# ICME for Creep of Ni-Base Superalloys in Advanced Ultra-Supercritical Steam Turbines

**Pengyang Zhao[1], Supriyo Chakraborty[1], Yunzhi Wang[1], and Stephen Niezgoda[1,2]**

[1]Department of Materials Science and Engineering, The Ohio State University

[2]Department of Mechanical and Aerospace Engineering, The Ohio State University

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NATIONAL ENERGY TECHNOLOGY LABORATORY

(DE-FE0027776)

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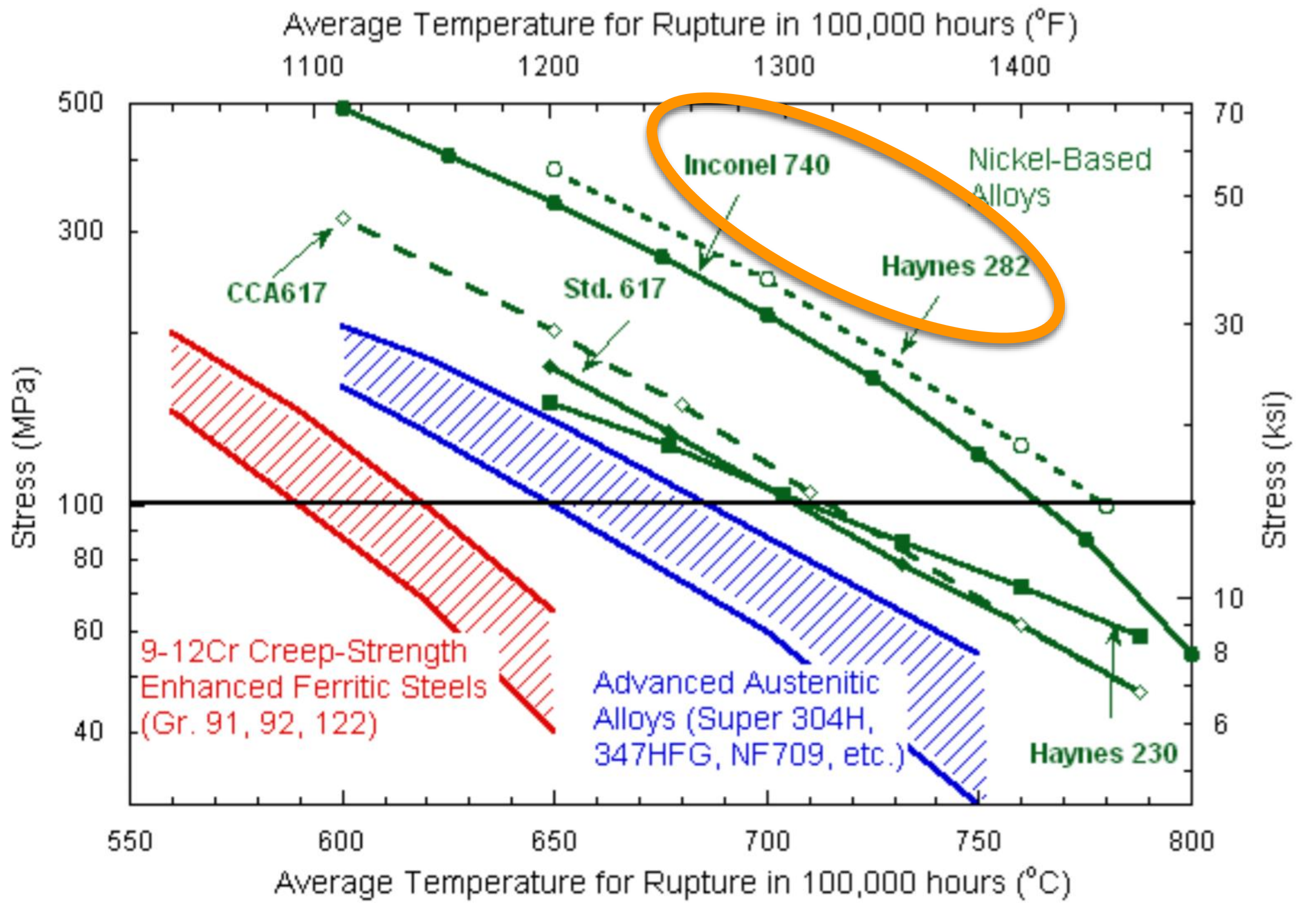
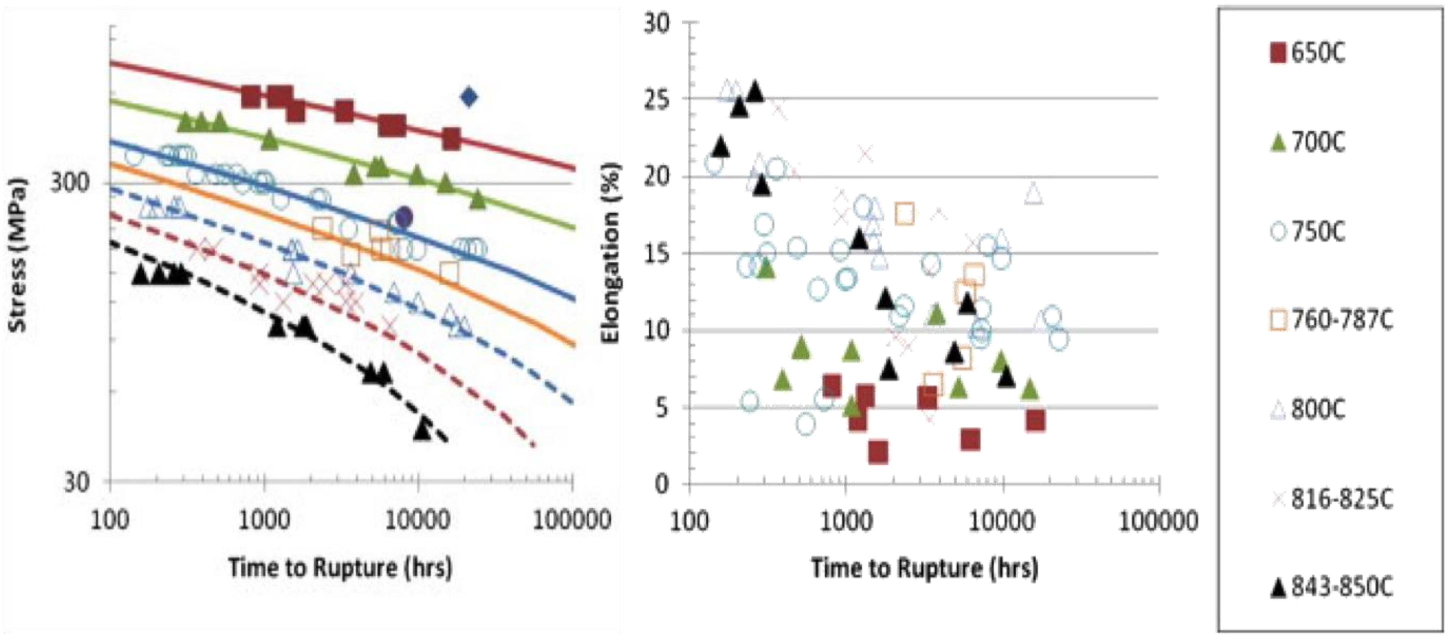
# Alloy Selection for A-USC conditions (>1400°F, >4ksi)




Shingledecker, et. al, 2014

# Large Data Scatter for Creep Performance

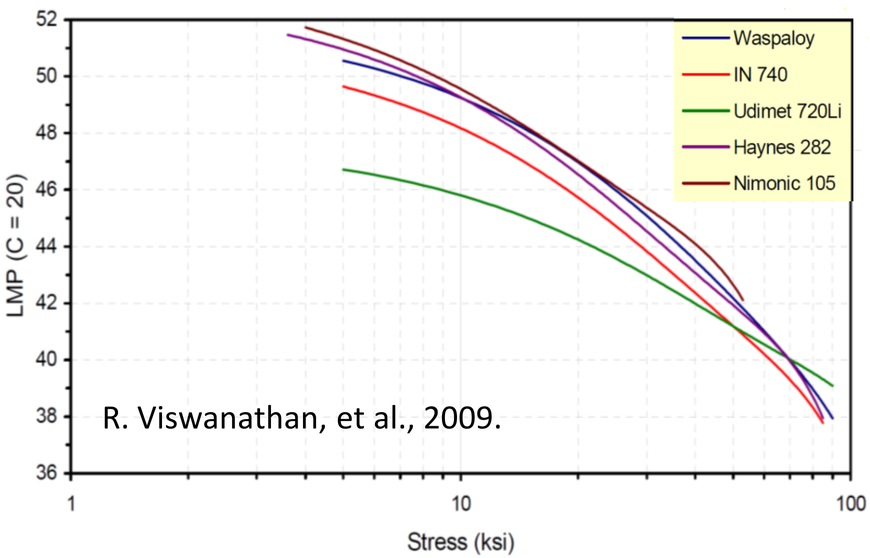



Rupture time vs. Stress/Elongation at various temperatures for Inconel 740 (Shingledecker, et. al, 2013)

- The scatter is primarily due to material variability at the microstructure level
- Critical analysis of the creep data and the development of creep model must explicitly account for and describe the microstructure variability.

# Current Creep Modeling of Ni-base Superalloys

*Larson-Miller parameter (LMP) vs stress for various Ni-base superalloys* ($C_{LM} = 20$)




Rupture time

$$T[C_{LM} + \log t_r] = LMP = f(\sigma)$$

LM constant

- Phenomenological in nature: simple analytical model by directly linking test conditions (e.g., stress) with creep measures (e.g., rupture time)
- No microstructure information is considered (The Larson-Miller constant is insensitive to the microstructure)
- No creep mechanisms are involved
- Cannot provide feedback on optimization of improving Ni-base superalloys
- Rely on sufficiently large amount of data (not efficient)

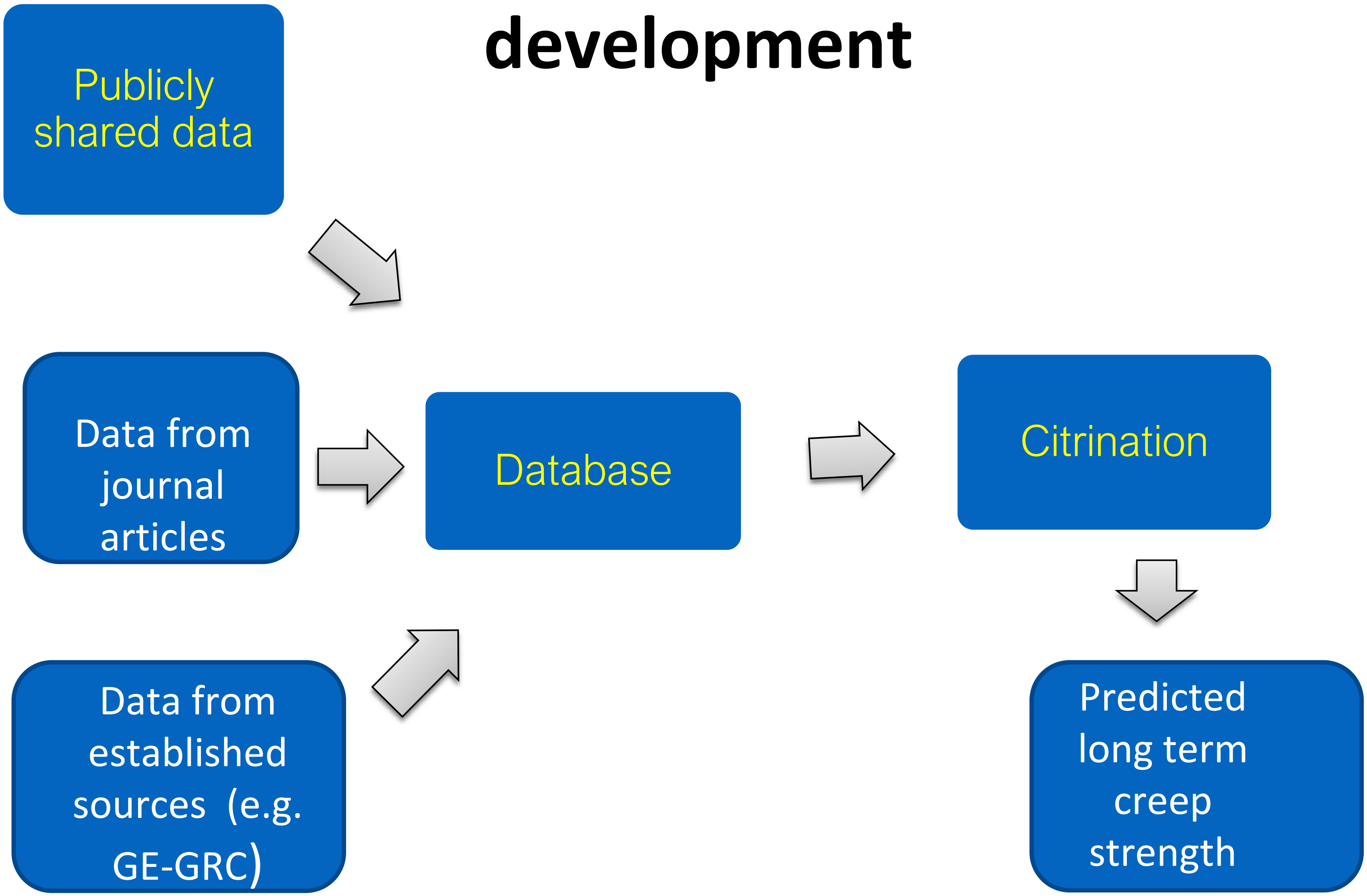
# Program Objectives

1. Application of advanced materials informatics for critical assessment of existing experimental data

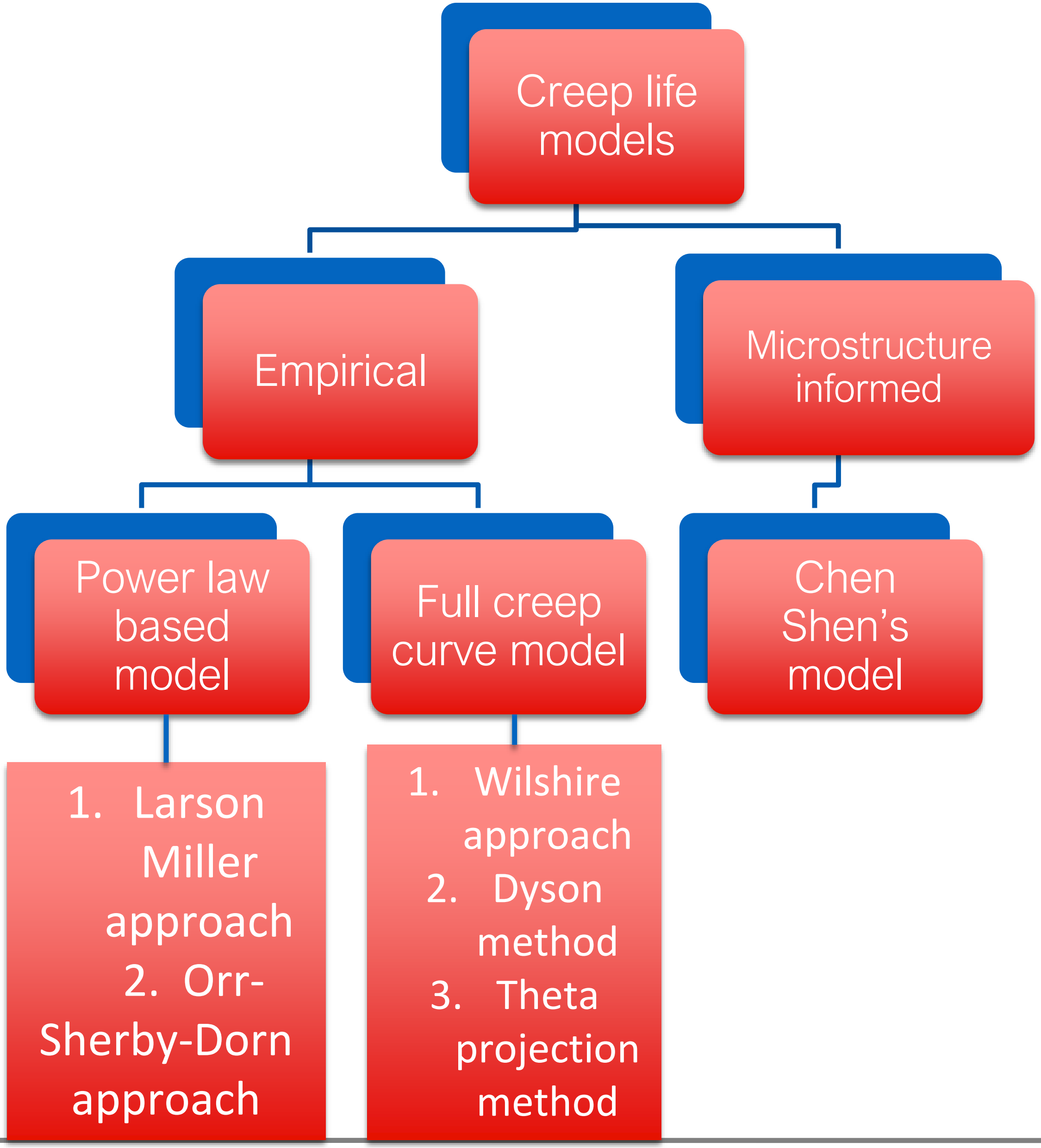
2. Critical assessment of existing modeling capabilities

