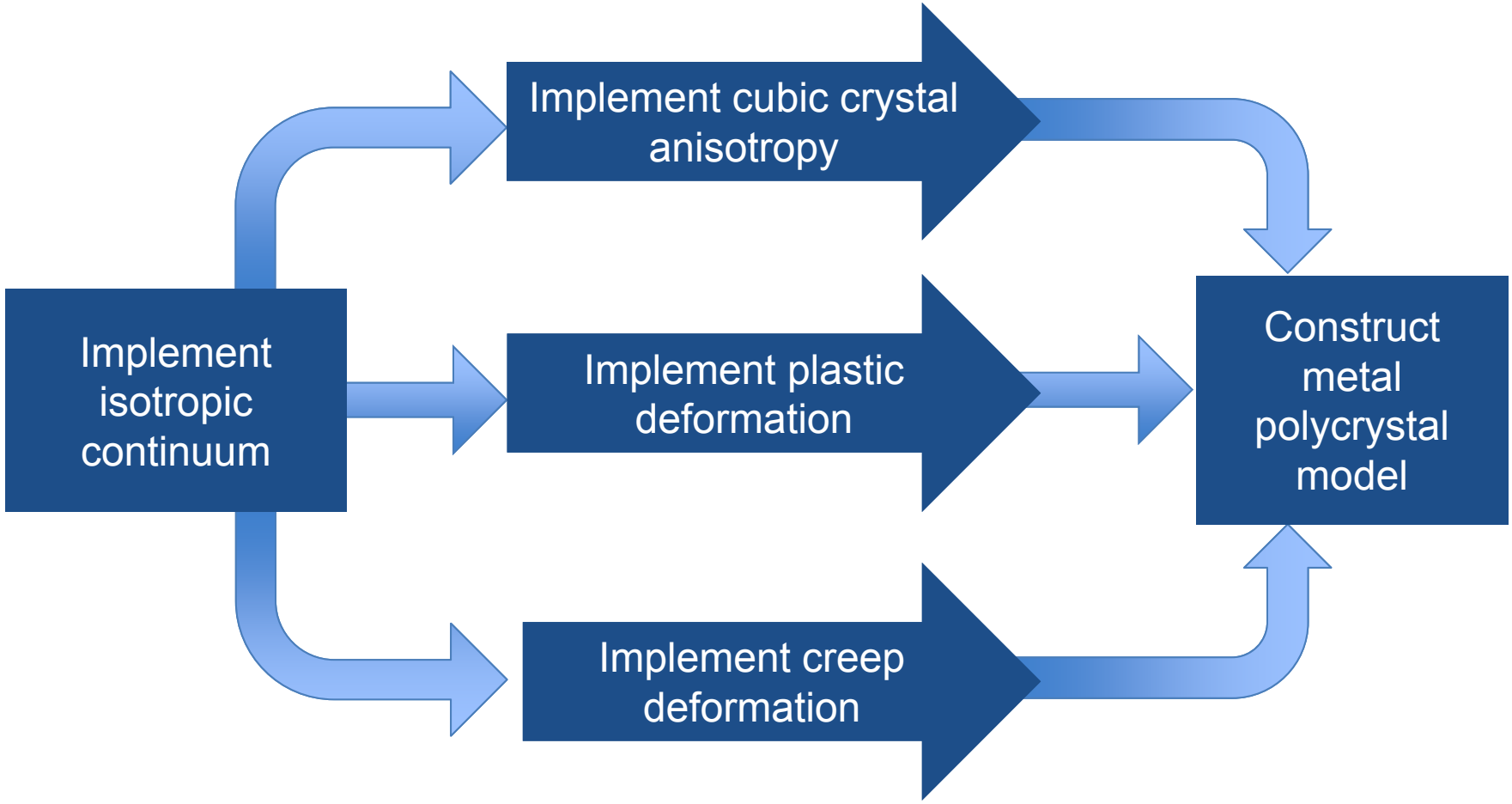
- **An element is a meso-scale domain**
  - e.g., a sub-grain or part of sub-grain

Hypothesis

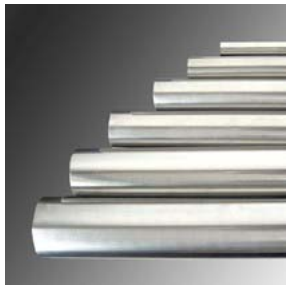
- We propose we can adapt DEM to correctly capture:
  - Polycrystal deformation
  - Microstructure evolution
  - Stochastic damage evolution



Developing the DEM model

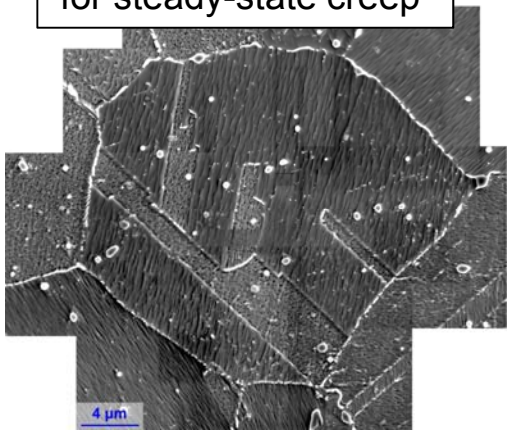


Material Selection



- Nimonic 75 chosen as model alloy
  - Simple Ni-20Cr solid solution microstructure represents many superalloys
    - Austenitic, solid solution grains
    - Chromium rich, globular grain-boundary carbides normally of the type $M_{23}C_6$

typical microstructure for steady-state creep



  - 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

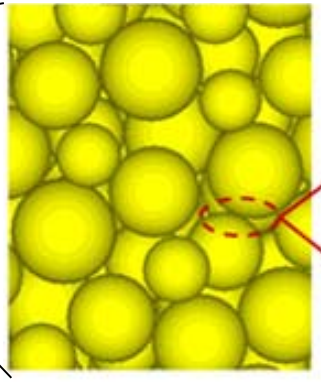
JRC EUROPEAN COMMISSION

irmm Institute for Reference Materials and Measurements

Adapting DEM for elastic anisotropy

Oregon sand dunes

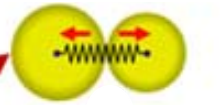
Particle Assembly

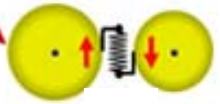


http://www.ngi.no/

Normal Stiffness

k_n

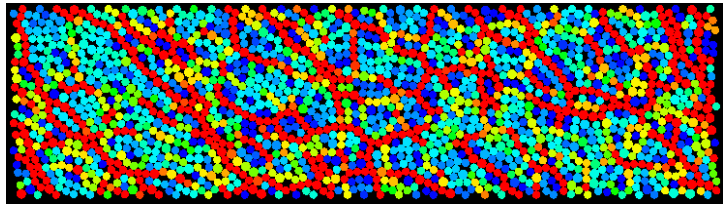




k_s

Shear Stiffness

But Sand is not homogeneously elastic!

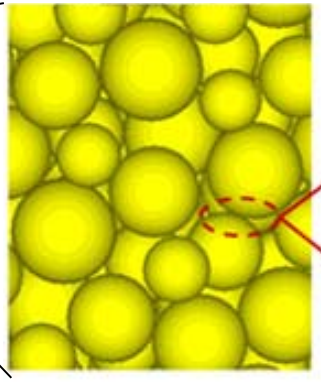


Intrinsic heterogeneous: force chains and jamming in granular materials (Image Banigan)

Adapting DEM for elastic anisotropy

Oregon sand dunes

Particle Assembly



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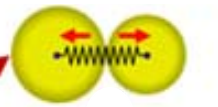
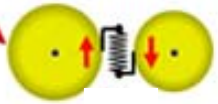
Normal Stiffness

k_n





k_s

Shear Stiffness

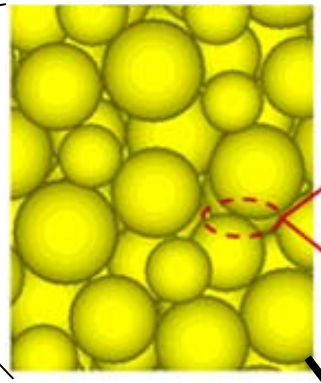
We must developing contact behaviors to make sand elastic

Homogeneous and isotropic in elastic response

Adapting DEM for elastic anisotropy

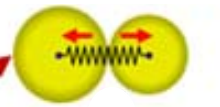
Oregon sand dunes

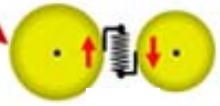
Particle Assembly



http://www.ngi.no/

Normal Stiffness k_n

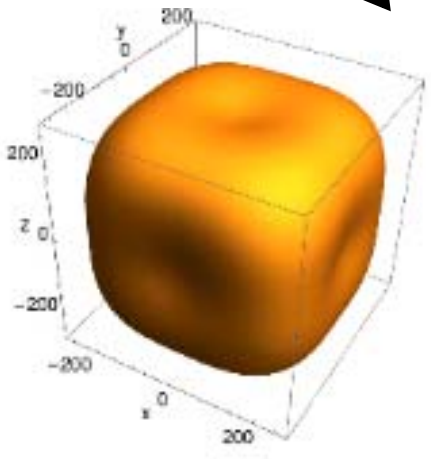




k_s Shear Stiffness

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

More than that we must make sand anisotropic elastic!



