

Models of Long-Term Creep Behavior of High Performance Structural Alloys

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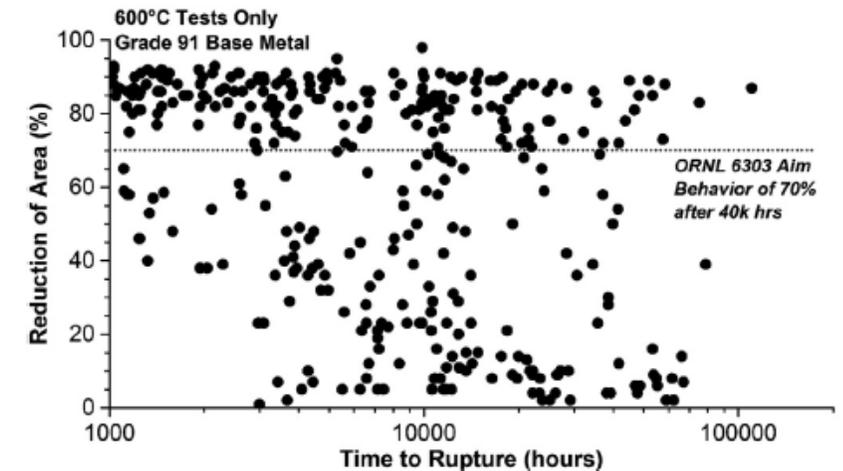
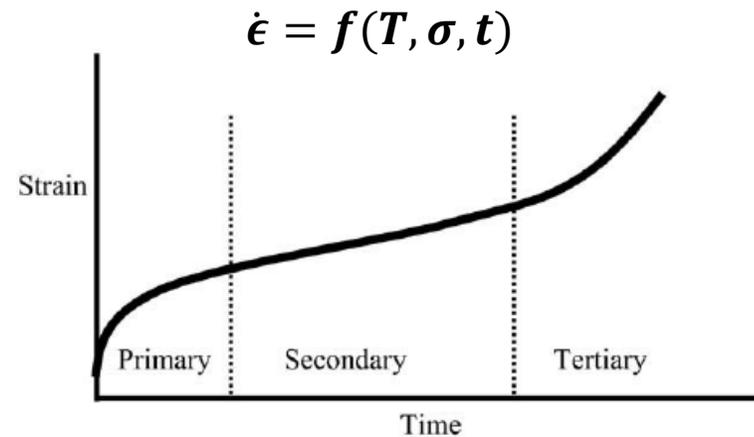
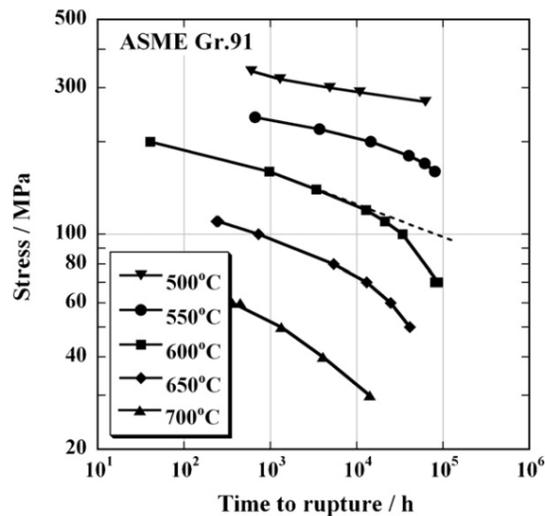
What do we want to model?

Creep Strength

- Answers **when** a material will fail
- Maximum allowable stress that will cause creep rupture in a given time
- Usually characterized as maximum allowable stress for a creep life of 100,000 hrs

Creep Ductility

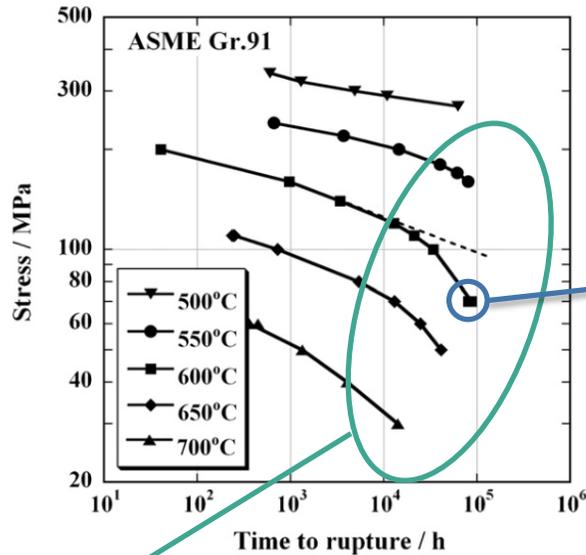
- Answers **how** a material will fail
- Characterized by reduction of area on fracture
- Low ductility failures can lead to catastrophic failures (Leak-before-break)



K. Sawada, et al., Mater. Sci. Eng. A (2011) 528

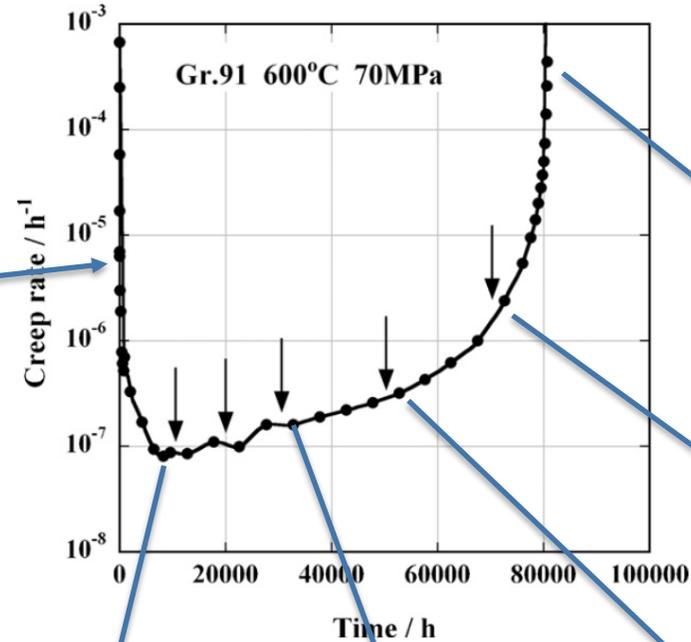
Siefert et al, 32 Intl. J. of Pressure Vessels and Piping 138 (2016) 31-44

CSEF steels and accelerated creep

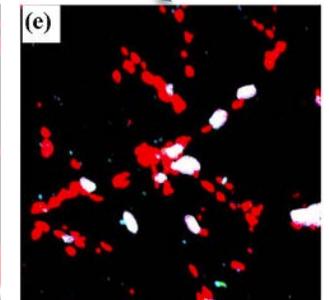
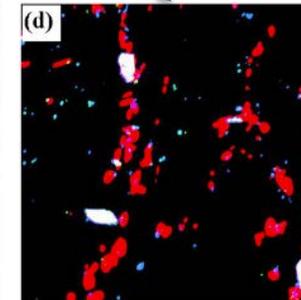
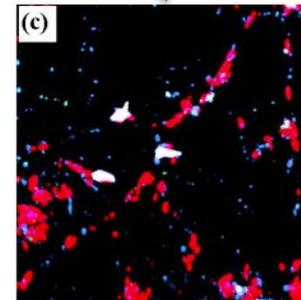
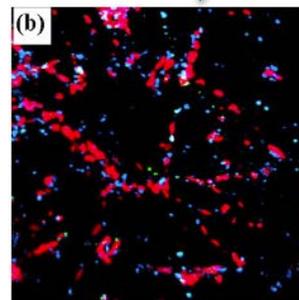
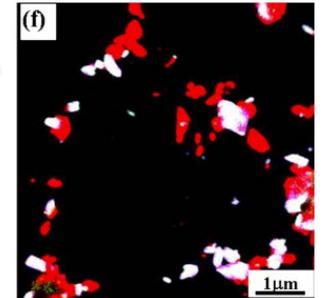


Accelerated strength reduction in long term creep

Accelerated strength reduction accompanied by microstructural degradation.