3. Development of new modeling capabilities that are critical but currently missing in predicting long-term creep behavior of Ni-base superalloys

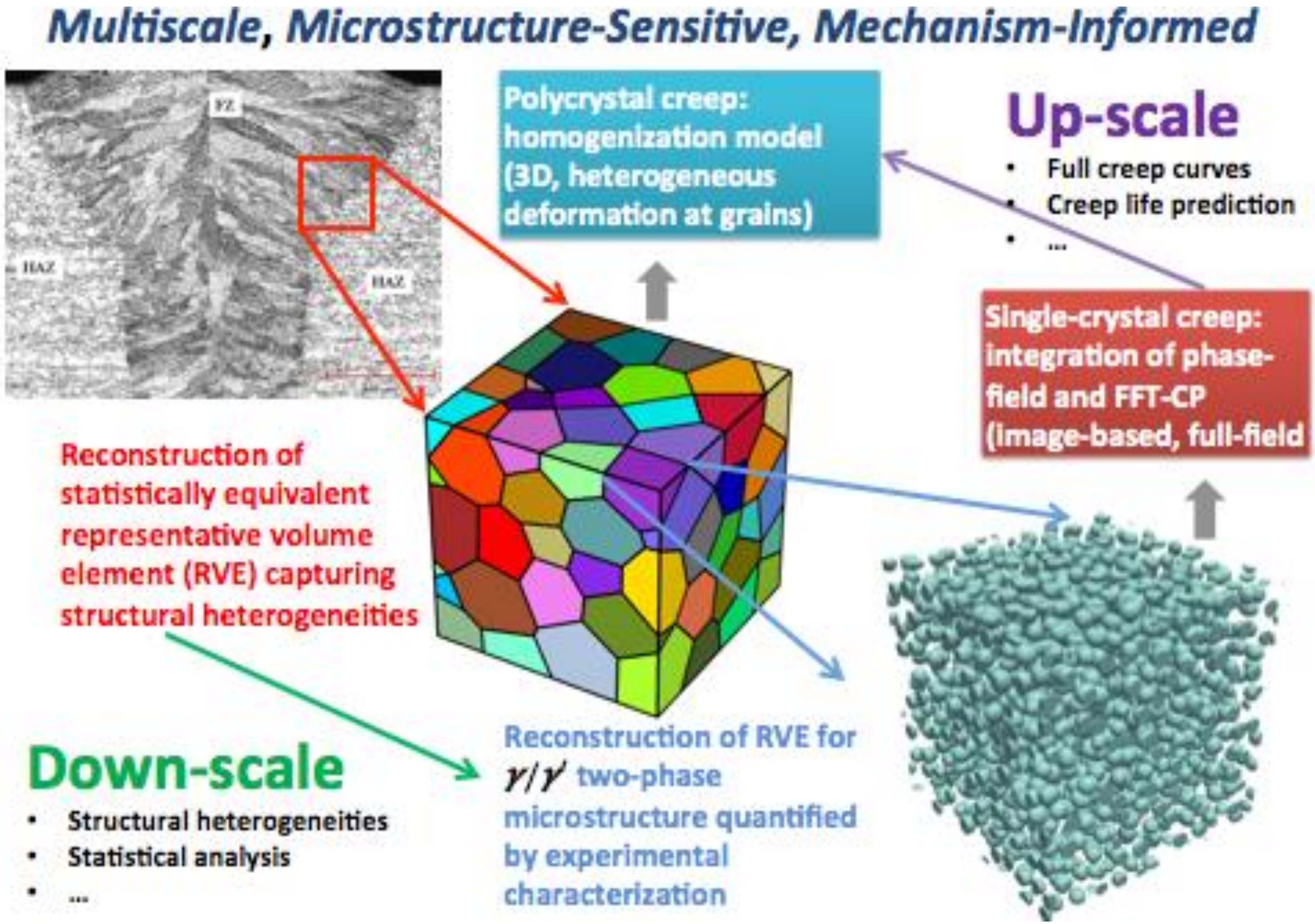
# Data assessment and database development



# Existing creep models



# An Integrated Modeling Scheme



# Outline

- **Development of a multiscale physics-based creep model for Ni-base superalloys**
  - Fast Fourier transform (FFT) based crystal plasticity (CP) model for $\gamma/\gamma'$ superalloys
  - Phase-field model for $\gamma/\gamma'$ structural evolution
  - Integration between FFT-CP and phase-field
  - Application to full-field modeling of creep of single crystal superalloys: interplay between microstructure and micromechanics
  - Application to H282

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# FFT based Micromechanical Solver

## Spectral (FFT) method

- Solutions are approximated by *global* Fourier series.
- Stress equilibrium is satisfied at every (image) sampling point in the *strong* form, i.e.,

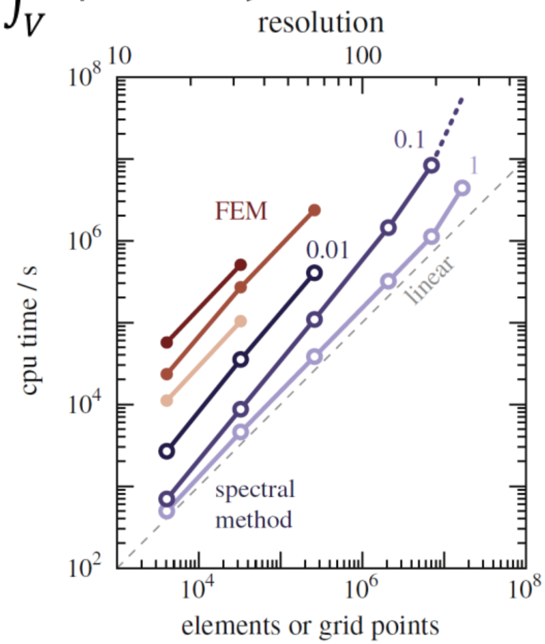
$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}$$

Lebensohn, R. A., et al. (2012). *IJP*.

## Finite element method

- Solutions are approximated by *localized* shape-functions
- Stress equilibrium is satisfied in over elements in the *weak* form, i.e.,

$$\int_V \delta\phi \cdot (\nabla \cdot \boldsymbol{\sigma})dV = \mathbf{0}$$

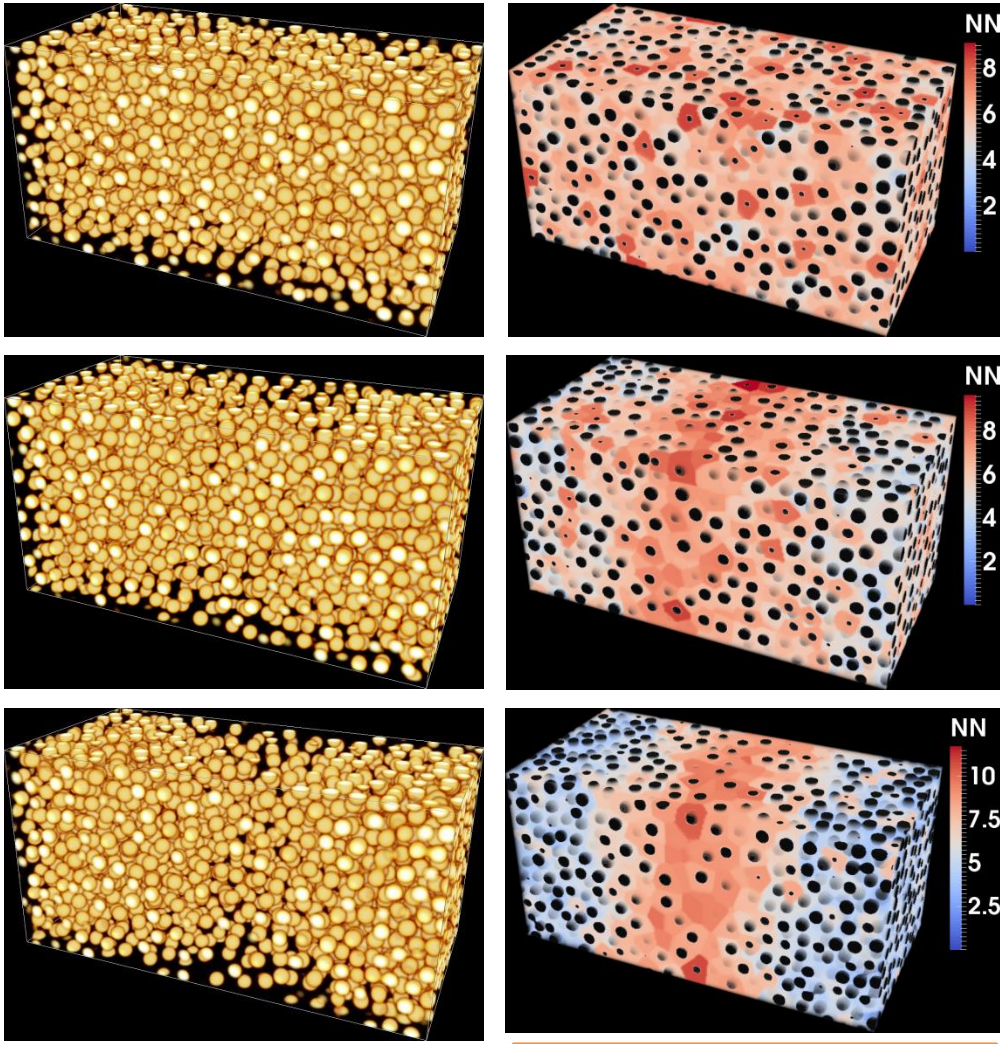



Eisenlohr, P., et al. (2013). *IJP*.

**Advantage of FFT method for this study:**

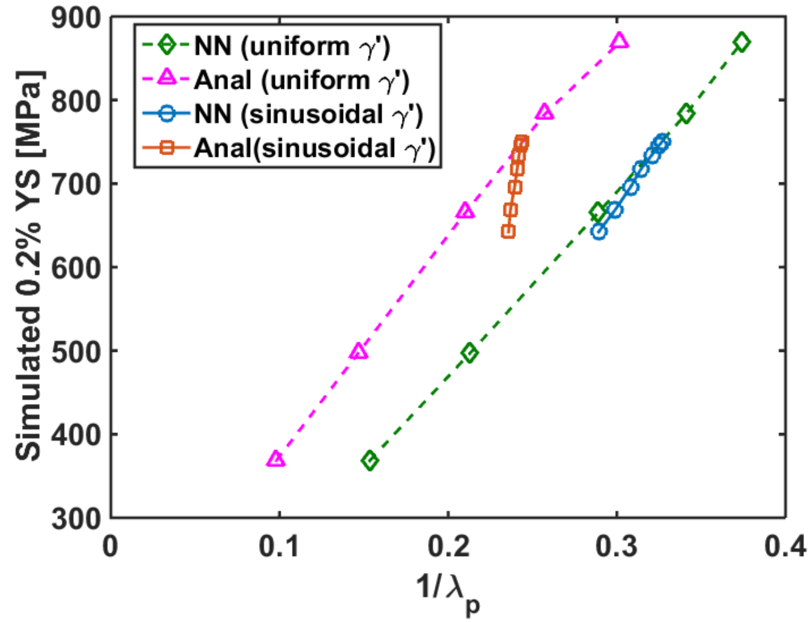
- Account for complex geometry of γ/γ’ microstructure
- Fast numerical implementation due to FFT algorithm
- Integration with phase-field

# Local Inter-Particle Spacing




**Phase-field generated HA282 with different sinusoidal $\gamma'$ variation**

**NN distance map generated based on geometric analysis**




- The local inter-particle spacing turns out to be a better microstructure descriptor than the conventional analytical method.
- The microstructure details can be effectively taken into account if the appropriate structure descriptor is employed

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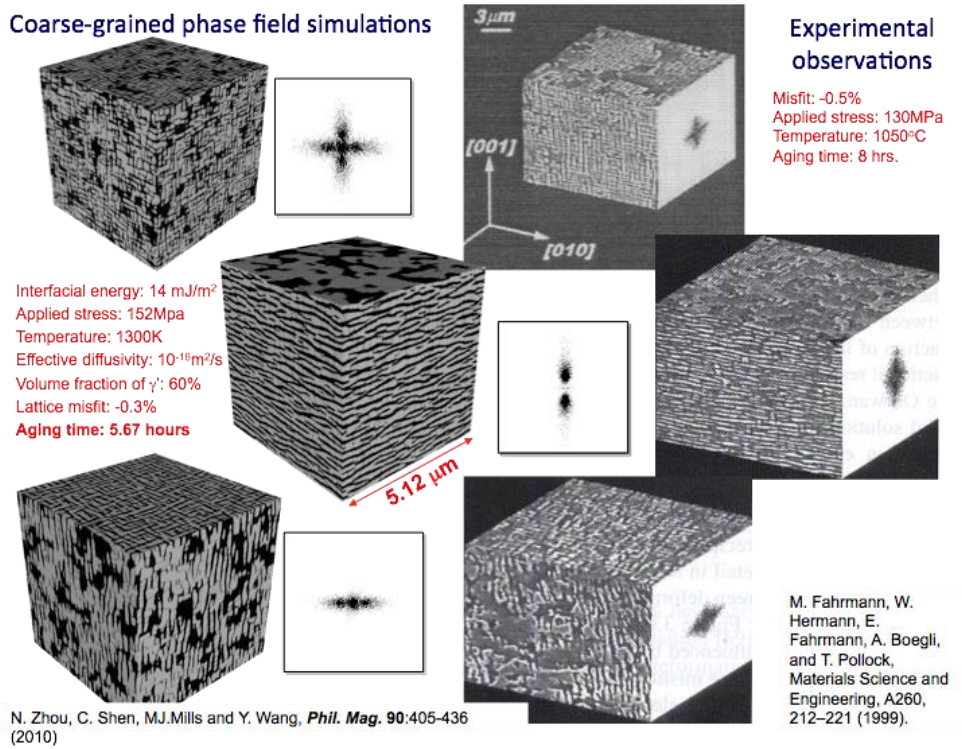
# Phase-Field Model for γ/γ' Microstructure



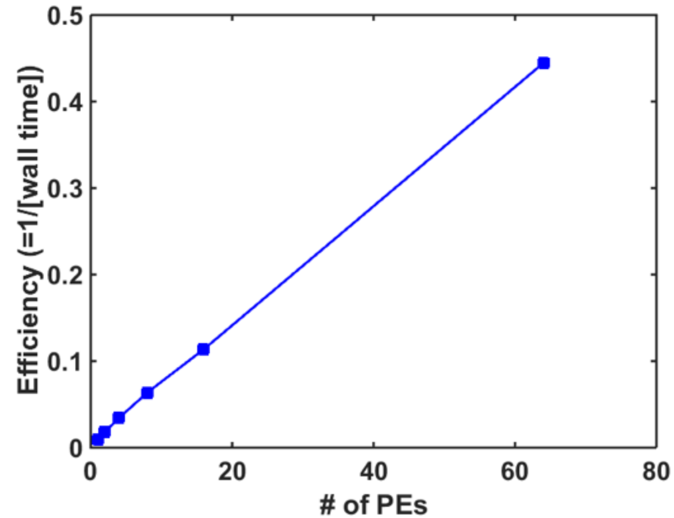

$$F = \int_V \left[ f\left(c(\mathbf{x}), \{\phi_i(\mathbf{x})\}_{i=1}^4\right) + \frac{\kappa^2}{2}\sum_{i=1}^{4}(\nabla\phi_i(\mathbf{x}))^2 \right] dV + E^{\text{elast}}$$

$$\frac{\partial c(\mathbf{x})}{\partial t} = \nabla\cdot\left[M\nabla\left(\frac{\delta F}{\delta c(\mathbf{x})}\right)\right]$$

$$\frac{\partial \phi_i(\mathbf{x})}{\partial t} = -L\frac{\delta F}{\delta\phi_i(\mathbf{x})}$$

