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

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2020 HIGH PERFORMANCE MATERIALS PROJECT REVIEW MEETING

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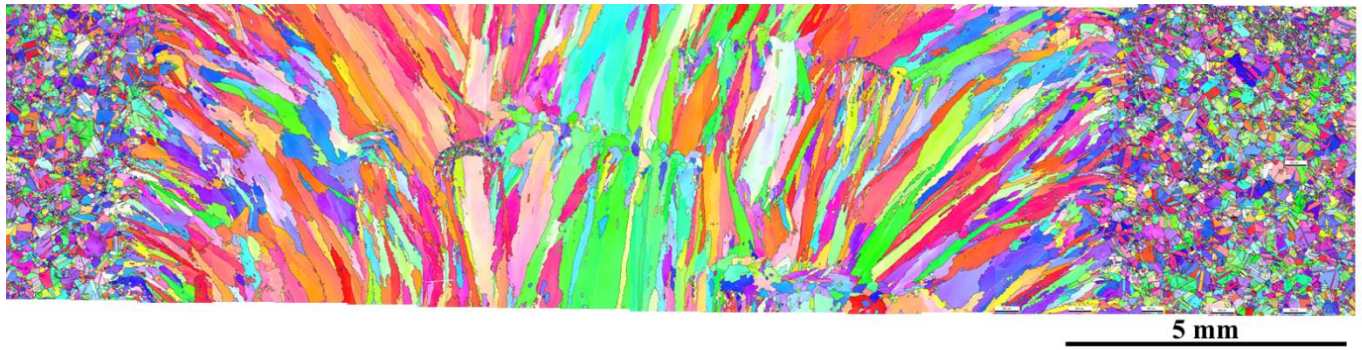

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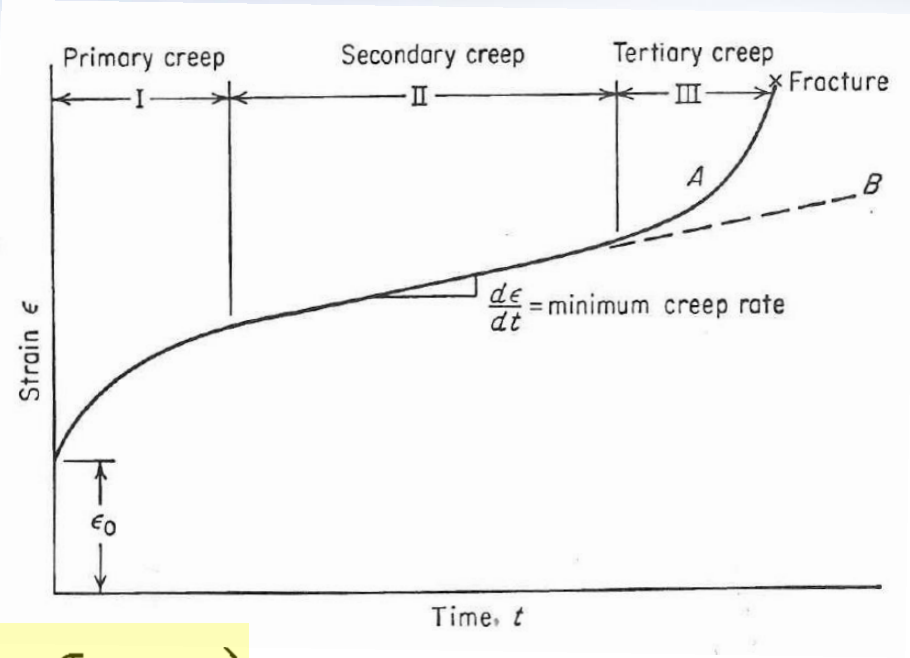
Background/Project Justification

Creep strain is described by:

$$\varepsilon^{creep} = \varepsilon^{disloc} + \varepsilon^{diffusion}$$



Creep rate due to dislocation motion:

$$\dot{\varepsilon}^{disloc} = \begin{cases} \rho A\, f(1-f)\left(\sqrt{\frac{\pi}{4f}} - 1\right) \sinh\left(C\frac{\sigma_{eff}-\sigma_B-\sigma_o}{MkT} b^2 \lambda\right) & \text{, if } \sigma_{eff} - \sigma_B - \sigma_o > 0 \\ 0 & \text{othewise} \end{cases}$$

Description of dislocation creep is empirical!

