Physics-based Creep Simulations of Thick Section Welds in High Temperature and Pressure Applications

Thomas M. Lillo, PI

Wen Jiang, Co-Investigator

Idaho National Laboratory

P.O. Box 1625

Idaho Falls, ID 83415

Thomas.Lillo@INL.gov

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5 mm

Project Goals and Objectives

Goal: Develop modeling and simulation capabilities to describe/predict the creep behavior of thick section welds in Alloy 740H

- Computational modeling development of physical processes involved in the creep of welds in Alloy 740H across length scales:
  - Diffusion
  - Dislocation motion and deformation
  - Microstructural evolution
  - Uniaxial creep specimen behavior

- Develop/modify individual computational "modules" to describe each physical process:
  - Dislocation glide/climb
  - Dislocation/γ' interaction
    - γ' shearing
    - Dislocation climb over γ' particles
    - Dislocation looping of γ'
  - Incorporate experimental microstructures and their evolution
  - Diffusional creep
  - Grain boundary sliding

# *Project Goals and Objectives – cont.*

- Experimental Validation
  - Creep tests – different stresses and temperatures
  - γ' aging
    - Weld
    - HAZ
    - Base metal (if necessary)
  - Threshold stress as a function of γ' evolution – dislocation/γ' interaction as a function of γ' radius
  - Microstructural characterization for the generation of synthetic microstructures
    - Weld
    - HAZ
    - Base metal

Presentation Outline

- Modeling and simulation approach
  - Overview of the MOOSE architecture
  - Power law creep – incorporation of dislocation climb
  - Dislocation interaction with γ' particles
    - Particle shearing
    - Dislocation climb bypass
    - Orowan looping

- Experimental Studies supporting modeling
  - Creep tests of weld
  - Microstructural characterization using EBSD
  - γ' Aging
  - Threshold stress determination

Modeling and Simulation Approach – MOOSE Architecture
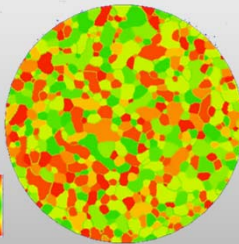
MOOSE
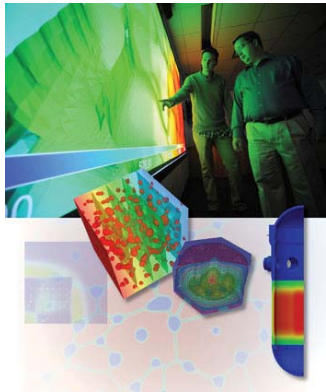
Framework → All of the code that forms the basis of the MOOSE framework
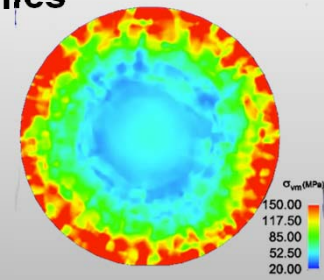
Modules →

Phase Field
- Cahn-Hilliard equation
- Allen-Cahn equations
- Free energy based development

Tensor Mechanics
- Linear elasticity
- Eigenstrains
- J2 Plasticity
- Crystal plasticity

R&D 100 2014 Winner

- MOOSE is a finite element, multiphysics framework that simplifies the development of advanced numerical applications.

- It provides a high-level interface to sophisticated nonlinear solvers and massively parallel computational capability.

- Open Source, available at http://mooseframework.org

Physical based Multi-scale Material Model Development

- Atomistic simulations identify critical mechanisms and determine parameters required for mesoscale model development.

- Mesoscale modeling and simulation is used to inform the development of analytical theory for engineering scale.
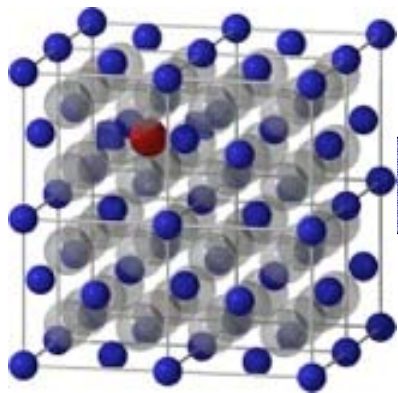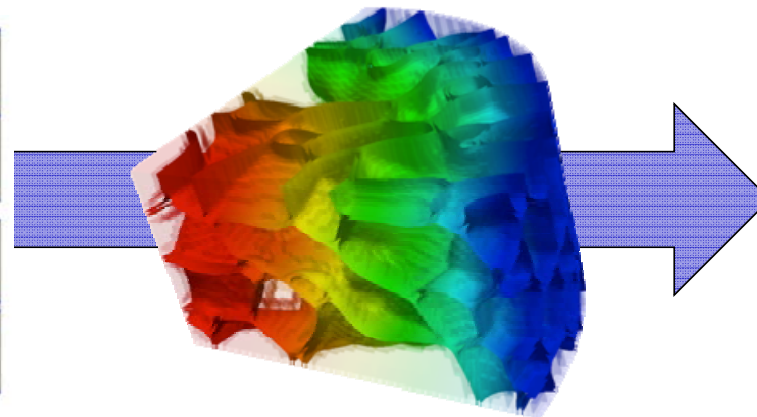

