

Award DE-FE0011722 August 2013 – August 2016 Program Manager: Briggs White

PI: Richard W. Neu GRAs: Ernesto A. Estrada Rodas, Sanam Gorgan Nejad and Anirudh Bhat

The George W. Woodruff School of Mechanical Engineering School of Materials Science & Engineering Georgia Institute of Technology Atlanta, GA 30332-0405 rick.neu@gatech.edu

University Turbine Systems Research Workshop Georgia Institute of Technology November 3-5, 2015

Hot Section Gas Turbine Materials

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering



Land-based gas turbines

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



Single Crystal Alloy being Investigated for IGT Applications

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

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



Thermomechanical Fatigue (TMF)

School of Materials Science and Engineering





Effect of T_{min} on OP TMF of CMSX-4

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

CMSX-4 [001]







[Arrell et al., 2004]







Life Modeling Approach

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

Damage Mechanism Modules





The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

- 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 Studies

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

- Conventional creep-fatigue (baseline)
 > ASTM E2714-09
- Long-term creep followed by fatigue
- Fatigue followed by long-term creep
- Impact of pre-aging
- Creep-fatigue interaction life analysis
- Orientations: <001>, <111>, <011>
- Application to TMF with long dwells









The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

In a creep-fatigue interaction test, life can be controlled by:

- Plastic strain range
- Environmental effects
- Influence of mean stress / stress range
- Creep damage (dwell)
- Microstructure / crystal orientation

Conventional Creep-Fatigue (baseline)



Conventional Creep-Fatigue (baseline)



Cycle Evolution

3

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

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



Crack Characteristics

The George W. Woodruff School of Mechanical Engineering

R = 0, T = 1100°C, $\Delta\epsilon = 0.8\%$ $N_f = 1420$



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

School of Materials Science and Engineering

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









Half-life at 1025 °C



Half-life at 1100 °C

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering





The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

- 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

Microstructure Evolution in Blades

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering





Distance from Root



Rafting and Coarsening of y'



The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering



[Epishin et al., 2008]

GeorgiaInstitute of Technology at 950° C/185MPa for different times

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering



[Matan, Cox, Rae, & Reed, 1999]

GeorgiaInstitute of Technology Stress-dependent Aging Study – CMSX-8

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

Objective: Obtain kinetic data to predict rafting and coarsening as a function of temperature,

stress, microstructure and time





CMSX-8 Rafted Microstructure



2-point Correlation Method

School of Materials Science and Engineering

The George W. Woodruff School of Mechanical Engineering

- 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.

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

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

$$= \frac{1}{S} |{}^{n}M_{\mathbf{k}}| |{}^{p}M_{\mathbf{k}}| e^{-i {}^{n}\theta_{\mathbf{k}}} e^{i {}^{p}\theta_{\mathbf{k}}}$$

[Niezgoda, Fullwood and Kalidindi,2008]



(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

The George W. Woodruff School of Mechanical Engineering





Kinetics of Rafting – CMSX-8 and CMSX-4

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering





	Α (μm/h)	Q (KJ/mol)	U _T (J/mol.Mpa.K ⁿ)	n
CMSX-8	2.0 x 10 ⁵	205.80	0.033	1.525
CMSX-4	9.31 x 10 ⁴	221.78	0.19	1.294

$$\dot{w}(T,\sigma) = A. exp\left[-\frac{Q - U(T).\sigma}{RT}\right]$$

 $U(T) = U_T (T - T_0)^n$ [Epishin et al., 2008]

Stress-free Aging – CMSX-8

The George W. Woodruff School of Mechanical Engineering





LSW model – Describe and Predict Coarsening Behavior

School of Materials Science and Engineering

The George W. Woodruff School of Mechanical Engineering

GeorgiaInstitute of Technology

 According to Lifshitz-Slyozov-Wagner (LSW) theory particle coarsening process involves growth of the larger particles at the expense of the smaller ones to dissolve, with the driving force of reduction in interfacial energy of the system.