Project Goals

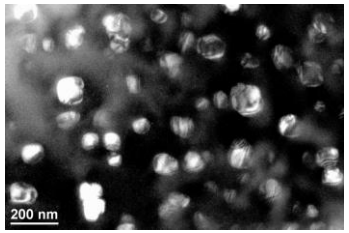
Project Goals

- Replace empirical description of dislocation creep with physics-based description/ mechanism
- Incorporate weld/base metal microstructure into the simulation
- Include multi-axial stress states
- Predict long-term creep behavior

Approach

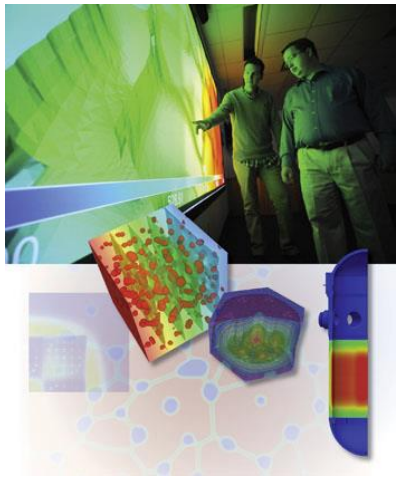
Simulations need to include

- Dislocation density-based crystal plasticity model w/ dislocation density evolution
- Orwan looping of γ' particles
- Diffusional creep mechanisms
  - Bulk diffusion
  - Grain boundary Diffusion
- Experimental microstructure of base metal and weld metal
  - EBSD characterization of grain characteristics and texture
  - Generation of synthetic microstructures with the same grain statistics using Dream3D
- Evolution of γ' distribution characteristics
  - Temperature-dependent volume fraction
  - Size evolution with time & temperature
- Use the Multi Object Oriented Simulation Environment (MOOSE)



Modeling and Simulation Approach – MOOSE Architecture

MOOSE



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

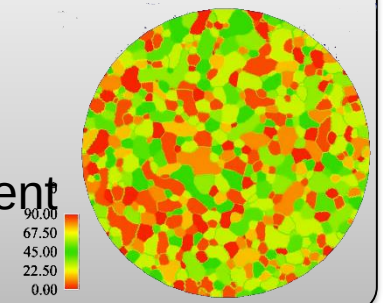
Framework

All of the code that forms the basis of the MOOSE framework

Modules

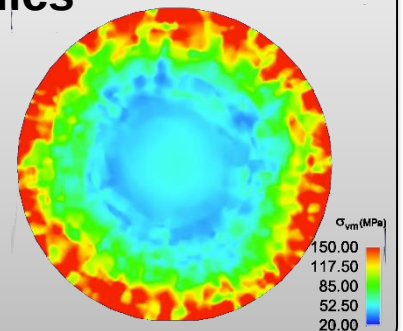
Phase Field

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

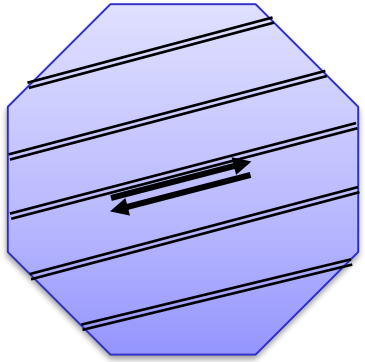


Tensor Mechanics

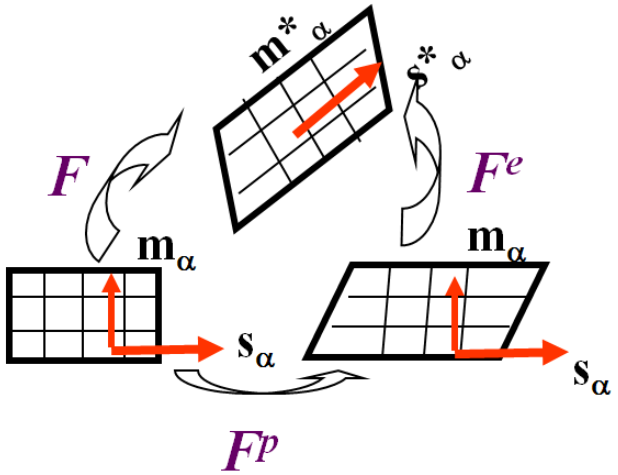
- Linear elasticity
- Eigenstrains
- J2 Plasticity
- Crystal plasticity