## Improvements

- C++, MPI parallelization

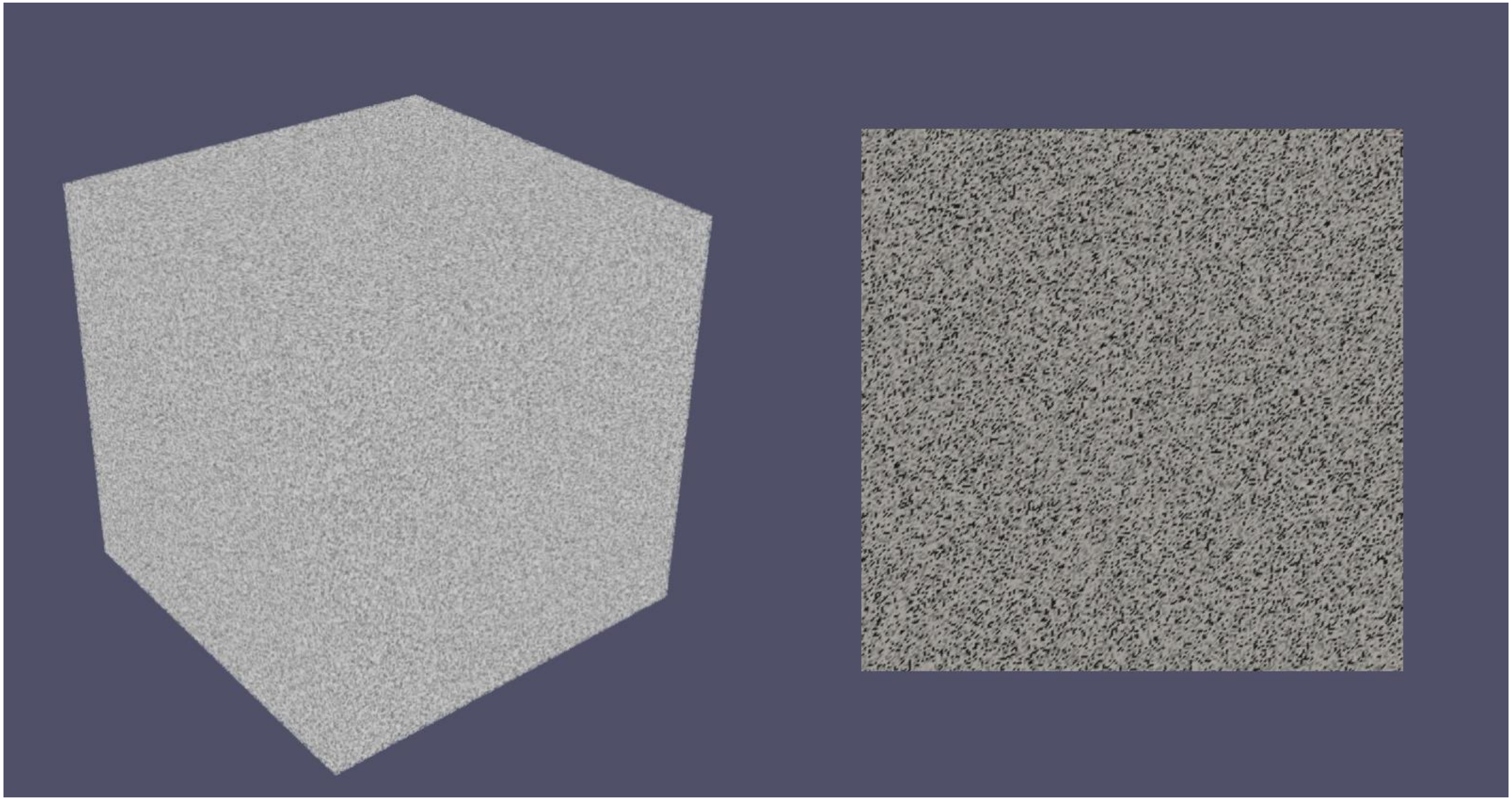



- Incorporate modulus mismatch

$$\begin{aligned} E^{\text{elast}} &= \frac{1}{2}\int_V \left[C^0_{ijmn}\Delta S_{mnpq}(\mathbf{x})C^0_{pqkl} - C^0_{ijkl}\right]\Delta\epsilon_{ij}(\mathbf{x})\Delta\epsilon_{kl}(\mathbf{x})dV \\ &+ \frac{1}{2}\int_V C^0_{ijkl}[\epsilon_{ij}(\mathbf{x}) + \Delta\epsilon_{ij}(\mathbf{x})][\epsilon_{kl}(\mathbf{x}) + \Delta\epsilon_{kl}(\mathbf{x})]dV - \bar{\varepsilon}_{ij}\int_V C^0_{ijkl}[\epsilon_{kl}(\mathbf{x}) + \Delta\epsilon_{kl}(\mathbf{x})]dV \\ &+ \frac{V}{2}C^0_{ijkl}\bar{\varepsilon}_{ij}\bar{\varepsilon}_{kl} - \frac{1}{2}⨍\frac{d^3k}{(2\pi)^3}[\tilde{\sigma}_{ij}(\mathbf{k}) + \Delta\tilde{\sigma}_{ij}(\mathbf{k})]\Gamma_{jikl}(\mathbf{n})[\tilde{\sigma}_{kl}(\mathbf{k}) + \Delta\tilde{\sigma}_{kl}(\mathbf{k})]^* \end{aligned}$$

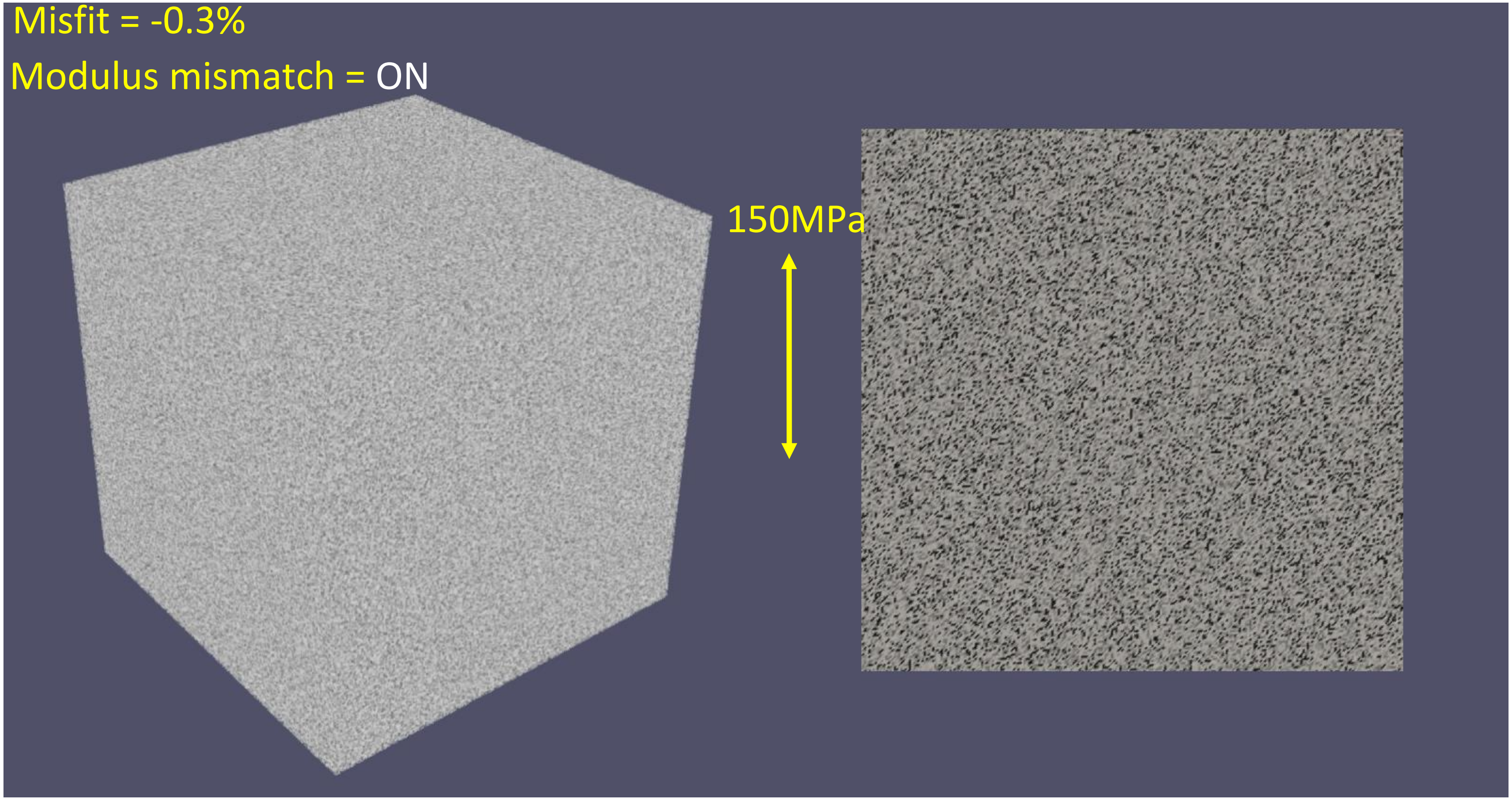
$$\begin{aligned} \frac{\delta E^{\text{elast}}}{\delta\phi_i} &= \frac{1}{2}C^0_{ijmn}\frac{d\Delta S_{mnpq}(\mathbf{x})}{d\phi_i}C^0_{pqkl}\Delta\epsilon_{ij}(\mathbf{x})\Delta\epsilon_{kl}(\mathbf{x}) \\ &+ \left[C^0_{ijmn}\Delta S_{mnpq}(\mathbf{x})C^0_{pqkl} - C^0_{ijkl}\right]\frac{d\Delta\epsilon_{ij}(\mathbf{x})}{d\phi_i}\Delta\epsilon_{kl}(\mathbf{x}) \\ &+ \left(\frac{d\epsilon_{ij}(\mathbf{x})}{d\phi_i} + \frac{d\Delta\epsilon_{ij}(\mathbf{x})}{d\phi_i}\right)\left[C^0_{ijkl}\epsilon^0_{kl}(\mathbf{x}) - C^0_{ijkl}\bar{\epsilon}^0_{kl} - \left\langle C^0_{mnij}\Gamma_{mnkl}(\mathbf{n})C^0_{klts}\tilde{\epsilon}^0_{ts}(\mathbf{k})\right\rangle_{\mathbf{x}} - \sigma^{\text{appl}}_{ij}\right] \end{aligned}$$

# Phase-Field Model for γ/γ’ Microstructure

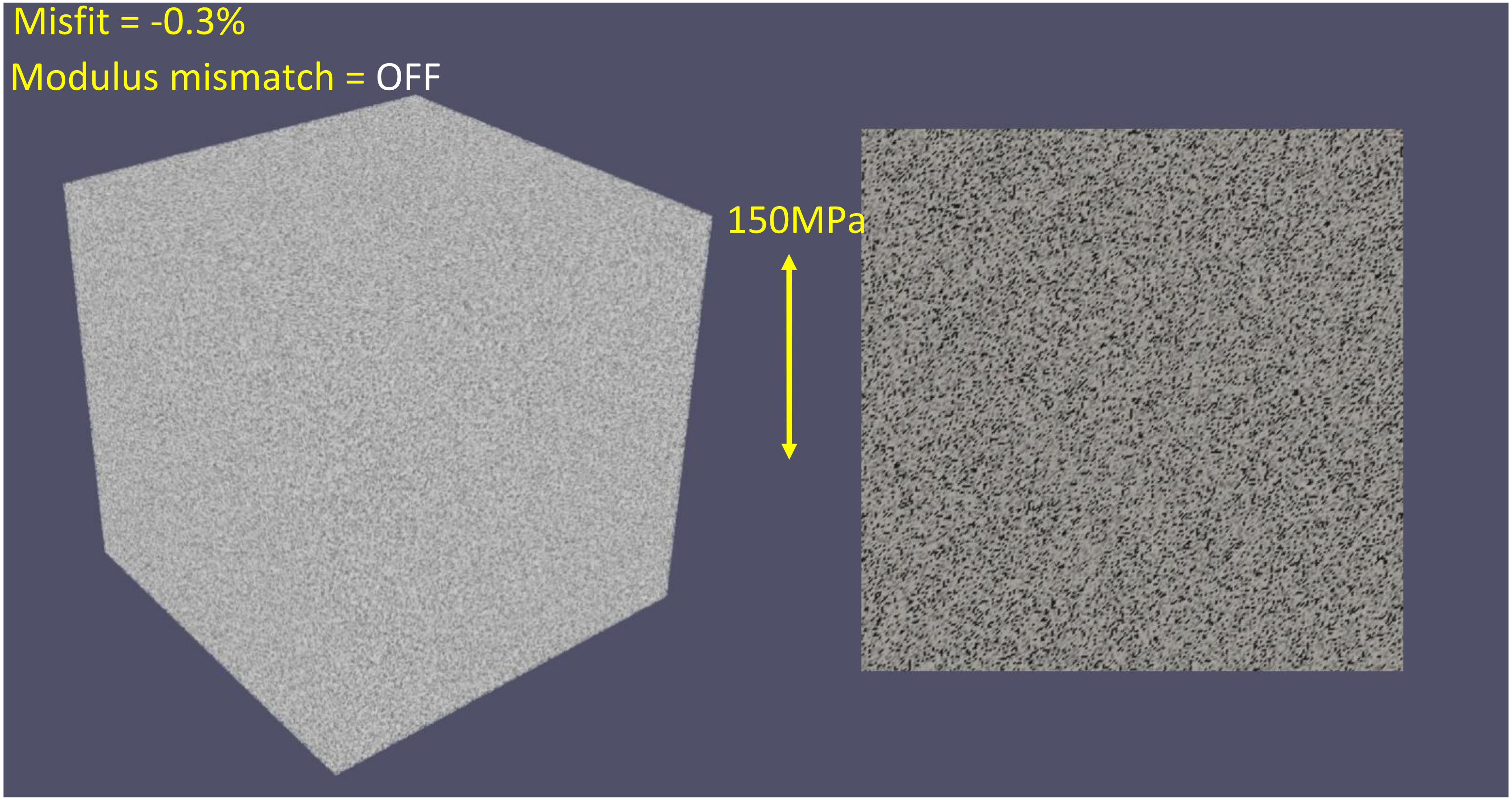


- Misfit -0.3%, inhomogeneous modulus
- 5.12μm^3 (256^3)
- simulation wall time = 1hr by using 64 computing nodes.