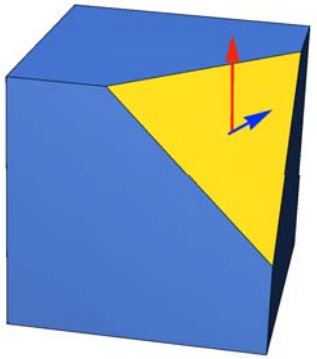
Ni-Cr: homogeneously elastic, but anisotropically elastic

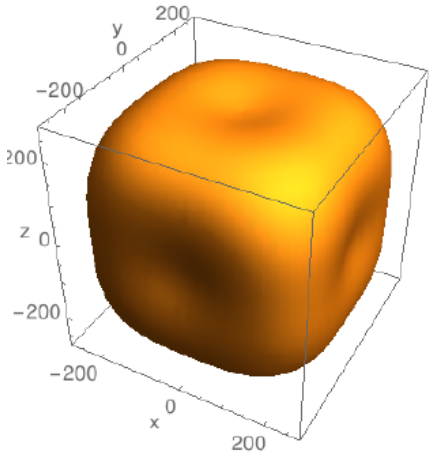
$$C_{ij} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

Adapting DEM for elastic anisotropy

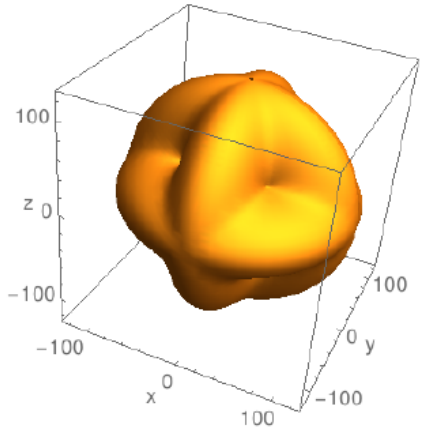
The subtleties of anisotropic elasticity...

- Directionally dependent elastic response of single crystal Ni

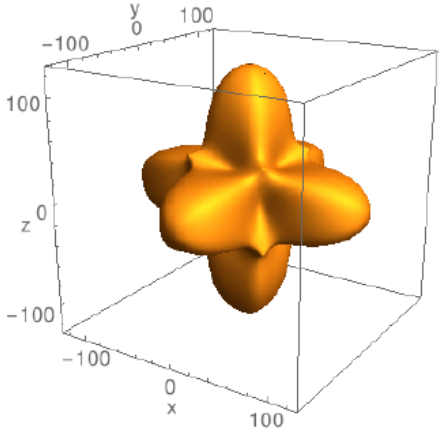




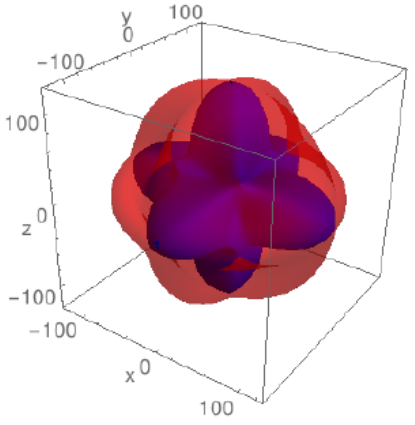
Directionally dependent normal stiffness



Shear stiffness in stiff direction



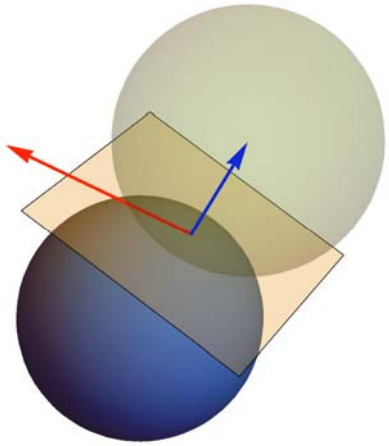
Shear stiffness in soft direction

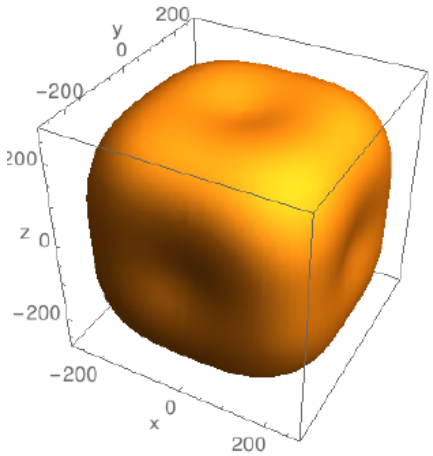


Stiff and soft shear stiffness overlaid

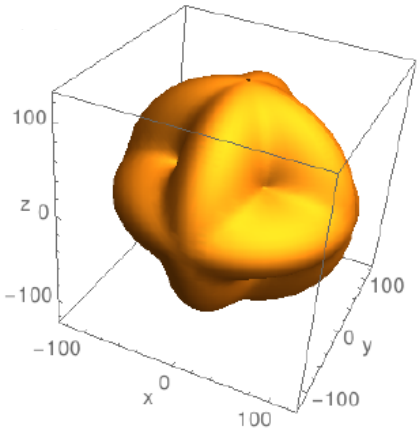
Adapting DEM for elastic anisotropy

Derive a set of contact interactions that produce this angular response.

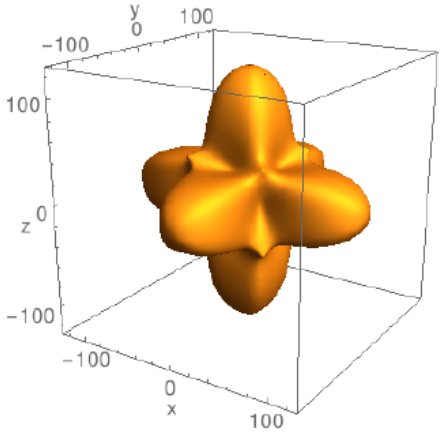




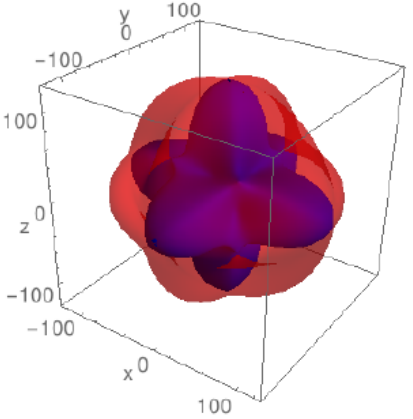
Directionally dependent normal stiffness



Shear stiffness in stiff direction



Shear stiffness in soft direction

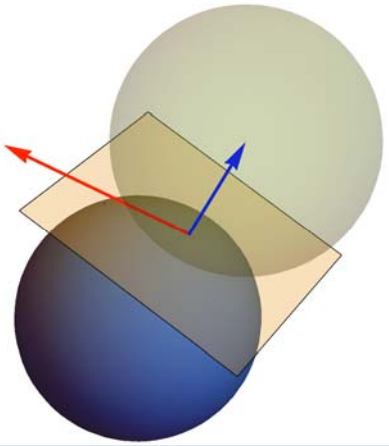


Stiff and soft shear stiffness overlaid

Adapting DEM for elastic anisotropy

Derive a set of contact interactions that produce this angular response.

Two different approaches to defining angularly dependent contact stiffness $k_n(\theta,\Phi)$ and $k_s(\theta,\Phi)$…



Emergent

- Simple form of $k_n(\theta,\Phi)$ and $k_s(\theta,\Phi)$
- Correct cubic symmetry
- Cubic elasticity emerges from collections of particles