nanometers
First Principles
- Identify critical bulk mechanisms
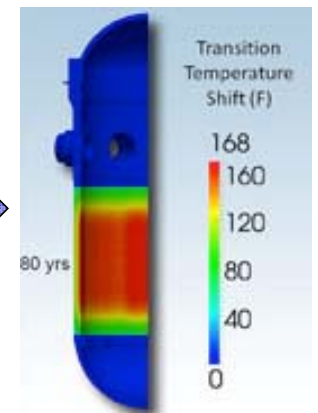- Determine bulk properties
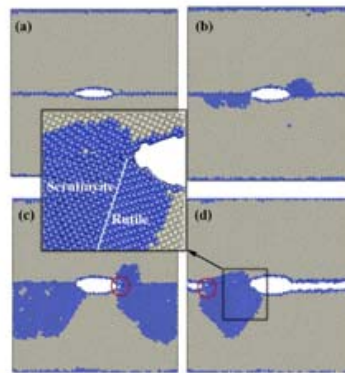
100's of nanometers
Molecular Dynamics
- Identify interfacial mechanisms
- Determine interfacial properties

microns
Mesoscale
- Predict microstructure evolution
- Determine impact on properties

millimeters and up
Engineering scale
- Use analytical theory
- Predict material performance

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Modeling Approach

- Polycrystalline length scale – region consisting of base metal, HAZ and fusion region
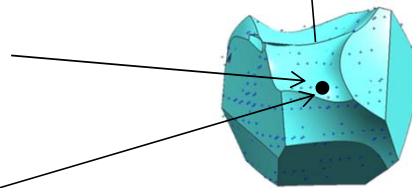
- FIB, EBSD, SEM – Grain size, orientation, misorientation distribution
- Reconstructed or synthetic microstructure satisfying the statistics
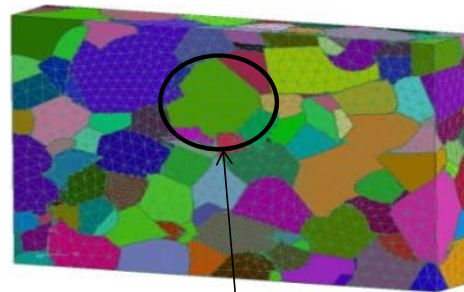
Representative Volume of polycrystalline microstructure
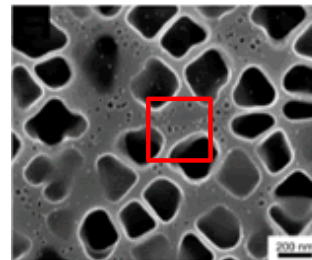
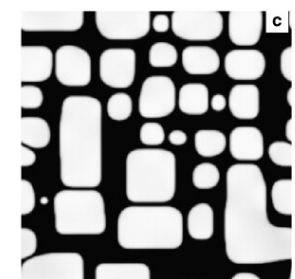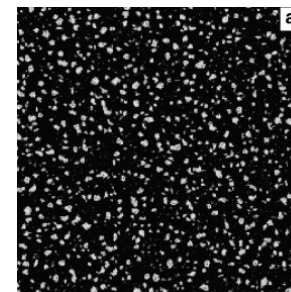**Diffusional creep:**
Vacancy generation/annihilation model

Dislocation creep:
Dislocation density based model considering APB shearing, Orowan loop and climb

Effect of γ' shape, size, volume fraction on APB shear - Homogenized model from micromechanics simulation

Evolution of γ' precipitate

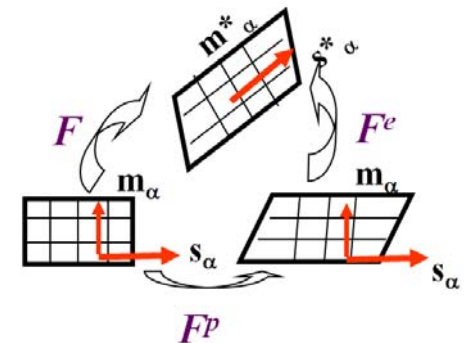# Crystal plasticity Model (dislocation density based)

- Crystal plasticity mechanistically represents plastic deformation by representing dislocation slip along slip planes
- Slip contributions are summed across all slip planes
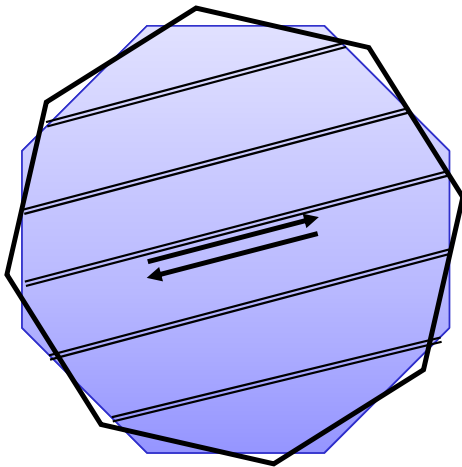
Dislocation motion defined by a flow rule

$$\dot{\gamma}^s = \tilde{\dot{\gamma}}^s \left(\tau^s, \tau_0^s \right)$$

$\boldsymbol{F} = \boldsymbol{F}^V \boldsymbol{F}^e \boldsymbol{F}^p$ Volumetric can account for residual strains

Plastic velocity gradient in the intermediate configuration

$$\dot{\boldsymbol{F}}^p \boldsymbol{F}^{p-1} = \sum_{\alpha} \dot{\gamma}_{glide}^{\alpha} \boldsymbol{S}_0^{\alpha} + \sum_{\alpha} \dot{\gamma}_{c\lim b}^{\alpha} \boldsymbol{N}_0^{\alpha}$$

$$\boldsymbol{S}_0^{\alpha} = \boldsymbol{s}^{\alpha} \otimes \boldsymbol{m}^{\alpha} \qquad \boldsymbol{N}_0^{\alpha} = \boldsymbol{s}^{\alpha} \otimes \boldsymbol{s}^{\alpha}$$

