# Microstructure-Sensitive Crystal Viscoplasticity for Ni-base Superalloys (with application to long-term creep-fatigue interactions)

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# **Hot Section Gas Turbine Materials**

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### Land-based gas turbines

- drive to increase service temperature to improve efficiency; increase life; with minimal increase in cost
- replace large directionallysolidified Ni-base superalloys with single crystal superalloys



# **Hot Section Gas Turbine Materials**

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Superalloys airfoils are subject to a continuation of "process" during service due to sustained hostile environment and loading. Understanding the influence of the microstructure and its evolution on TMF, creep and fatigue and their interactions is key to delivering better turbine designs



### **PSPP Map for Ni-base Superalloy Airfoils**

PERFORMANCE

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### GeorgiaInstitute of Technology Microstructure, Properties, & Performance

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PERFORMANCE

**PROPERTIES** 

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 PROCESS
 STRUCTURE



### **Role of Chemical Composition**

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# Single Crystal Alloy being Investigated for IGT Applications

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CMSX-8: 1.5% Re "alternative 2<sup>nd</sup> gen alloy" replacing 3.0% Re containing alloys (e.g., CMSX-4, PWA1484)

Alloy	Cr	Co	Mo	W	Al	Ti	Ta	Re	Hf	С	В	Zr	Ni
Mar-M247LC-DS	8.4	10.0	0.7	10.0	5.5	1.0	3.0	-	1.5	0.07	0.015	0.05	Bal
CM247LC-DS	8.1	9.2	0.5	9.5	5.6	0.7	3.2	-	1.4	0.07	0.015	0.01	Bal
CMSX-4	6.5	9.0	0.6	6.0	5.6	1.0	6.5	3.0	0.1	-	-	-	Bal
SC16	16	0.17	3.0	0.16	3.5	3.5	3.5	-	-	-	-	-	Bal
PWA1484	5.0	10.0	2.0	6.0	5.6	-	9.0	3.0	0.1	-	-	-	Bal
CMSX-8	<mark>5.4</mark>	<mark>10.0</mark>	<mark>0.6</mark>	<mark>8.0</mark>	<mark>5.7</mark>	<mark>0.7</mark>	<mark>8.0</mark>	1.5	<mark>0.2</mark>	-	-	-	<mark>Bal</mark>



### Influence of Temperature, Loading Direction and Crystal Orientation on Modulus and Strength

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# **Thermomechanical Fatigue (TMF)**







# Effect of T<sub>min</sub> on OP TMF of CMSX-4

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### CMSX-4 [001]













# Life Modeling Approach

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### Damage Mechanism Modules





- Creep-fatigue interaction experiments on CMSX-8
- Influence of aging on microstructure and creep-fatigue interactions
- Microstructure-sensitive, temperaturedependent crystal viscoplasticity to capture the creep and cyclic deformation response

# **Major Activities and Accomplishments**

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Experimentally establish the creep-fatigue interactions in a single-crystal Ni-base superalloy that is being targeted for use in industrial gas turbines (CMSX-8)

- Characterize creep-fatigue interactions on CMSX-8
  - Creep-fatigue
  - Thermomechanical fatigue
  - Creep (either tension or compression) followed by fatigue
  - Fatigue followed by creep
- Characterize the influence of aging on microstructure and creepfatigue interactions





# **Conventional Creep-Fatigue (baseline)**



# **Conventional Creep-Fatigue (baseline)**



# **Cycle Evolution**

Cycle 1

Cycle 3

Cycle 2

Cycle 4

2.5

3

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# T = 1100 °C, R = 0, $\Delta \epsilon$ = 1.0 %



# **Crack Characteristics**

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# R = 0, T = 1100°C, $\Delta\epsilon$ = 0.8% $N_{f}$ = 1420



$$\epsilon \int_{t} R = 0$$

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# $$\label{eq:relation} \begin{split} R = -\infty, \ T = 1100^{o}C, \ \Delta \epsilon = 0.8\% \\ N_f = 980 \end{split}$$









### Half-life at 1025 °C



# Half-life at 1100 °C

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- Creep-fatigue interaction experiments on CMSX-8
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# **Major Activities and Accomplishments**

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Experiments & Models to Predict Current State of Microstructure (Service Process-Structure Linkages)