Dislocation density-based Crystal plasticity model



dislocation slip along slip planes



Elastic and plastic deformation gradient

$$\boldsymbol{F} = \boldsymbol{F^e F^p}$$

Plastic velocity gradient in the intermediate configuration

$$\dot{\boldsymbol{F}}^{\boldsymbol{p}} \boldsymbol{F}^{\boldsymbol{p-1}} = \sum_{\alpha=1}^{N_S} \dot{\gamma}^a_{glide} \boldsymbol{S}_{\boldsymbol{0}}^{\boldsymbol{\alpha}} + \sum_{\alpha=1}^{N_C} \dot{\gamma}^a_{climb} \boldsymbol{N}_{\boldsymbol{0}}^{\boldsymbol{\alpha}}$$

$\boldsymbol{S}_{\boldsymbol{0}}^{\boldsymbol{\alpha}} = \boldsymbol{m}_{\boldsymbol{0}}^{\boldsymbol{\alpha}} \otimes \boldsymbol{n}_{\boldsymbol{0}}^{\boldsymbol{\alpha}}$ Glide direction

$\boldsymbol{N}_{\boldsymbol{0}}^{\boldsymbol{\alpha}} = \boldsymbol{m}_{\boldsymbol{0}}^{\boldsymbol{\alpha}} \otimes \boldsymbol{m}_{\boldsymbol{0}}^{\boldsymbol{\alpha}}$ Climb direction

s - Slip direction *m* - normal in reference configuration

Glide rate :

$$\dot{\gamma}^a_{glide} = (1 - \phi_p) \rho^\alpha_M b v^\alpha_g$$

- ϕ_p : precipitate volume fraction. The glide is limited to the matrix channels
- ρ_M : mobile dislocation density

Climb rate :

$$\dot{\gamma}^a_{climb} = -\phi_p \rho^\alpha_M b v^\alpha_c$$

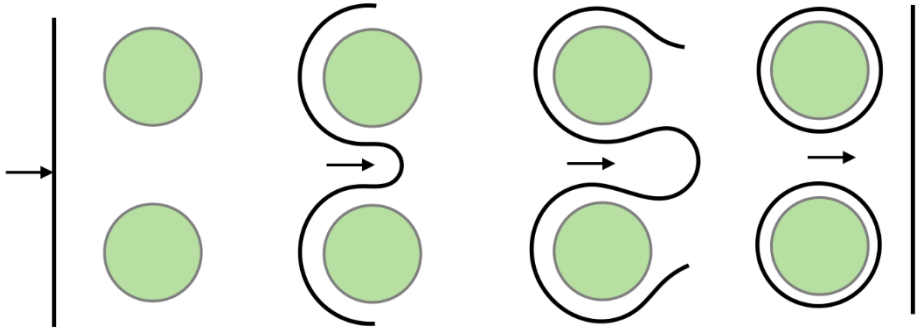
The mobile dislocation in contact with precipitates is: $\phi_p \rho^\alpha_M$

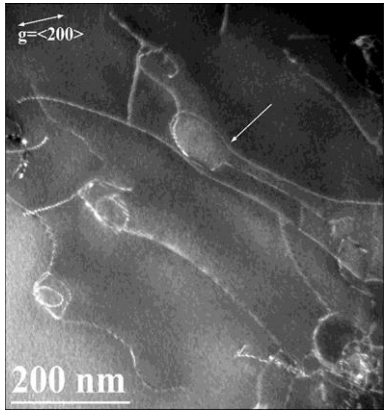
Climb velocity:

$$v^\alpha_c = -\frac{2\pi D}{b \log(r^\alpha_\infty / r_c)} \left(c^\alpha_{eq} - c_0\right)$$

Orowan Looping

Orowan looping Orowan looping occurs when the stress required for a dislocation to bow between precipitates is less than the stress required for the dislocation to penetrate precipitates





γ' particle bypass by dislocation looping (Alloy 617)

Stress above which looping will occur was determined by

$$\tau_{looping} = \frac{Gb}{L_s}$$

Spacing between precipitates $L_s = \sqrt{\frac{8}{3\pi\phi_p}} r_p - r_p$

The athermal resistance is increased by the Orowan looping :

