MEANS 2: Development of Microstructure- and Micromechanism-Sensitive Property Models and Their Integration Into the Design of Advanced Turbine Disk and Blade Systems

CAMM (OSU): Mills, Daehn, Wang, Li, Flores, Williams, Ghosh, Pollock (U of M), Hemker (JHU)
AFRL (Woodward, Dimiduk, Larsen), GEAE (Whitis), P&W (Schirra)

Objectives:

Target several pacing materials issues with hot-section materials:

(1) Creep mechanisms and microstructure stability of disks and blades, and delivery of physically-based deformation models for creep of both.

(2) Determine the local plasticity mechanisms during fatigue at high temperature, and build on the creep models to account for the multiple mechanisms that will be active near stress risers leading to crack initiation (focus on blades).
Ni-Based Superalloys

- $\gamma$ (FCC solid solution) matrix

- $\gamma'$ (ordered L1$_2$ structure) precipitates

CMSX-4 Single Crystal
Dlouhy (1998)

- a/2[110]

Rene 88 Polycrystal
Sarosi (2003)

- a/2[110]
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Understanding of Micromechanical Processes: Experiment + Modeling

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Mechanisms of Creep in Disk Alloys

- APB Shearing
- Dislocation Looping
- Isolated Faulting
- Microtwinning
- Dislocation Bypass
- Tertiary γ Dissolution
MEANS 2 (AFOSR): Materials Engineering for Affordable New Systems

Proposed General Framework for Developing Time-Dependent Constitutive Models
Experimental Thrusts

- Complete elucidation of micromechanisms and transitions:
  - ME3 Disk alloy (OSU)
  - MX4 Blade alloy (Pollock)
- Transient creep testing for activation parameters
- Strain mapping (Pollock)
- Tension/compression asymmetry and crystal snisotropy of flow in disk alloys using single crystals and high temp microsample testing (Hemker)
First Principles and Atomistic Modeling

1/6<112> pairs

Matrix (L1₂)

GB Source

Twin

Orthorhombic

Cubic (L1₂)

For Disks:
- Fault energies (as function of T)
- Modeling of elementary processes:
  - Reordering for microtwinning and SESF formation
**First Principles and Atomistic Modeling**

For Blades:
- Diffusion-mediated climb/glide of dislocations in $\gamma$

For Blades:

\[ b_1 = a/2[011] \]
\[ b_2 = a/2[0\bar{1}1] \]
\[ b_T = a[001] \]
Phase Field Modeling

Microstructure Evolution (Disks)

- Realistic spatial distributions
- Coarsening kinetics

Coarsening f(t, T)

- Statistical Strength Modeling
  - Model dislocation/twin motion in large statistical arrays of obstacles w/multi-mechanisms.
  - Use dislocation dynamics or cellular automaton.

- Crystal Plasticity Modeling
  - From parameterized slip plane plasticity develop anisotropic forms with load shedding for backstresses

- Computational efficient constitutive laws for AIM tools including measures of variability

Increasing Length Scale

RCA 1 Activities

RCA 4 Activities

Structure Evolution Laws (Exp'l and Phase Field)

- Microstructure Evolution
  - Coarsening
  - Phase evolution
  - Ratting

- Dislocation Structure
  - Dislocation generation
  - Dislocation Annihilation
  - Pattern Formation

Fundamental Kinetics (RCA 3)

- Viscous Laws
- Barrier Laws (discrete release)

Evaluation Methods
- Experimental
- Simulation
- Both

Experimental Observations (RCA 2 output)

- Mechanisms
- Strength (rate, temp)
- Transient Response
- Microstructures

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Phase Field Modeling
Dislocation Dynamics

- Channel filling and $\gamma'$ cutting
- Shockley partial nucleation for isolated faulting
Phase Field Modeling

Microstructure Evolution (Blades)

- Realistic spatial distributions
- Coarsening kinetics
- Rafting in blades
  - Requires treatment of diffusion and channel filling processes

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Phase Field Modeling

Dislocation Dynamics

- Channel filling and γ' cutting

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Statistical Strength Modeling

Phase Field Modeling

- Dislocation dynamics through simulated microstructures
**Statistical Strength Modeling**

- Dealing with barriers of multiple barriers and evolution.
- Scaling should match other models.
- CA modeling in large statistical arrays (intra- and intergranular processes)