# γ' Precipitation subject to Stress



# γ' Precipitation subject to Stress



# Effect of Elastic Modulus Mismatch on γ' Evolution subject to Stress

**W/O modulus mismatch**

**W/ modulus mismatch**

- **In the elastic regime, modulus mismatch and applied stress controls rafted structure.**
- **Similar conclusion has been drawn by many previous works.**

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# Dynamic coupling of phase-field and FFT-CP

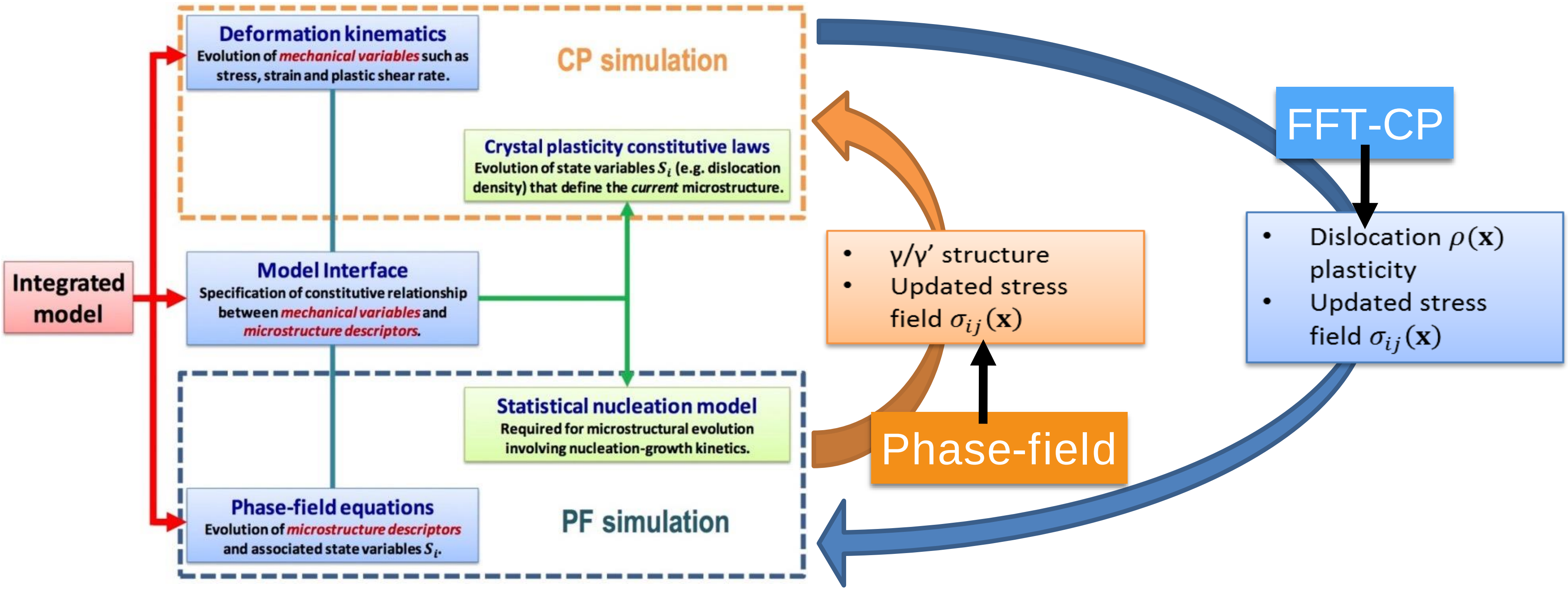
**Elastic strain**
- Satisfy the stress-equilibrium equation

**Transformation strain** (microstructure)
- Use LROs and composition fields to describe the evolution

**Plastic strain** (plasticity)
- Use dislocation density fields to describe the evolution

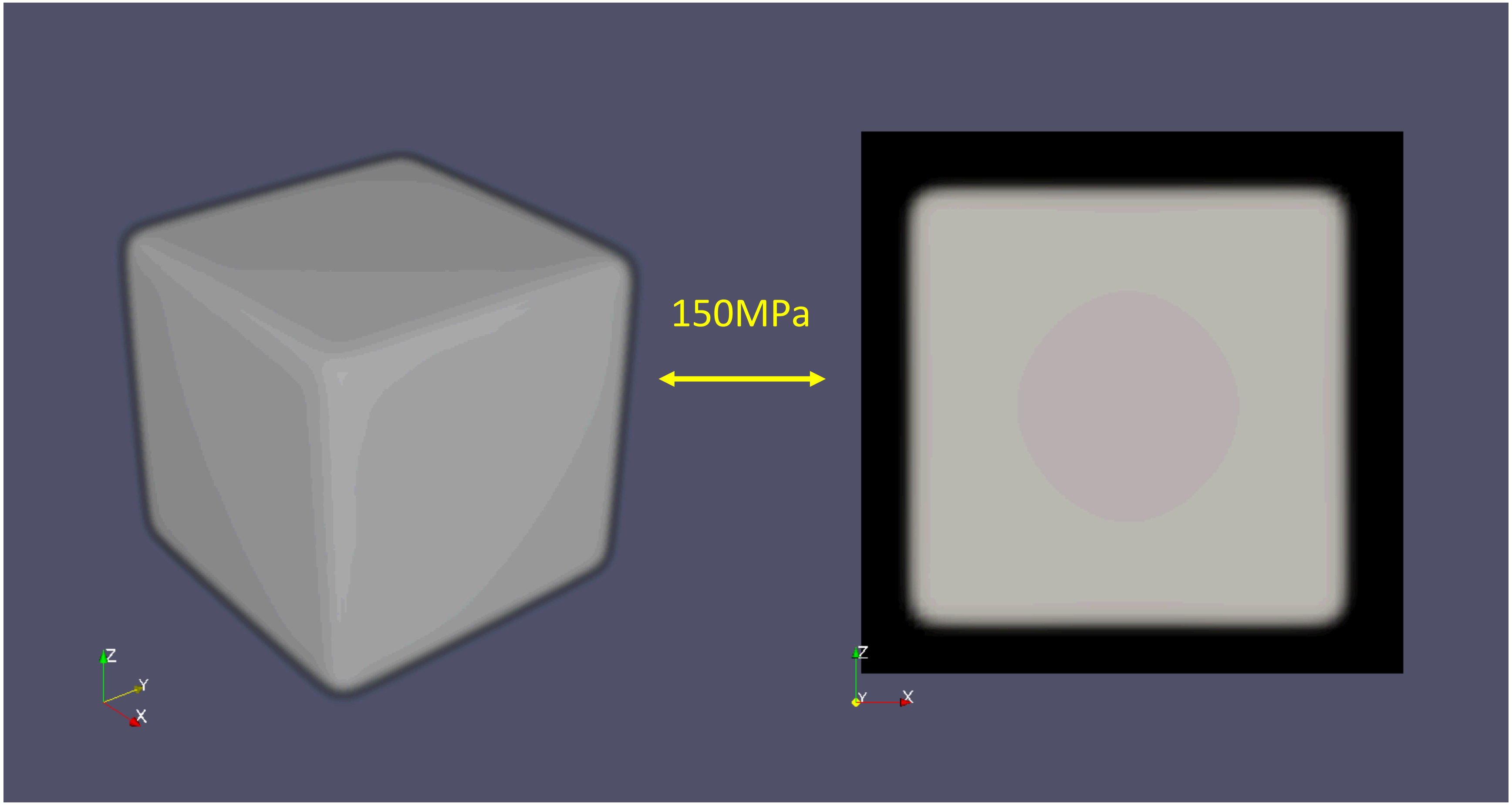
$$\varepsilon_{ij}(\mathbf{x}) = e_{ij}(\mathbf{x}) + \epsilon^{t}_{ij}(\mathbf{x}) + \epsilon^{p}_{ij}(\mathbf{x})$$

Cottura, M., et al. *JMPS*, 94 (2016): 473.




Zhao, Low, Wang, and Niezgoda IJP, 80(2016): 38

# Integrating Modeling: W/O Plasticity



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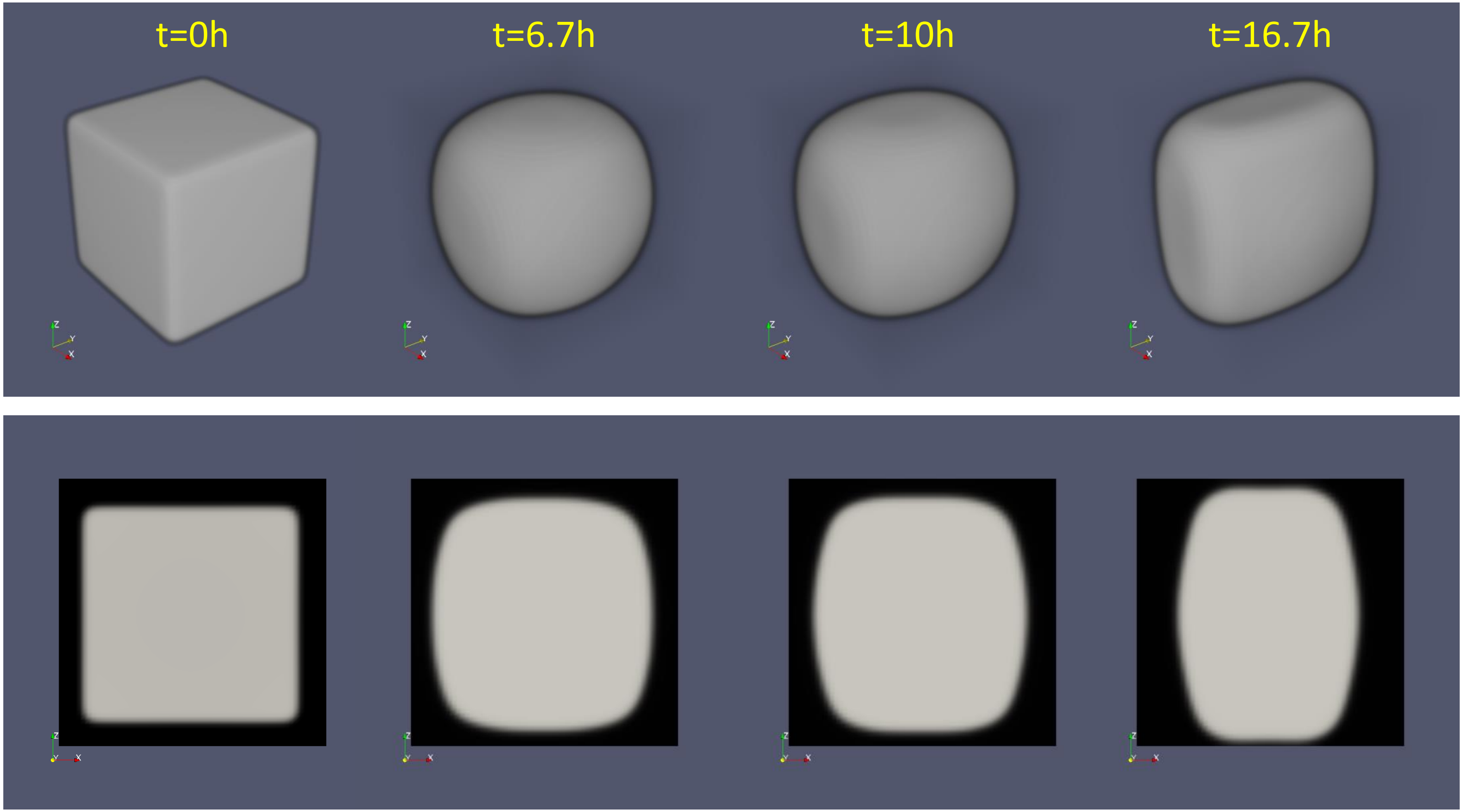
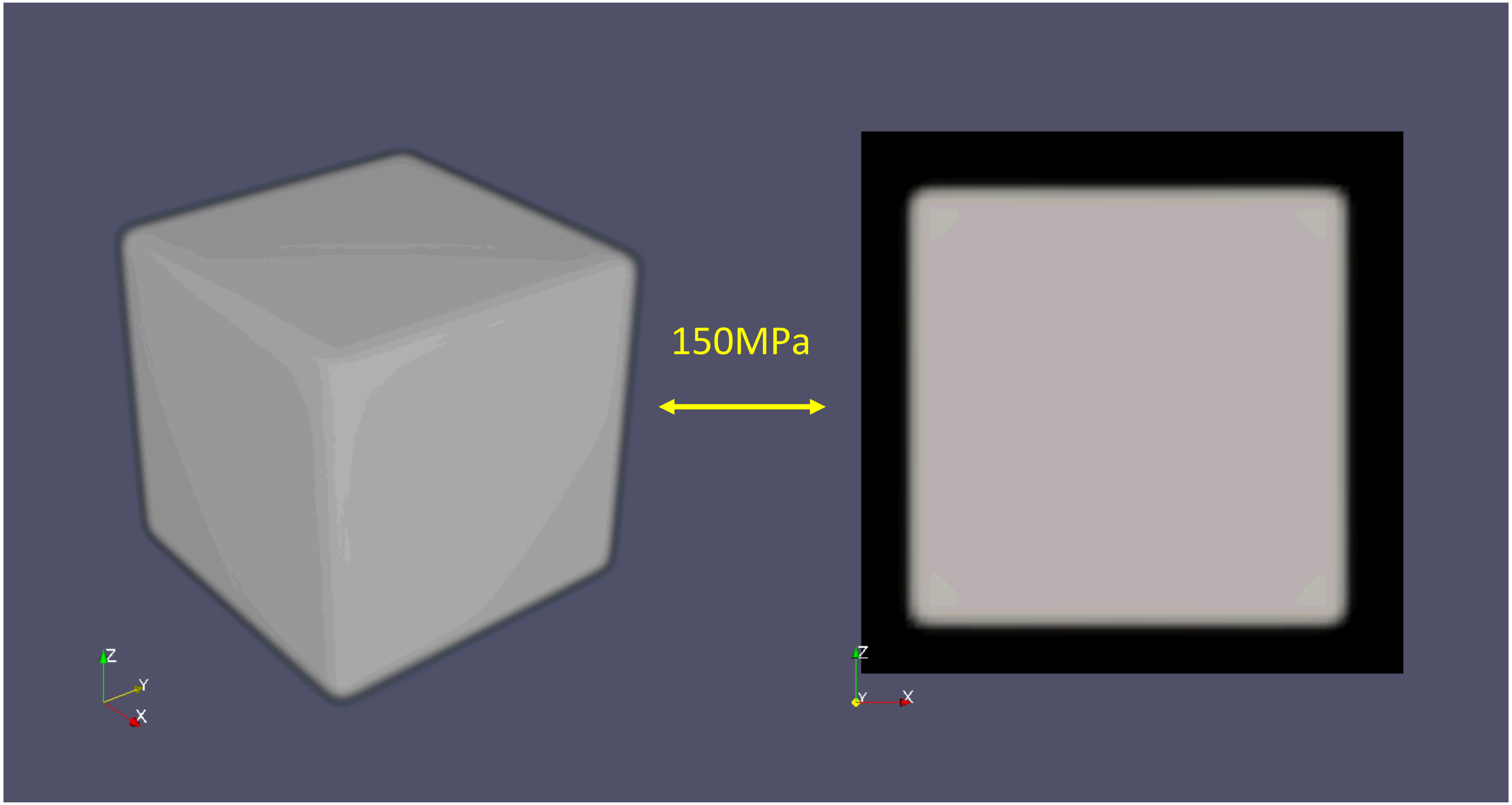
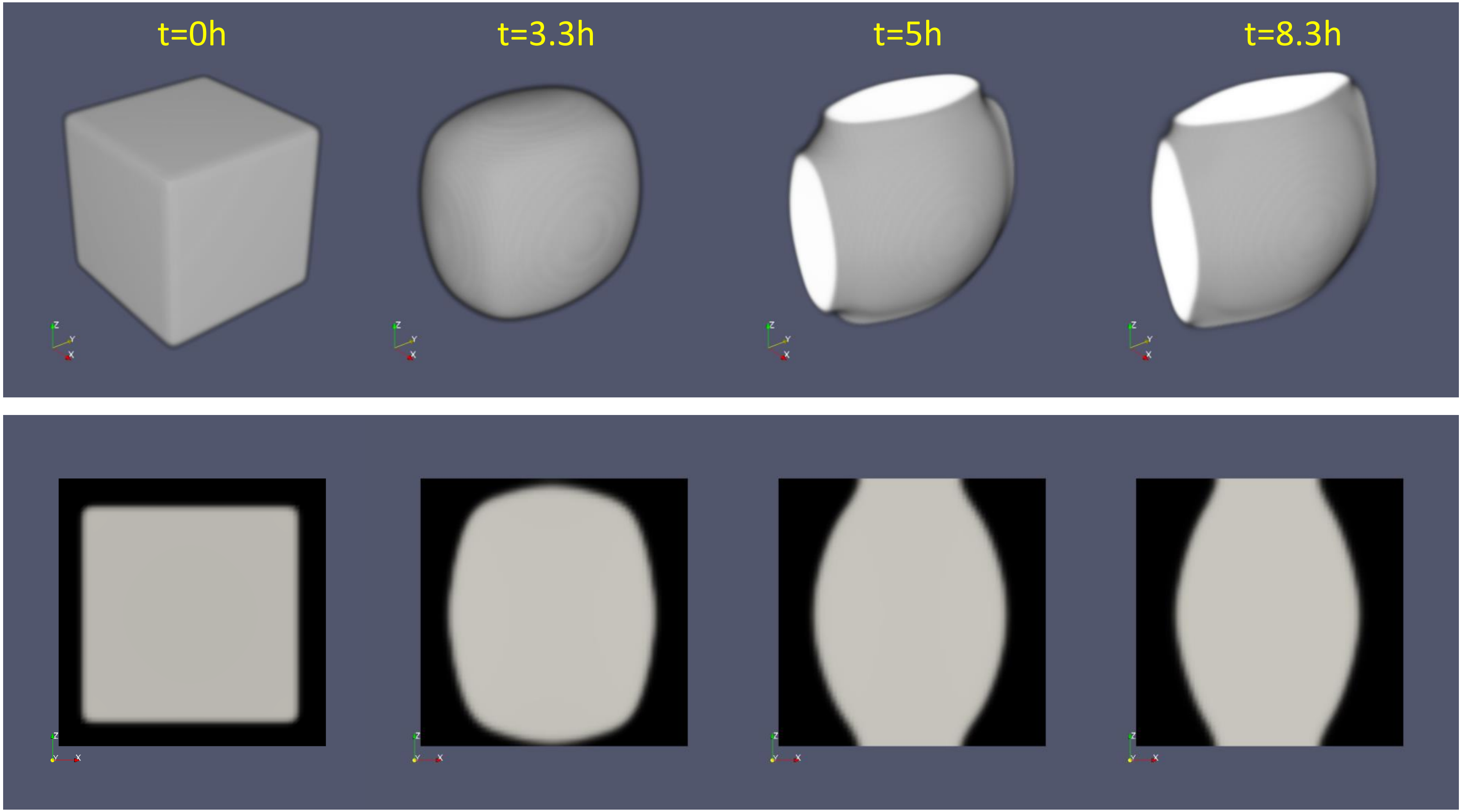



- To have a complete raft structure takes over 20h
- The final raft has a flat γ/γ' interface perpendicular to the tensile axis.