- Stress-free and stress-assisted (rafting) aging experiments under tensile and compressive stresses
- Establishing process-structure linkages using physical models, 2-point statistics and PCA



Microstructure-sensitive Crystal Viscoplasticity (CVP) Model to Determine Service "Process"-Structure-Property Linkages

$$\mathbf{L}^{in} = \dot{\mathbf{F}}^{in} \, \mathbf{F}^{in^{-1}} = f_{\gamma} \left( \sum_{\alpha=1}^{12} \dot{\gamma}_{\gamma}^{in(\alpha)} \left( \hat{\mathbf{d}}^{(\alpha)} \otimes \hat{\mathbf{n}}^{(\alpha)} \right) \right) + f_{\gamma} \left( \sum_{\alpha=13}^{24} \dot{\gamma}_{L1_2}^{in(\alpha)} \left( \hat{\mathbf{d}}^{(\alpha)} \otimes \hat{\mathbf{n}}^{(\alpha)} \right) \right)$$

γ deformation







Sensitivity of Local Composition on Diffusivity for Input in Aging and Viscoplasticity Models

> Thermo-Calc DICTRA Databases: TCNi5 / MOBNi2

- Composition segregation in γ and γ' phase
- Determination of composition sensitive effective diffusivity to characterize aging activation energy and diffusivity parameter in viscoplasiticity models





# **Microstructure Evolution in Blades**

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# **Distance from Root**



# Rafting and Coarsening of y'

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# **High-Throughput Stress-assisted Aging**



### **Aged Microstructure under Compressive Stress**

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**Compression Creep Frame** 

Ceramic Compression Creep Extensometer



# **Physical Models to Describe Aging Behavior**

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# **2-point Correlation Method**

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- 2-point correlation A statistical representation of the microstructure that provides a magnitude measure in addition to the associated spatial correlation.
- 2-point correlations f(h, h' | r) capture the probability density associated with finding an ordered pair of specific local state at the head and tail of a randomly placed vector r into the microstructure.
- Cross-correlation

Defined by  $f(h, h' \neq h | r)$ . The function gives the probability that a random vector of length x start in one phase and end in the other.

$$\Gamma(h, h'|\mathbf{r}) = \frac{1}{vol(\Omega)} \int_{\Omega} m(\mathbf{x}, h) m(\mathbf{x} + \mathbf{r}, h'd\mathbf{x})$$

$${}^{np}F_{\mathbf{k}} = \Im({}^{np}f_{\mathbf{t}}) = \frac{1}{S} {}^{n}M_{\mathbf{k}}^{*} {}^{p}M_{\mathbf{k}}$$
  
$$= \frac{1}{S} |{}^{n}M_{\mathbf{k}}| |{}^{p}M_{\mathbf{k}}| e^{-i {}^{n}\theta_{\mathbf{k}}} e^{i {}^{p}\theta_{\mathbf{k}}}$$





(a) An example of two phase microstructure (b) Crosscorrelation for the black and white phases at the head and tail of a vector [Fullwood, Niezgoda, Adams, Kalidindi, 2010].

Distance along [0 0 1] [µm]

# **2-point Correlation Application to CMSX-8**

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# **Quantifying the Current Aged State**

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# **Influence of Variation in Composition**

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Y

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Composition segregation Thermo-Calc



# **Influence of Composition on Diffusivity**

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Interdiffusion coefficients of Ni-x binary systems DICTRA Composition variation (Re) effect on effective diffusivity of the complex Superalloy system DICTRA





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- Creep-fatigue interaction experiments on CMSX-8
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- Microstructure-sensitive, temperaturedependent crystal viscoplasticity to capture the creep and cyclic deformation response

# Microstructure-sensitive Crystal Viscoplasticity for Single-Crystal Ni-base Superalloys

strain [%]



# **Crystal Viscoplasticity – Kinematic Relations**

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Kinematic relations including temperature dependence

**Deformation gradient** 

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \mathbf{F}^e \cdot \mathbf{F}^p \cdot \mathbf{F}^\theta$$

Velocity gradient  $\mathbf{L} = \mathbf{F} \cdot \mathbf{F}^{-1}$ 

Macroscopic plastic velocity gradient

$$\mathbf{L}^{p} = \mathbf{F}^{p} \mathbf{F}^{p^{-1}} = \sum_{\alpha=1}^{N_{slip}} \boldsymbol{\chi}^{(\alpha)} \left( \mathbf{s}_{o}^{(\alpha)} \otimes \mathbf{n}_{o}^{(\alpha)} \right)$$