Dislocation generation and pile-up accounted for by increasing slip resistance with a hardening law

s^a - Slip direction m^a - normal in reference configuration

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Glide model

Numerical example

- 75 x 75 x 75 μm unit cube
- 27 grains randomly oriented
- 3375 elements
- Uniaxial tension with symmetric boundary condition
- Non-calibrated parameters

Glide rate in matrix $\quad \dot{\gamma}^{\alpha}_{glide} = \rho^{\alpha}_{M} b v^{\alpha}_{glide}$

(ρ_M – Potentially mobile dislocation density)

Glide velocity:

$$v^{\alpha}_{glide} = \begin{cases} l\nu\exp\left(-\frac{\Delta F_{glide}}{KT}\left(1-\left(\frac{\left|\tau^{\alpha}\right|-g^{\alpha}_{athermal}}{g^{\alpha}_{thermal}}\right)^{p}\right)^{q}\right)\mathrm{sgn}\left(\tau^{\alpha}\right); \text{ for } \left|\tau^{\alpha}\right| > g^{\alpha}_{athermal} \\ 0 \end{cases}$$

Resolved shear stress $\quad \tau^{\alpha} = \boldsymbol{T}^{*} : S^{\alpha}_{0}$

Athermal resistance: $\quad g^{\alpha}_{athermal} = \sqrt{\left(\tau^{\alpha}_{disloc-disloc}\right)^{2}}$
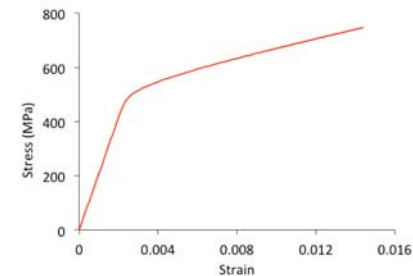
$$\tau^{\alpha}_{disloc-disloc} = q_{\rho}Gb\sqrt{\sum A^{\alpha\xi}\rho^{\xi}}$$
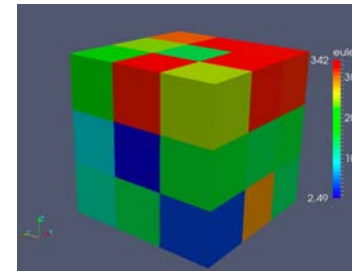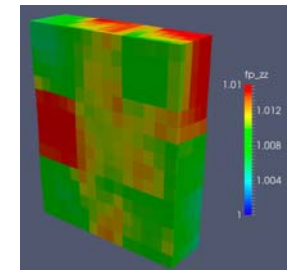

Euler Angle (θ)
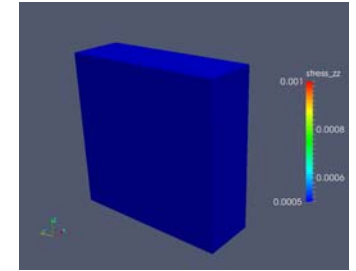
Stress Evolution

Stress strain

Anisotropic plastic deformation

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Climb model

Edge component of dislocation will climb

Climb stress $\quad \tau^\alpha = \boldsymbol{T}^* : \boldsymbol{N}_0^\alpha = \dfrac{RT}{V_m}\ln\left(\dfrac{c^{*\alpha}}{c}\right)$

c^* - vacancy concentration at dislocation core
c - vacancy concentration in surrounding matrix

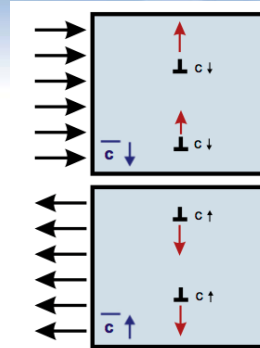Equilibrium concentration at dislocation core $\quad c^{*\alpha} = c_0 \exp\left(\dfrac{k\tau^\alpha V_m}{RT}\right)$

k : *factor that depends on precipitate size, shape, etc*

Climb velocity $\quad v_c^\alpha = -\dfrac{2\pi D}{b\log(r_\rho/r_c)}\left(c^{*\alpha} - c_0\right)$

Effect of dislocation density on effective radius $\quad r_\rho = \dfrac{1}{2\sqrt{\sum\left(\rho_M^\alpha + \rho_I^\alpha\right)}}$

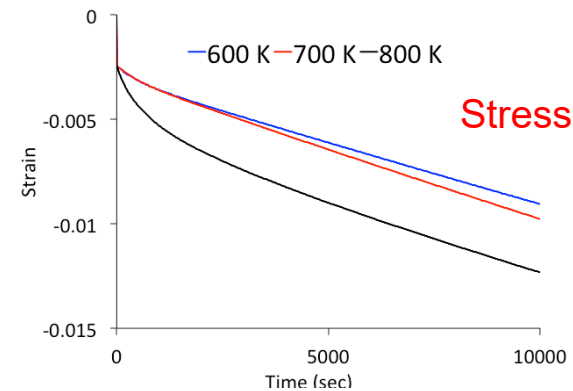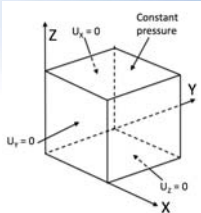Core radius $r_c = 4b$ $\quad r_\rho$ = radius where $c^* \sim c$