# Integrating Modeling: W/ Plasticity

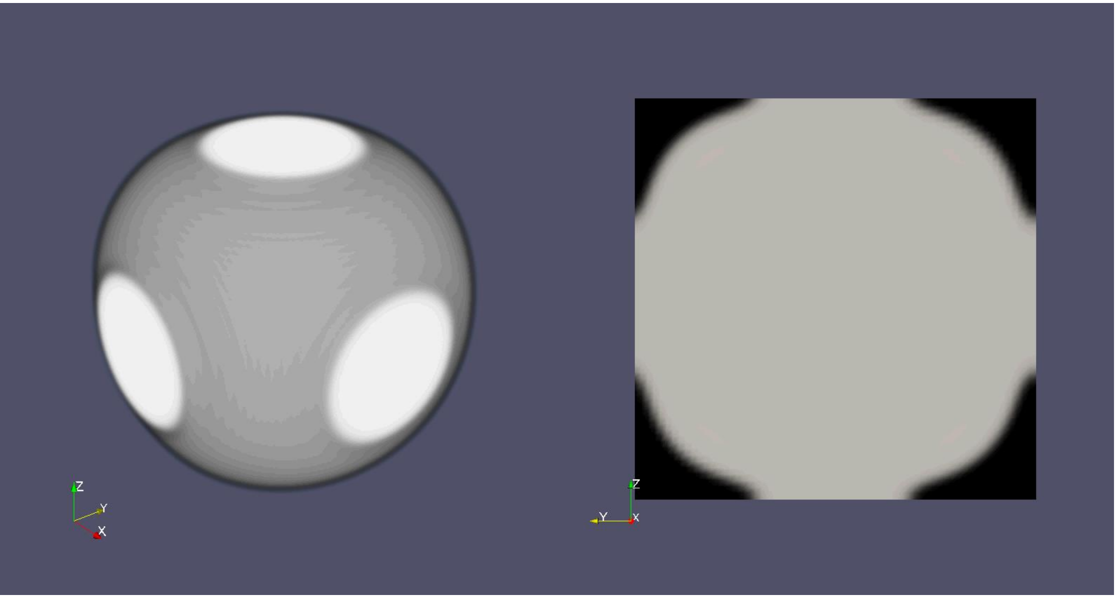


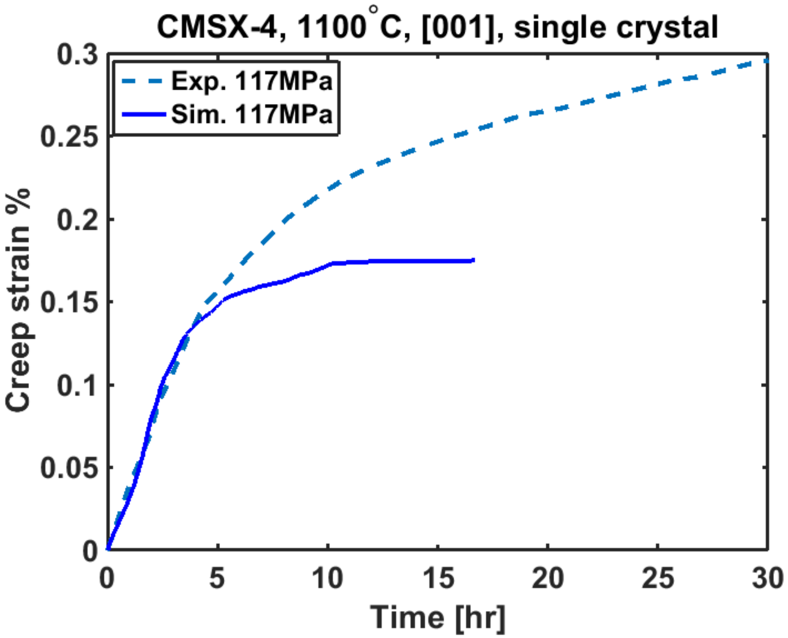
# Integrating Modeling: W/ Plasticity




- **Rafting process is accelerated by ~3 times**
- **The final raft has a wavy γ/γ' interface**

# Quantitative Example: CMSX-4 (ongoing)






- **The primary creep can be faithfully captured by the current integrated model.**
- **Transition to secondary creep in alloys with high volume fraction of γ’ requires particle shearing mechanisms.**
- **More realistic RVE is needed for future studies.**

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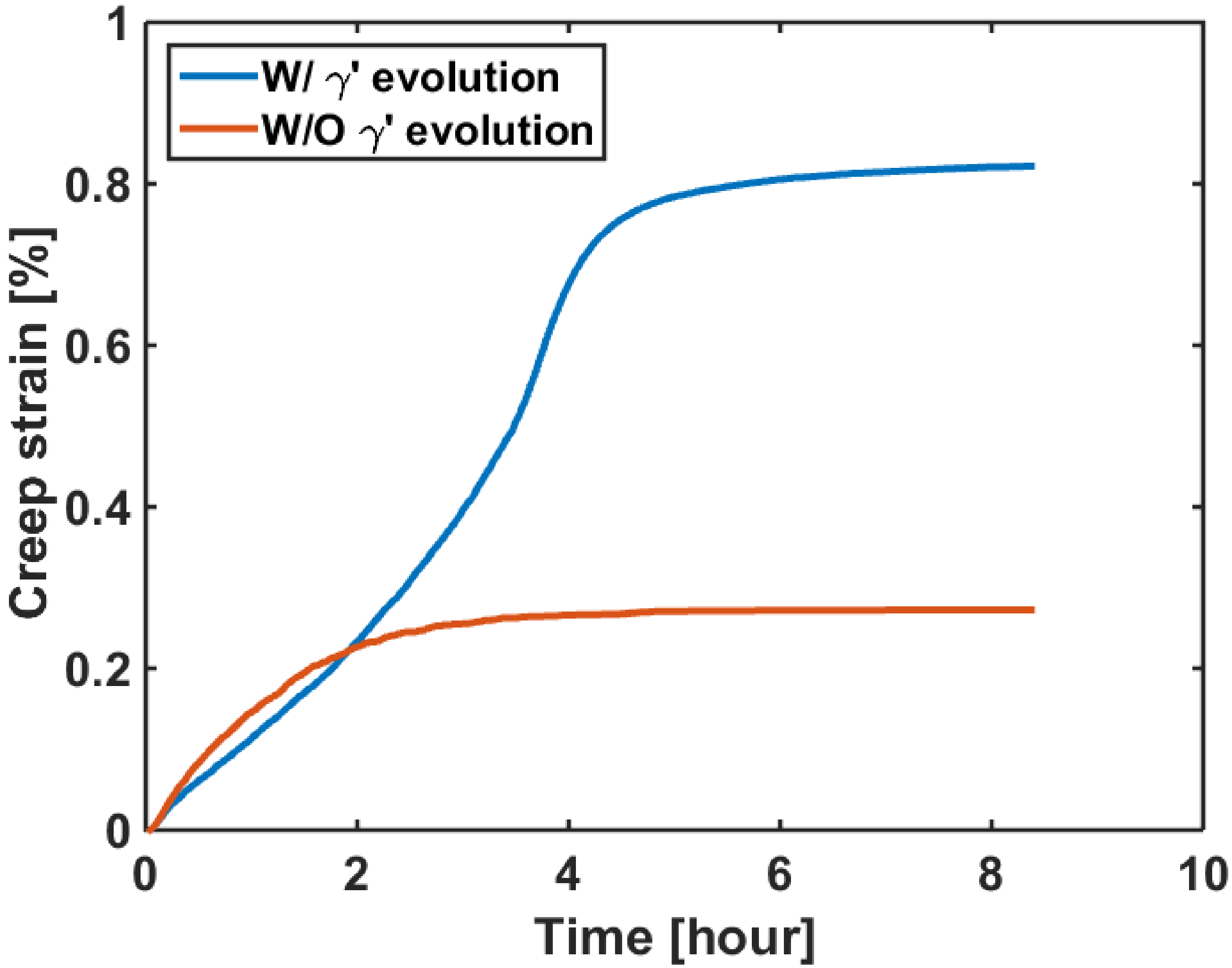
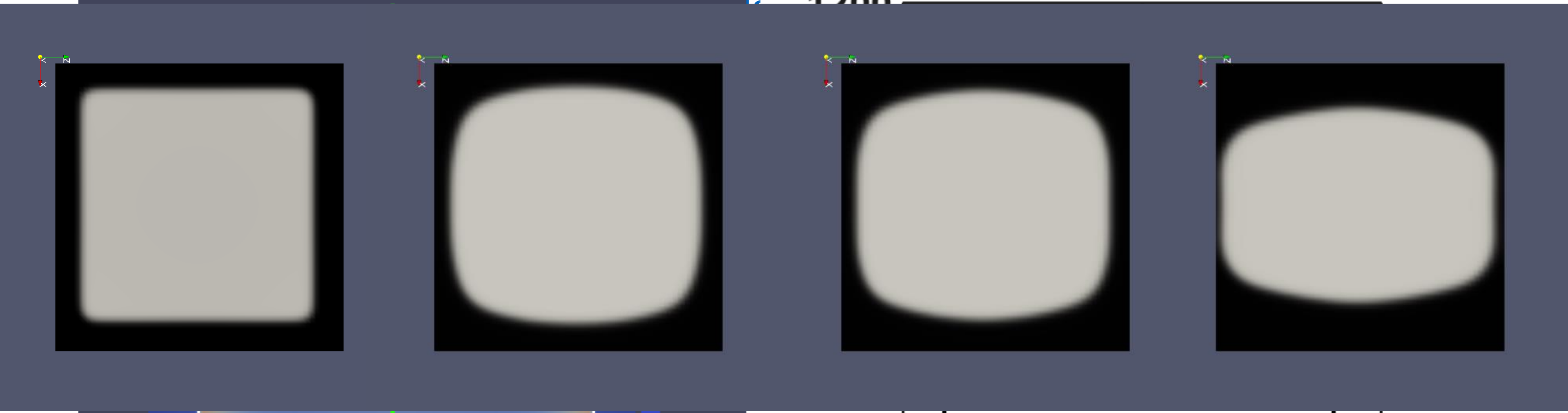
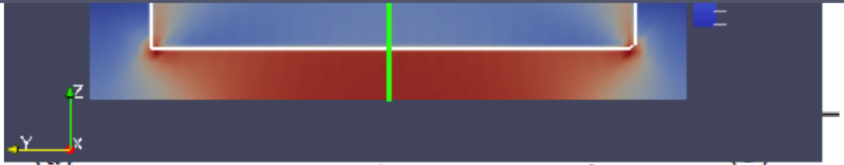
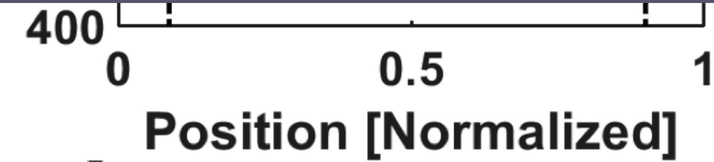
# γ’ Evolution Can Accelerate Creep







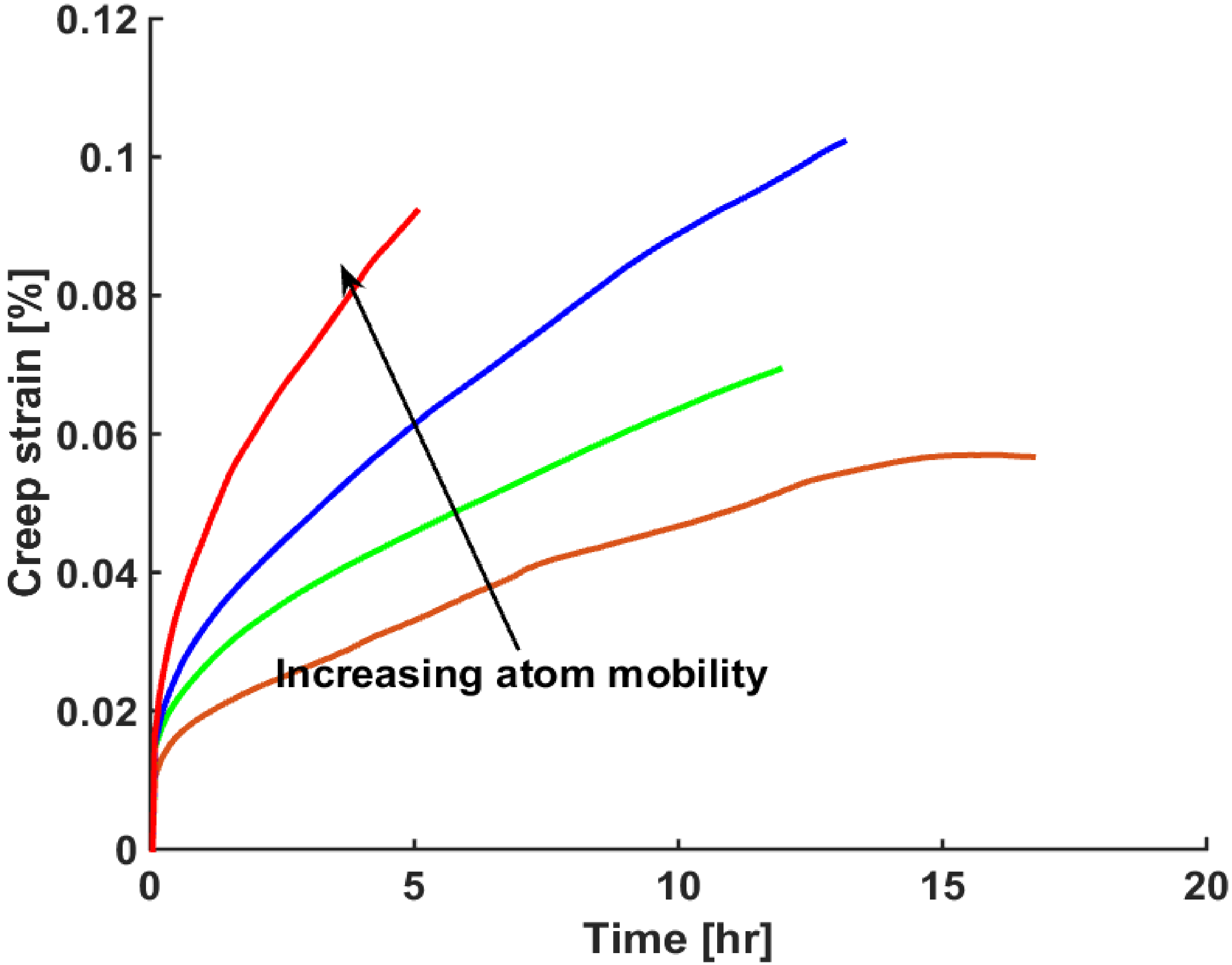



Negative lattice misfit
(Kamaraj, 2003.)

