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

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University Turbine Systems Research Workshop Pittsburgh November 1-2, 2017

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



Complexities in evaluating creep-fatigue interaction



Lengths scales in the Ni-base superalloys



PSPP Map for Ni-base Superalloy Airfoils

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Georgia Institute of Technology Microstructure, Properties, & Performance

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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 2nd 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>	<mark>1.5</mark>	<mark>0.2</mark>	-	-	-	<mark>Bal</mark>



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

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- 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

Creep-Fatigue Interaction Experiments

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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
 TMF life: R = 0 (IP) vs. R = -1 (OP)





Conventional Creep-Fatigue (baseline)



Conventional Creep-Fatigue (baseline)





Half-life at 1100 °C

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







Fatigue Lifetime Models - I

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Ostergren Model

- Energy-based life prediction model based on the net hysteretic energy.
- Accounts for the mean stress and cycle time (frequency) effect.
- The accuracy of prediction relies on precision of inelastic strain measurement.







Fatigue Lifetime Models - II

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Zamrik and Renauld Model

- Introducing hold-time and elevated temperature function to account for creep effect and exponentially increasing creep/or environmental damage with increasing temperature, respectively.
- Substituting inelastic strain with maximum tensile strain range.

$$N = A \left[\left(\frac{\varepsilon_{ten}}{\varepsilon_f} \right) \left(\frac{\sigma_{max}}{\sigma_u} \right) \right]^B \left(1 + \frac{t_h}{t_c} \right)^C exp \left(\frac{-Q}{R(T_{max} - T_0)} \right)$$

- σ_{max} : maximum tensile stress in mid-life hysteresis loop
- $m{arepsilon_{ten}}$: tensile strain range in mid-life hysteresis loop for which the stress is tensile

[Zamrik and Renauld, 2000]

- σ_u : ultimate strength measured under monotonic tensile loading
- $oldsymbol{arepsilon}_f$: elongation to failure measured under monotonic tensile loading
- *t_h*: length of compressive hold-time
- t_c : length of total time including hold-time
- **Q**: activation energy for high temperature damage



Fatigue Lifetime Models - III

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Kulawinski et al. Model

- The model is based on Zamrik model and the energy density term includes:
 - Zamrik damage parameter
 - Inelastic strain range
 - Stress range
 - Arrhenius term

$$N_{f} = A \left[\Delta \sigma_{eq} \cdot \Delta \varepsilon_{eq}^{in} \cdot W_{zam} \cdot exp\left(\frac{-Q}{RT}\right) \right]^{B}$$

$$\mathbf{W}_{\mathsf{Kul}}$$

- The goodness of fit plot shows majority of life predictions using Kulawinski model lie within the scatter band of factor two.
- 95% of the variance of the low cycle fatigue (LCF) and creep-fatigue (CFI) life data is captured by this lifetime model.



[Kulawinski et al., 2015]



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Microstructure Evolution in Blades

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Distance from Root



Microstructures Generated by Additive Manufacturing

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 SX Height Melt Depth I
 Deposit Height

 Original Substrate Height





500 μm —

As-built



500 nm **-**

After Heat Treatment



500 nm •

[Basak and Das (Georgia Tech), 2017]

Rafting and Coarsening of y'

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[Epishin et al., 2008]

High-Throughput Stress-assisted Aging



Aged Microstructure under Compressive Stress

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Compression Creep Frame

Ceramic Compression Creep Extensometer



Aging Behavior of CMSX-8



[Gorgannejad, Estrada Rodos, and Neu, Materials at High Temperature, 2016]



Influence of Variation in Composition

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Y'









Influence of Re Content on Diffusivity

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- Effective diffusivity of system is equivalent to effective diffusivity in *γ* channels.
- Diffusivity of Ni-m binary systems computed from mobility databases using DICTRA from Thermo-Calc.



$$D_{eff} = D_{0,eff} exp\left(-\frac{Q_{eff}}{kT}\right)$$



[Mushongera et al. 2015]

 C_m : atomic concentration of element m



[Estrada Rodas, Gorgannejad, Neu, et al., Superalloys 2016]





Employing Data Science to Predict Aged Structure

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microstructure as a result of various aging histories is generated

Tracking Microstructure Evolution

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- The 2-point statisical correlation is a rigorous quantification method that describes spatial correlation and critical structural information with microstructure reconstruction capability.
- It is computed based on the probability density associated with finding an ordered pair of specific phase at the head and tail of a randomly placed vector *r* into the microstructure.

•





Large Dimensional Dataset generated by 2-point statistical spatial correlation

Data Visualization of Aged CMSX-8 in PC Space

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- Application of PCA to the high dimension 2-point spatial correlation results in a reduced-order representation of microstructure ensemble.
- The axes are ordered descendingly by the extent of variation each explain.

Powerful classification and visualization tool:

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- PCA is a linear approach to dimensionality reduction by coordinate transform.
- The axes are defined by the directions of the highest variance



Effect of Aging on Creep-Fatigue



Role of Microstructure on LCF – Three Critical Temperature Regimes to Study

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Influence of Microstructure $R_{\epsilon} = 0$ versus $R_{\epsilon} = -\infty$ at 1100 °C

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No notable microstructure influence when $R_{\epsilon} = -\infty$.

Fatigue-environment interaction likely explanation when $R_{\epsilon} = -\infty$.