$$s_a^{\alpha} = \sqrt{\tau_{disloc-disloc}^{\alpha\ 2} + \tau_{looping}^2}$$

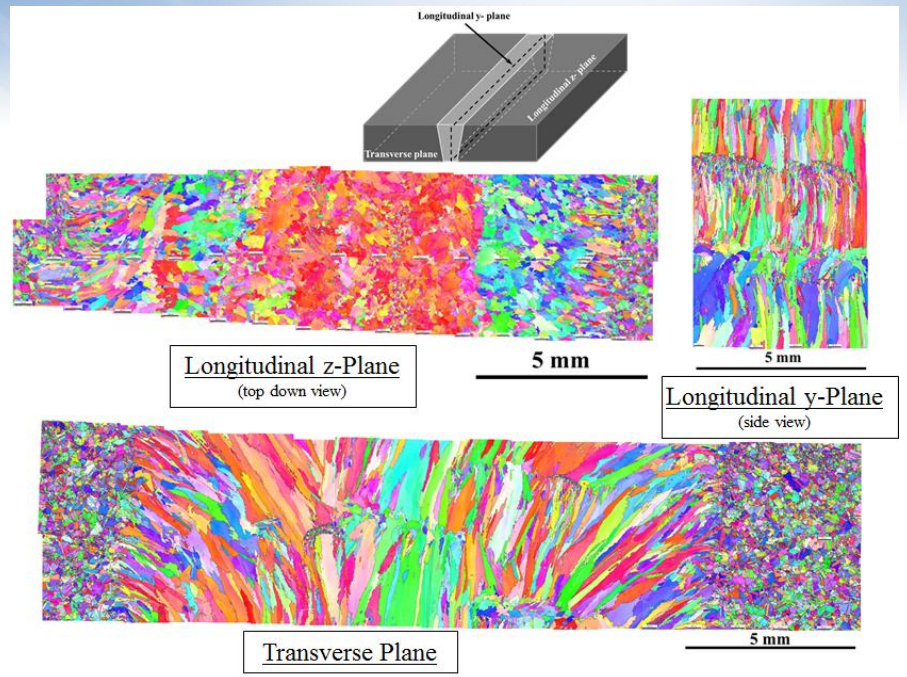
L_s = spacing between precipitates
f_p = volume fraction of precipitates
r_p = radius of precipitates

Synthetic Microstructures

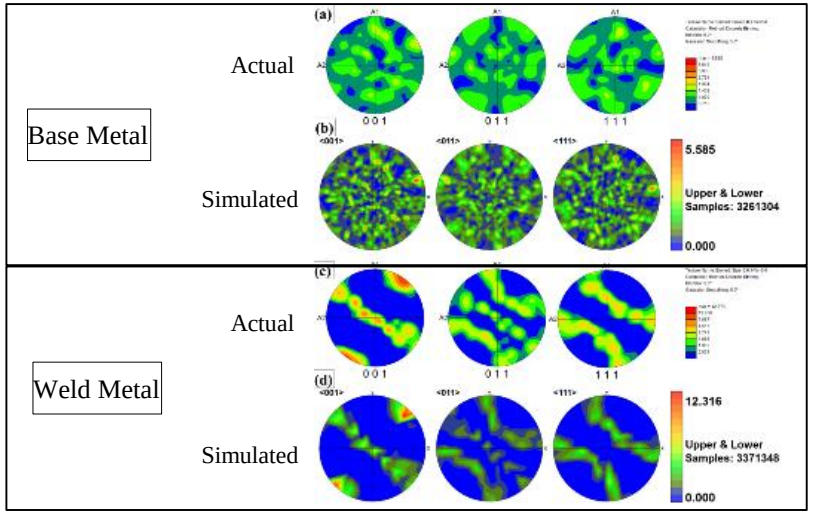
- 3D volume needed for simulations
- EBSD on three orthogonal surfaces
- Reconstructed in Dream 3D
  - Morphology
  - Orientation statistics

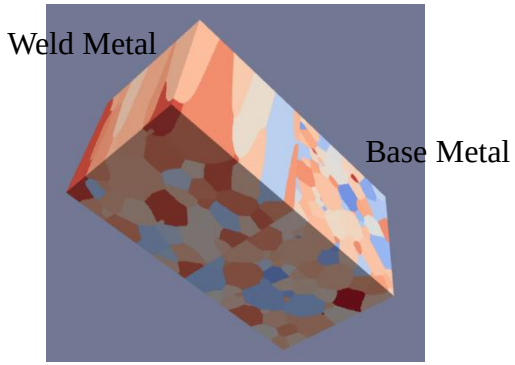
Issues

- Scale of weld requires multiple, large data files for base and weld metal
- Dream 3D cannot stitch the two microstructures together
  - Voxel approach
  - Serial EBSD



EBSD Data





Reconstructed

γ' Aging in the Weld

Concerns:

- γ' growth during creep
- Weld metal (compositional effects?)