Blue/Green: MX
Red: M₂₃C₆
White: Z-Phase

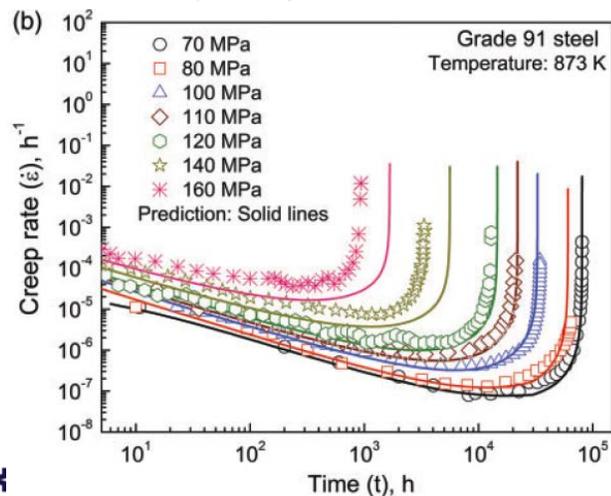


Comparison of Creep Models

Hyperbolic Sine Model

- State-of-the-art solution to model creep behavior
- Phenomenological model involving direct fitting to experimental data
- Extension to other materials would require the same amount of data used in the first fitting

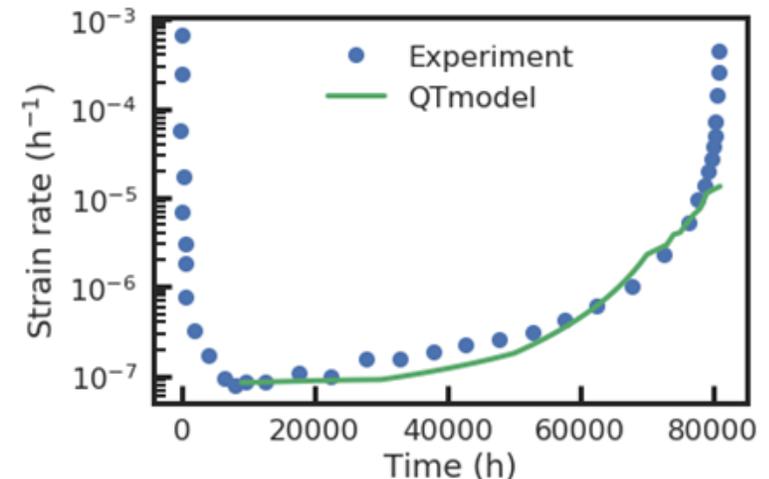
$$\dot{\epsilon} = \dot{\epsilon}_0 \frac{D_d}{1 - \left(1 - \frac{c_c}{c_0}\right) D_s} \sinh \left[\frac{\sigma(1-H)}{\sigma_0(1-DC)} \right]$$



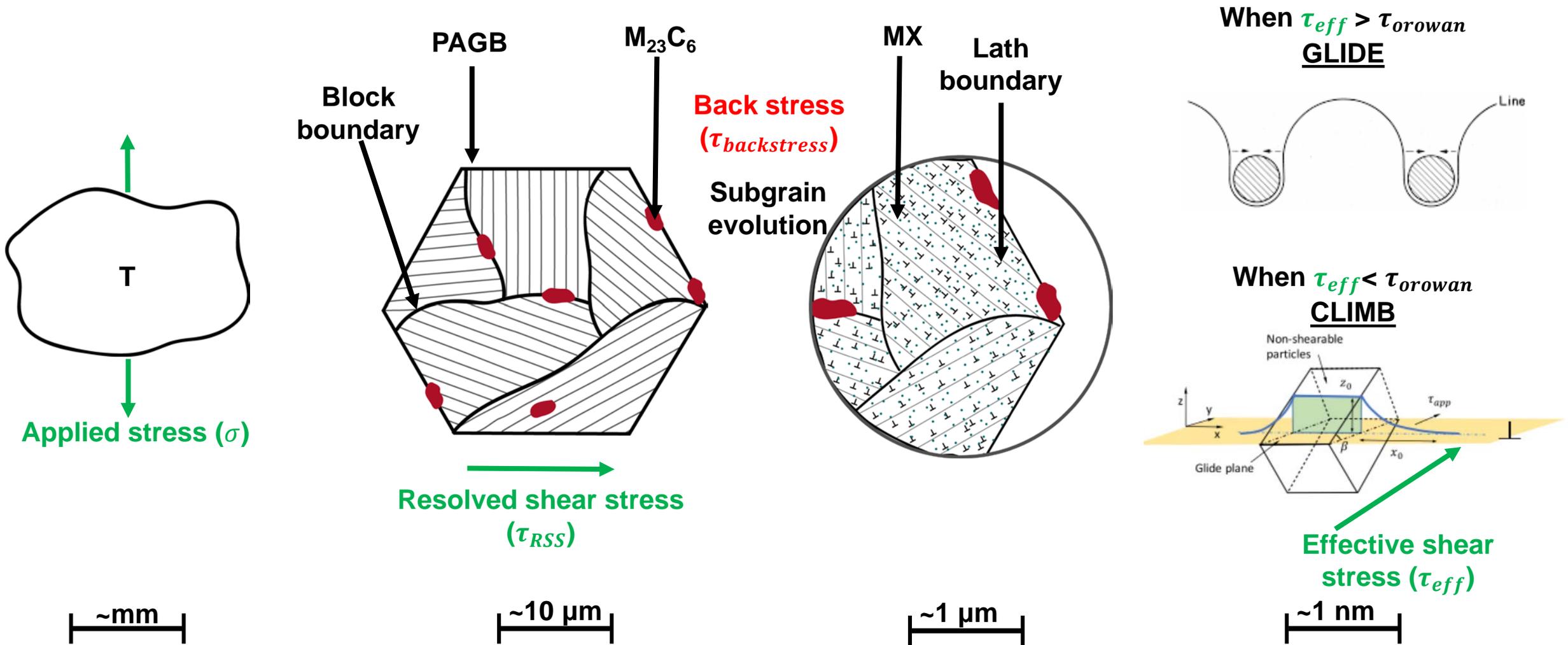
QuesTek's Creep Model

- Mechanistic model capturing the climb mechanism in play
- Easy extension to same material with different compositions or even other materials

$$\dot{\epsilon} = \rho_m b v = \rho_m b \frac{\lambda}{t} = \rho_m b \frac{\lambda}{t_c + t_g}$$



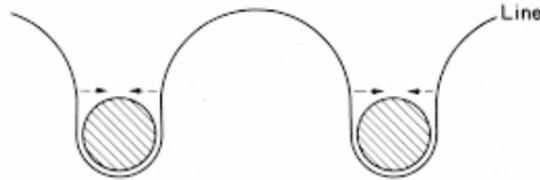
QuesTek's creep model – Dislocation creep



QuesTek's Creep Model: Cont.

