Discrete element method for deformation and microstructure evolution modeling

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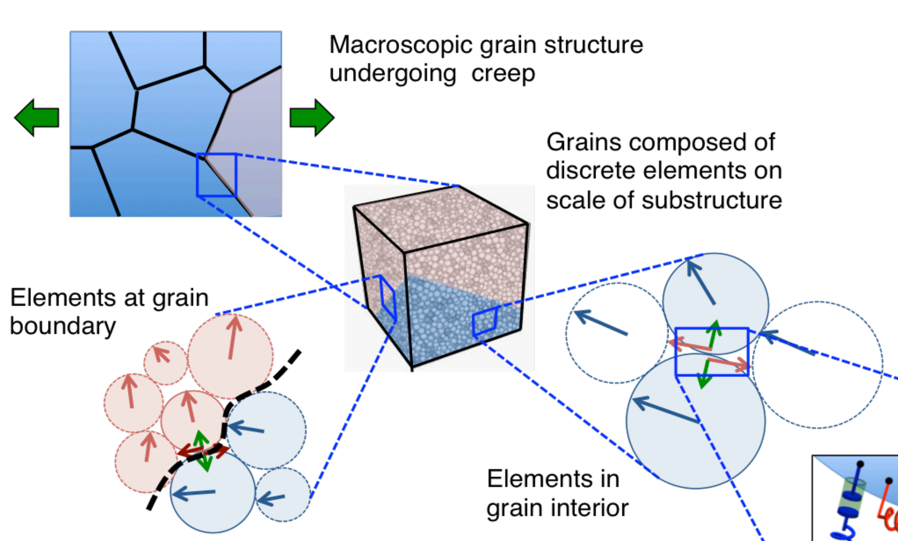
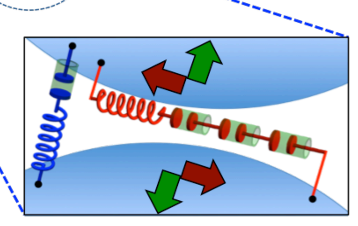
Introduction

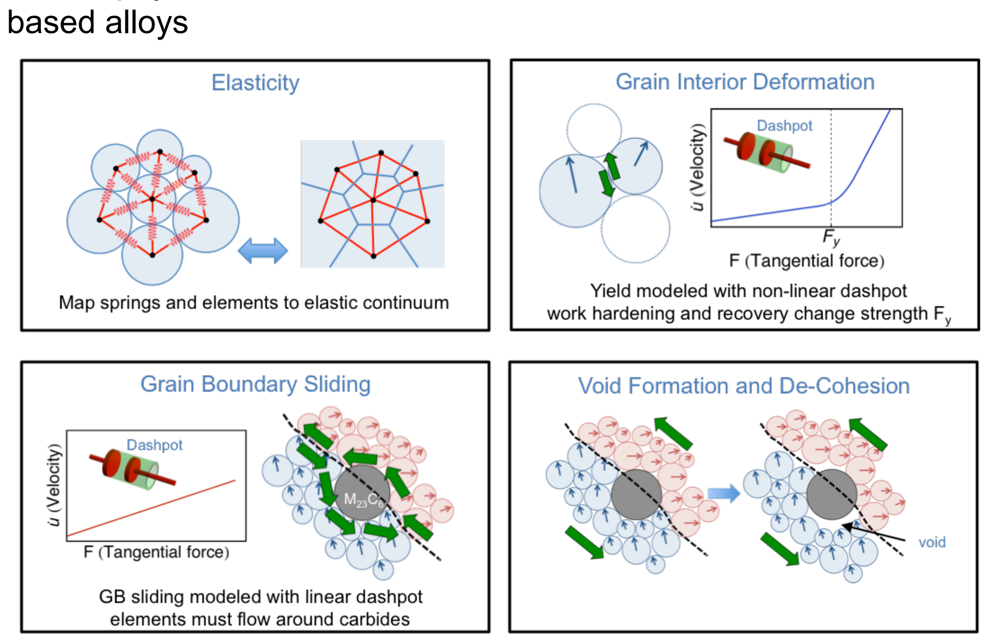
Our objective is to create and validate a robust, multiscale, mechanism-based model that quantitatively predicts elevated temperature mechanical properties and microstructure evolution for nickel-based alloys. The last 40+ years of materials science research has developed a multitude of mechanistic microplasticity models of deformation. We plan to embed our mechanistic understanding within a discrete element method (DEM) model framework to create a predictive system with a sound mechanistic foundation. We believe DEM is well suited to fill the meso-scale gap between micro/nano-scale mechanistic modeling and continuum modeling.