Climb rate: $\quad \dot{\gamma}_c^\alpha = (\rho_M^\alpha + \rho_I^\alpha)bv_c^\alpha$
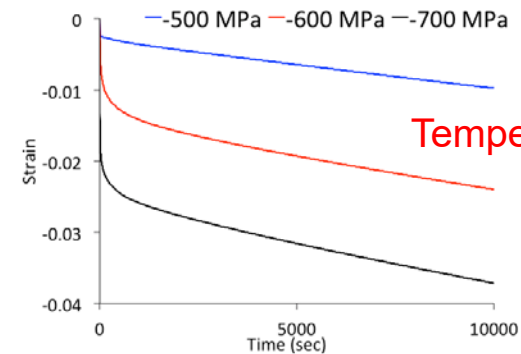
Geers, et. al. 2014

Numerical example

- 1 x 1 x 1 μm unit cube
- Single crystal with one element
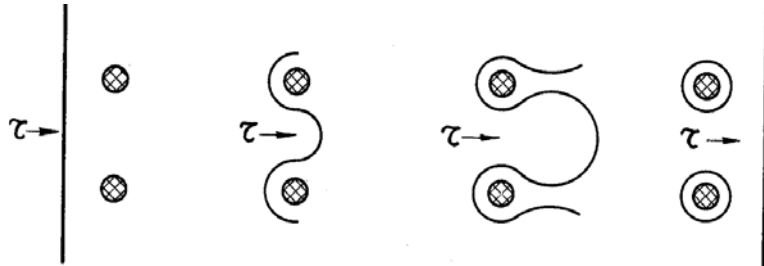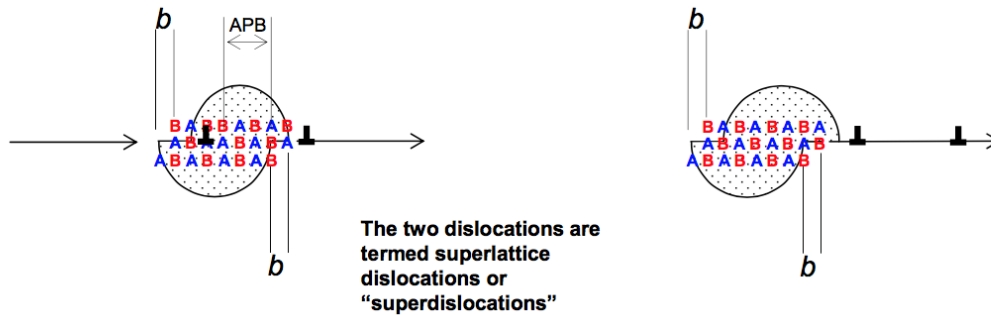- Creep compression with symmetric boundary condition

Constant pressure

Stress = -500 MPa

—600 K —700 K —800 K

Temperature = 700 K

—-500 MPa —-600 MPa —-700 MPa

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APB (Shearable) and Looping (Nonshearable)

The two dislocations are termed superlattice dislocations or "superdislocations"

- APB formation modifies the atomic structure of the ordered γ'
- Orowan looping occurs when looping is easier than cutting.

Slip resistance:

$$\tau_{disloc-ppt} = \frac{1}{2b^2 r}\sqrt{\frac{3f\overline{F}}{\pi G \beta}}$$

Shearable: $r < r_c$

$$\overline{F} = 2\beta Gb^2\left(\frac{r}{r_c}\right)$$

Non-shearable: $r > r_c$

$$\overline{F} = 2\beta Gb^2$$

r_c : critical radius of precipitate

Athermal resistance:

$$g^{\alpha}_{athermal} = \sqrt{\left(\tau^{\alpha}_{disloc-disloc}\right)^2 + \left(\tau^{\alpha}_{disloc-ppt}\right)^2}$$

Dislocation density evolution

Dislocation density evolution

$$\dot{\rho}^{\alpha} = \dot{\rho}^{\alpha}_{M} + \dot{\rho}^{\alpha}_{I}$$
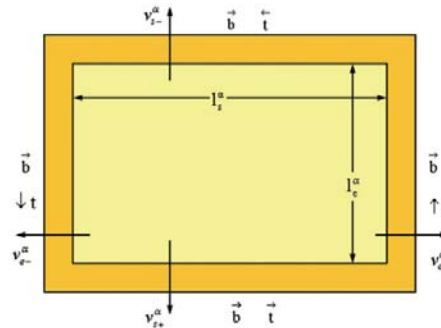
Evolution of mobile dislocation density

$$\dot{\rho}^{\alpha}_{M} = \frac{k_{mul}}{b}\sqrt{\sum_{\beta}\rho^{\beta}_{M}}\left|\dot{\gamma}^{\alpha}_{glide}\right| - \frac{2R_{c}}{b}\rho^{\alpha}_{M}\left|\dot{\gamma}^{\alpha}_{glide}\right| - \frac{1}{b\lambda^{\alpha}}\left|\dot{\gamma}^{\alpha}_{glide}\right| + C_{1}\left|\dot{\gamma}^{\alpha}_{c\lim b}\right| + C_{2}\left|\dot{\gamma}^{\alpha}_{ppt}\right|$$

Dislocation multiplication from Frank-Read source and loop expansion	Annihilation of dislocations of opposite signs	Dislocation trapping	Mobilization of Dislocations