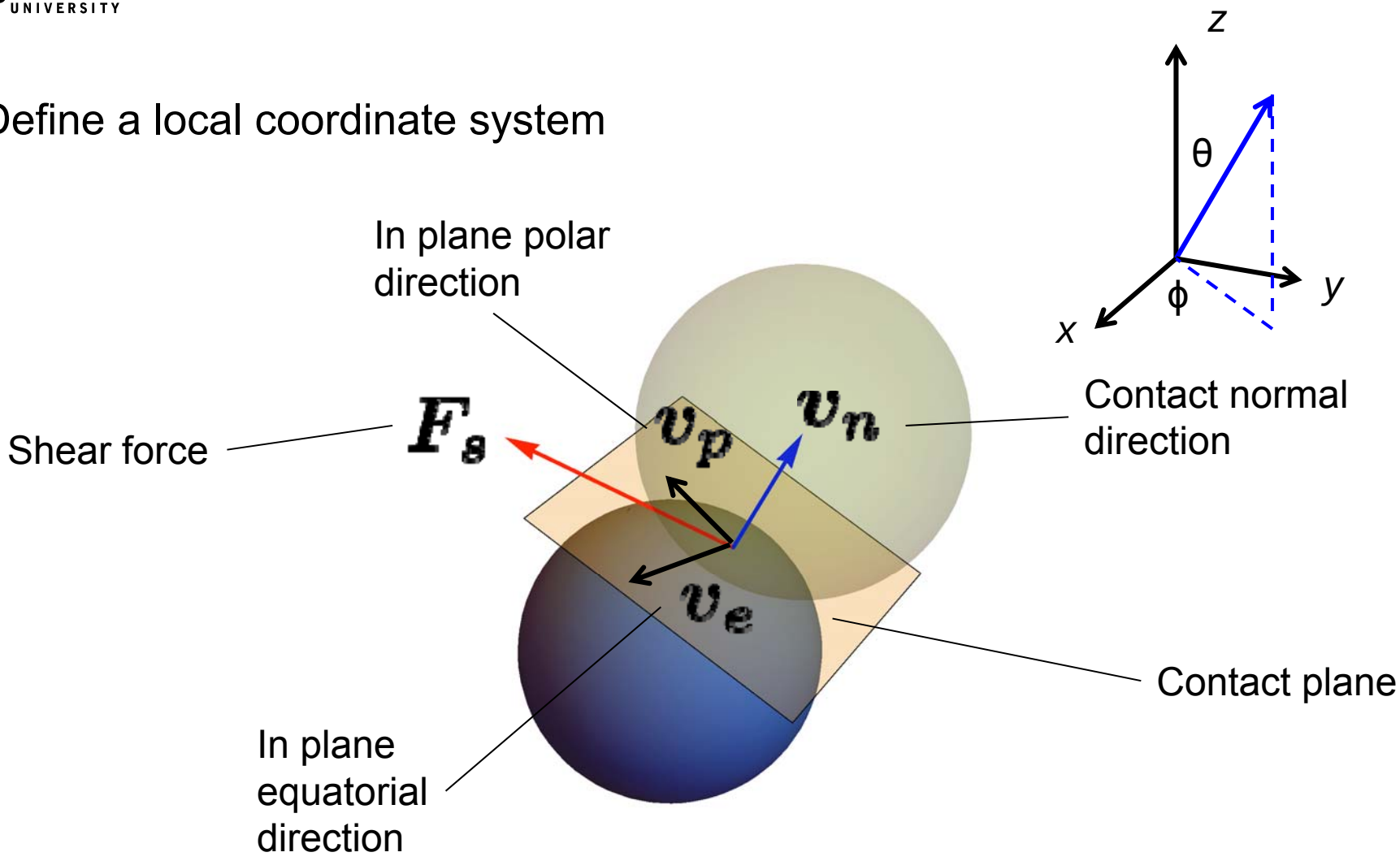
Imposed

- More complex form of $k_n(\theta,\Phi)$ and $k_s(\theta,\Phi)$
- Correct cubic symmetry
- Each contact mimics cubic elasticity

We have developed both approaches

Adapting DEM for elastic anisotropy

Define a local coordinate system



Adapting DEM for elastic anisotropy

Define bond contact laws based on coordinate system

$$K(\theta,\phi) = \frac{1}{2}\pi R_c C_{11}^* \begin{bmatrix} A & F & E \\ F & B & D \\ E & D & C \end{bmatrix}$$

$$\alpha = \frac{2C_{44}^*}{C_{11}^* - C_{12}^*}$$

$$\beta = \frac{C_{44}^*}{C_{11}^*}$$

$$A = \frac{\left(-(\alpha-1)\beta\left(8\sin^4(\theta)\cos(4\phi) + 4\cos(2\theta) + 7\cos(4\theta)\right) + 11(\alpha-1)\beta + 16\alpha\right)}{16\alpha}$$

$$B = \frac{\beta\left(-8(\alpha-1)\sin^2(\theta)\cos^2(\theta)\cos(4\phi) + 7(\alpha-1)\cos(4\theta) + 9\alpha + 7\right)}{16\alpha}$$

$$C = \frac{\beta\left(2(\alpha-1)\sin^2(\theta)\cos(4\phi) + (\alpha-1)\cos(2\theta) + 3\alpha + 1\right)}{4\alpha}$$

$$D = \frac{(\alpha-1)\beta\sin^2(\theta)\cos(\theta)\sin(4\phi)}{2\alpha}$$

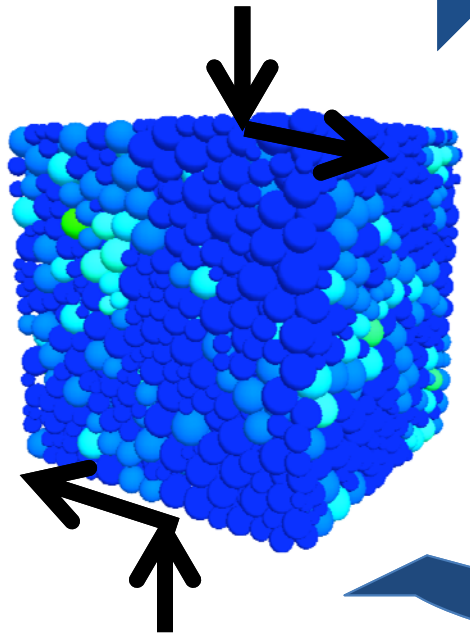
$$E = -\frac{(\alpha-1)\beta\sin^3(\theta)\sin(4\phi)}{2\alpha}$$

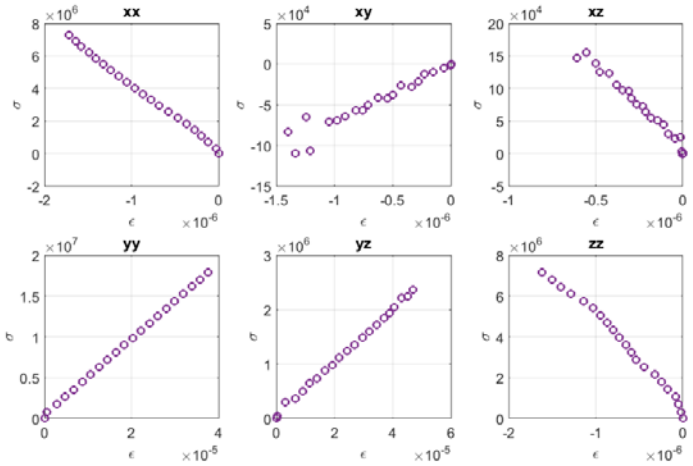
$$F = \frac{(\alpha-1)\beta\left(8\sin^3(\theta)\cos(\theta)\cos(4\phi) - 2\sin(2\theta) - 7\sin(4\theta)\right)}{16\alpha}$$

Adapting DEM for elastic anisotropy

- Optimization routine is used to find bond property constants α, β, C^*_{11} that give desired assembly response:

Shear and compress element assembly → Determine anisotropic elastic response → Update bond properties α, β, C_0





$$K(\theta,\phi) = \frac{1}{2}\pi R_c C_{11}^* \begin{bmatrix} A & F & E \\ F & B & D \\ E & D & C \end{bmatrix}$$

$$\alpha = \frac{2C_{44}^*}{C_{11}^* - C_{12}^*}$$

$$\beta = \frac{C_{44}^*}{C_{11}^*}$$

Adapting DEM for elastic anisotropy

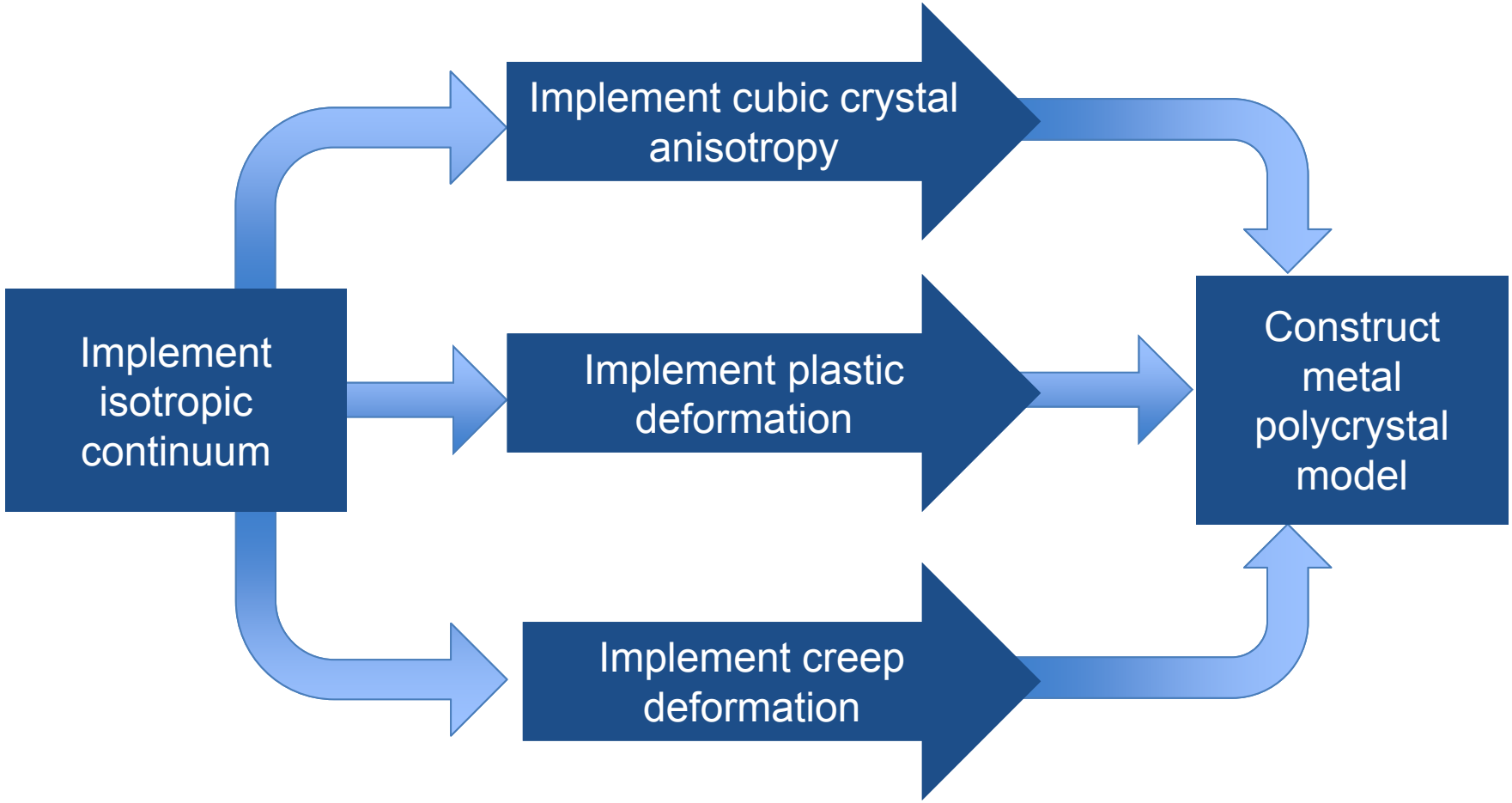
- Progress to date:

	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
Current Model	**237**	**77**	**73**
Ni	251	150	124
Ni (600°C)	221	145	102
Fe	231	116	135
Cr	340	99	59
Si	166	80	64

C_{11} in line with Ni-alloys

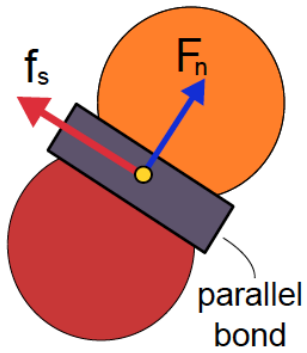
C_{12} and C_{44} in line with Si

Developing the DEM model

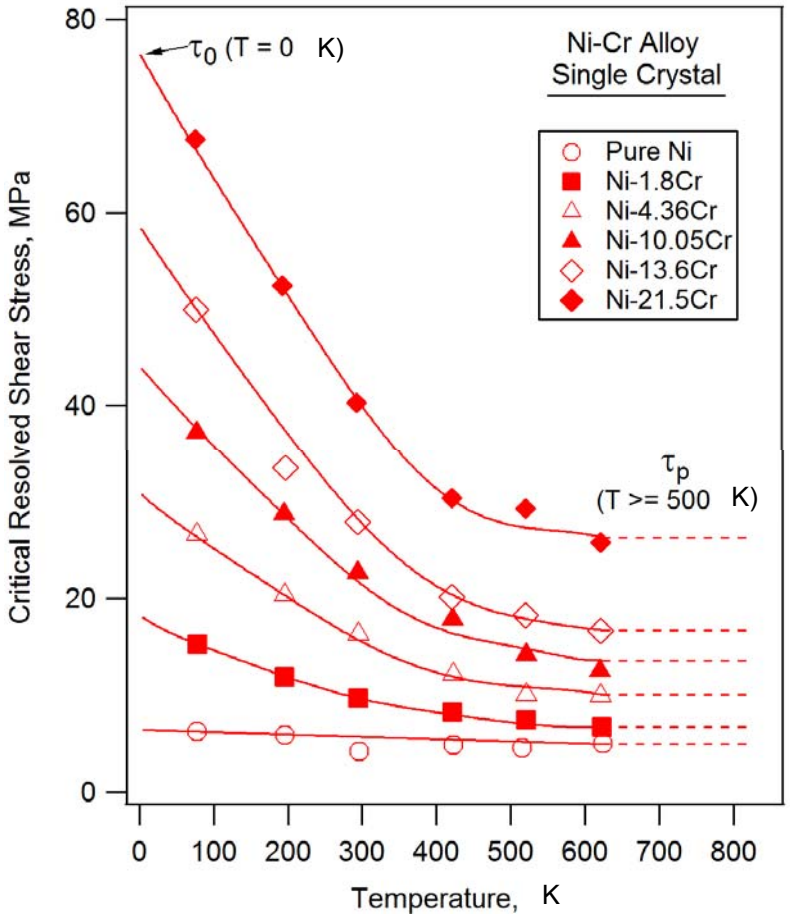


Plastic behavior of Ni-20Cr

- Critical resolved shear stress has a minimum plateau above ~500 K
- Literature data is being used to define parallel bond shear strengths in DEM model



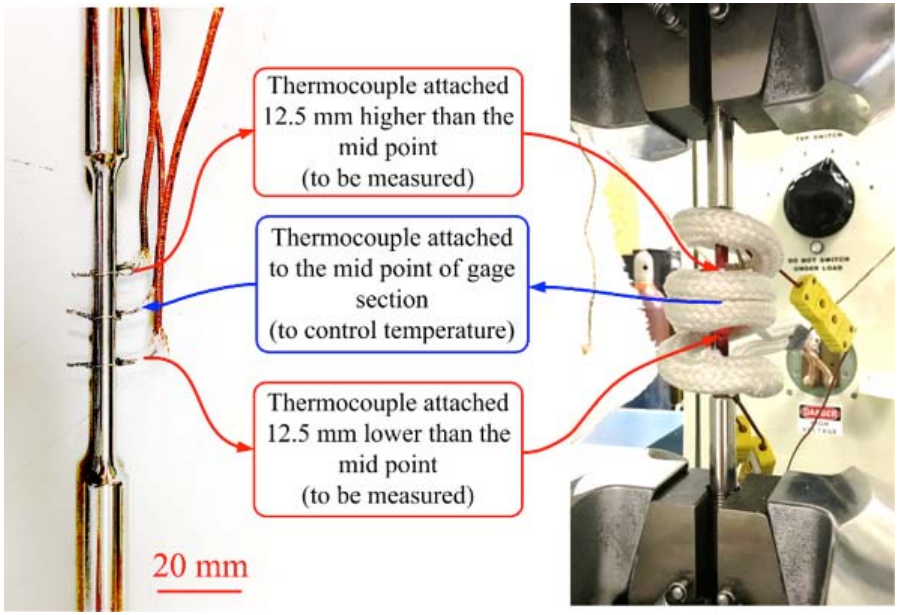
Various Ni-Cr alloys

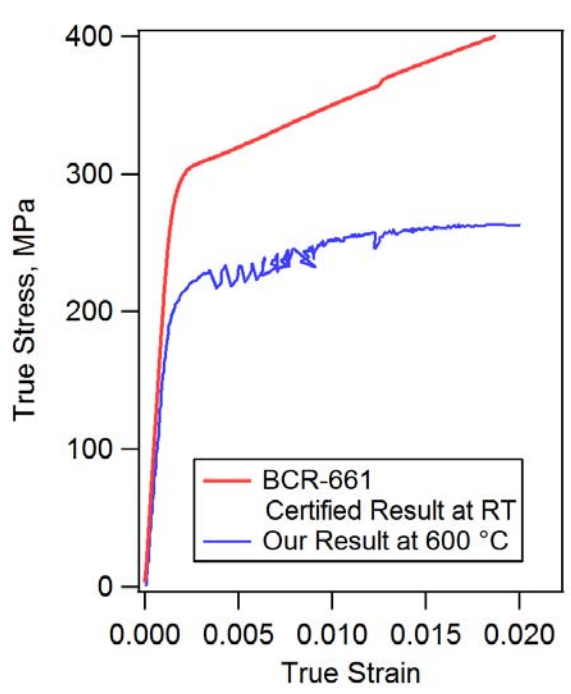


(Akhtar & Teghtsoo, 1971)

Plastic behavior of Nimonic 75

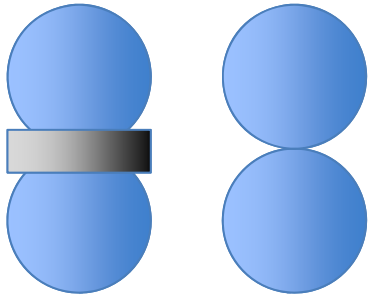
- Tensile testing underway on Nimonic 75
  - Determine hardening behavior at 600°C
  - Determine dynamic softening during stress relaxation at 600°C