Contacts between grains modeled with springs and series dashpots

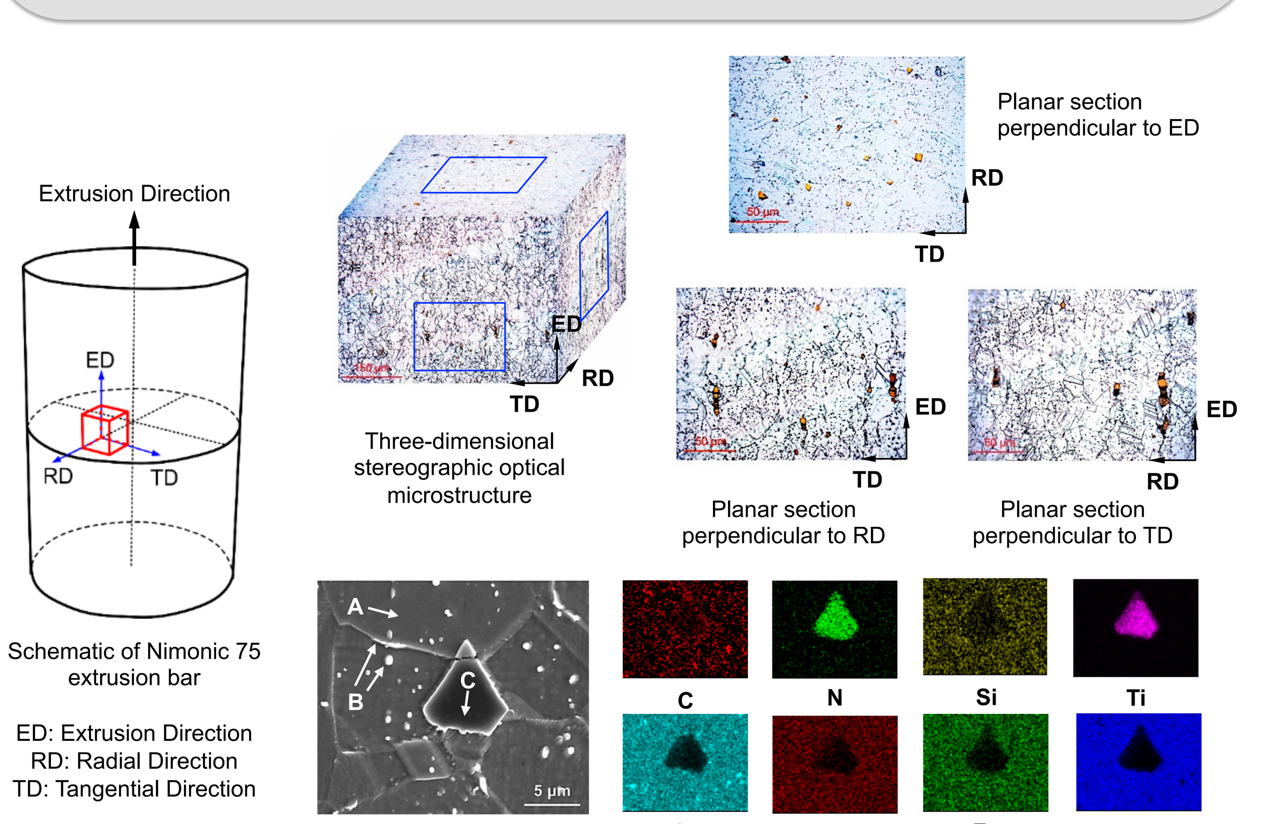
Above: Schematic representation of the proposed DEM model. Crystal grains will be represented using discrete elements that interact and move to allow deformation and microstructure evolution. The element interaction laws will be defined to represent the physical mechanisms involved for nickel based alloys



Above: Schematic representation of initial micro-mechanisms to be considered.