Fracture surface topology – Low cycle fatigue at 1100°C





Low Cycle Fatigue Response of CMSX-8 [001] $R_{c} = 0$, strain rate = 1 x 10⁻³ 1/s

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First 10 cycles – RT and 750 °C



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Fracture Surfaces

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Low Cycle Fatigue at Room Temperature

As-heat-treated



As-heat-treated



Low Cycle Fatigue at 750 ° C

Pre-aged



Pre-crept



Pre-crept





Crack Propagation Paths

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LCF at Room temperature

Pre-aged microstructure





10 μm		
開設		
5 μm		

CFI at **750** °C

As –heat – treated microstructure



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Creep Deformation REGIMES

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

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



Primary – γ' 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)

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



time [hrs] Tertiary creep: 950 °C, Stress = 400 MPa

time [hrs] Primary creep: 750 °C, Stress = 680 MPa

Crystal Viscoplasticity – Kinematic Relations

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Kinematic relations including temperature dependence

Deformation gradient

$$\mathbf{F} = \frac{\P \mathbf{x}}{\P \mathbf{X}} = \mathbf{F}^e \times \mathbf{F}^p \times \mathbf{F}^q$$

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

Macroscopic plastic velocity gradient

$$\mathbf{L}^{p} = \dot{\mathbf{F}}^{p} \mathbf{F}^{p^{-1}} = \mathop{\bigotimes}_{\partial=1}^{N_{slip}} \dot{\mathcal{G}}^{(\partial)} \left(\mathbf{s}_{o}^{(\partial)} \stackrel{\mathcal{H}}{\wedge} \mathbf{n}_{o}^{(\partial)} \right)$$





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

$$\dot{\gamma}_{\gamma}^{in(\alpha)} = \rho^{(\alpha)}_{\gamma} \ b \ \lambda_{\gamma}^{(\alpha)} F_{attack} sign\left(\tau^{(\alpha)} + \tau^{(\alpha)}_{mis} - \chi^{(\alpha)}\right) \exp\left\{\frac{-Q_{slip}^{110} + \left(\left|\tau^{(\alpha)} + \tau^{(\alpha)}_{mis} - \chi^{(\alpha)}\right| - \tau^{(\alpha)}_{\gamma}\right) - \tau^{(\alpha)}_{r}\right)}{kT}\right\}$$

$$\dot{\gamma}_{L1_2}^{in(\alpha)} = \rho_{L1_2}^{(\alpha)} b \ \lambda_{L1_2}^{(\alpha)} F_{attack} sign\left(\tau^{(\alpha)} - \chi^{(\alpha)}\right) \exp\left\{\frac{-Q_{slip}^{112} + \left(\left|\tau^{(\alpha)} - \chi^{(\alpha)}\right| - \tau^{(\alpha)}_{L1_2 pass} - \tau_{APB}\right) V_{c2}^{(\alpha)}}{kT}\right\}$$

$\begin{aligned} \mathbf{Dislocation Density Evolution Equations} \\ & \left[\dot{\rho}_{\gamma}^{(\alpha)} = \frac{1}{b} \left[\frac{c_{mult1}}{\lambda_{\gamma}^{(\alpha)}} - c_{annh1} \rho_{\gamma}^{(\alpha)} \right] \dot{\gamma}_{\gamma}^{in(\alpha)} \right] \\ & \dot{\rho}_{L1_2}^{(\alpha)} = c_{mult21} \rho_{pb}^{(\alpha)} \Gamma + \frac{c_{mult22}}{b \lambda_{\gamma'}^{(\alpha)}} \dot{\gamma}_{\gamma'}^{(\alpha)} - c_{annh2} \rho_{\gamma'}^{(\alpha)} \dot{\gamma}_{\gamma'}^{(\alpha)} \right] \\ & \dot{\rho}_{pb}^{(\alpha)} = \frac{c_{mult}^{pb}}{b L_{\gamma}} \dot{\gamma}_{\gamma}^{in(\alpha)} - c_{pb}^{pb} \rho_{pb}^{(\alpha)} \dot{\gamma}_{\gamma}^{in(\alpha)} \right] \end{aligned}$



Evolution of dislocation densities

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multiplication annihilation $\frac{c_{mult1}}{\lambda_{\gamma}^{(\alpha)}} - c_{annh1} \rho_{\gamma}^{(\alpha)} \left| \dot{\gamma}_{\gamma}^{in(\alpha)} \right|$ $\dot{\rho}_{\gamma}^{(\alpha)}$

 $\dot{\rho}_{pb}^{(\alpha)} = \frac{c_{mult}^{po}}{bL_{m}} \left| \dot{\gamma}_{\gamma}^{in(\alpha)} \right| - c_{annh}^{pb} \rho_{pb}^{(\alpha)} \left| \dot{\gamma}_{\gamma}^{in(\alpha)} \right|$

 $\dot{\rho}_{L1_{2}}^{(\alpha)} = c_{mult21} \rho_{pb}^{(\alpha)} \Gamma + \frac{c_{mult22}}{b \lambda_{wl}^{(\alpha)}} \left| \dot{\gamma}_{\gamma'}^{(\alpha)} \right| - c_{annh2} \rho_{\gamma'}^{(\alpha)} \left| \dot{\gamma}_{\gamma'}^{(\alpha)} \right|$

Creep in different orientations

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Various Creep Predictions

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Effect of Channel Size on Creep

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Effect of APB Energy on Creep

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Primary and Tertiary Creep

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TMF validation

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Very good agreement predicting TMF

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Since Re segregates almost exclusively in the γ channels, the Activation energy in the γ 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]

Intellectual Impacts

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Creep-Fatigue Interaction Experiments and Lifetime Models



Experiments & Models (both physically-based and data analytics) 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

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

γ deformation

y' deformation





Established Method to Determine 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







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