Evolution of immobile dislocation density

$$\dot{\rho}^{\alpha}_{I} = \frac{1}{b\lambda^{\alpha}}\left|\dot{\gamma}^{\alpha}_{glide}\right| - C_{3}\left|\dot{\gamma}^{\alpha}_{c\lim b}\right| - C_{4}\left|\dot{\gamma}^{\alpha}_{ppt}\right|$$

Dislocation trapping	Mobilization of Dislocations

Mean trapping distance $\quad \frac{1}{\lambda^{\alpha}} = \beta_{\rho}\sqrt{\rho^{\alpha}} + \beta_{ppt}\sqrt{Nd}$

Modular model development
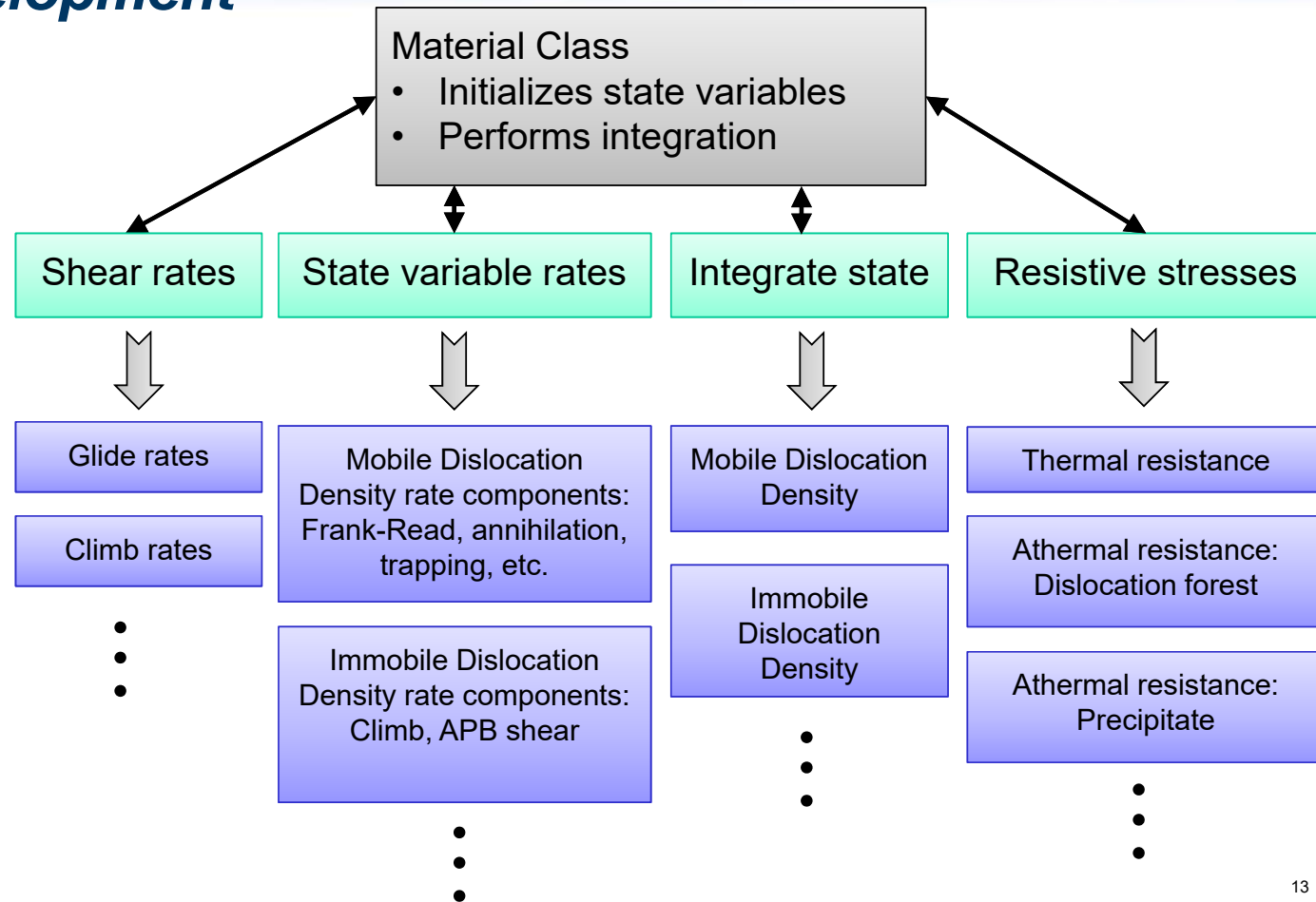
Integration at every material point

- Newton-Raphson for stress

$$T_{n+1}^{i+1} - \tilde{T}_{n+1}^{i+1}\left(F_{n+1}^{p,i+1}, y_{n+1}^{j}\right) = 0$$

- Fixed-point iteration for state

$$y_{n+1}^{j+1} = f\left(T_{n+1}^{i+1}, F_{n+1}^{p,i+1}, y_{n+1}^{j}\right)$$

till $\quad \left| y_{n+1}^{j+1} - y_{n+1}^{j} \right| < \eta$

Material Class
- Initializes state variables
- Performs integration

Shear rates

State variable rates

Integrate state

Resistive stresses

Glide rates

Climb rates

Mobile Dislocation Density rate components: Frank-Read, annihilation, trapping, etc.