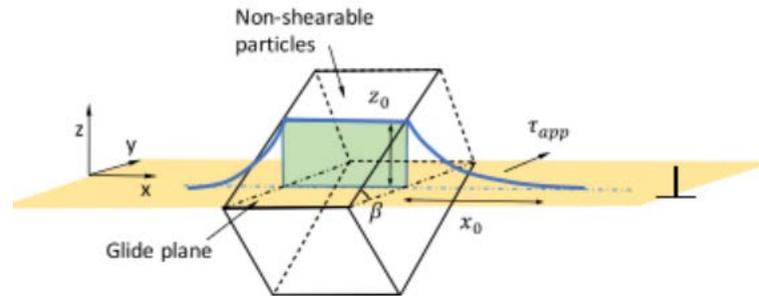
Decreasing stress

When $\tau_{eff} > \tau_{orowan}$: Glide



$$v_g = f(T, \tau)$$

When $\tau_{eff} < \tau_{orowan}$: Climb

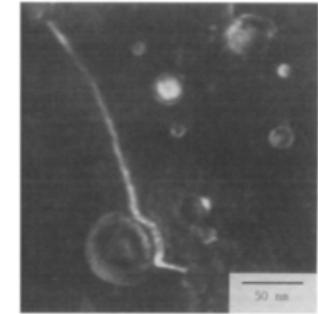


$$t_c = \int_{y_{min}}^{y_{max}} \frac{dy}{dy/dt}$$

$$\frac{dy}{dt} = C_i \frac{\mu}{dA/dy} =$$

Driving force for adding vacancies
Number of vacancies required to climb

When $\tau_{eff} < \tau_{threshold}$: No climb (or glide)



$$\tau_{threshold} = f(T, \tau)$$

$$t_{detach} = 1 / \frac{3D_v}{b^2} \exp \left(- \frac{Gb^2 r [(1-k) (1 - \frac{\tau_{eff}}{\tau_d(T)})]^{3/2}}{k_B T} \right)$$

- J Rosler, et al., Acta Metal. (1988)
- E Arzt, et al., Acta Metal. (1988)
- J Zhao, et al., Acta Mater. (2018)

Overall Dislocation creep

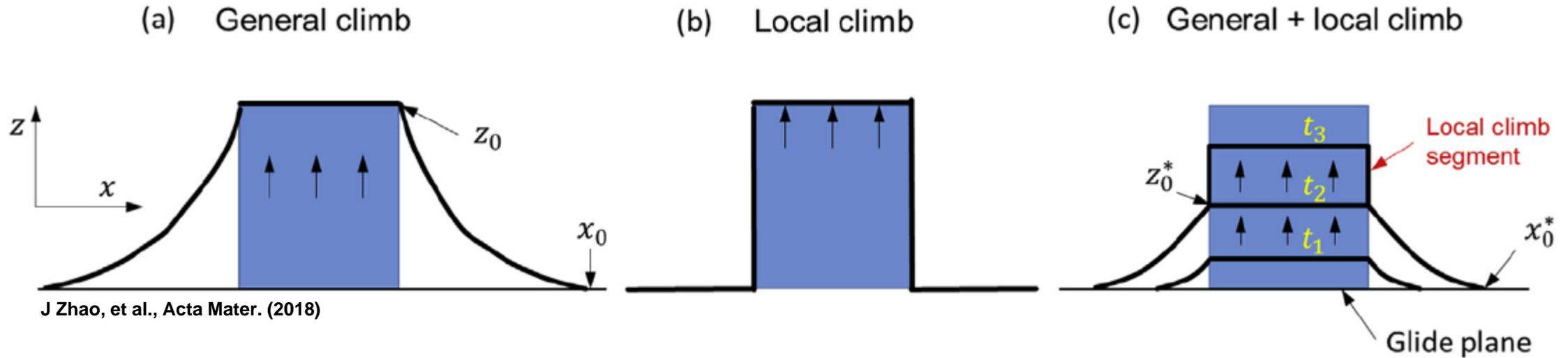
$$\epsilon_{dis} = \rho_m b v = \rho_m b \frac{\lambda}{t} = \rho_m b \frac{\lambda}{t_c + t_g + t_{detach}}$$

+

Diffusional creep (Coble)

$$\epsilon_{diff} = A \left(\frac{D_{gb}}{d^3} \right) \sigma$$

General climb and local climb modes



General Climb

- Enabled at low stress
- Larger driving force
- More vacancies needed
- Usually slower

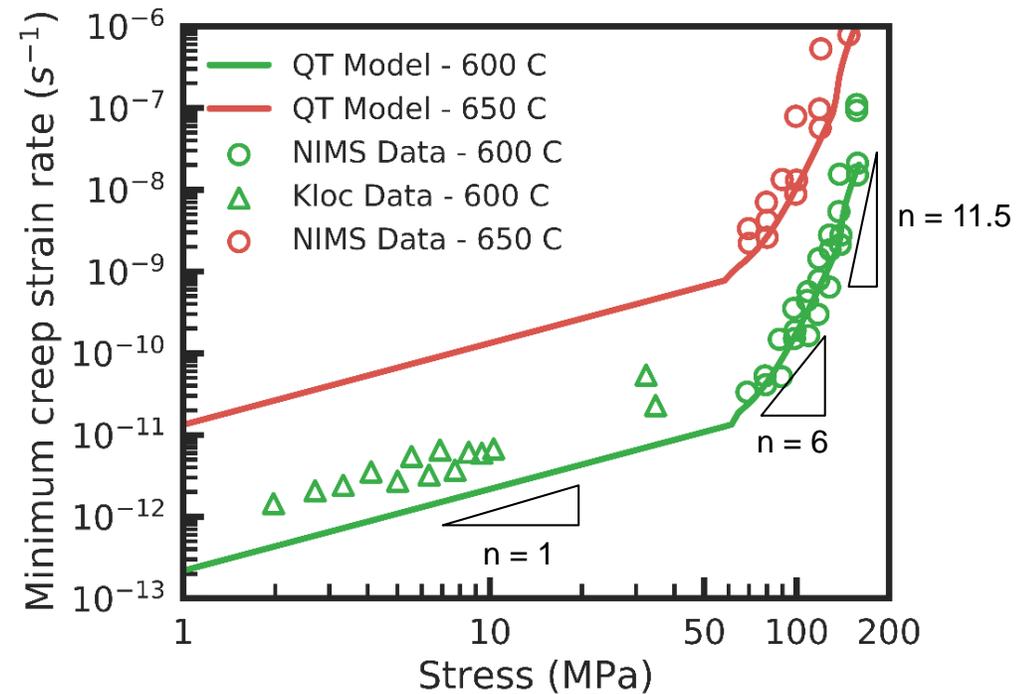
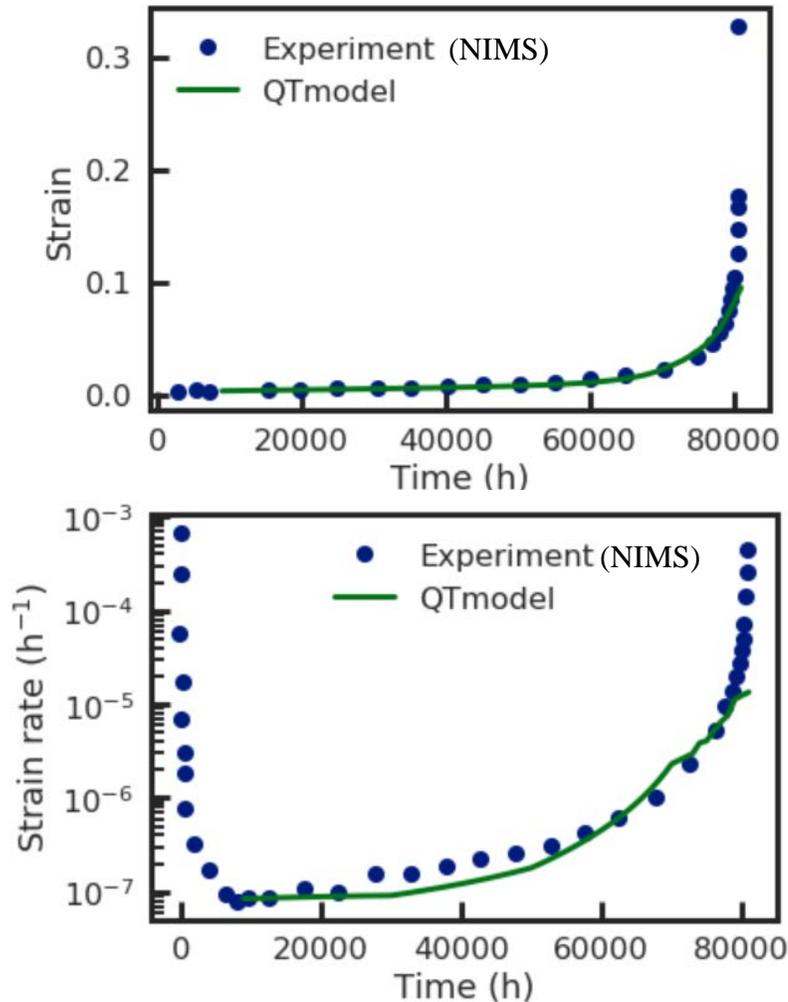
Local Climb