Cube rate law indicates the volume diffusion

Aged Microstructure under Compressive Stress

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

Compression Creep Frame

Ceramic Compression Creep Extensometer



Composition Sensitive Effective Diffusivity

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

Flux of all n components in CMSX-8 system during a diffusion controlled process can be described by the **effective diffusion coefficient**, D_{eff}

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

$$Q_{eff} = \sum_{i=1}^{n} x_i Q_{Ni-i}$$
 [Ai et al., 2015]

Prediction of Aging

Effective diffusion coefficient term embedded in LSW model of isotropic coarsening,

$$r^{3} - r_{o}^{3} = K(t - t_{o})$$

$$K = \frac{64D_{eff}C_{\infty}\sigma\Omega^{2}}{9RT}$$
Coarsening
activation energy
$$D_{eff} = D_{0,eff} \left(-\frac{Q_{eff}}{RT}\right)$$

Temperature-Dependent Constitutive Models

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_{0} \Theta(T) \left\langle \frac{\tau_{o}^{\alpha}}{D^{\alpha}} \right\rangle^{n} \exp\left\{ B_{0} \left\langle \frac{\tau_{o}^{\alpha}}{D^{\alpha}} \right\rangle^{n+1} \right\} \operatorname{sgn}(\tau^{\alpha} - \chi^{\alpha})$$

$$\Theta(T) = \exp(-\frac{Q_{0}}{RT})$$

Composition dependent
diffusivity parameter

Inter-diffusion coefficient of Ni-m binary system can be determined by DICTRA software

Effective Activation Energy for CMSX-8

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering



$$Q_{eff} = \sum_{i=1}^{n} x_i \, Q_{Ni-i}$$

Effective Activation energy / Coarsening Activation energy

= 275.89 kJ/mol

The influence of perturbations in composition on aging and diffusioncontrolled processes is feasible with this methodology.



The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

- 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

Length Scales in Ni-base Superalloys

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering



Crystal Viscoplasticity – Kinematic Relations

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

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

Macroscopic plastic velocity gradient

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



Creep Deformation Mechanisms of Superalloys

The George W. Woodruff School of Mechanical Engineering

Influence of stress and temperature on modes of creep deformation



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

School of Materials Science and Engineering

Rafting – transport of matter constituting the γ 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 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)

Crystal Viscoplasticity (CVP) – Rate Eqn

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

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

r

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





Microstructure Sensitivity

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

CMSX-4 Model Predictions

Tertiary creep 950° C/400MPa Primary creep 750°C/770MPa



Deformation along [001] Volume fraction of © fixed at 0.7

[Ma, Dye, and Reed, 2008]



Orientation Sensitivity

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

CMSX-4 Model Predictions



Initial Calibration to CMSX-8 Creep Data

The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering







The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

- Directional coarsening is roughly a constant volume process
- Stress-free coarsening maintains proportionality between all precipitate/channel dimensions
- Microstructure uniqueness is defined by 2 independent dimensions

$$\begin{array}{l} \text{Rafting: } \dot{w}_{i}^{raft}(T, \boldsymbol{\sigma}) = -\left(\frac{3Aw_{i}}{2w_{o}}\right) \left(\frac{\sigma_{i}^{dev}}{\sigma_{VM} + \delta}\right) exp\left(-\frac{Q_{raft} - \sigma_{VM}U(T)}{RT}\right) \\ \text{[Tinga, Brekelmans, and Geers, 2009]} \end{array}$$



The George W. Woodruff School of Mechanical Engineering

School of Materials Science and Engineering

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:

$$\dot{\gamma}_{\gamma}^{in(\alpha)} = \Theta(T) \rho^{(\alpha)}{}_{\gamma} b \lambda_{\gamma}^{(\alpha)} F_{attack} sign(\tau^{(\alpha)} + \tau^{(\alpha)}{}_{mis} - \chi^{(\alpha)}) \exp\left\{ \frac{-Q_{slip}^{110} + \left(\left|\tau^{(\alpha)} + \tau^{(\alpha)}{}_{mis} - \chi^{(\alpha)}\right| - \tau^{(\alpha)}{}_{\gamma pass} - \tau^{(\alpha)}{}_{oro}\right) V_{c1}^{(\alpha)}}{kT} \right\}$$

$$\dot{\gamma}_{L1_{2}}^{in(\alpha)} = \rho_{L1_{2}}^{(\alpha)} b \lambda_{L1_{2}}^{(\alpha)} F_{attack} sign(\tau^{(\alpha)} - \chi^{(\alpha)}) \exp\left\{ \frac{-Q_{slip}^{112} + \left(\left|\tau^{(\alpha)} - \chi^{(\alpha)}\right| - \tau^{(\alpha)}{}_{L1_{2} pass} - \tau_{APB}\right) V_{c2}^{(\alpha)}}{kT} \right\}$$

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]