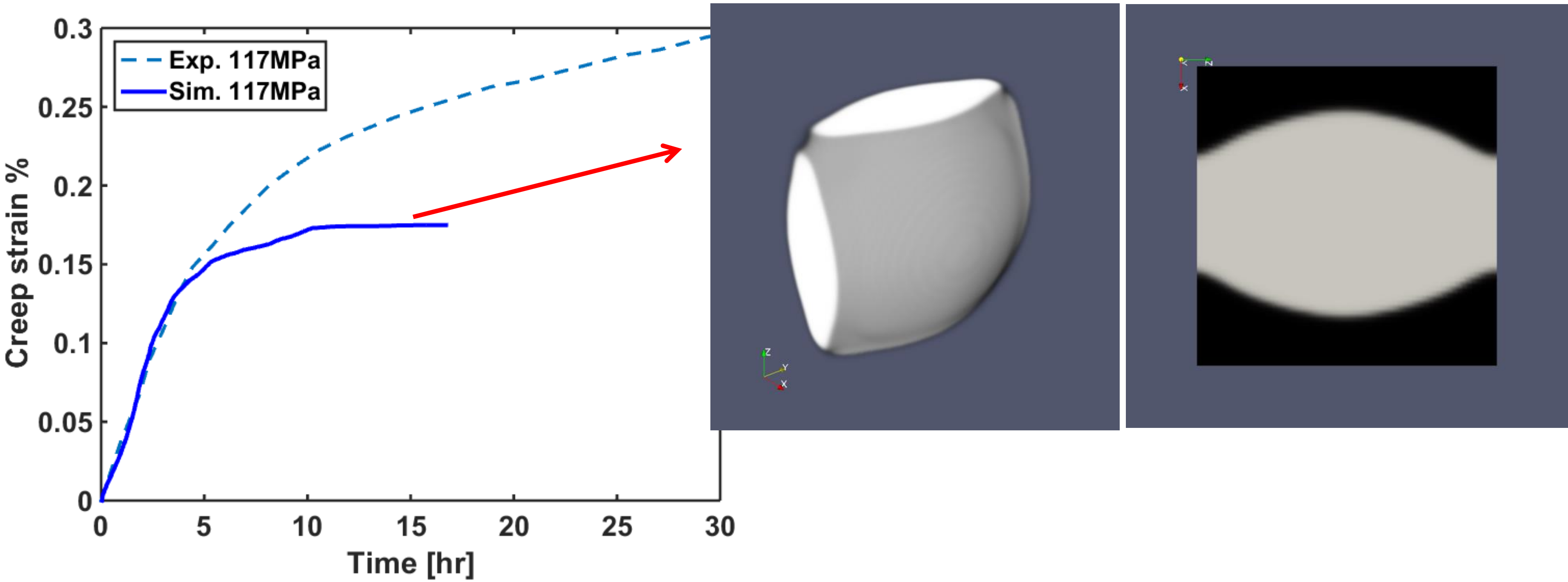
## The interplay between plasticity and microstructure:

- Dislocation glide should primarily occur in the horizontal channels
- The γ' directional coarsening eliminates the vertical channels and widen the horizontal channels.
- The increase of horizontal channel volume fraction accelerates dislocation glide, leading to the experimentally observed high primary creep rate.

# Parametric Study: Effect of Atomic Mobility



# Wavy γ/γ' Interface Stabilized by Plasticity



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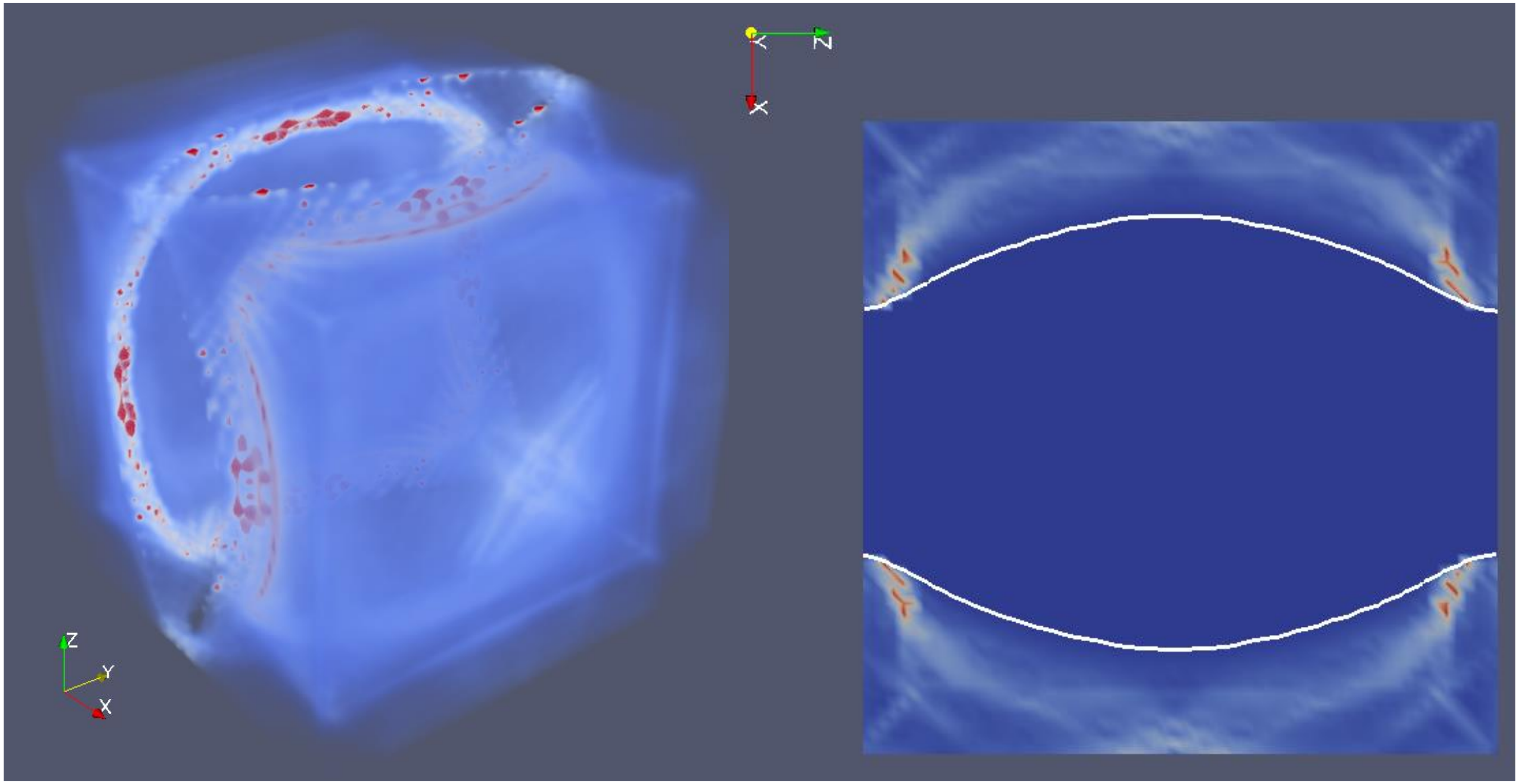
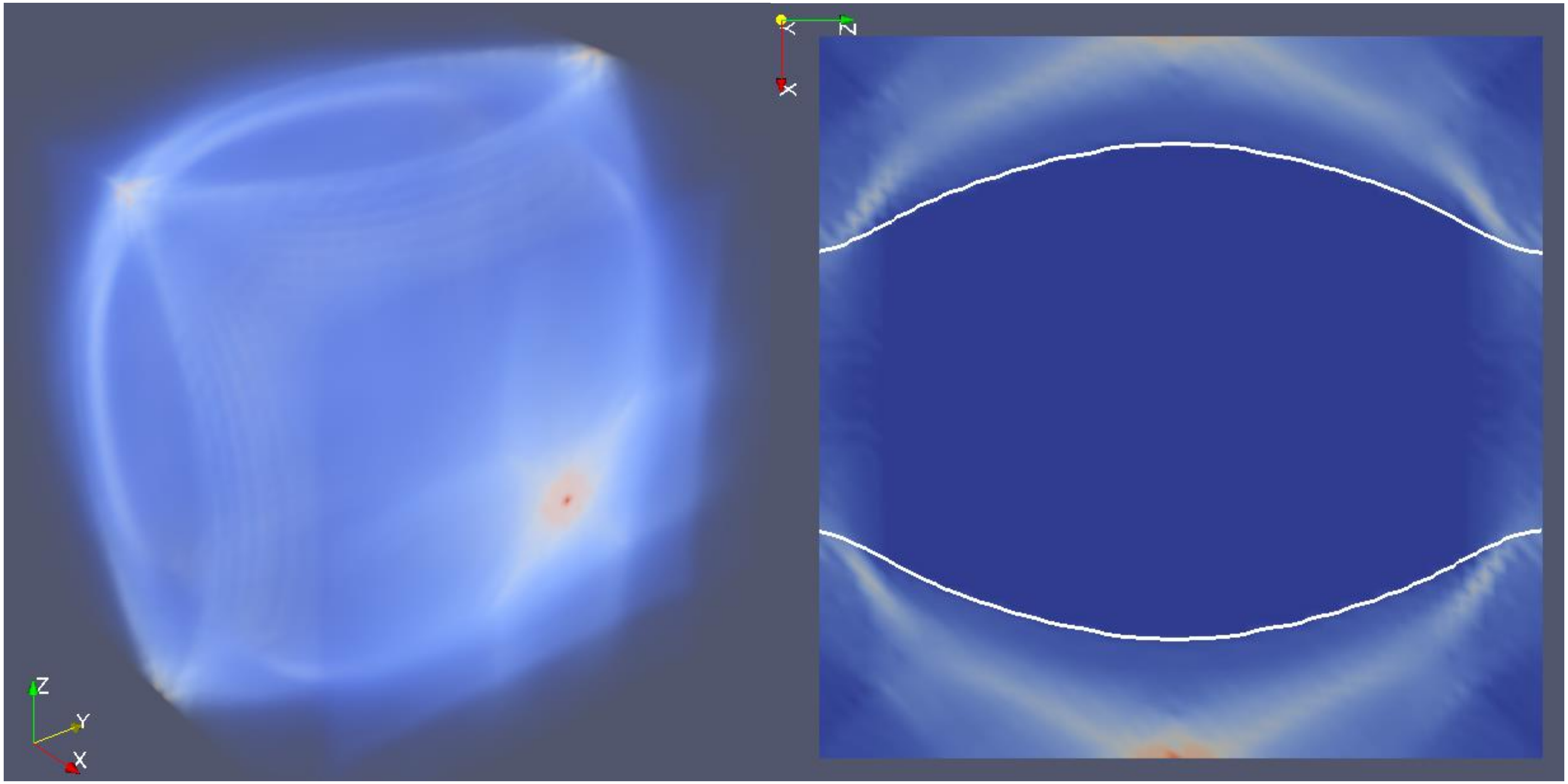


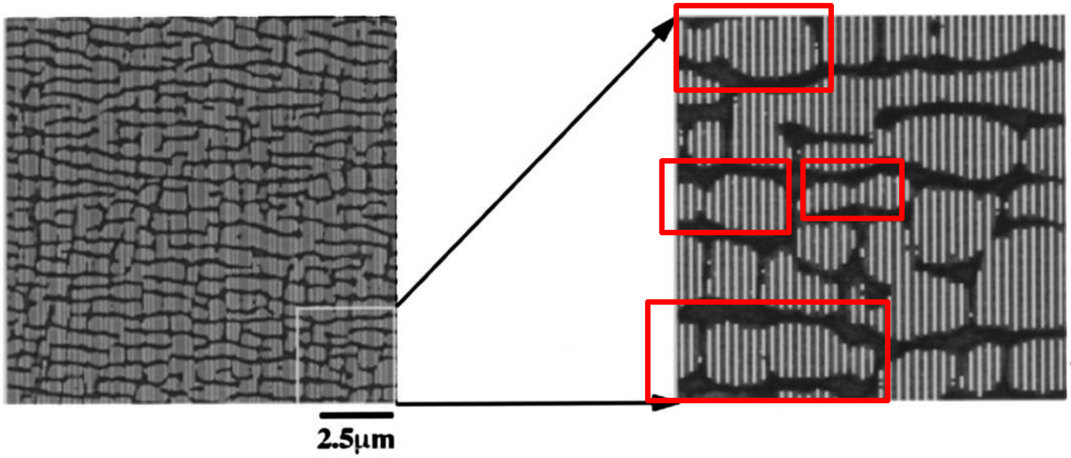

**Geometrically necessary dislocation (GND) density**

# Wavy γ/γ' Interface Stabilized by Plasticity

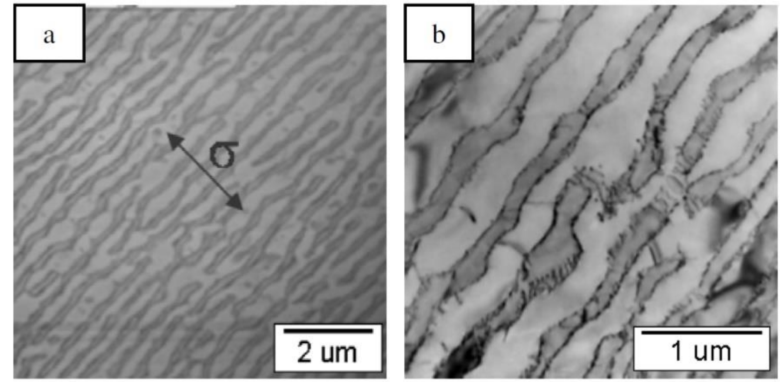



**Plastic strain distribution**

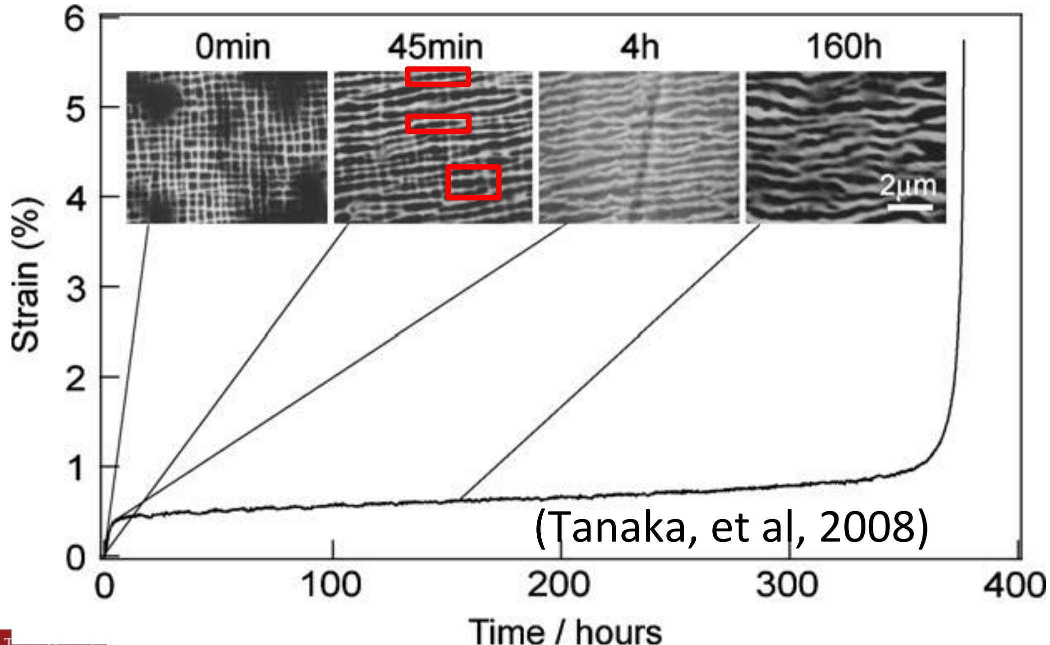
# Wavy γ/γ' Interface in Experiments



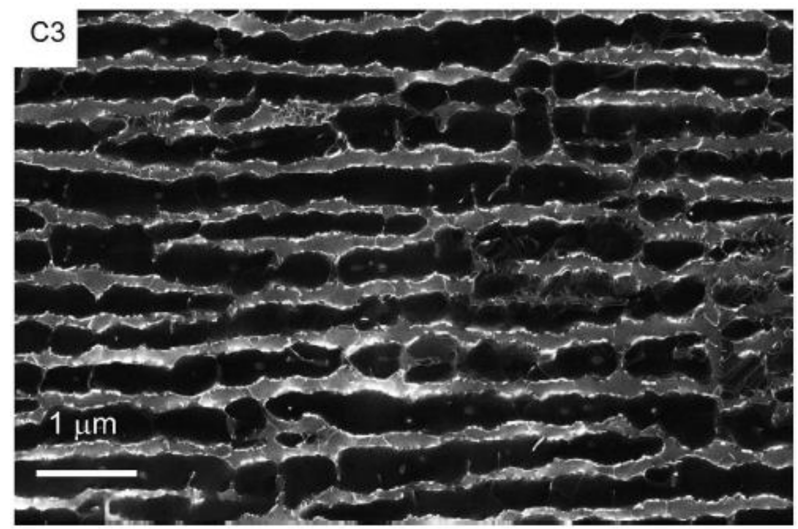

CMSX-4, 0.27% creep strain (Matan, Reed, et al, 1999)



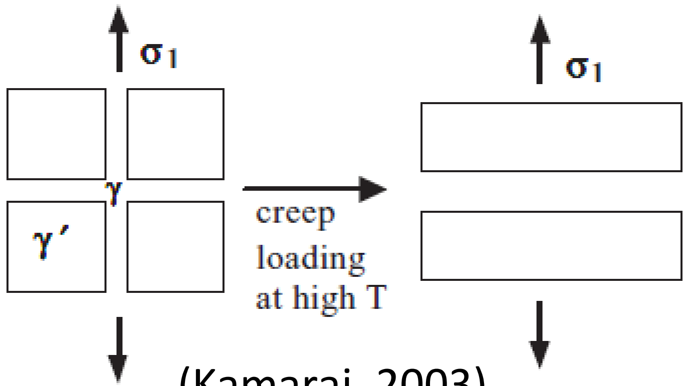

PWA1484, 1.0% creep strain
(Czyrska-Filemonowicz, et al, 2007)