- Enabled at high stress
- Low driving force
- Fewer vacancies needed
- Usually faster

General + Climb

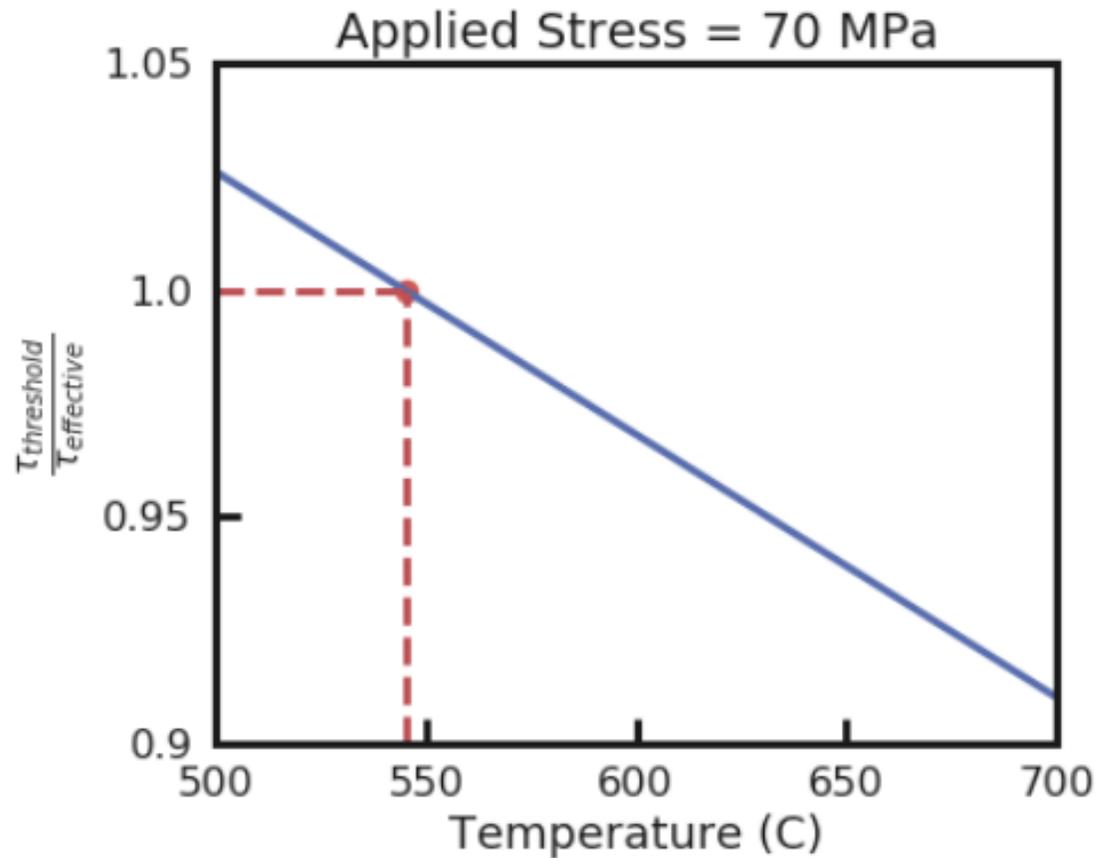
- Used in this model
- Captures both modes
- Needs to find equilibrium/transition point

Model application to Grade 91 steel

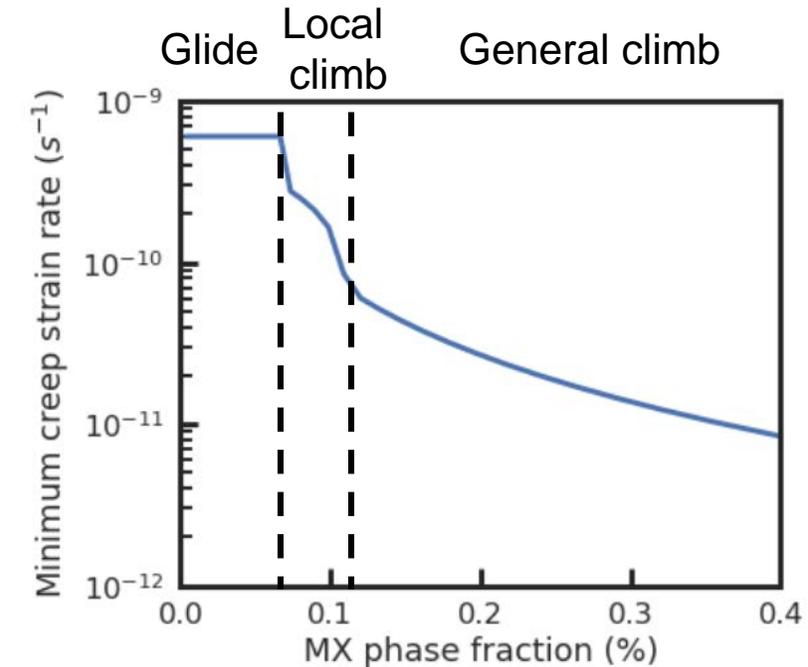
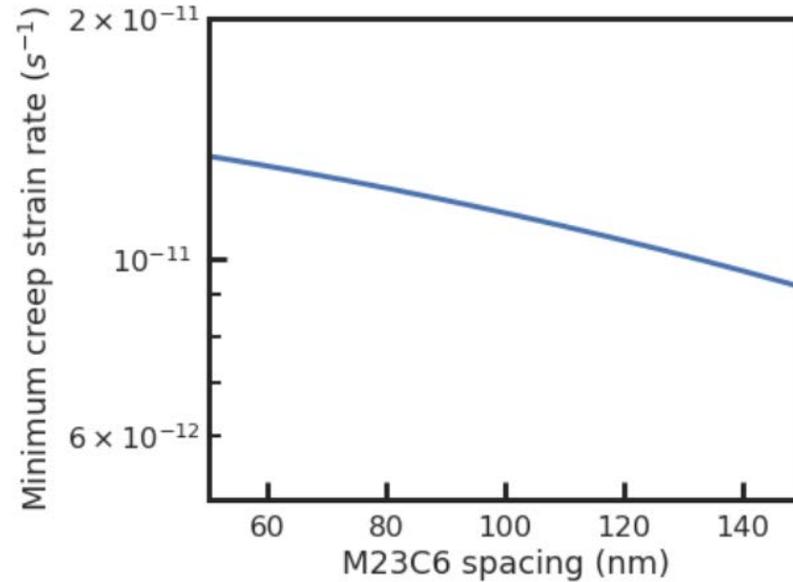
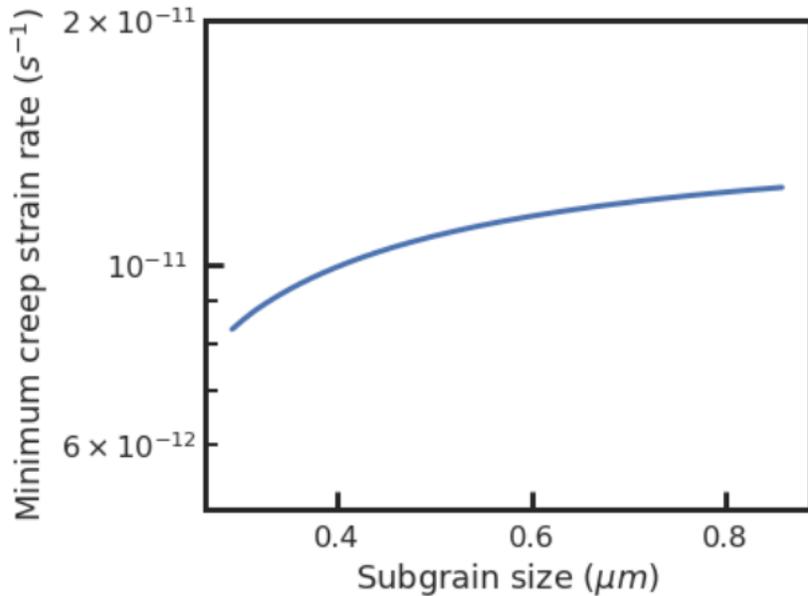