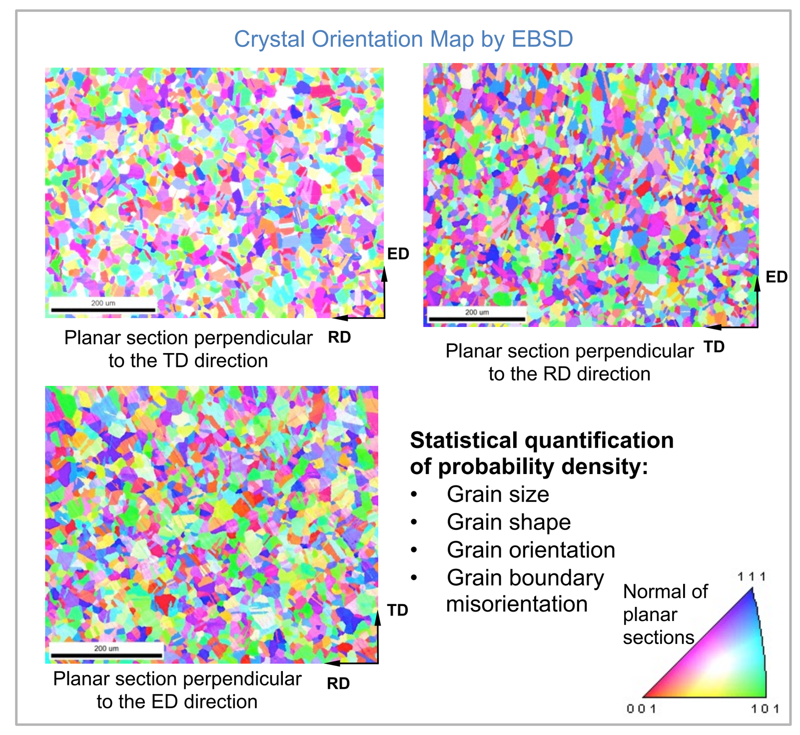
Material Selection and Microstructure

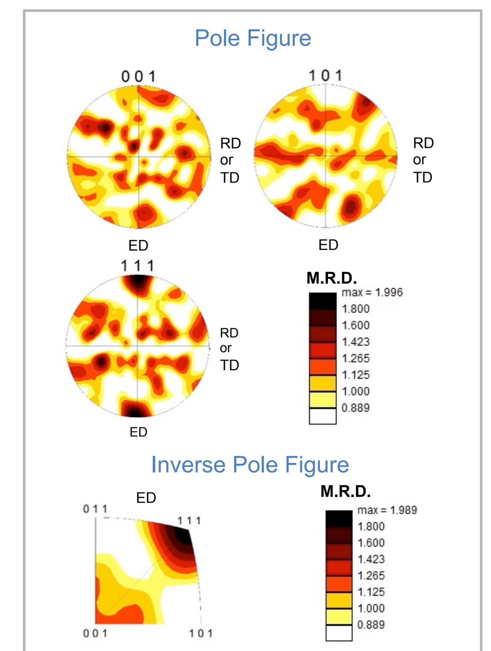
We selected a relatively simple, model solid solution Ni-20Cr alloy (Nimonic 75). Nimonic 75 is also ideal for this study because it is a certified creep reference material [1]. To build an accurate model, microstructure characterization is currently being carried out by electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM).



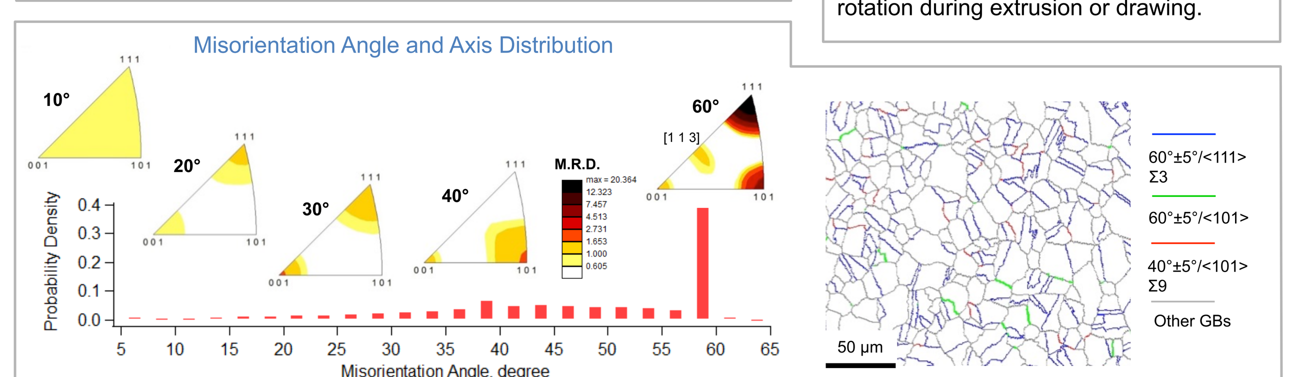
Phase identification by SEM/Energy-dispersive X-ray spectroscopy (EDS) mapping: Arrow A–Ni-20%Cr matrix phase; Arrow B–Intergranular and intragranular Cr-rich carbide; Arrow C–Intergranular titanium nitride.