(Tanaka, et al, 2008)




(Ram, et al, 2016)




(Kamaraj, 2003)

## Diffusion-driven boundary migration

Diffusion potential defined in our model

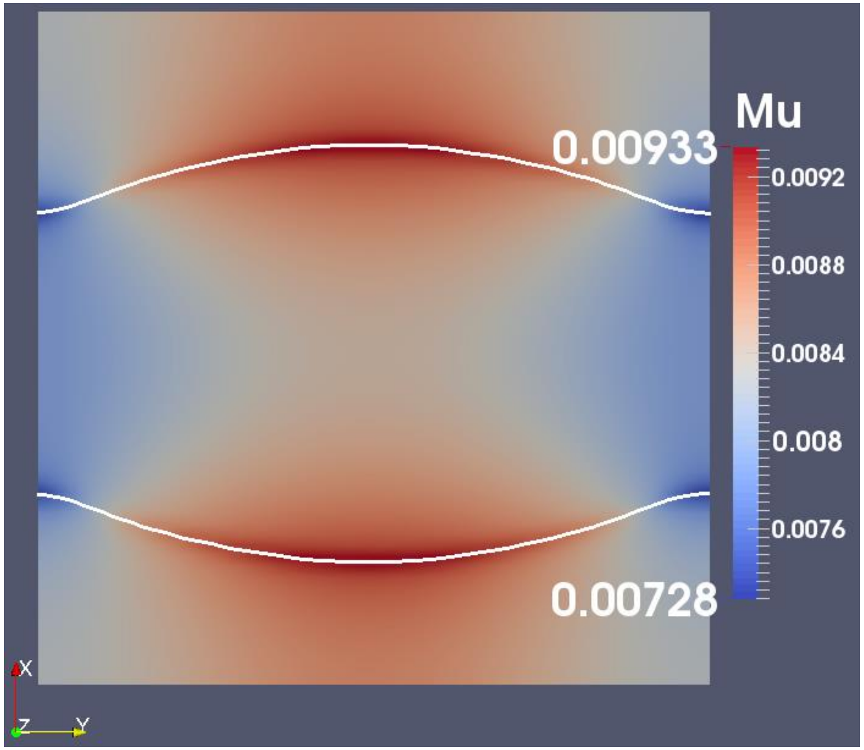
$$F = \int_V \left[ f\left(c(\mathbf{x}), \{\phi_i(\mathbf{x})\}_{i=1}^{4}\right) + \frac{\kappa^2}{2} \sum_{i=1}^{4} \left(\nabla\phi_i(\mathbf{x})\right)^2 \right] dV + E^{\mathrm{elast}}$$

$$\mu^{\mathrm{diff}}(\mathbf{x}) = \frac{\delta F[c(\mathbf{x}), \phi_i(\mathbf{x})]}{\delta c(\mathbf{x})} = \frac{2f_0}{V_m}\left[c(\mathbf{x}) - c_e^{\mathrm{m}} - h[\phi_i(\mathbf{x})]\Delta c_e^0\right]$$

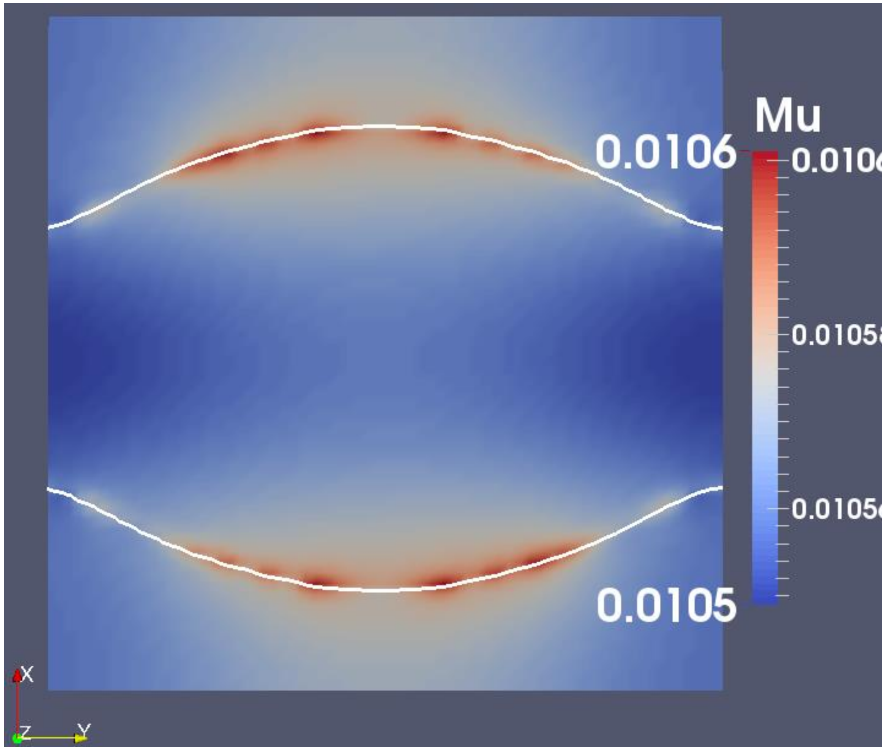
- The dependence of diffusion potential on elasticity is implicit, but significant as to be shown.

# $\mu^{\text{diff}}$ from Simulations

W/O plasticity




W/ plasticity

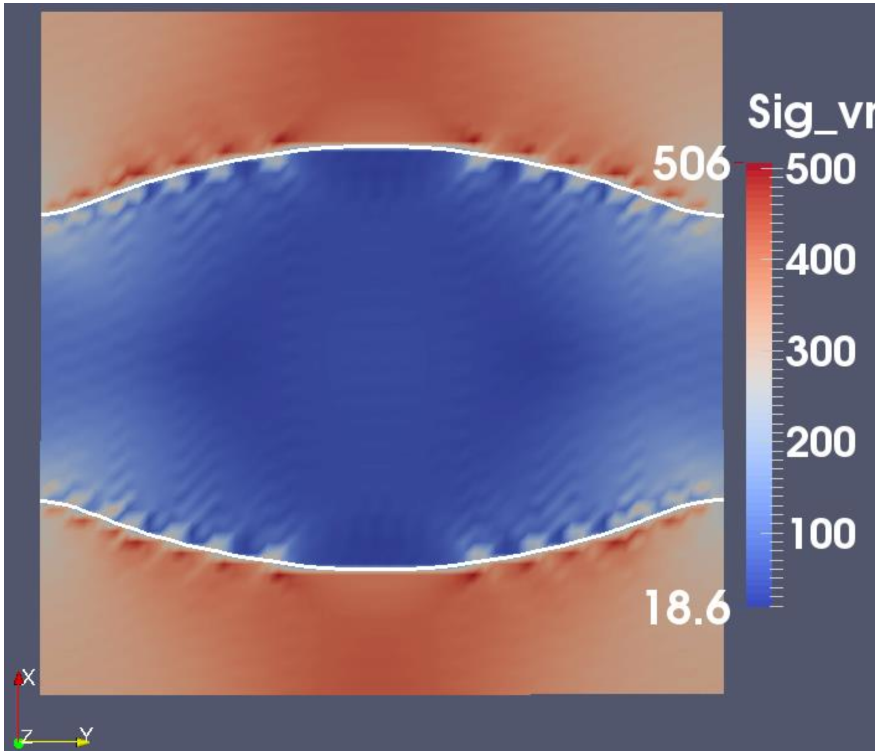



$$\frac{\max(\mu^{\text{diff}}) - \min(\mu^{\text{diff}})}{\min(\mu^{\text{diff}})} = 28.2\%$$

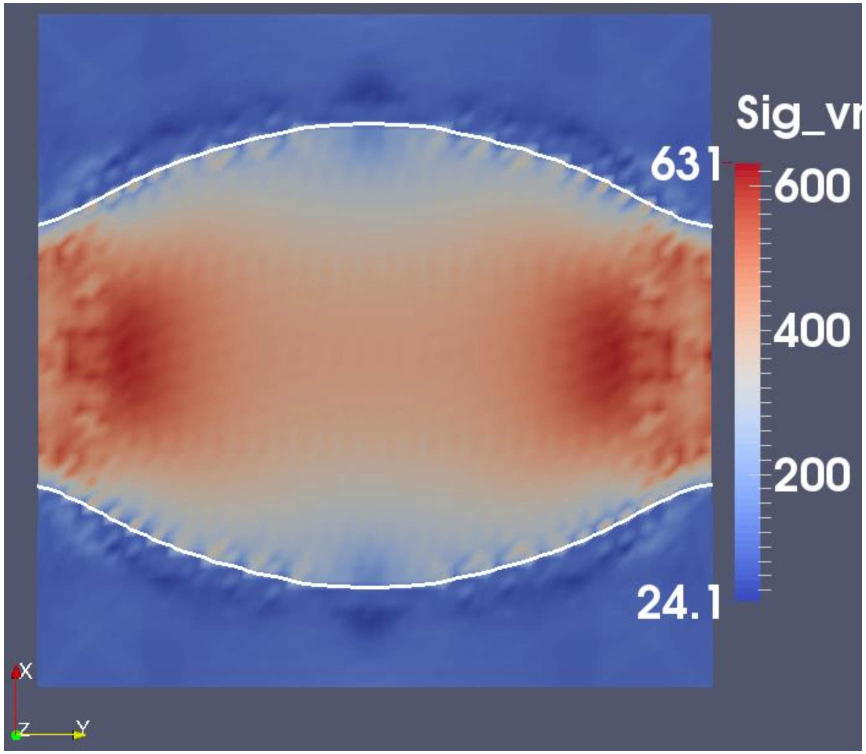
$$\frac{\max(\mu^{\text{diff}}) - \min(\mu^{\text{diff}})}{\min(\mu^{\text{diff}})} = 1.0\%$$

# Stress from Simulations

W/O plasticity




W/ plasticity




- Stress is drastically different when relaxation via plasticity is allowed.

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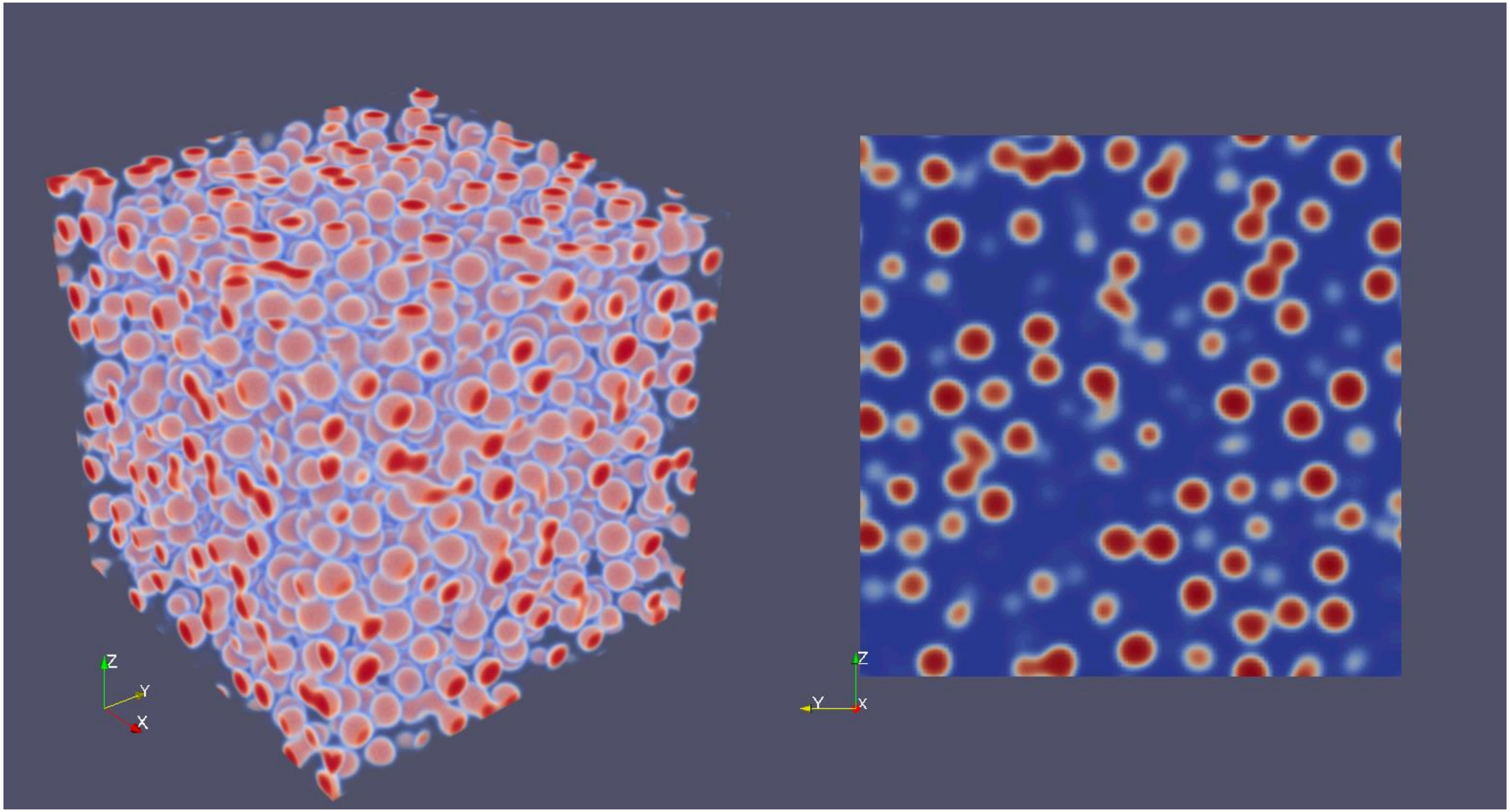
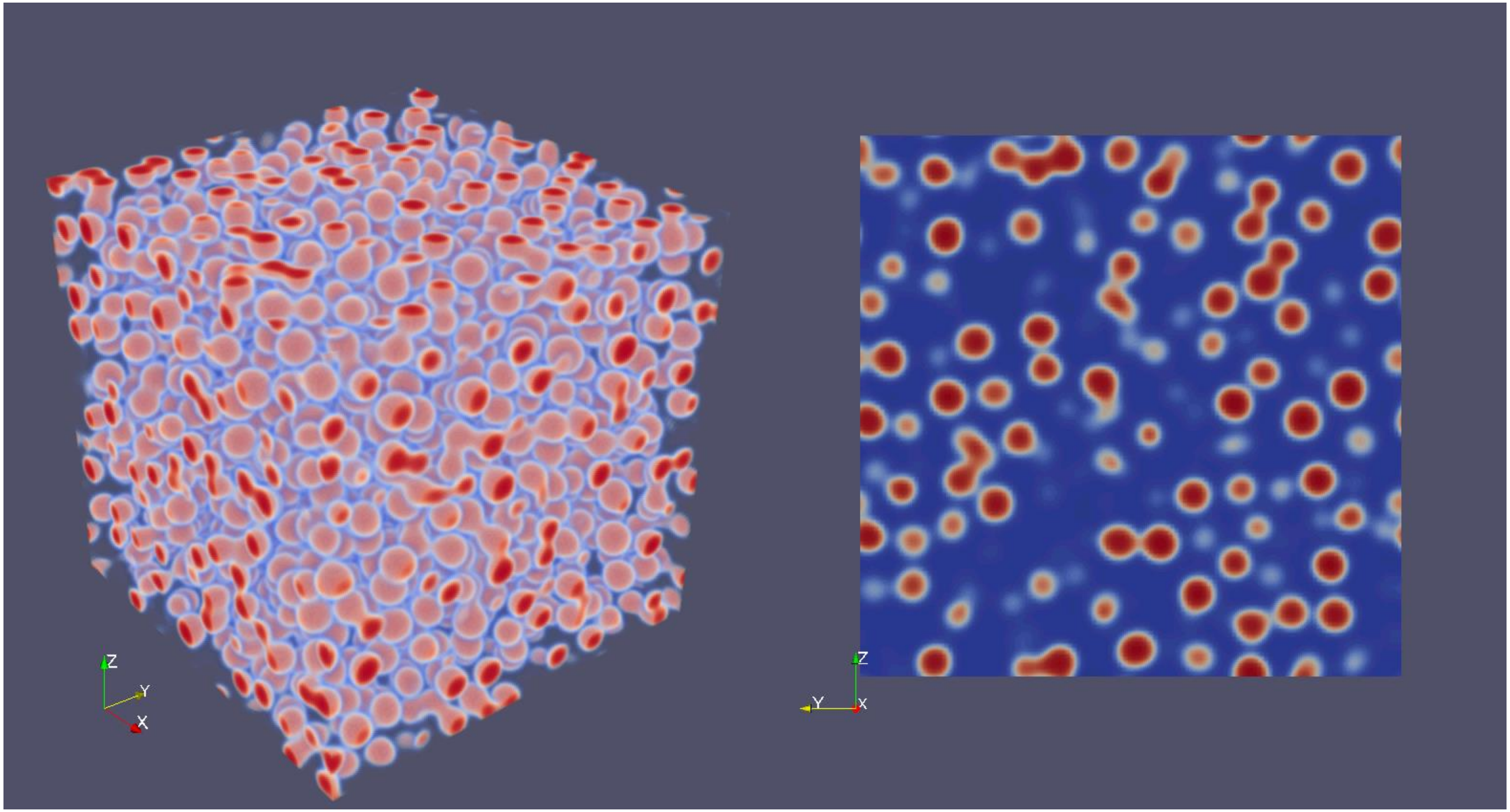
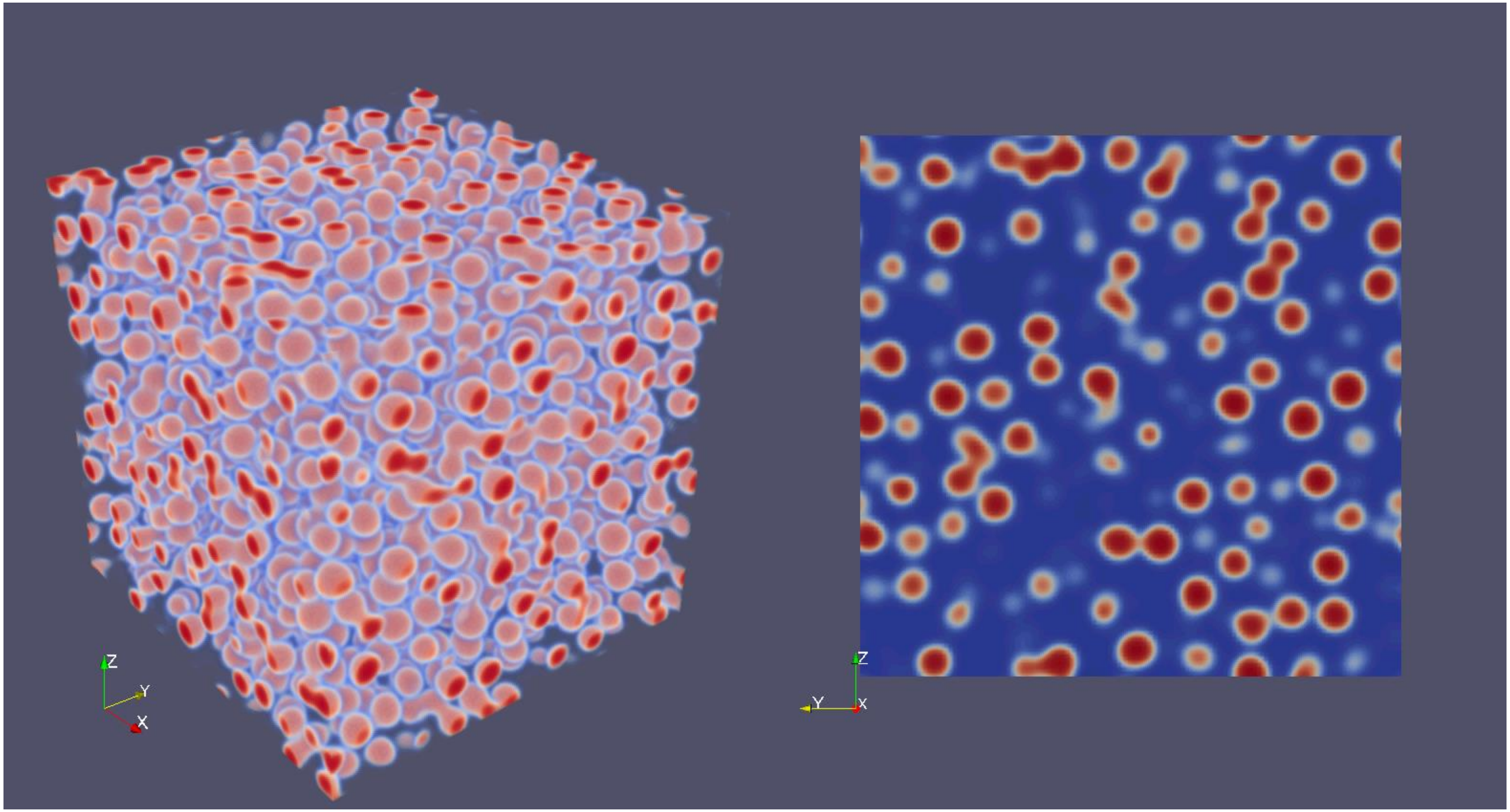
# H282, static aging (W/O stress)