- Accurate prediction of strain and creep rate at 70 MPa
- Prediction made using experimental data from [1]
- Tertiary creep region was modeled by a necking model
- Captures stress dependence in min. creep rate predictions
- Transition from general \rightarrow local climb mode observed

Transition from dislocation to diffusional creep

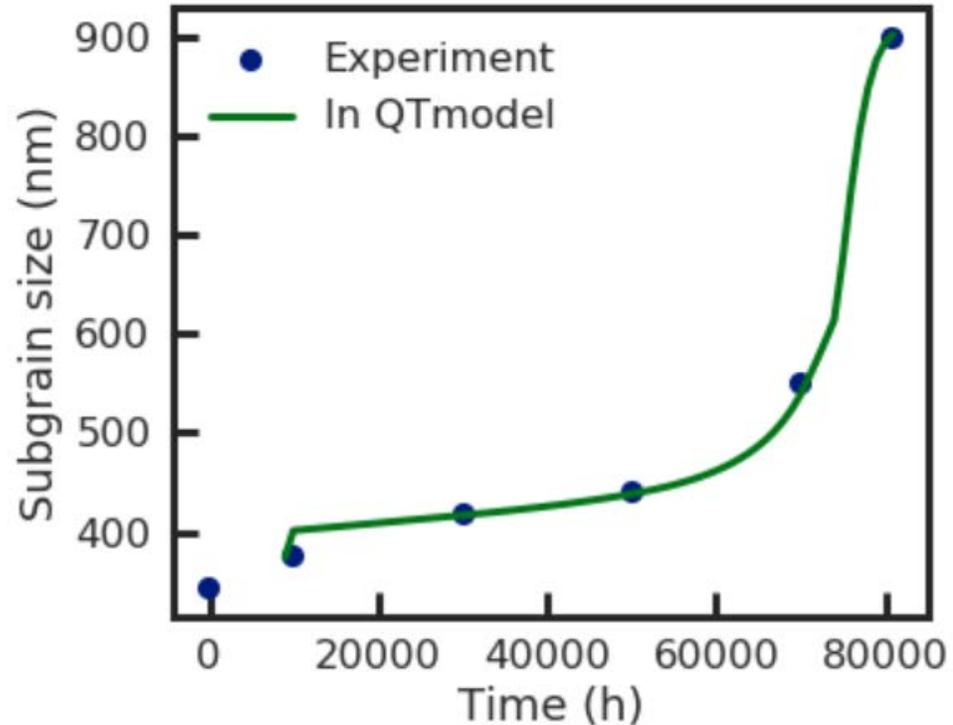


Effect of different microstructural variables



- Creep strain rate most sensitive to MX phase fraction
- Microstructurally sensitive model enables application to different conditions (eg – weld regions)

Modeling microstructural evolution



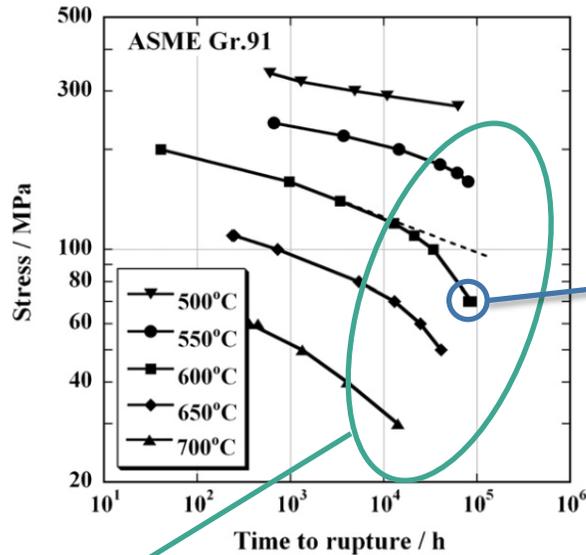
Subgrain size model [1]

$$\ln\left(\frac{d}{d_{ST}}\right) = \ln\left(\frac{d_0}{d_{ST}}\right) \exp\left(-\frac{\varepsilon}{k_{sg}}\right)$$

Dislocation number density

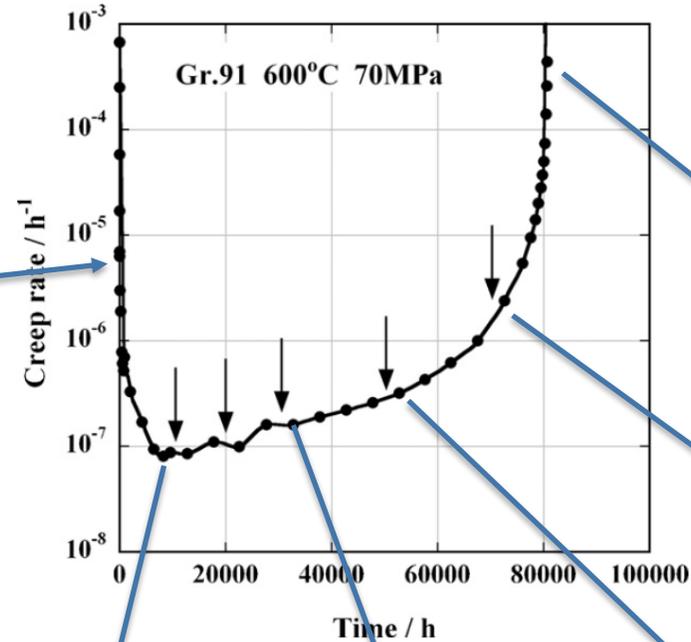
- Currently using experimental data values
- Working on dislocation evolution model

Accelerated creep deformation

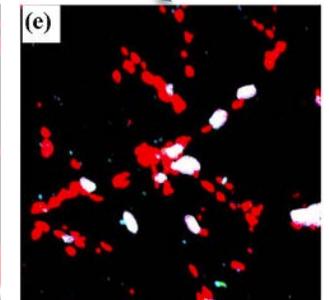
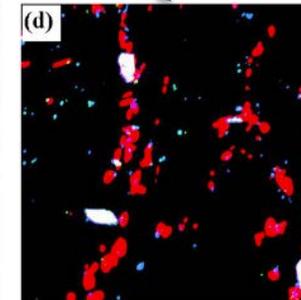
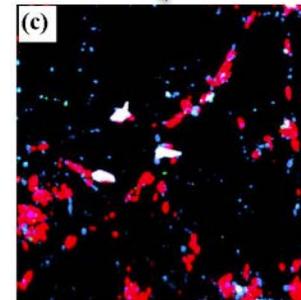
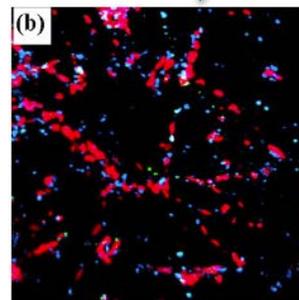
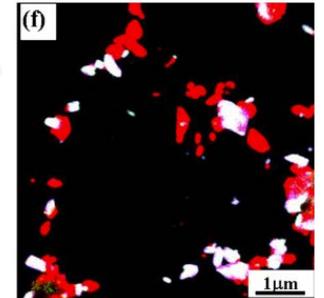