Goal:

- Determine growth constant for γ' as a function of temperature, *k(T)*, for modeling effort:

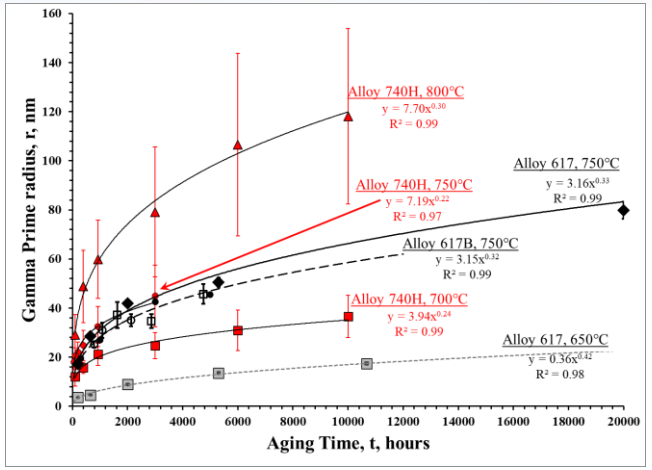
$$r^3 - r_o^3 = k(T)t$$

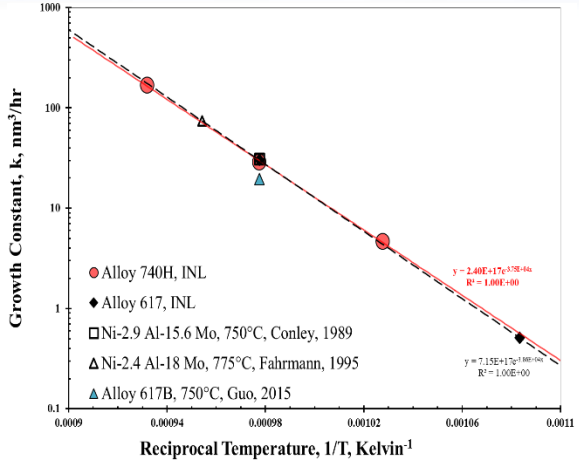
Experimental:

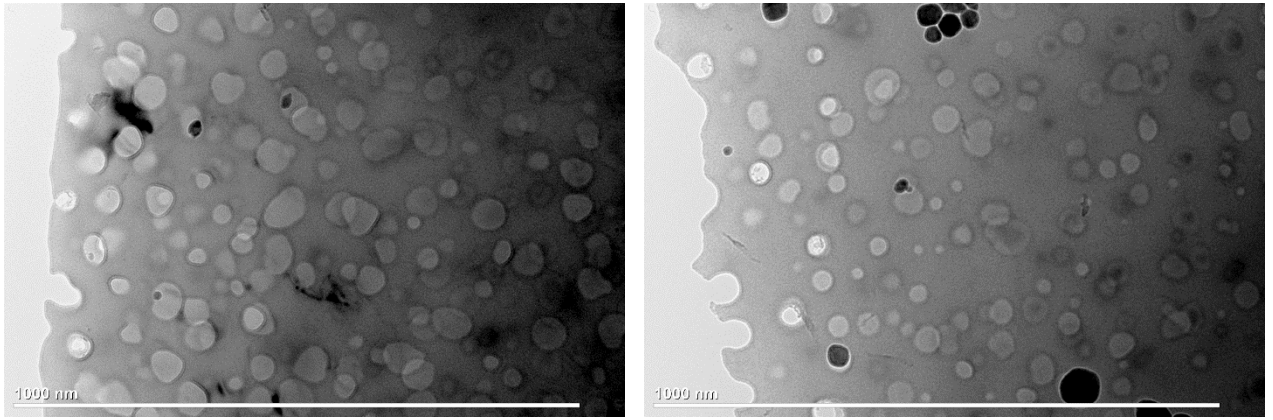
- Temperatures: 700, 750, 800°C
- Aging times up to 10,000 hrs
- TEM with image analysis

Results:

- γ' growth behavior at 750°C follows that of Alloy 617
- More statistical variation of γ' size in weld