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Crystal Plasticity Modeling

Experimental Observations
(RCA 2 output)
Mechanisms
Strength (rate, temp)
Transient Response
Microstructures

Fundamental Kinetics
(RCA 3)
Viscous Laws
Barrier Laws (discrete release)

Evaluation Methods
Experimental
Simulation
Both

Structure Evolution Laws (Exp’I and Phase Field)

Microstructure Evolution
- coarsening
- phase evolution
- rating

Dislocation Structure
- Dislocation generation
- Dislocation Annihilation
- Pattern Formation

Statistical Strength Modeling
Model dislocation/twin motion in large statistical arrays of obstacles w/multi-mechanisms. Use dislocation dynamics or cellular automaton.

Crystal Plasticity Modeling
From parameterized slip plane plasticity develop anisotropic forms with load shedding for backstresses

Computationally efficient constitutive laws for AIM tools including measures of variability

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### Table 1.1: Enhancement of AIM Toolset by this MEANS-2

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<tr>
<th>Feature</th>
<th>Present AIM</th>
<th>Enhanced Capabilities after MEANS2</th>
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<td>Alloys</td>
<td>Rene88 (supersolvus) IN100 (subsovls)</td>
<td>Rene104 (supersolvus) MX4 (single crystal)</td>
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<td>Microstructure (application)</td>
<td>Polycrystalline (disk)</td>
<td>Single Crystal (blades)</td>
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<td>GE Proprietary, PrecipiCalc (temporal)</td>
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<td>Micromechanics-Based Property Models</td>
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<td>Macro-mechanical Behavior</td>
<td>Microsamples–slip system response</td>
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<td>Microstructure Basis for Variability Prediction</td>
<td>Average features</td>
<td>Spatial correlations and distributions</td>
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<td>Confidence for Extension to New Alloys</td>
<td>Moderate</td>
<td>High</td>
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Key Initial Issues

Disk Alloys:

1. Aging and microstructure coarsening

2. Microtwinning mechanism

3. Isolated faulting mechanism

4. Transition between 2 and 3
Dramatic Effect of Microstructure Scale On Creep Response

• Strong effect of tertiary volume fraction of creep strength
• Coarsening of tertiary population occurs at these temperatures
  • *Different mechanisms* active for two microstructures
Disk Alloys:

1. Aging and microstructure coarsening

2. Microtwinning mechanism

3. Isolated faulting mechanism

4. Transition between 2 and 3
Deformation Structure (Cooling Rate 400F/min)

Creep Tested at 1200F / 121.6ksi / 0.5% strain

- Faults associated with shearing of both secondary and tertiary γ′
- Continuous faults dominate, some isolated faulting
- Very low dislocation density
Nature of Continuous Faulting

- Fault contrast in precipitates and matrix
- Partial dislocations lying on the same or parallel (111) planes
- Subtle +g /-g effects on the contrast for partial dislocations on faults
Faulting Occurs by Motion of $1/6[11-2]$ Partials

- Fault contrast

- Shockley partial not visible for both $+/-\ g[-111]$
Faulting Occurs by Motion of 1/6[11-2] Partials

- Faults out of contrast
- *Pairs* of identical Shockley partials visible

\[ |g \cdot b| = \frac{2}{3} \text{ for: } \frac{1}{6}[11-2] \]
\[ |g \cdot b| = 0 \text{ for: } \frac{1}{6}[1-21] \]
HRTEM Reveals that Continuous Faults are Microtwins!

Estimating Strain due to Microtwinning . . .

\[ \Delta = n | b_p | = n a_o \left( \frac{\sqrt{3}}{6} \right)^2 \]

- Present HRTEM indicates
  \( n_{\text{ave}} \sim 5-10: \)

\[ \gamma = \frac{N_{\text{twin}} \Delta_{\text{ave}}}{L} \]

\( \gamma_{\text{est}} = 0.5 - 1.0\% \quad \gamma_{\text{actual}} = 1\% \)

Microtwinning is the dominant deformation process!