Immobile Dislocation Density rate components: Climb, APB shear

Mobile Dislocation Density

Immobile Dislocation Density

Thermal resistance

Athermal resistance: Dislocation forest

Athermal resistance: Precipitate

Initial calibration of Alloy 617

C11	C12	C44	G
170.64Gpa	108.39Gpa	77.82Gpa	77.82Gpa

p	q	Activation Entropy(J)	Thermal Resistance
0.78	1.15	5.148×10^{-19}	0.5

Barrier factor	Self harden Factor	Latent harden factor	Multiplication factor
0.045	0.052	0.052	0.01

Euler Angle (θ)

26MP, 900C
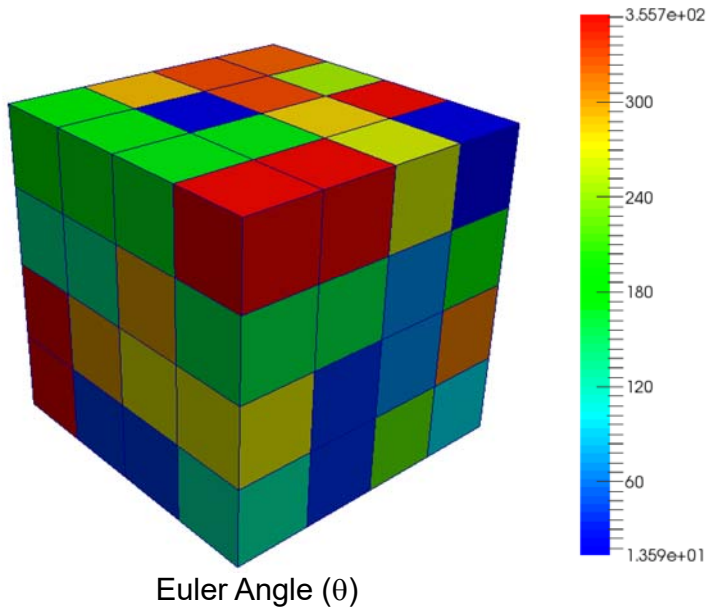
16MP, 1000C
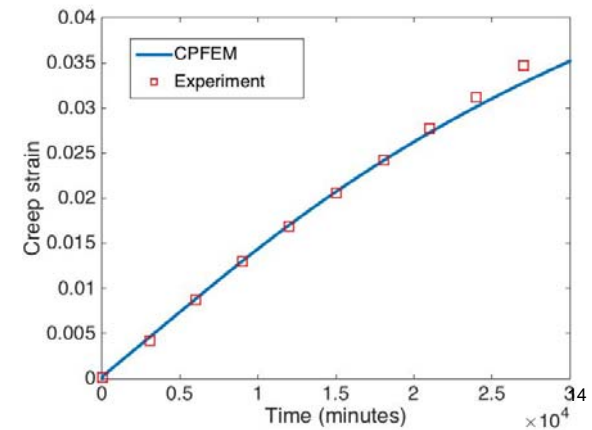

- 500 x 500 x 500 μm unit cube
- 64 grains randomly oriented
- Uniaxial tension with symmetric boundary condition
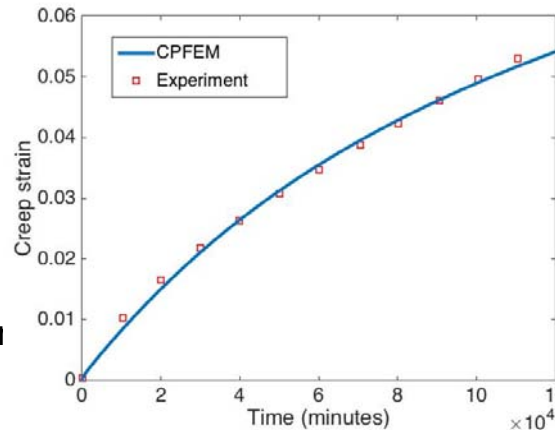
# *Experimental Studies – Creep Testing*

- Creep tests will be carried out at or below the aging temperature
  - Short/intermediate term creep tests – support modeling and validation of modules
    - All-weld metal gage section
      - Longitudinal
      - Transverse – compression creep sample
    - Transverse gage section
    - Creep stresses to yield test duration between 200-2000 hrs (Larson-Miller plot, Special Metals datasheet for Alloy 740H implies 140 - 400 MPa for welds)
  - Long term creep test – validate simulation
    - 141 MPa, 750°C, ~9700 hrs (expected)
    - 83 MPa, 800°C, ~9700 hrs (expected)
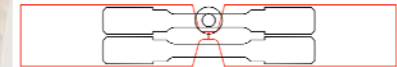
| Specimen ID	Test temperature, °C	Test type	Initial Stress, MPa	Orientation	Expected rupture life, hrs	Start date	Finish date	Rupture life, Hrs
740-Q1-01	700	Rupt	413	CW*	200	8/24/2016	9/21/2016	639
740-Q1-08	700	Rupt	413	CW	500	11/28/2016	12/27/2016	670.8
740-Q1-06	700	Rupt	395	CW	1000	01/09/2017		
	700	Rupt	344	CW	1000			
740-Q1-03	750	Rupt	350	CW	200	9/29/2016	10/07/2016	184
740-Q1-05	750	Rupt	305	CW	500	10/18/2016	11/06/2016	450
	750	Rupt	213	CW	1000			
740-Q1-04	800	Rupt	240	CW	200	10/10/2016	10/15/2016	123.6
740-Q1-02	800	Rupt	200	CW	500	11/08/2016	11/22/2016	326.8
	800	Rupt	138	CW	1000			
	700	Rupt	400	AWM**	500			
	750	Rupt	248	AWM	500			
	800	Rupt	144	AWM	500			