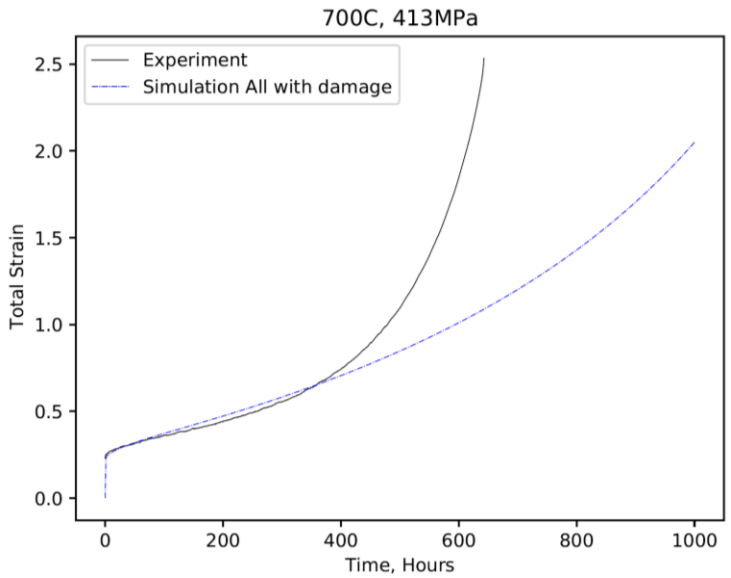


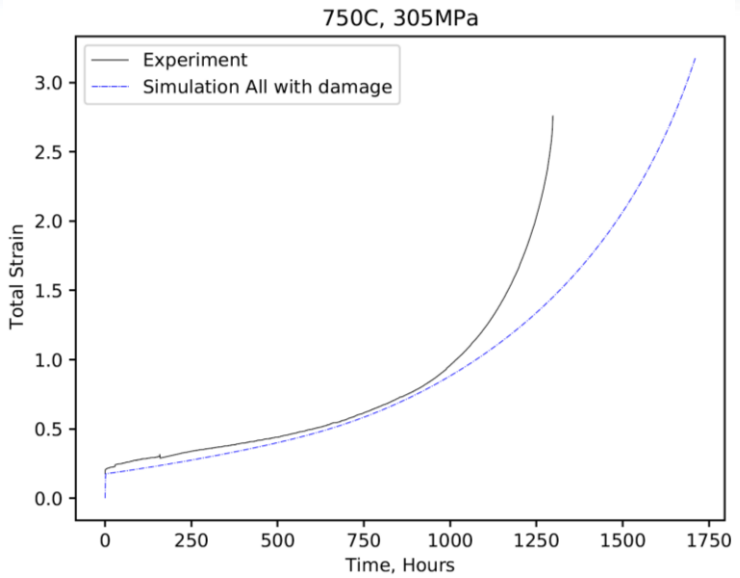


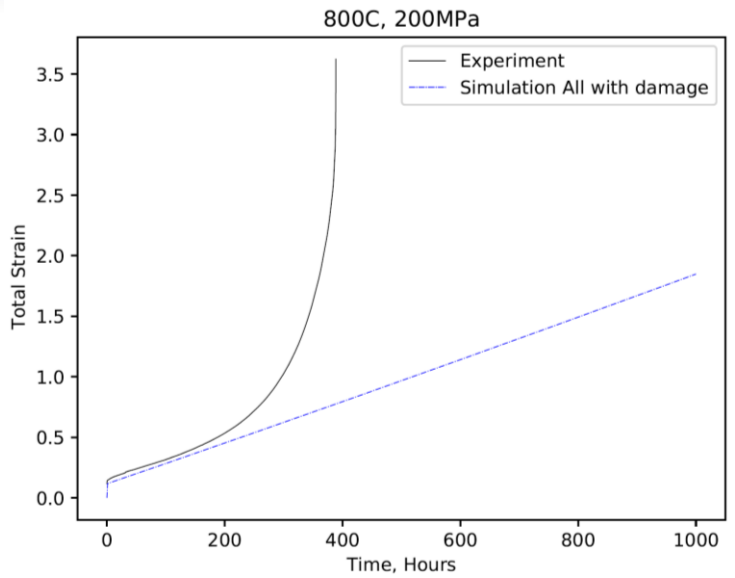
γ' fraction variation in weld (Aged - 750°C, 400 hrs)