# **Creep Deformation Mechanisms of Superalloys**

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Influence of stress and temperature on modes of creep deformation



[Reed, 2006; Ma, Dye, and Reed, 2008, CMSX-8 Data]

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**Rafting** – transport of matter constituting the  $\gamma$  phase out of the vertical channels and into the horizontal ones (tensile creep case)



[Ma, Dye, and Reed, 2008]

**Tertiary** – dislocation activity restricted to a/2 < 110 > form operating on {111} slip planes in the  $\gamma$  channels



**Primary** –  $\gamma$ ' particles are sheared by dislocation ribbons of overall Burgers vector a<112> dissociated into superlattice partial dislocations separated by a stacking fault; shear stress must above threshold stress (about 550 MPa)

# Crystal Viscoplasticity (CVP) – Rate Eqn

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### **Inelastic Velocity Gradient**

$$\mathbf{L}^{in} = \dot{\mathbf{F}}^{in} \mathbf{F}^{in^{-1}} = f_{\gamma} \left( \sum_{\alpha=1}^{12} \dot{\gamma}_{\gamma}^{in(\alpha)} \left( \hat{\mathbf{d}}^{(\alpha)} \otimes \hat{\mathbf{n}}^{(\alpha)} \right) \right) + f_{\gamma'} \left( \sum_{\alpha=13}^{24} \dot{\gamma}_{L_{1_2}}^{in(\alpha)} \left( \hat{\mathbf{d}}^{(\alpha)} \otimes \hat{\mathbf{n}}^{(\alpha)} \right) \right)$$

### **Inelastic Shear Strain Rate**

$$\begin{split} \dot{\gamma}_{\gamma}^{in(\alpha)} &= \rho^{(\alpha)}_{\gamma} \ b \ \lambda_{\gamma}^{(\alpha)} F_{attack} sign\left(\tau^{(\alpha)} + \tau^{(\alpha)}_{mis} - \chi^{(\alpha)}\right) \exp\left\{\frac{-\mathcal{Q}_{slip}^{110} + \left(\left|\tau^{(\alpha)} + \tau^{(\alpha)}_{mis} - \chi^{(\alpha)}\right| - \tau^{(\alpha)}_{\gamma pass} - \tau^{(\alpha)}_{oro}\right) V_{c1}^{(\alpha)}}{kT}\right\} \\ \dot{\gamma}_{L1_2}^{in(\alpha)} &= \rho_{L1_2}^{(\alpha)} b \ \lambda_{L1_2}^{(\alpha)} F_{attack} sign\left(\tau^{(\alpha)} - \chi^{(\alpha)}\right) \exp\left\{\frac{-\mathcal{Q}_{slip}^{112} + \left(\left|\tau^{(\alpha)} - \chi^{(\alpha)}\right| - \tau^{(\alpha)}_{L1_2 pass} - \tau_{APB}\right) V_{c2}^{(\alpha)}}{kT}\right\} \end{split}$$

### **Evolution Equations**

1

$$\begin{vmatrix} \dot{\rho}_{\gamma}^{(\alpha)} = \frac{1}{b} \left( \frac{c_{mult1}}{\lambda_{\gamma}^{(\alpha)}} - c_{annh1} \rho_{\gamma}^{(\alpha)} \right) \left| \dot{\gamma}_{\gamma}^{in(\alpha)} \right| \\ \dot{\rho}_{L1_{2}}^{(\alpha)} = c_{mult21} \rho_{pb}^{(\alpha)} \Gamma + \frac{c_{mult22}}{b \lambda_{\gamma'}^{(\alpha)}} \left| \dot{\gamma}_{\gamma'}^{(\alpha)} \right| - c_{annh2} \rho_{\gamma'}^{(\alpha)} \left| \dot{\gamma}_{\gamma'}^{(\alpha)} \right| \\ \dot{\rho}_{pb}^{(\alpha)} = \frac{c_{mult}^{pb}}{b L_{\gamma}} \left| \dot{\gamma}_{\gamma}^{in(\alpha)} \right| - c_{annh}^{pb} \rho_{pb}^{(\alpha)} \left| \dot{\gamma}_{\gamma}^{in(\alpha)} \right| \end{aligned}$$