Accelerated strength reduction in long term creep

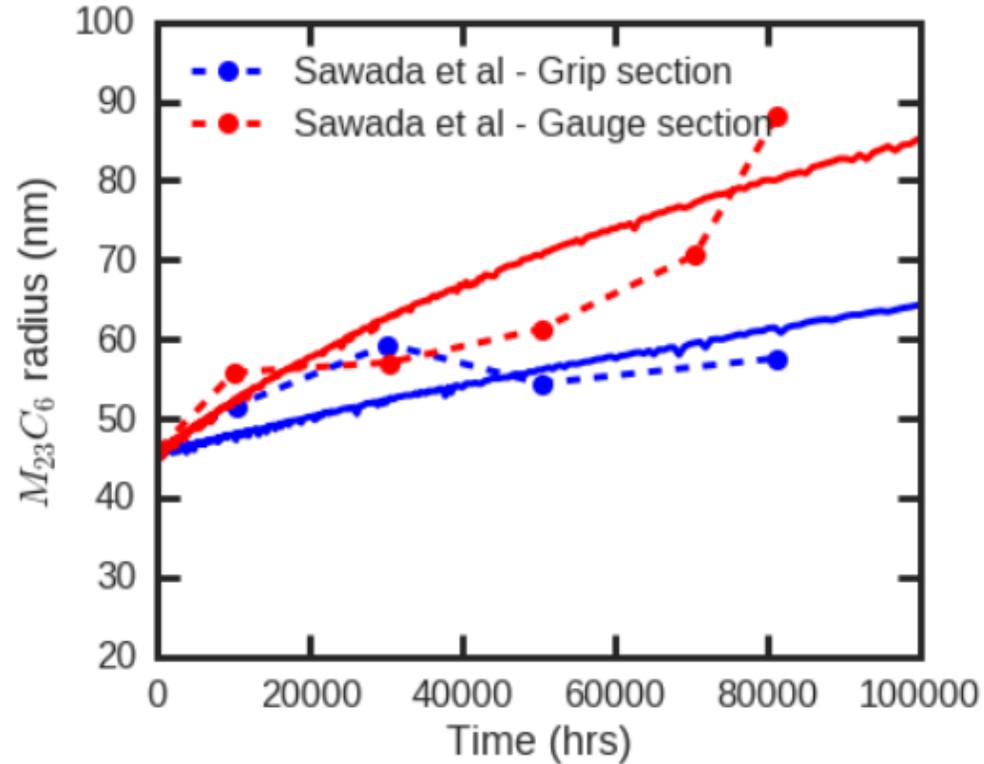
Accelerated strength reduction accompanied by microstructural degradation.



Blue/Green: MX
Red: M₂₃C₆
White: Z-Phase

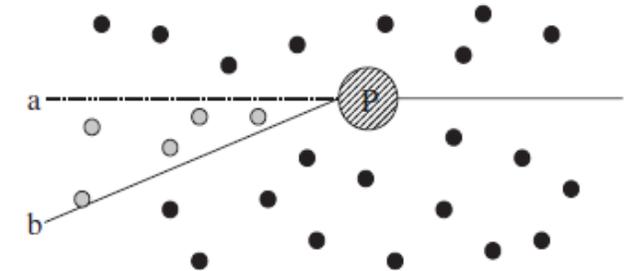


Evolution of $M_{23}C_6$ precipitate



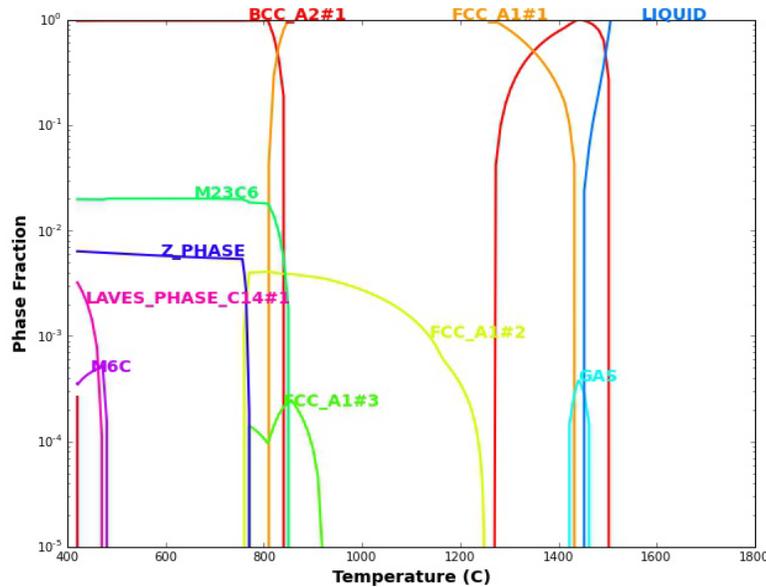
$$D_{eff} \propto \dot{\epsilon}$$

Scavenging effect^[1]



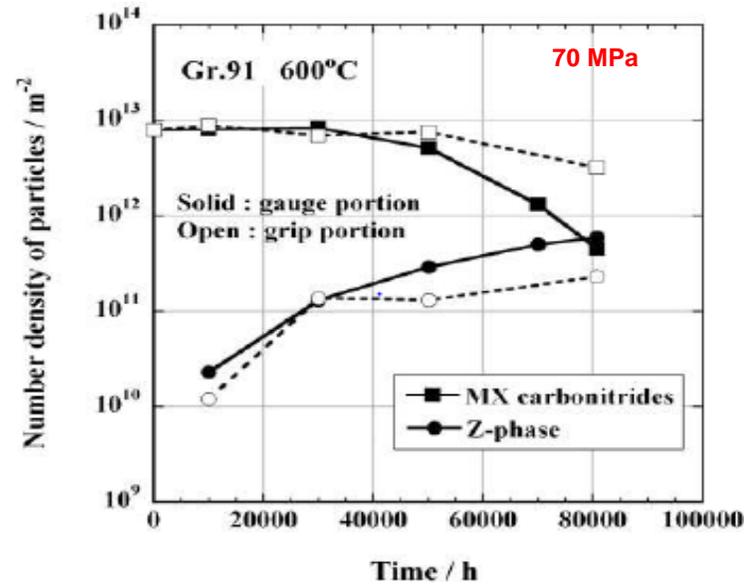
- Accelerated coarsening explained by increase in diffusion coefficients due Scavenging effect
- A closed loop simulation between creep model and precipitation model will be more accurate

Evolution of MX → Z-Phase precipitation



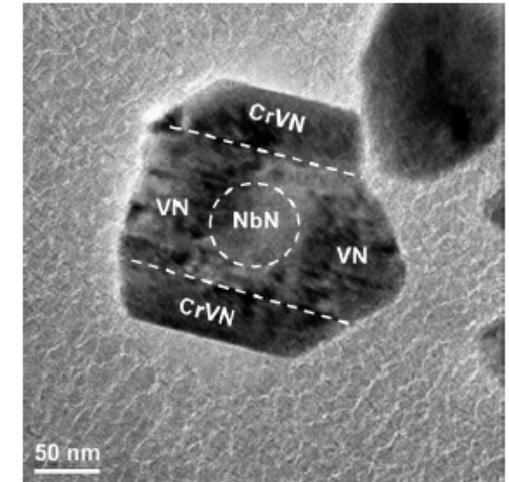
Z-Phase is a thermodynamically stable phase.

K. Sawada, et al., Mater. Sci. Eng. A (2011) 528



Z-Phase Precipitation consumes beneficial MX precipitates.