Current Model Calibration Results

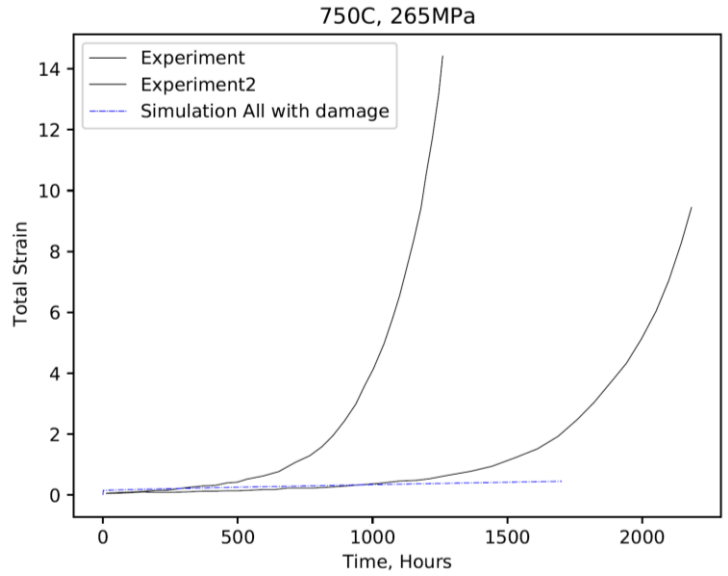
Weld Metal Only

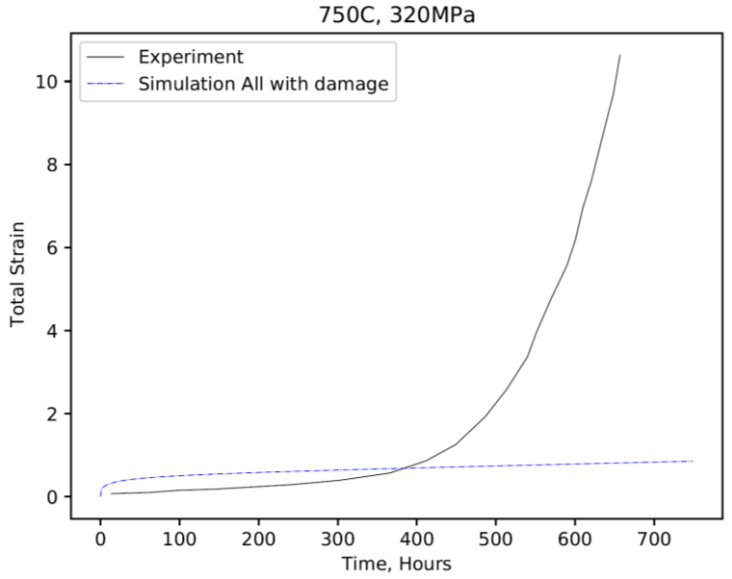


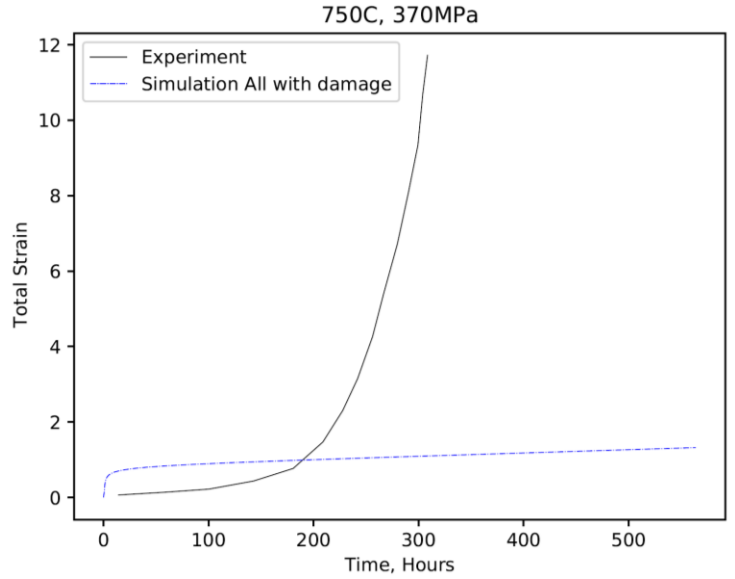




Base Metal Only

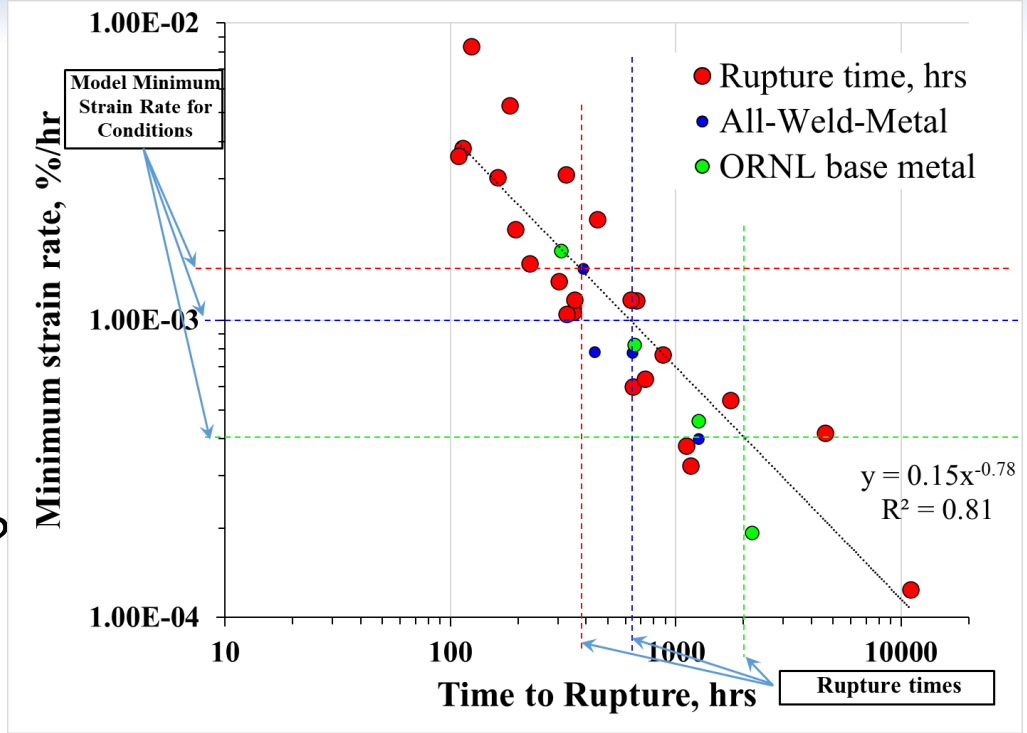






Tertiary Creep Transition Issue

- Primary and secondary creep are simulated quite well
- Transition to tertiary creep is inconsistent
- Physical processing occurring during transition are not known with confidence – can't develop the physics-based model for tertiary creep transition
- Model uses a damage model for transition to tertiary creep following Shen, 2015 – Wrong damage model?