* CW = Cross weld
** AWM = All Weld Metal
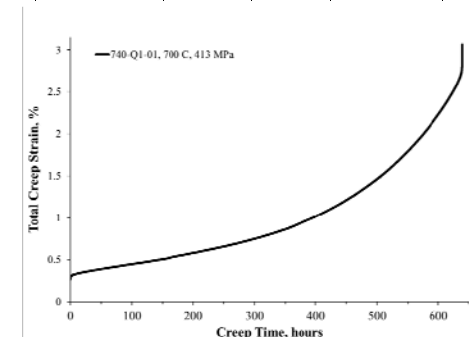
# *Microstructural Characterization*

- Optical metallography and EBSD on three orthogonal surfaces

- Includes base metal, HAZ and weld metal

- Grain Morphology

- Orientation and misorientation statistics

- Supports generation of synthetic microstructures

- Solidification segregation in the weld metal

- γ' size & volume fraction -TEM
  - Base metal
  - HAZ
  - Weld metal


Longitudinal y-plane

Longitudinal z-plane
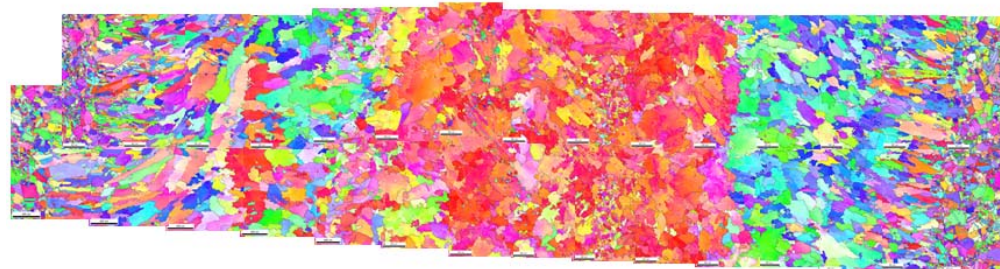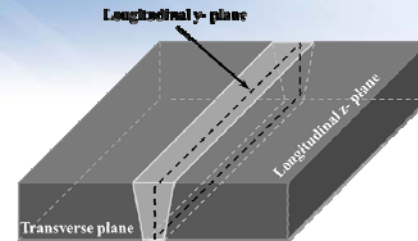
Transverse plane

Longitudinal y-Plane
(top down view)

5 mm

Longitudinal z-Plane
(side view)

5 mm

Transverse Plane

5 mm
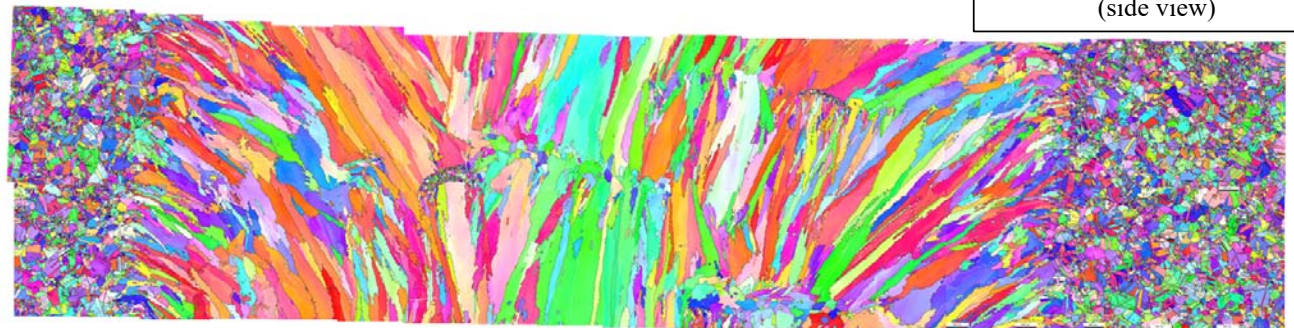
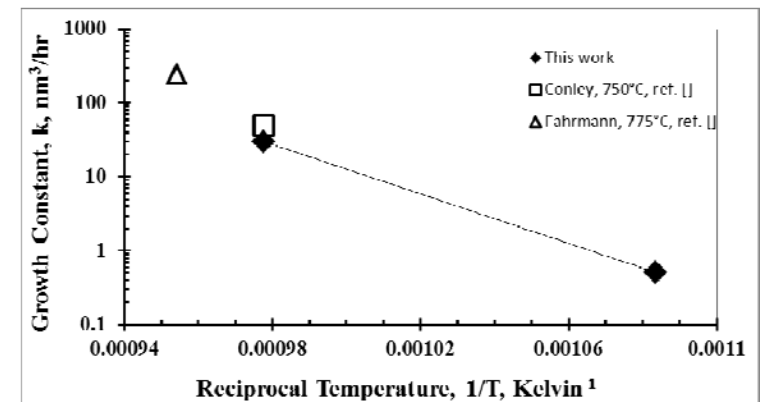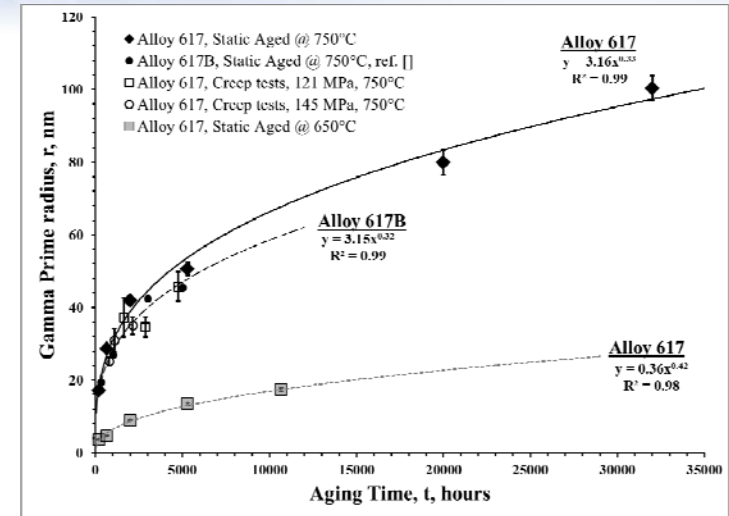# γ' *Aging*