![](_page_35_Figure_10.jpeg)

# **Orientation Sensitivity**

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# **CMSX-4 Model Predictions**

![](_page_36_Figure_5.jpeg)

# **Creep in different orientations**

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Temp = 950[°C], Stress = 250[MPa] 40 Data <001> CVP <111> 35 CVP <001> Т. CVP <112> L Т 30 ..... CVP <101> н CVP <212> CVP <102> 25 creep strain [%] 20 15 1 10 5 0 200 800 1200 1400 0 400 600 1000 1600 time [hrs]

![](_page_37_Figure_4.jpeg)

# **Primary and Tertiary Creep**

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![](_page_38_Figure_4.jpeg)

![](_page_38_Figure_5.jpeg)

# **TMF** validation

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![](_page_39_Figure_4.jpeg)

![](_page_39_Figure_5.jpeg)

[100-850-100] °C, R = - $\infty$ ,  $\dot{T} = 2.83[$  °K/s]

Very good agreement predicting TMF

# **TMF** validation

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Experiment

Simulation

BIRITARIA.

-1

![](_page_40_Figure_4.jpeg)

[100-1100-100] °C, R = 0,  $\dot{T} = 2.83[$  °K/s]

Stabilized hysteresis: OP-TMF [100-850-100] °C, R = - $\infty$ ,  $\dot{T}$  = 2.83[°K/s]

mechanical strain [%]

-0.5

0

Very good agreement predicting TMF

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Since Re segregates almost exclusively in the  $\gamma$  channels, the Activation energy in the  $\gamma$  phase can be modified to account for Re content as follows:

$$\begin{split} \dot{\gamma}_{\gamma}^{in(\alpha)} &= \Theta\left(T\right)\rho^{(\alpha)}_{\gamma} \ b \ \lambda_{\gamma}^{(\alpha)} F_{attack} sign\left(\tau^{(\alpha)} + \tau^{(\alpha)}_{mis} - \chi^{(\alpha)}\right) \exp\left\{\frac{-Q_{slip}^{110} + \left(\left|\tau^{(\alpha)} + \tau^{(\alpha)}_{mis} - \chi^{(\alpha)}\right| - \tau^{(\alpha)}_{\gamma pass} - \tau^{(\alpha)}_{oro}\right) V_{c1}^{(\alpha)}}{kT}\right\} \\ \dot{\gamma}_{L1_{2}}^{in(\alpha)} &= \rho_{L1_{2}}^{(\alpha)} b \ \lambda_{L1_{2}}^{(\alpha)} F_{attack} sign\left(\tau^{(\alpha)} - \chi^{(\alpha)}\right) \exp\left\{\frac{-Q_{slip}^{112} + \left(\left|\tau^{(\alpha)} - \chi^{(\alpha)}\right| - \tau^{(\alpha)}_{L1_{2} pass} - \tau_{APB}\right) V_{c2}^{(\alpha)}}{kT}\right\} \end{split}$$

If we considering activation energy for plastic flow  $Q_0$  a function of %Re, the diffusivity parameter could take the form of:

$$\Theta(T) = \exp\left(-\frac{Q_o}{RT}\right) \quad \text{for } T \ge \frac{T_m}{2} \qquad \qquad \Theta(T) = \exp\left(-\frac{2Q_o}{RT}\left[\ln\left(\frac{T_m}{2T}\right) + 1\right]\right) \quad \text{for } T \le \frac{T_m}{2}$$

[Miller, 1976; Shenoy et al., 2005]

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- Exercise new CVP codes
  - (1) displacement-controlled algorithm coded in FORTRAN as UMAT for ABAQUS (suitable for 3D analysis of detailed features, but computationally expensive)
  - (2) stress-controlled algorithm coded in MATLAB (limited to 1D loadings, but computationally cheap; utility in alloy design; early design iterations)
- Characterize aged microstructure and its analysis
  - Establish protocols for reduced-order modeling of the current state of the microstructure using spatial correlations and principal component analysis
  - Develop PSP linkage models using PC values for describing current state
     of the microstructure
- Creep-fatigue interaction life analysis relationships using all new data
- Disseminate research
  - Archival journal articles
  - Intern with Siemens Energy
  - Workshops and Conferences (UTSR, ASME, ...)
- Ernesto Estrada Rodas complete Ph.D. studies in 2017