- Use physics-based model to predict minimum creep rate and Grant-Monkman plot to predict rupture time

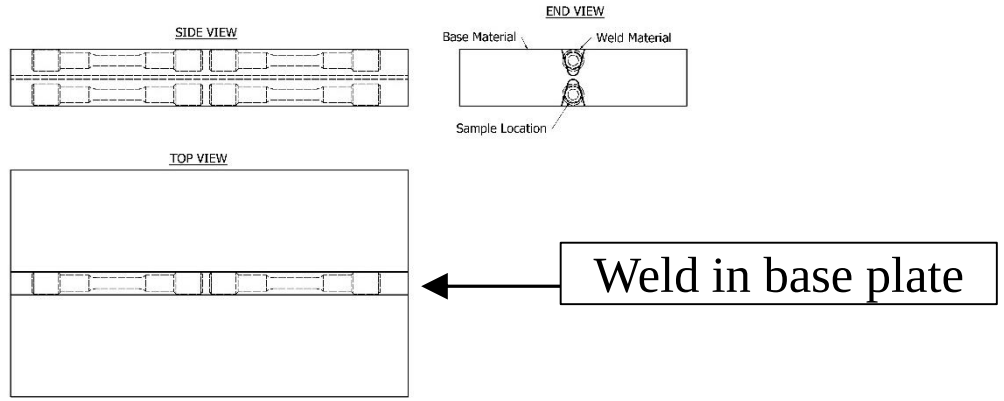


Temperature, °C	Stress, MPa	Actual Rupture Time, Hrs	Grant- Monkman Rupture Time, Hrs
700	413	643	610
750	305	1261	2000
800	200	400	390

Current status

- Experimental data collection and analysis is complete
- Currently determining model calibration parameters for base metal and for weld metal, separately

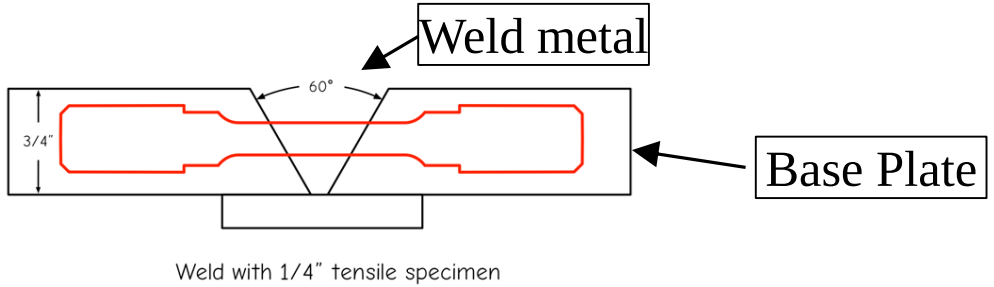
Weld-Metal-Only Specimens



Weld in base plate

- Will run simulations on uniaxial creep specimen – base metal + weld metal

Cross-weld creep Specimens



- Final report

Questions

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