Above: Qualitative snapshot of the microstructure of Nimonic 75 on three orthotropic planar sections by optical microscopy (OM) and scanning electron microscopy (SEM). Three phases are identified: (1) Ni-20%Cr matrix phase in the form of equi-axed grains containing abundant annealing twins; (2) Small and spherical Cr-rich carbide particles which are densely distributed at grain boundaries and within grains; (3) Large and polyhedron-shaped titanium nitride inclusions that are elongated in the extrusion direction and sparsely distributed at grain boundaries (more frequently at triple joints).



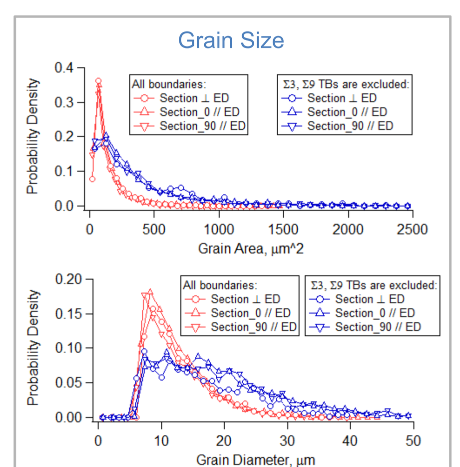


Axisymmetric <111>-<100> fiber texture typical for FCC metals results from crystal rotation during extrusion or drawing.

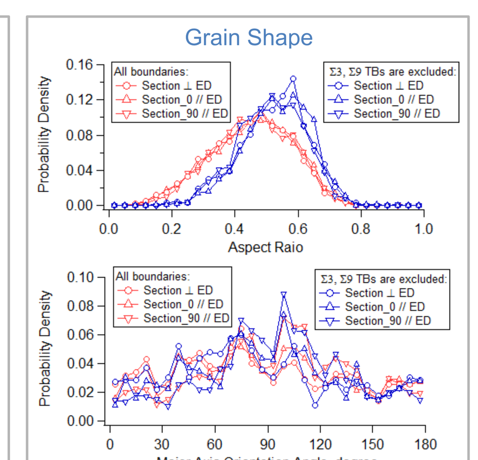


Probability density of misorientation angle shows two peaks at 40° and 60°. Peak distribution of misorientation axes is found in the <111> and <101> directions. Most of the misorientation axes with the misorientation angle of 40° are distributed in the <101> direction.

Boundary map:
- 60°±5°/<111> Σ3 primary annealing twin
- 40°±5°/<101> Σ9 2nd annealing twin
- 60°±5°/<101> GB



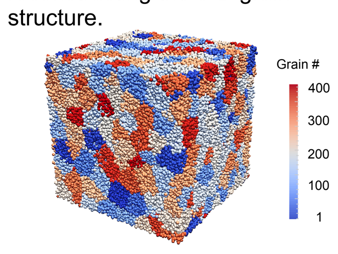
Grain size: 1) grain area (pixel counts within a grain – accurate); 2) grain diameter (assuming grain as a circle – inaccurate when grains are elongated or have irregular shape). Probability density are plotted with consideration of all the boundaries and those without Σ3 and Σ9 twin boundaries.



Grain fragment is best fitted by an ellipse. Grain shape: 1) aspect ratio; 2) major axis orientation (angle between major axis and horizontal line). Probability density are plotted with consideration of all the boundaries and those without Σ3 and Σ9 twin boundaries.