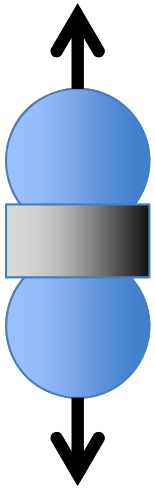
Adapting DEM for plasticity

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

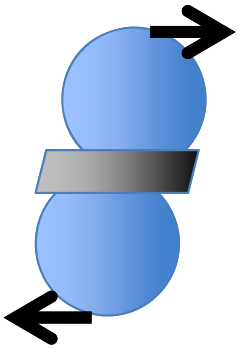


Potential Bond Breaking Phenomena

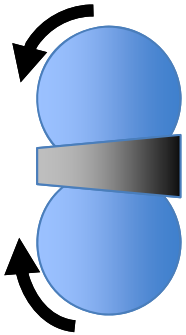
Normal stretch



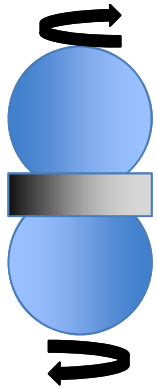
Shear stretch



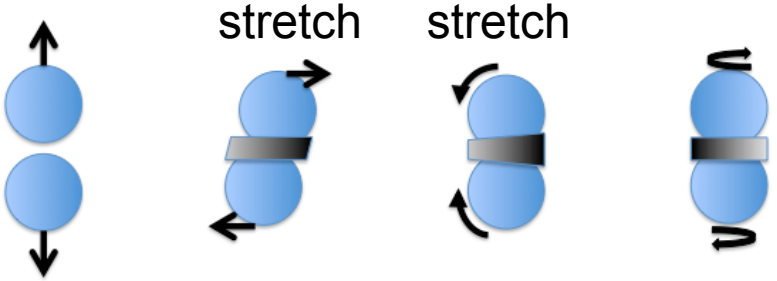
Tilt stretch



Twist stretch

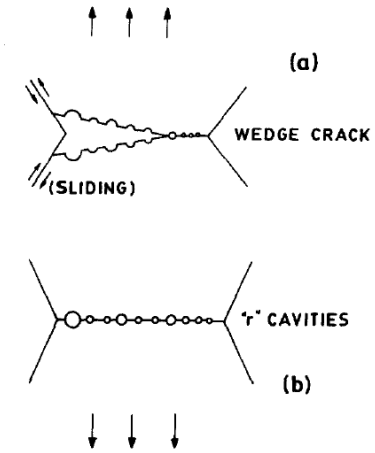


Adapting DEM for plasticity

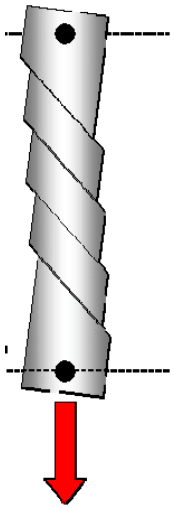


Corresponding Physical Phenomena

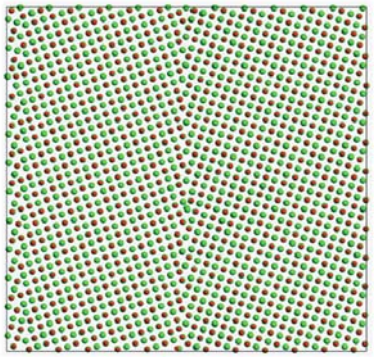
Crack or Void Formation



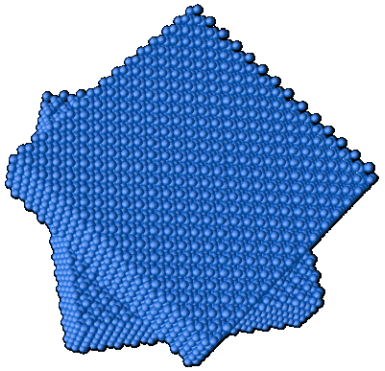
Plastic slip



Tilt Boundary Formation



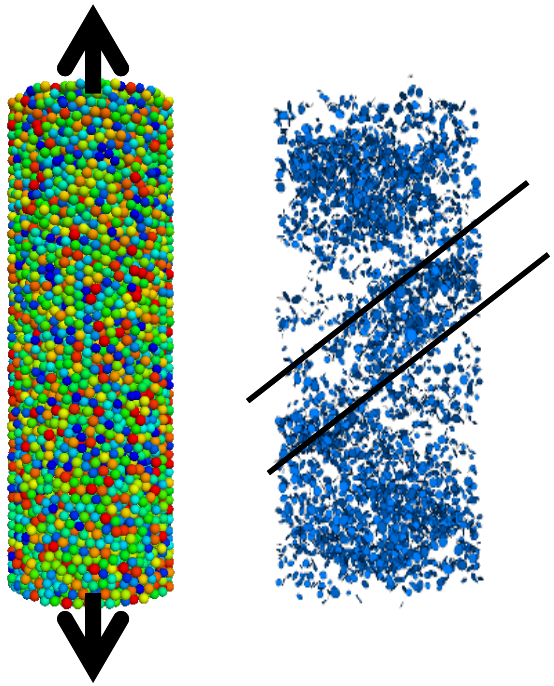
Twist Boundary Formation

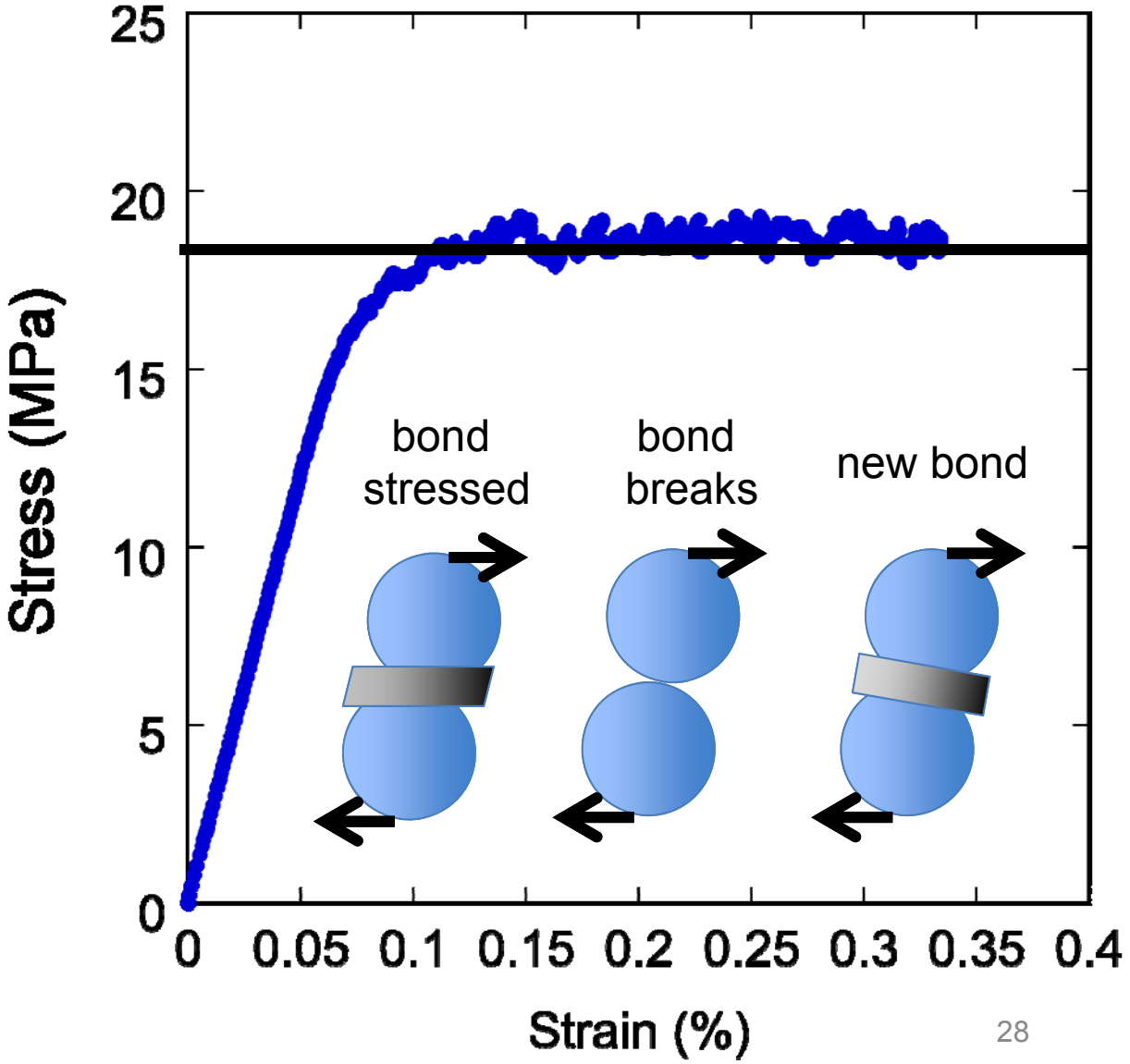


sub-grain evolution

Adapting DEM for plasticity

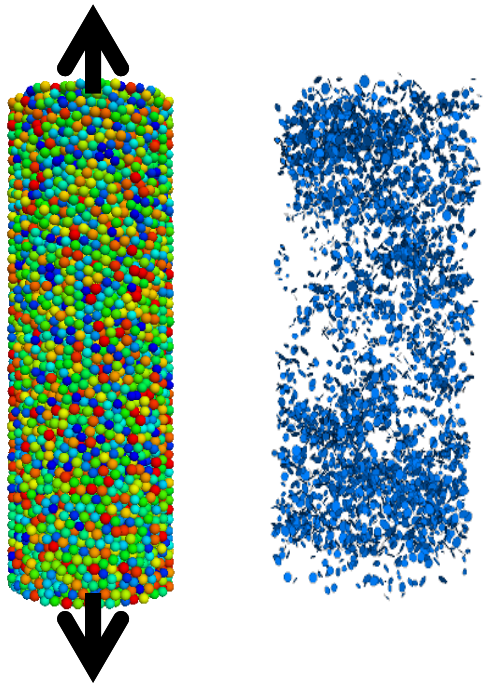
- Non-hardening deformation
  - perfect plasticity
  - shear localization evolves