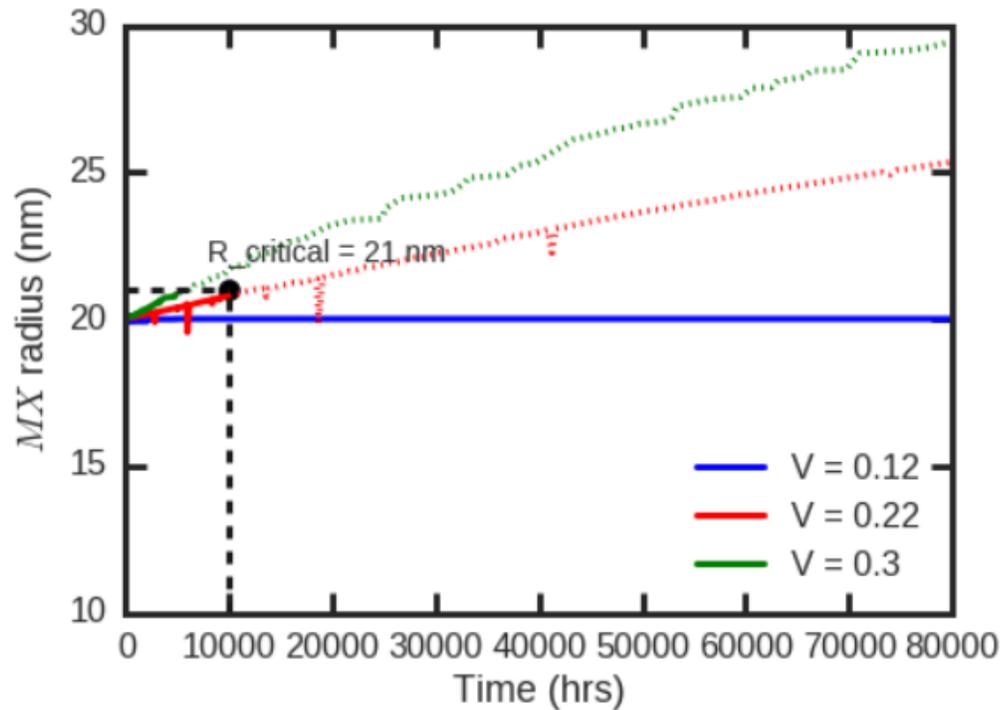
H. K. Danielsen, Mater. Sci. Tech. (2016) 32



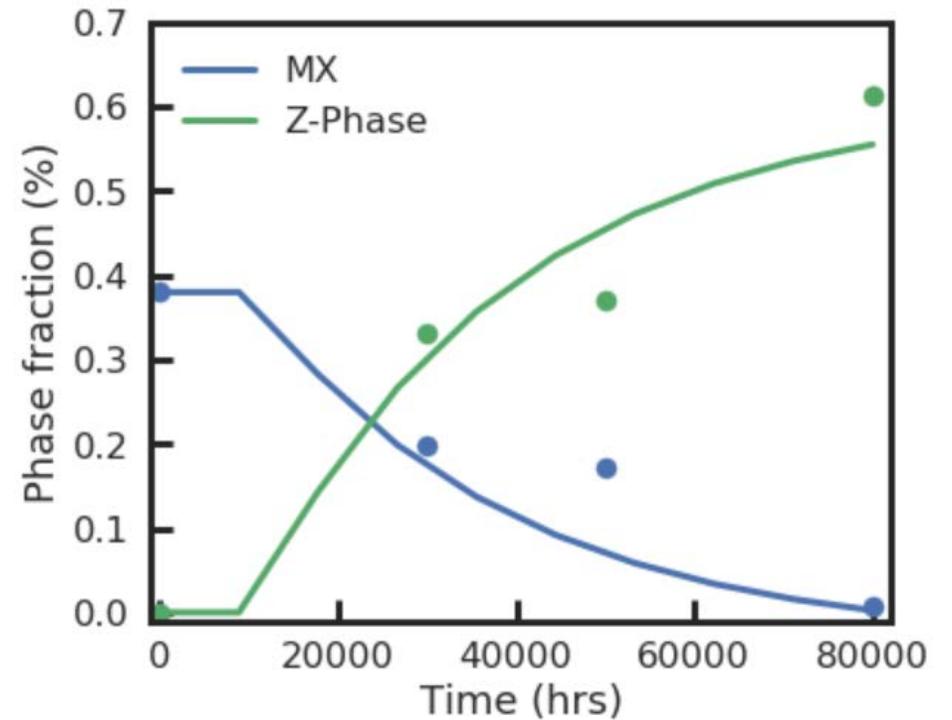
Heterogeneous nucleation on MX precipitates

MX → Z-Phase precipitation

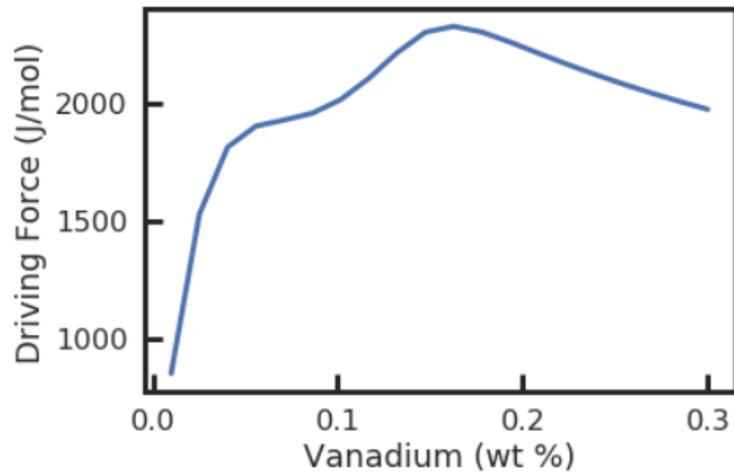
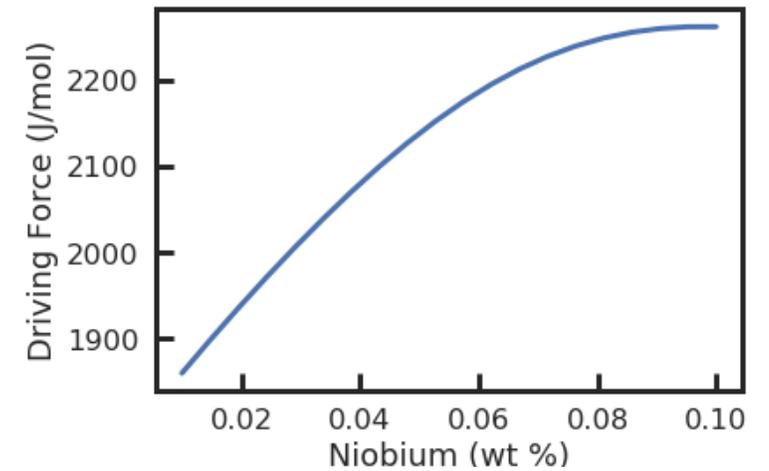
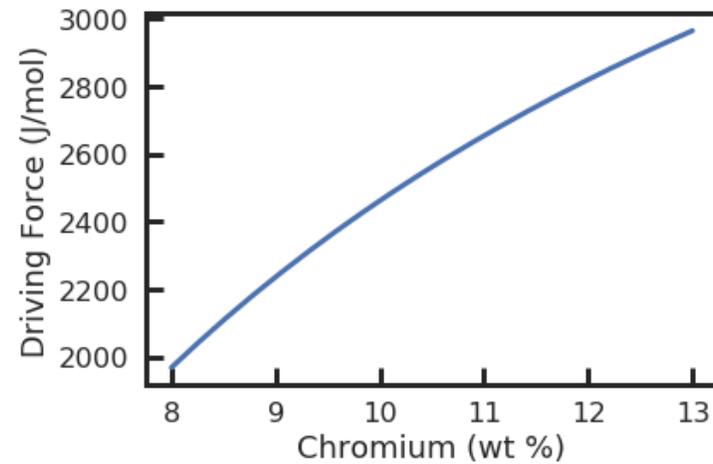
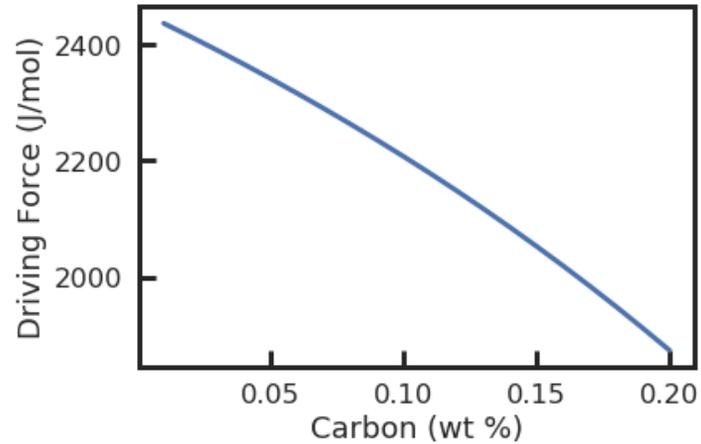
Critical radius for Z-phase nucleation