3-D Grain Structure for DEM by Voronoi Tessellation Algorithm

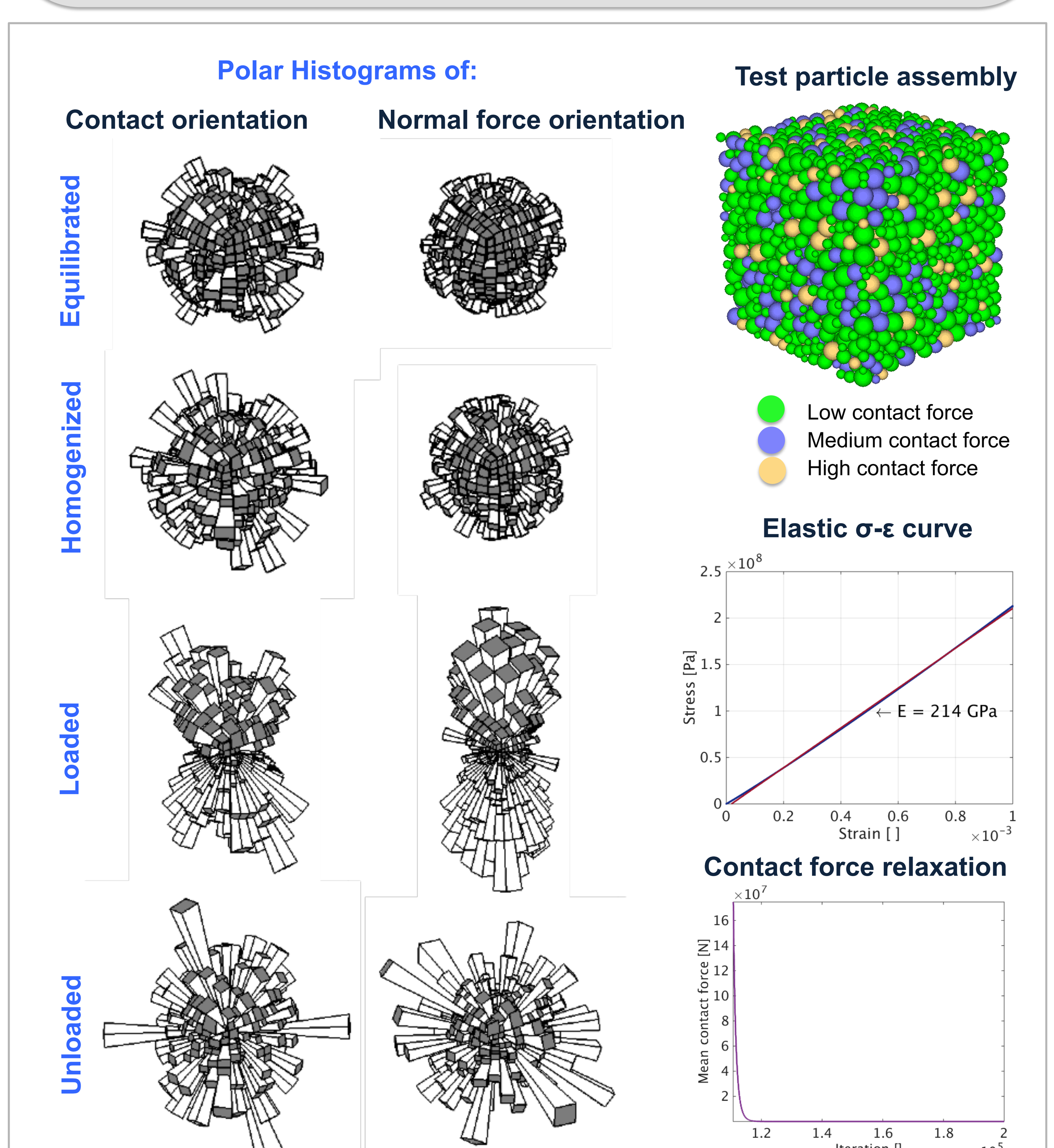
Grain structure tessellated by 3-D Voronoi algorithm captures the 2-D EBSD characterized distributions of grain size, grain orientation, and grain boundary misorientation. As Σ3 and Σ9 annealing twin boundaries are unlikely to be initiation sites for creep damage [2], these boundaries are excluded for reconstructing the 3-D grain structure.



