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

Jay Kruzic, Matt Evans (OSU)  
Alex Greaney (UCR)
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- Postdoctoral researchers:
  - Dr. Qin Yu
  - Dr. Agnieszka Truszkowska

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

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• 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

• Not easily extendible outside measured ranges
  
  – Longer lifetimes
  – Variable operating conditions

\[ \varepsilon = A t \sigma^n \exp \left( \frac{-Q}{RT} \right) \]

\[ \sum_j \left( \frac{n}{N_d} \right)_j + \sum_k \left( \frac{\Delta t}{T_d} \right)_k \leq D \]
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

- 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

Oregon sand dunes

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

DEM Model:
Cone crack emerges under indent in silica glass

Hedjazi et al. (2012)

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

Macroscopic grain structure undergoing creep

Grains composed of discrete elements on scale of substructure

Contacts between grains modeled with springs and series dashpots
Hypothesis

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

Implement cubic crystal anisotropy

Implement plastic deformation

Implement creep deformation

Construct metal polycrystal model

Implement isotropic continuum
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 $M_{23}C_6$
  – 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
Adapting DEM for elastic anisotropy

But Sand is not homogeneously elastic!

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

Particle Assembly

Oregon sand dunes

Normal Stiffness

Shear Stiffness

\[ k_n \]

\[ k_s \]

http://www.ngi.no/
We must developing contact behaviors to make sand elastic.

Homogeneous and isotropic in elastic response.
More than that we must make sand anisotropic elastic!

Ni-Cr: homogeneously elastic, but anisotropically elastic

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

$$C_{ij} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$
Adapting DEM for elastic anisotropy

The subtleties of anisotropic elasticity...

• Directionally dependent elastic response of single crystal Ni
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
Define a local coordinate system

- Shear force
- In plane polar direction
- In plane equatorial direction
- Contact plane
- Contact normal direction

Formula: $F_s$
Adapting DEM for elastic anisotropy

Define bond contact laws based on coordinate system

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

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

\[ \beta = \frac{C_{44}^*}{C_{11}^*} \]

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

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

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

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

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

\[ F = \frac{(\alpha - 1)\beta \left(8\sin^3(\theta)\cos(\theta)\cos(4\phi) - 2\sin(2\theta) - 7\sin(4\theta)\right)}{16\alpha} \]
Adapting DEM for elastic anisotropy

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

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

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

$$\beta = \frac{C^*_{44}}{C^*_{11}}$$
Adapting DEM for elastic anisotropy

• Progress to date:

<table>
<thead>
<tr>
<th></th>
<th>$C_{11}$ (GPa)</th>
<th>$C_{12}$ (GPa)</th>
<th>$C_{44}$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Current Model</strong></td>
<td>237</td>
<td>77</td>
<td>73</td>
</tr>
<tr>
<td>Ni</td>
<td>251</td>
<td>150</td>
<td>124</td>
</tr>
<tr>
<td>Ni (600°C)</td>
<td>221</td>
<td>145</td>
<td>102</td>
</tr>
<tr>
<td>Fe</td>
<td>231</td>
<td>116</td>
<td>135</td>
</tr>
<tr>
<td>Cr</td>
<td>340</td>
<td>99</td>
<td>59</td>
</tr>
<tr>
<td>Si</td>
<td>166</td>
<td>80</td>
<td>64</td>
</tr>
</tbody>
</table>

$C_{11}$ in line with Ni-alloys

$C_{12}$ and $C_{44}$ in line with Si
Developing the DEM model

- Implement cubic crystal anisotropy
- Implement plastic deformation
- Implement creep deformation
- Construct metal polycrystal model
- Implement isotropic continuum
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

Typical deformations:
- Normal stretch
- Shear stretch
- Tilt stretch
- Twist stretch

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

![Graph showing stress vs. strain]
Adapting DEM for plasticity

- Hardening deformation
  - Strain hardening
  - Localization suppressed
Adapting DEM for plasticity

- Elastic and plastic models are coupled.

- At right:
  - No bond hardening in this model.
  - Artificial hardening emerges from different elastic model.
  - Bond texture evolves into stiffer configuration.
  - Shear localization emerges.
  - Bond stressed, breaks, and forms in stiffer orientation.
  - Bond texture evolves.

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*Graph showing stress vs. strain with annotations.*

- Stress (MPa) axis ranging from 0 to 70.
- Strain (%) axis ranging from 0 to 0.4.
- Blue line and dots representing stress-strain behavior.
- Arrows indicating bond stress, breakage, and formation in stiffer orientation.
- Text annotations for shear localization and bond texture evolution.
Creating a DEM Polycrystal

- EBSD used to quantify grain structure
  - Presence of twins skews apparent distributions
  - $\Sigma 3$ and $\Sigma 9$ annealing twin boundaries are unlikely damage sites (Zhang & Field, 2013)
  - Initially a twin-free microstructure is created for our DEM model
Creating a DEM Polycrystal

- A 3-D Voronoi algorithm for crystal plasticity has been adapted for making a polycrystalline 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 on 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
Questions?
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 $C_{11}$

<table>
<thead>
<tr>
<th>Material</th>
<th>Equilibrium lattice parameter, $a$, Å</th>
<th>Bulk modulus $B$, GPa</th>
<th>Zener’s modulus $C’$, GPa</th>
<th>$C_{11}$, GPa</th>
<th>$C_{12}$, GPa</th>
<th>$C_{44}$, GPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pure Ni (2x2x2 supercell)</td>
<td>3.518</td>
<td>200.1</td>
<td>55.7</td>
<td>274.3</td>
<td>163.0</td>
<td>128.8</td>
</tr>
<tr>
<td>Ni-20Cr (2x2x2 SQS supercell)</td>
<td>3.523</td>
<td>204.1</td>
<td>60.0</td>
<td>284.1</td>
<td>164.1</td>
<td>131.7</td>
</tr>
</tbody>
</table>
MD simulations at $T > 0\,\text{K}$ using embedded atom method and a $3 \times 3$ 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 $600\,\text{°C}$ will verify extrapolation.

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

$C_{ij}$ at $0\,\text{K}$

$\sim$Debye temperature

$\sim$Gruneisen parameter