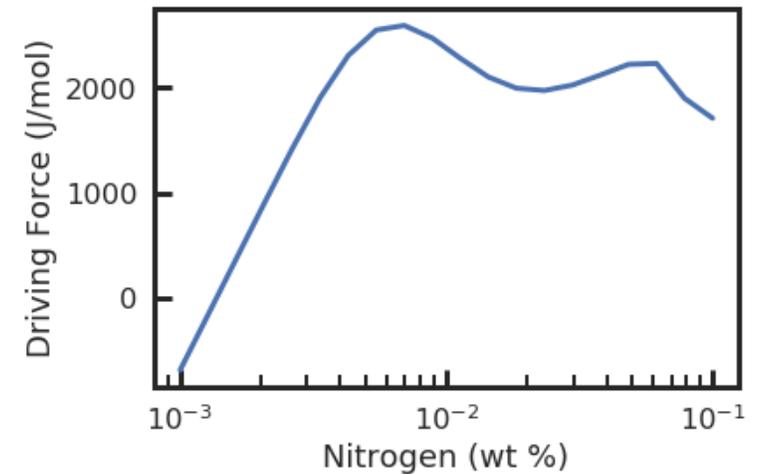
Once critical radius is reached, phase fraction is modeled using a JMAK equation with driving force of Z-Phase as input



Effect of composition on Z-phase driving force



**CALPHAD method enables prediction
of Z-Phase stability as a function of
composition**



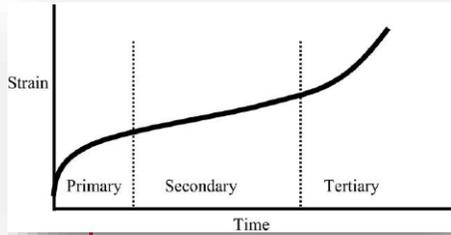
Modeling creep ductility

- Important to model the tertiary creep region accurately to get accurate prediction of creep ductility
- Kachanov-type damage evolution most widely used method for describing tertiary creep

$$\dot{D}_{CV} = C \cdot \dot{\epsilon}_{eq}^{cr} \left(\frac{\sigma_1}{\sigma_{eq}} \right)^\nu$$

- Damage evolution governed by maximum principle stress
- Phenomenological approach not based on actual creep cavitation and growth mechanism
- QuesTek's efforts will be based on developing damage evolution model using an extension of Gurson-type model (GTN model) for modeling ductile failure in porous material
- Plastic deformation in Gurson model can directly be replaced by creep deformation. Void nucleation and growth relation will be taken from Needleman and Tvergaard formulation of Gurson model
- Such a mechanistic approach will enable prediction of damage evolution as a function of composition, specifically the inclusion content. (Strong dependence of inclusion on void nucleation reported by EPRI)

Landscape of long term creep modeling for CSEF steels



PRIMARY CREEP

SECONDARY CREEP

TERTIARY CREEP

Dislocation density evolution

Dislocation climb and glide

Creep cavitation

Precipitate evolution

Martensite microstructure evolution

Mechanism

State-of-art modeling approach

Hardening parameter

Hyperbolic sine model with damage parameters

Cavitation damage parameter (Kachanov-type damage model)

Precipitate damage parameter

QuesTek's modeling approach

Hardening parameter or dislocation density evolution model

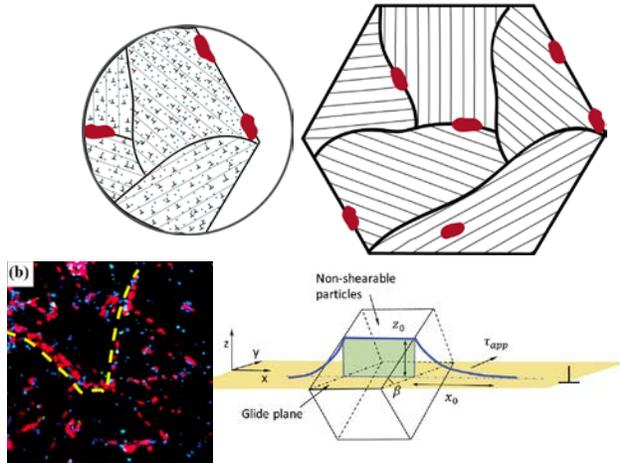
Dislocation dynamics based microstructure sensitive model

Gurson-type damage evolution model

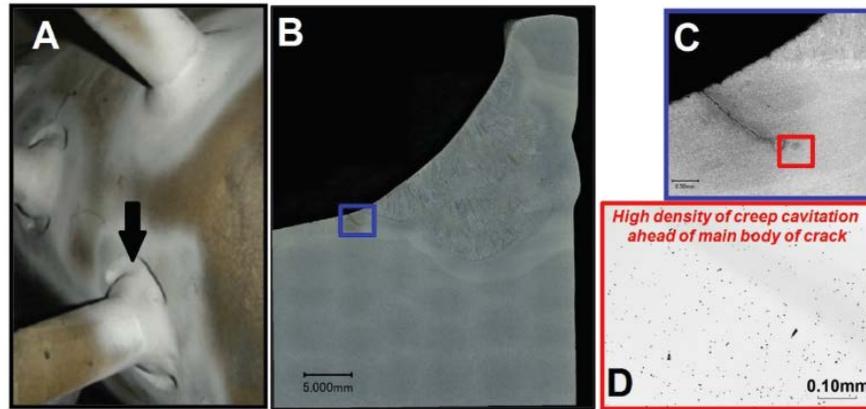
Precipitation model

Subgrain evolution model

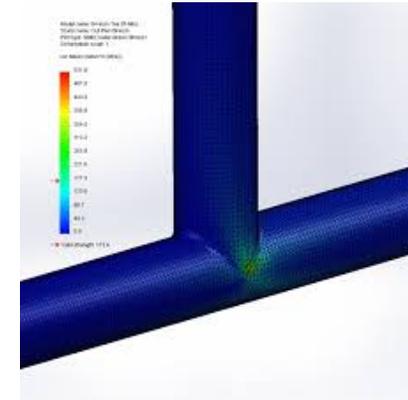
A multiscale modeling framework



K. Sawada, et al., Mater. Sci. Eng. A (2011) 528



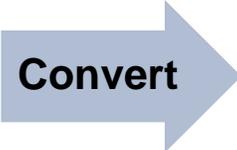
EPRI 3002003472 (2014)



QT creep strain rate model
+ microstructure evolution model



QT creep damage evolution
model



Composition dependent
CDM models

Summary

- **QuesTek's creep model**
 - Captures diffusional and power law creep behavior for Grade 91 steels
 - Good agreement with experiments
 - Mechanistic approach enables easy application to other (CSEF) alloys
- **Ongoing efforts at QuesTek**
 - Application of model to weld metal and HAZ
 - Creep damage evolution model
 - QT model to CDM model converter
- **Contacts**
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 - Jiadong Gong (PI), jgong@questek.com



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