An example of 3-D grain structure containing 400 grains

DEM model development

DEM models are typically used to simulate discontinuous materials with a high degree of spatial heterogeneity. This is approach quite powerful, but implementation for continuum modeling is challenging. Of particular note is the need for force homogenization and equilibration across the sample space. We have developed an algorithm that iterates forces in the assembly towards a constant value, as exhibited in the figures below.

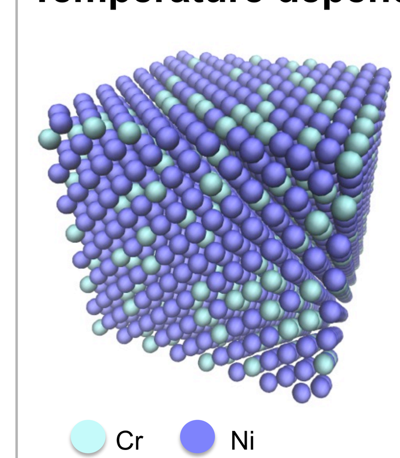


Determination of model parameters

A combination of mechanical testing and multi-scale modeling will be used to determine the needed model parameters. An initial set of parameters and the methods used is listed below:

- Temperature dependent elastic constants
- Grain boundary sliding viscosity
- Work hardening & Temperature softening rates (future)
- Void nucleation rate (future)

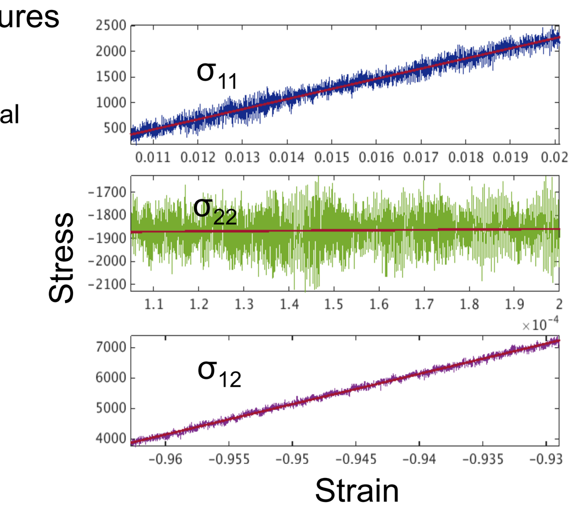
Temperature dependent elastic properties



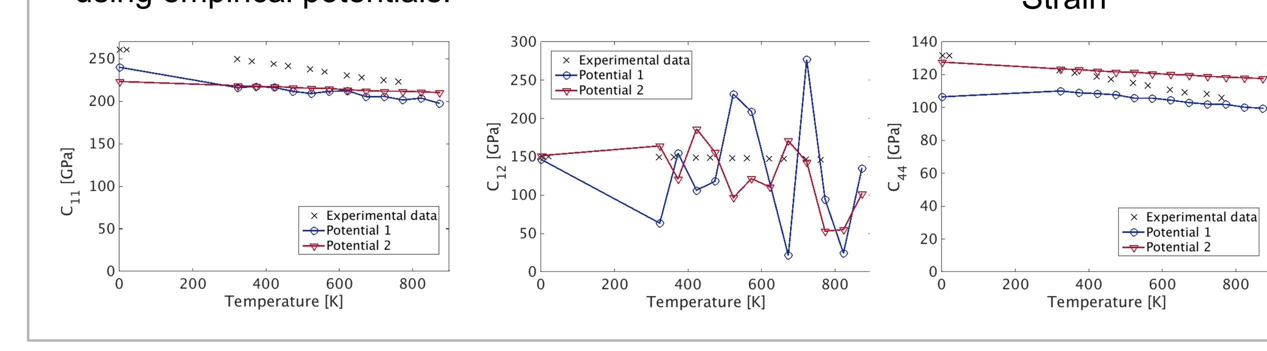
Anisotropic elastic constants of Ni-20Cr solution will be predicted using quantum molecular dynamics of special quasi-random structures

Simulate in the canonical ensemble while slowly deforming along strain path:

$$\begin{vmatrix} \varepsilon & \varepsilon/2 & 0 \\ \varepsilon/2 & 0 & 0 \\ 0 & 0 & 0 \end{vmatrix}$$



Testing the approach from [3] using empirical potentials:



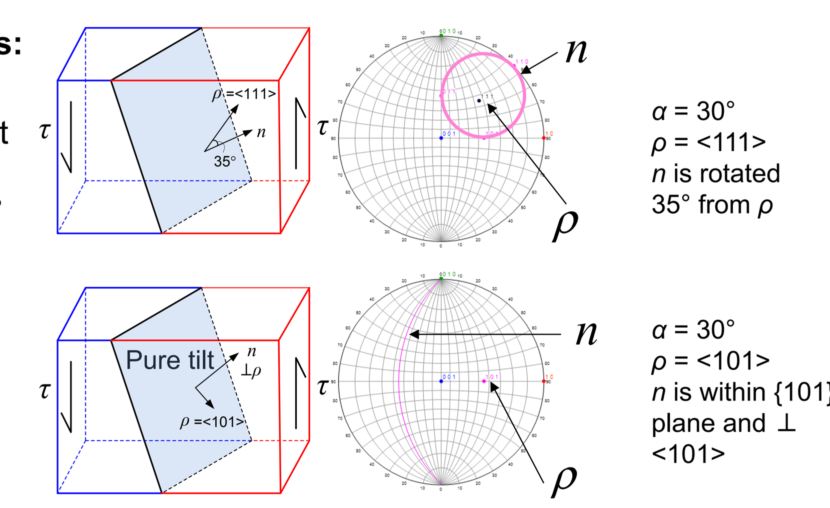
Grain Boundary Viscosity

Literature [2] reports of creep-damaged grain boundaries in similar FCC Ni-Cr alloy

α = misorientation angle
ρ = misorientation axis
n = grain boundary normal

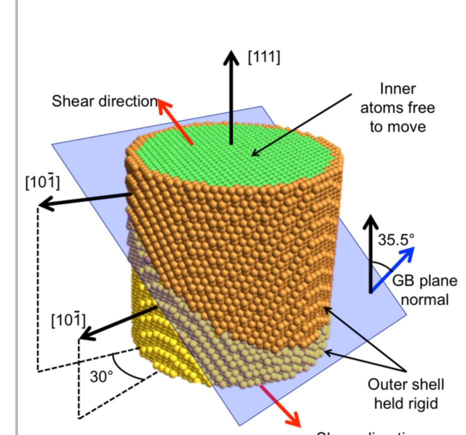
Two important boundaries:

1. 30° misorientation about <111> with normal of boundary plane at 35.5° to misorientation axis
2. 30° pure tilt boundary with tilt axis along <101>



α = 30°
ρ = <111>
n is rotated 35° from ρ

α = 30°
ρ = <101>
n is within {101} plane and ⊥ <101>

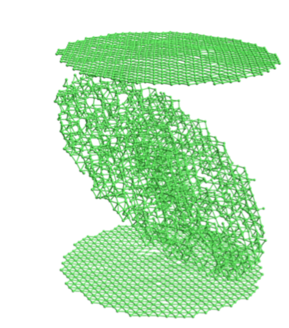


Simulation setup

For 30° misorientation about <111> with GB normal 35.5° to misorientation axis

Crystals are aligned along irrational direction and thus are perfectly non-commensurate

GB structure is several atom layers thick



Atomic structure of GB (only atoms with large centrosymmetry shown)

Conclusions thus far…

- Initial microstructure of Ni-20Cr alloy is fully characterized
- DEM algorithm is developed for isotropic elastic continuum

Next steps…

- DEM will be extended to capture the anisotropic elastic constants
- Sliding processes added to DEM model
- Compute T dependent anisotropic elastic constants and validate by high temperature nanoindentation
- Nanoindentation used to measure local work hardening & softening rates
- MD used to obtain the grain boundary sliding viscosity
- 3-D polycrystalline grain structure for DEM input will be reconstructed by high-energy diffraction microscopy (HEDM)
- Macroscopic high T creep and creep-fatigue testing to validate DEM model prediction

References

[1] D. Gould, M. Loveday, The Certification of Nimonic 75 Alloy as a Creep Reference Material, Commission of the European Communities, Directorate-General Science, Research and Development, 1990.

[2] F. Zhang, D. P. Field, Characterization of Creep-Damaged Grain Boundaries of Alloy 617, Metallurgical And Materials Transactions A, Volume 44A, 2013, pp. 4927-4936.

[3] P. Steneteg *et al.*, Temperature dependence of TiN elastic constants from *ab initio* molecular dynamics simulations, Physical Review B, Volume 87, 2013, pp. 094114.

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