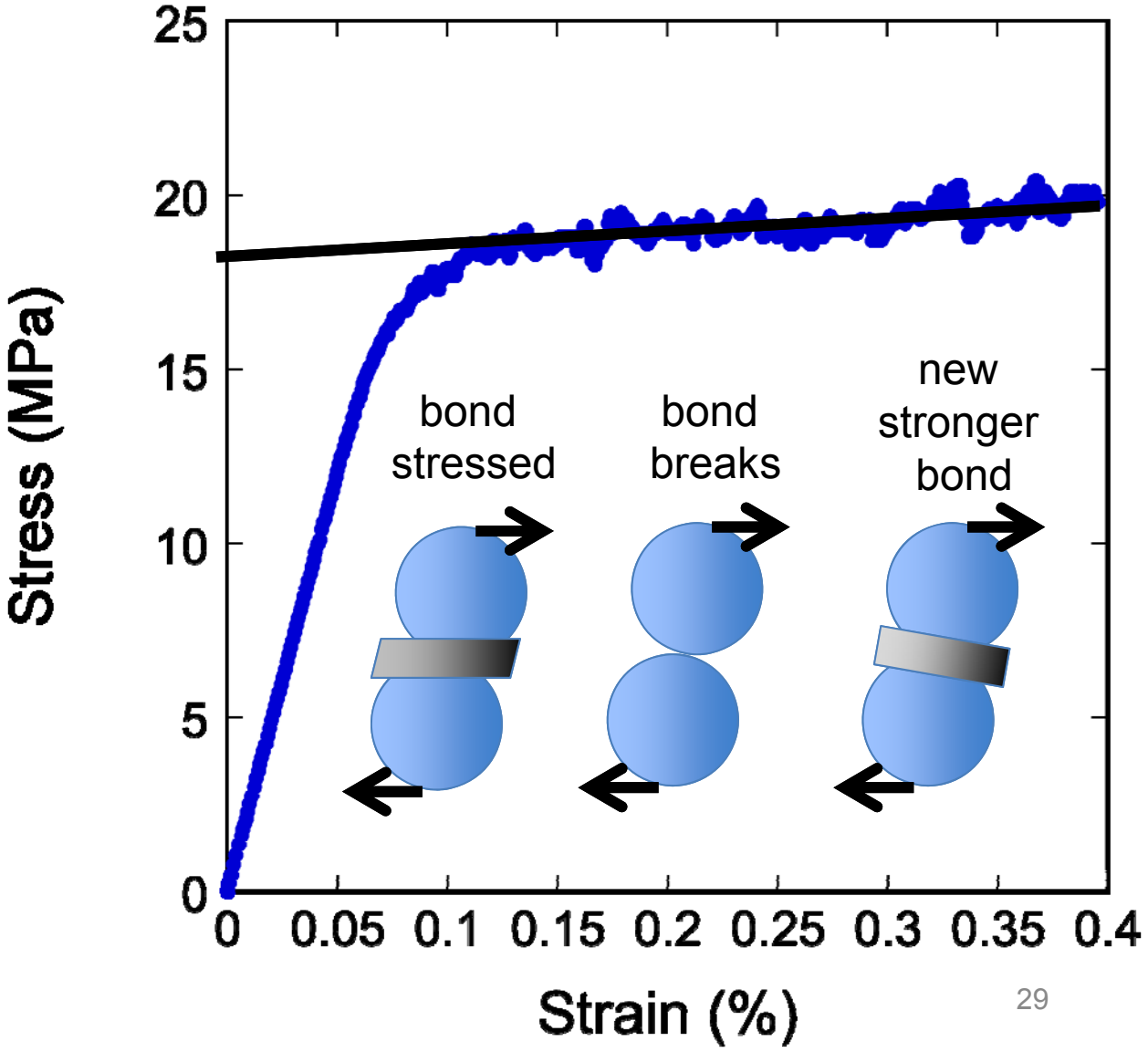




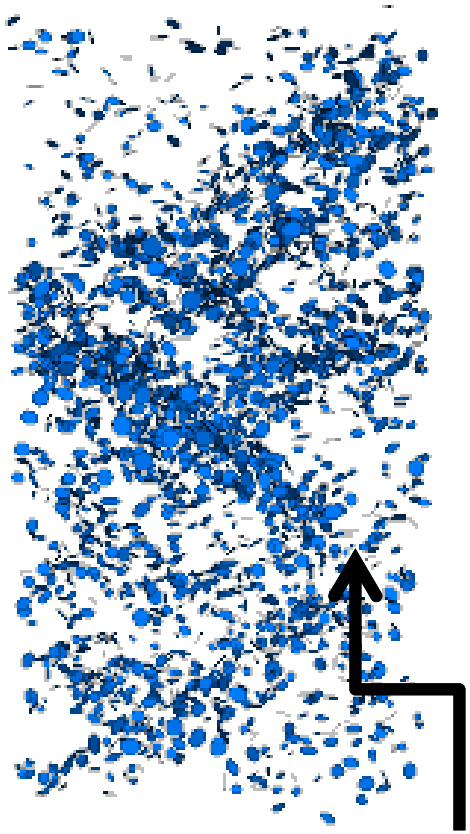
Adapting DEM for plasticity

- Hardening deformation
  - Strain hardening
  - localization suppressed

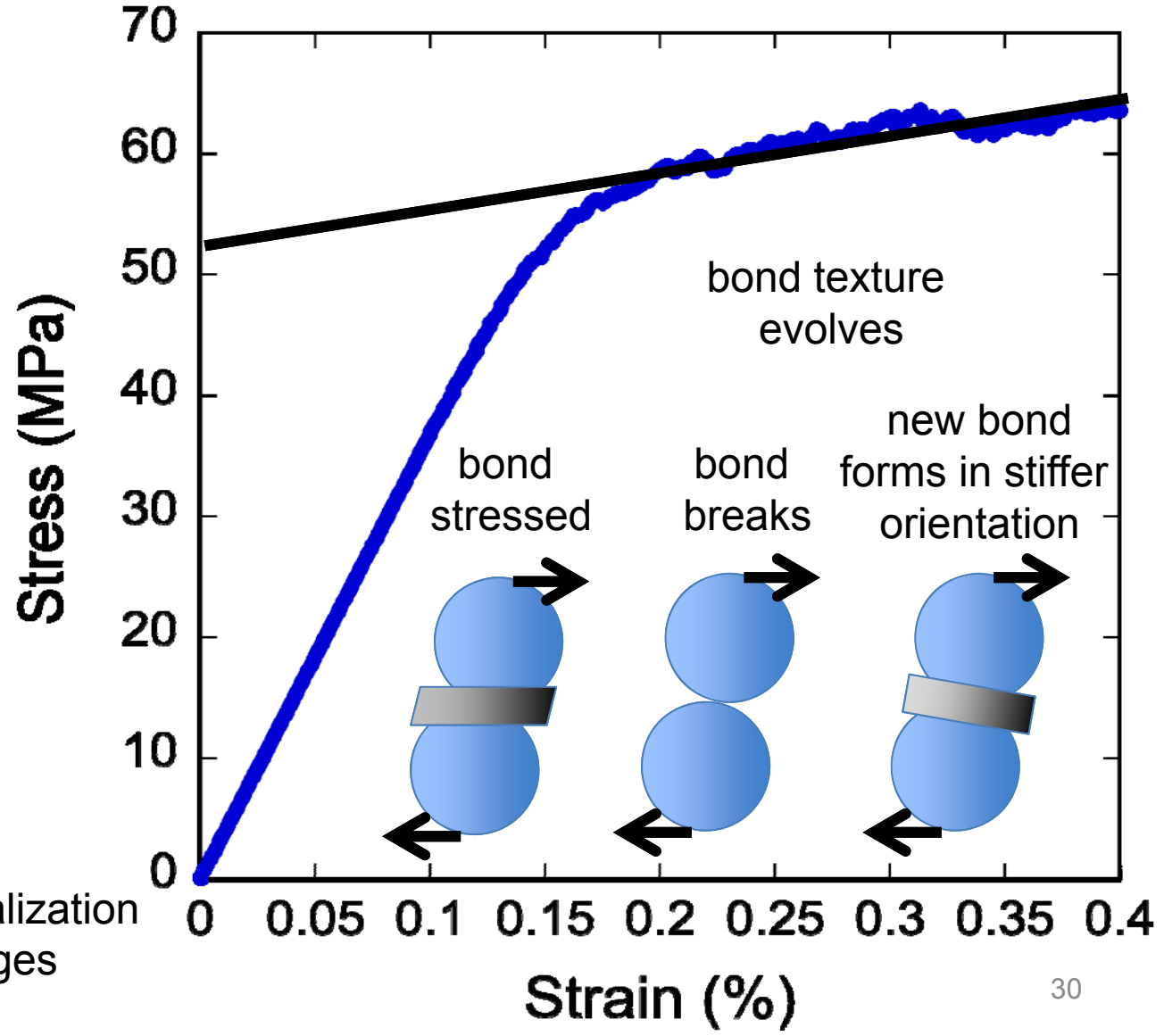




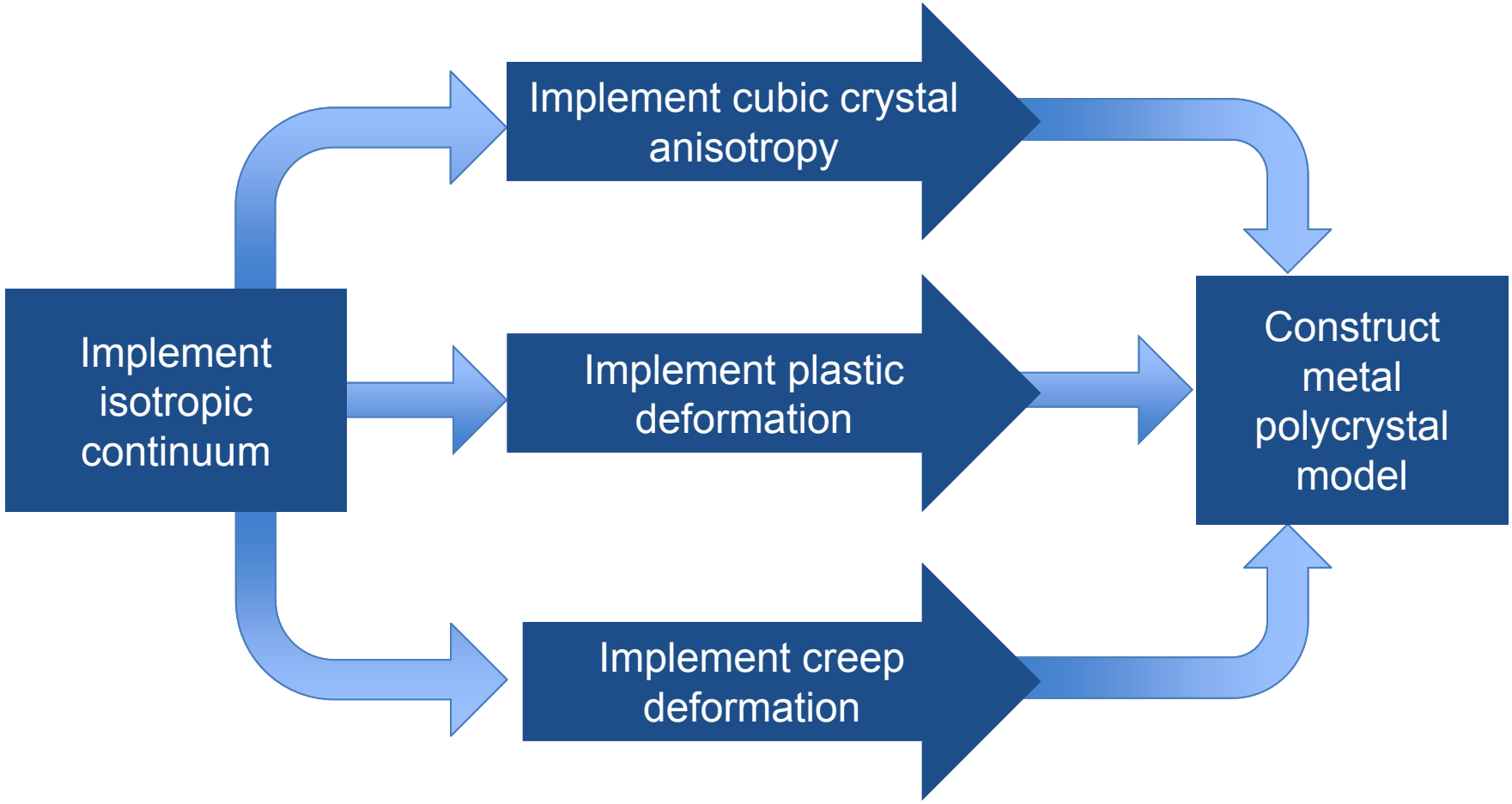
Adapting DEM for plasticity



shear localization emerges

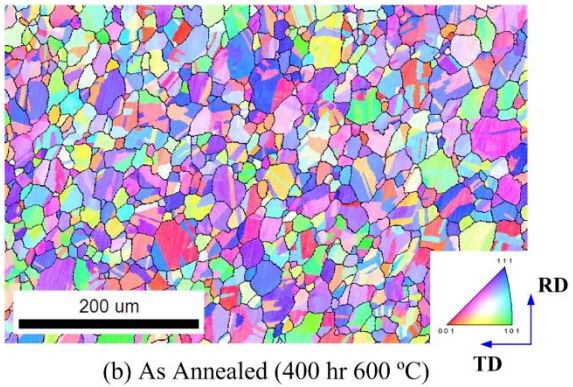


Developing the DEM model