1\( \mu \text{m} \mid 1 \text{nm} \)
Microtwin Mechanisms in L₁₂ Structure

Using 1/3[-12-1] Partials:
- L₁₂ structure preserved
- Larger Burgers vector must be nucleated

Using 1/6[11-2] Partials:
- Very high energy CSF-like faults formed
- L₁₂ structure not preserved in process

Sequence of Partials On (111) Plane

Creates “Pseudotwin” with Orthorhombic Structure!
HRTEM of Microtwin Structure
Within Secondary $\gamma'$

Creep Tested at 1200F / 121.6ksi / 0.2% strain

- True-twin structure observed
- Re-ordering to L1$_2$ must occur during partial motion
Mechanism For Thermally-Activated Microtwinning

- Swapping of atom positions to recreate L1₂ structure (Kolbe, 2001)
- Conservative process requiring local, closed-circuit diffusion

• Qualitative explanation for temperature/time dependence of process

![Diagram showing the mechanism of microtwinning in Ni₃Al, including the swapping of atom positions and the reordering from orthorhombic to cubic (L1₂) structure.](diagram.png)
Velocity for Diffusion-Mediated Glide of Partials

\[ \nu_{tp} = \frac{D_{ord}}{x^2} \cdot b_{tp} \ln \left[ \frac{f_2 \cdot (\gamma_{pt} - \gamma_{tt})}{(\tau_{eff} \cdot b_{tp} - f_2 \cdot \gamma_{tt})} \right] \]

Assumptions:
- Energy penalty due to twin decreases exponentially with time
- Shear of secondary \( \gamma' \) is thermally assisted while shear of tertiary \( \gamma' \) is athermal
- Effective stress driving shear of secondary \( \gamma' \) is given by:
  \[ \tau_{eff} = \tau - \tau_{tertiary} - \tau_{friction} \]
  \[ \tau_{tertiary} = \frac{f_3 \cdot \gamma_{pt}}{b_{tp}} \]

Strain Rate:
\[ \dot{\gamma}_{twin} = \rho_{tp} b_{tp} \nu_{tp} \]

Microstructure Parameters:
- Obtain from direct TEM measurements

Key Model Parameters:
- Obtain from transient creep experiments or modeling
Key Initial Issues

Disk Alloys:

1. Aging and microstructure coarsening
2. Microtwinning mechanism
3. Isolated faulting mechanism
4. Transition between 2 and 3
Dramatic Effect of Microstructure Scale On Creep Mechanisms

Deformation substructures after 0.5% Strain (121 Ksi at 650°C)

Coarse Structure (75F/min)

- Isolated shearing of individual secondary γ'
- 1/2<110> matrix dislocations

Fine Structure (400F/min)

- Continuous faults through precipitates and matrix
- 1/2<110> dislocations absent
Mechanism of Isolated Faulting of Secondary γ'

Coarse Structure
(75°F/min)
121 ksi at 1200°F
0.5% Strain

- \( \frac{1}{2}<110> \) dislocations in matrix
- Contrast analysis indicates the faults are Superlattice Extrinsic Stacking Faults (SESFs)
Mechanism of Isolated Faulting of Secondary $\gamma'$

- Requires reordering of two-layer CSF to lower energy SESF
Key Initial Issues

Disk Alloys:

1. Aging and microstructure coarsening

2. Microtwinning mechanism

3. Isolated faulting mechanism

4. Transition between 2 and 3
Transition in Mechanism with Stress

Coarse Structure: 
*Isolated Faulting*

Fine Structure: 
*Microtwinning*
What Drives the Change in Mechanism?
Important Role of Tertiary . . .

75F/min:
Smaller
γ’ vol. fraction

400F/min:
Larger
γ’ vol. fraction

Difference in
Effective friction stresses. . .
What Drives the Change in Mechanism?  
Important Role of Tertiary . . .

\[ \Delta \sigma_{\text{fault}} = \frac{2 f_{\text{tertiary}} \gamma_{\text{fault}}}{b} \]

- Suggests operative mechanism depends directly on tertiary volume fraction and fault energies
Modeling Challenges

Disk Alloys:

1. Aging and microstructure coarsening
   • Coarsening kinetics, interaction between secondary and tertiary populations

2. Microtwinning mechanism
   • CSF/SESF fault energies and reordering kinetics as function of temperature

3. Isolated faulting mechanism
   • Partial nucleation mechanisms, effect of precipitate volume fraction and spatial distribution