- γ' growth and compositional homogenization

- Base metal and weld metal (compositional effects?)

- Determine growth constant for γ' for modeling effort:

$$r^3 - r_o^3 = kt$$

- Temperatures: 700, 750, 800°C

- Times: 50, 100, 200, 400, 1000, 3000, 6000 and 10,000 hrs
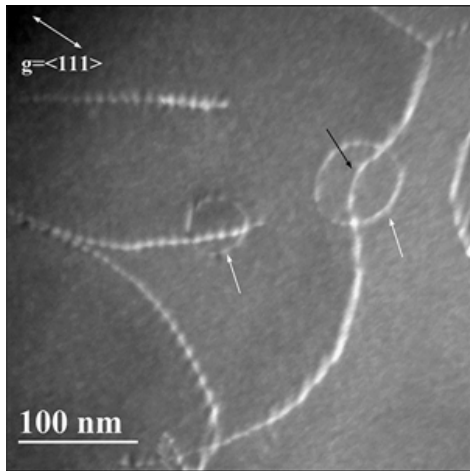
- TEM with image analysis
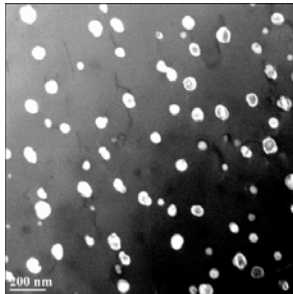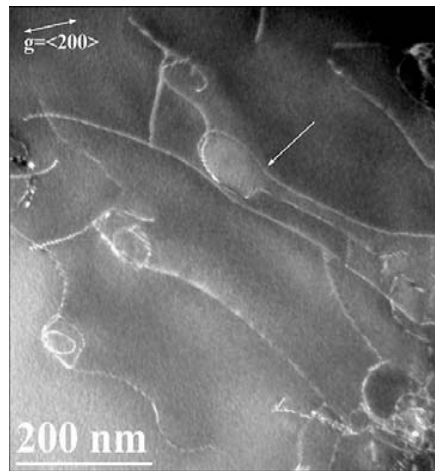

Alloy 617, 750°C,
145 MPa, e=5%,
~1083 hrs

Threshold Stress Determination

- Threshold stress is determined by primary dislocation bypass mechanism of the γ' particles
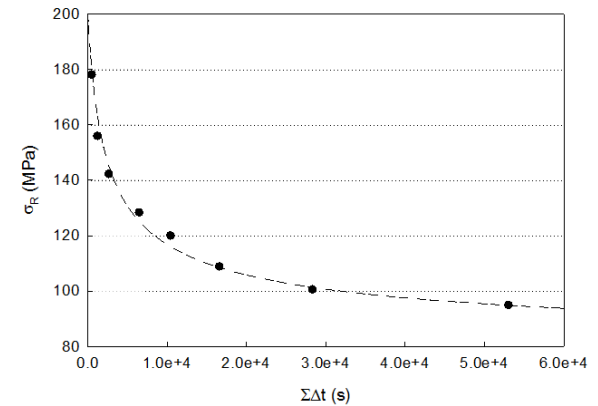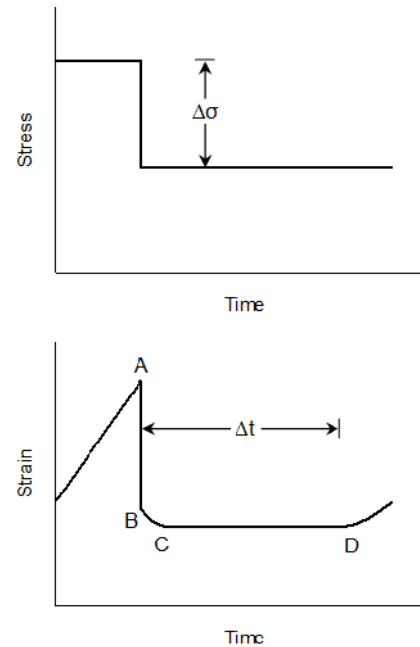- Threshold stress determined by stress drop creep tests

γ' particle bypass by dislocation climb

γ' particle bypass by dislocation looping

Bypass mechanisms in Alloy 617

$$\Sigma\Delta t = \frac{\mu^2 b^2}{K}\left[(\sigma_R - \sigma_0)^{-2} - (\sigma_\ell - \sigma_0)^{-2}\right]$$

Questions

Contact Information

- Thomas Lillo:
    - Thomas.Lillo@inl.gov
    - (208)526-9746

- Wen Jiang:
    - Wen.Jiang@inl.gov
    - (208)526-1586