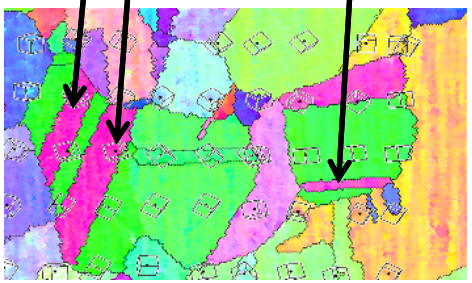
Creating a DEM Polycrystal

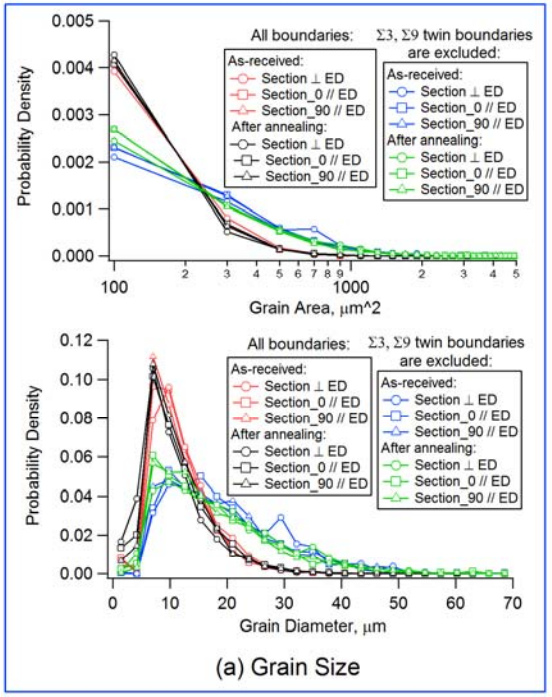
- EBSD used to quantify grain structure
  - Presence of twins skews apparent distributions
  - Σ3 and Σ9 annealing twin boundaries are unlikely damage sites (Zhang & Field, 2013)
  - Initially a twin-free microstructure is created for our DEM model



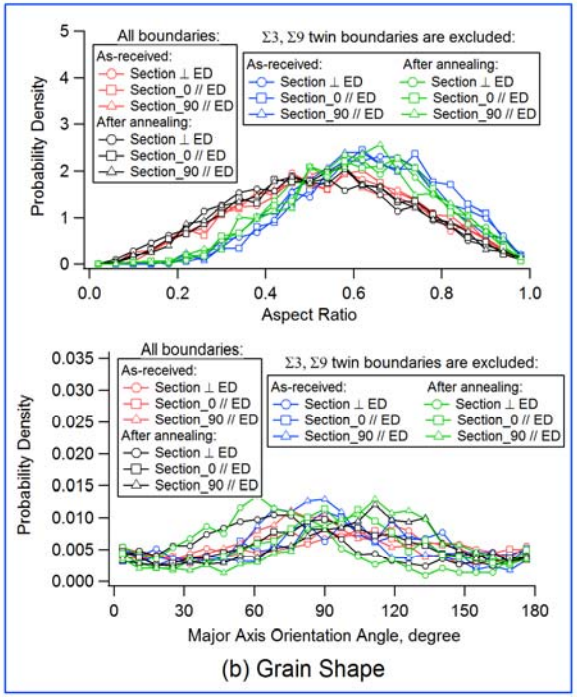
(b) As Annealed (400 hr 600 ºC)

Twins are prevalent





(a) Grain Size

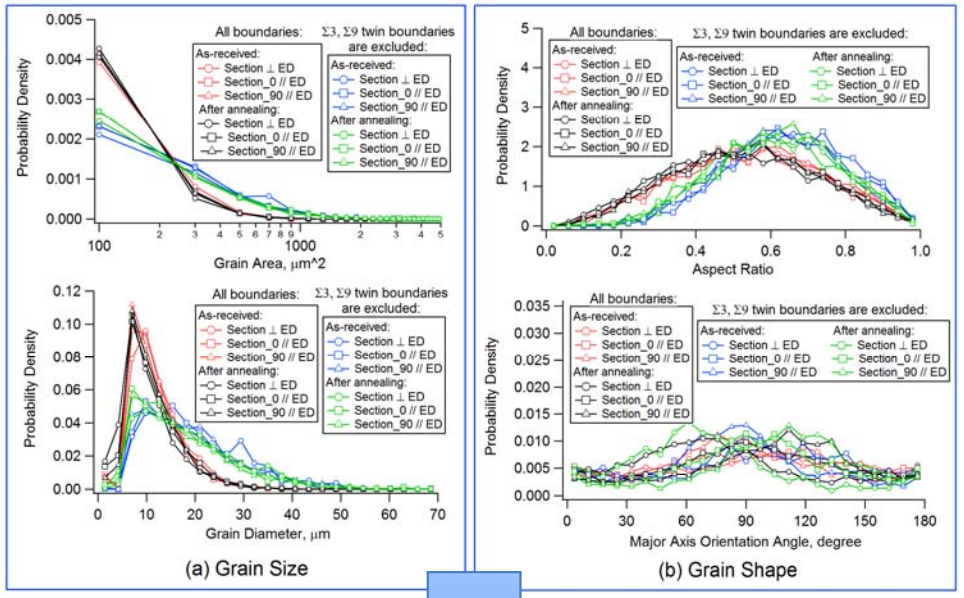


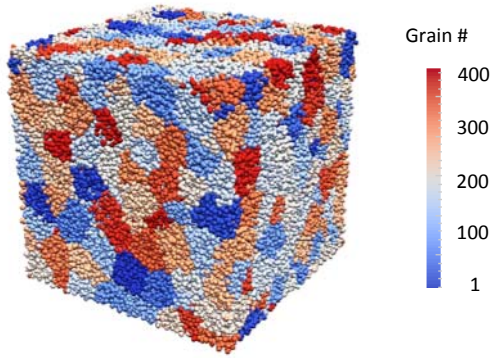
(b) Grain Shape

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

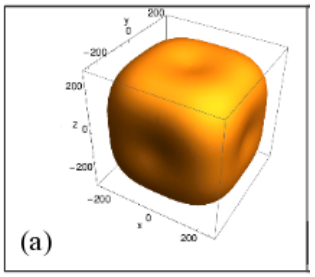
creep samples tested at NETL

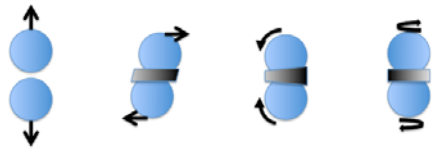


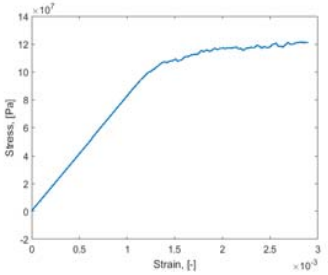


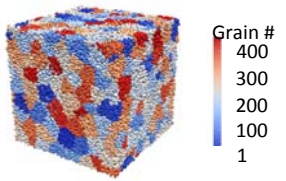
Conclusions

- An anisotropic elasticity formulation can be developed to mimic cubic anisotropy
  - We will tweak formulation to access the exact desired stiffness tensor
- Bond breaking and reforming can be used to simulate metal plasticity
  - Elastic and plastic behavior is coupled based our initial results
  - Will refine model to capture desired strength, hardening, and slip plane orientation behavior



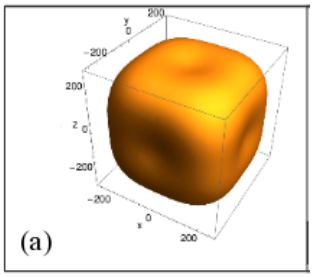




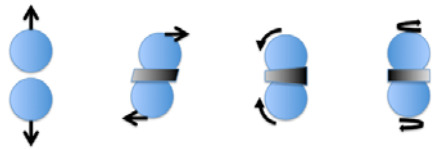


Steps to Project Completion

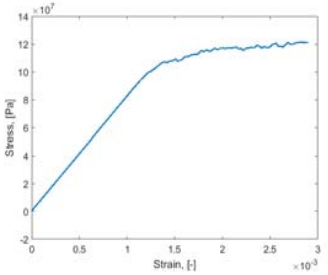
- Elastic Anisotropy:
  - Run large DFT-MD simulation to verify constants at 600°C for Ni-20Cr
  - Refine element stiffness formulation to get correct tensor for Ni-20Cr alloy



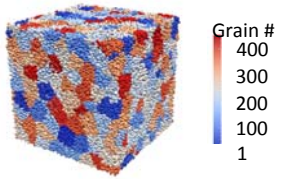
- Plasticity:
  - Determine strain hardening law at 600°C for Nimonic 75 using tensile samples as function of strain rate
  - Refine bond breaking and reforming scheme to capture desired strength, hardening, and slip plane orientation behavior



- Creep:
  - 600°C creep response well known from literature
  - Determine softening laws at 600°C for Nimonic 75 using tensile stress relaxation experiments
  - Develop time dependent bond breaking and reforming scheme to capture creep behavior



- Final Model Assembly:
  - Combine above elements into a crystal plasticity DEM model for Nimonic 75
  - Validate and refine model based on experimental creep results



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Questions?

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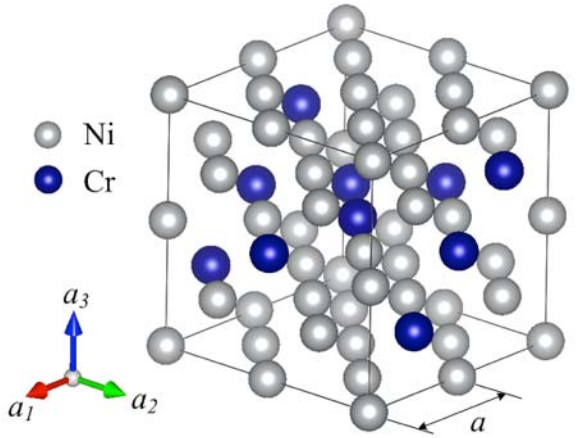
Cubic Anisotropy for Nimonic 75

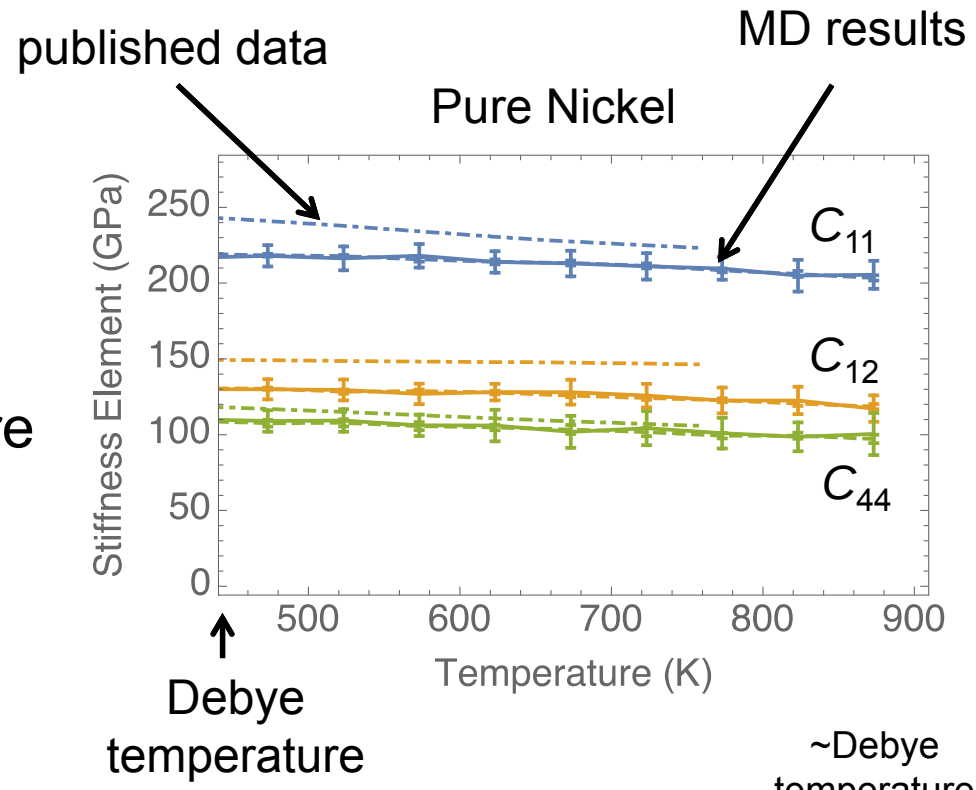
- Density Functional Theory (DFT) used to calculate C_{11}, C_{12}, C_{44} for Ni-20Cr at 0 K
  - Special quasi-random structure (SQS) supercell
  - Only small deviation from pure Ni seen in C_{11}



Material	Equilibrium lattice parameter, a, Å	Bulk modulus B, GPa	Zener's modulus C', GPa	C_{11}, GPa	C_{12}, GPa	C_{44}, GPa
Pure Ni (2x2x2 supercell)	3.518	200.1	55.7	274.3	163.0	128.8
Ni-20Cr (2x2x2 SQS supercell)	3.523	204.1	60.0	284.1	164.1	131.7

Cubic Anisotropy at 600°C

- MD simulations at T > 0K using embedded atom method and a 3 x 3 SQS supercell
- For pure Ni, we can compare elastic softening of C_{11}, C_{12}, C_{44} to published data
- In both cases, fitting elastic softening to Watchman functional is appropriate
- Future DFT-MD simulation at 600°C will verify extrapolation



~Debye temperature

$$C_{ij}(T) = C_{ij}^{T=0} - B_{ij} T \exp\left(-\frac{T_M}{T}\right)$$

C_{ij} at 0K

~Gruneisen parameter