# H282, stress aging (W/O plasticity)

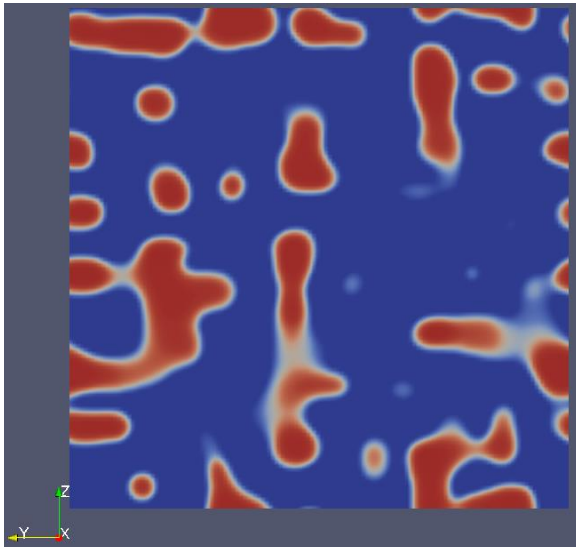


# H282, stress aging (W/ plasticity)

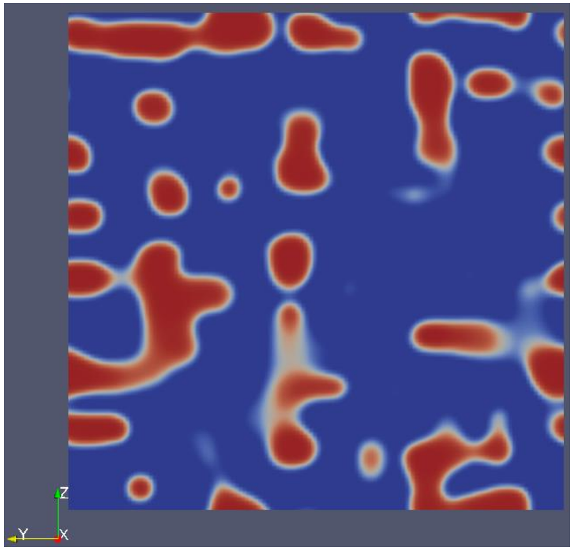


# Plasticity Can Stabilize Small Precipitates

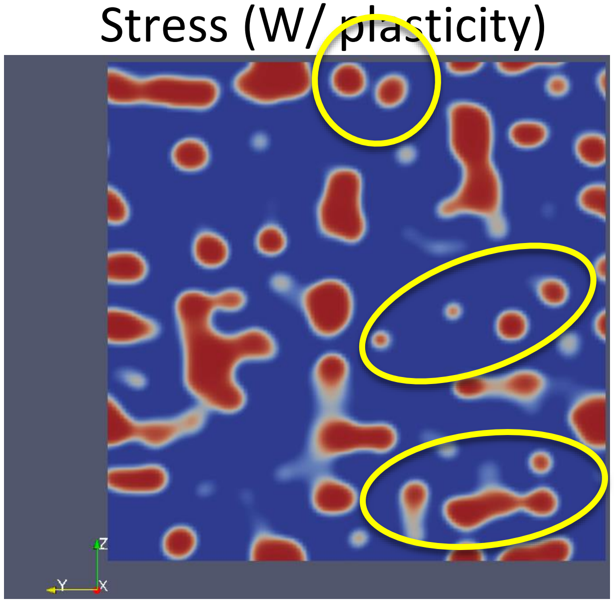
Static (W/O stress)




Stress (W/O plasticity)




Stress (W/ plasticity)



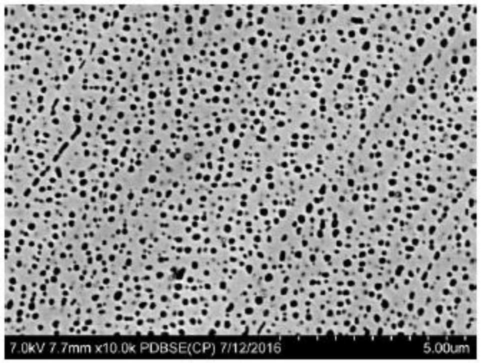

- **The dynamics of static and stress W/O plasticity are approximately the same in terms of number of γ' particles.**
- **The number of γ' particles for stress W/ plasticity is apparently larger than the other two cases.**

# Experiments on H282

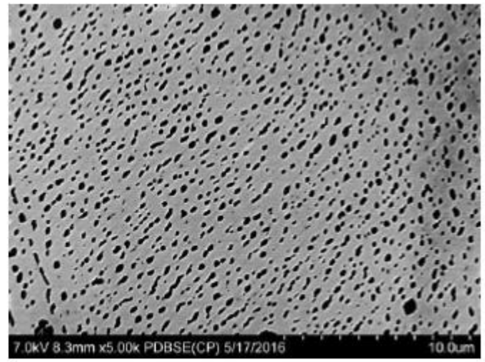
## Intragranular γ′ Evolution: Static Exposure vs Creep

**Creep**

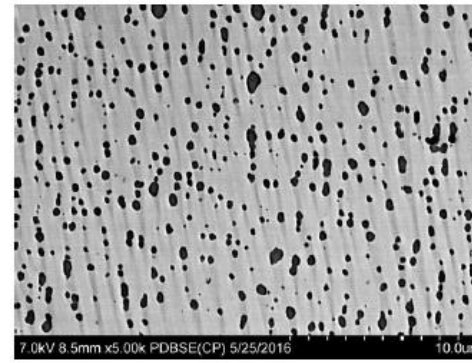
1500F/25ksi/1606hrs




1600F/15ksi/1678hrs

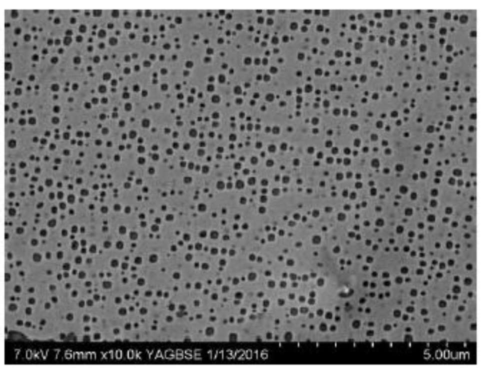



1700F/8ksi/1000hrs

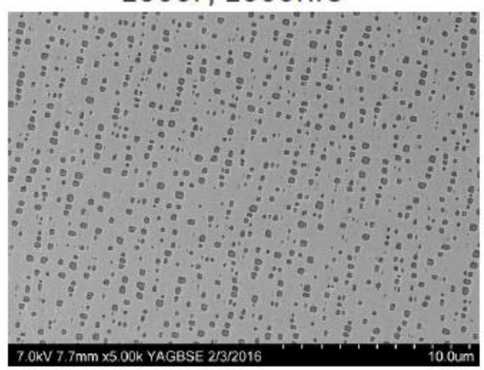



**Static Exposure**

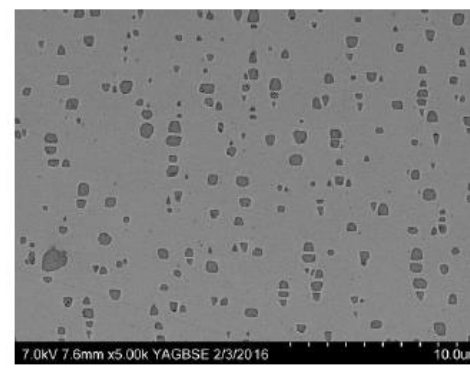
1500F, 1000hrs




1600F, 1000hrs

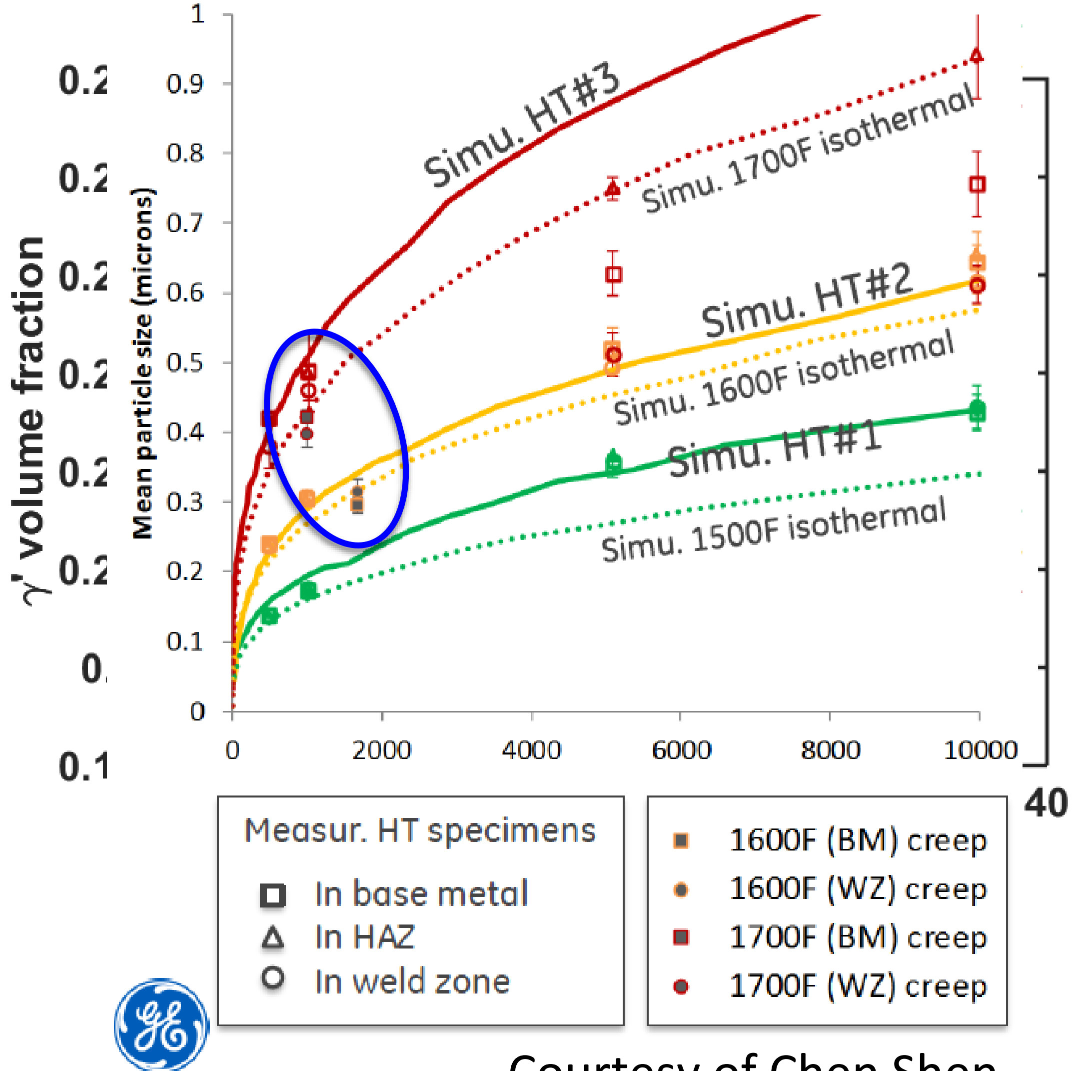



1700F, 1000hrs




Courtesy of Chen Shen

# Plasticity Leads to Smaller Average γ' Size




Courtesy of Chen Shen

- **Adding plasticity promotes more dissolution of γ'**
- **Combined with the (seemingly) increased number density due to plasticity, the average γ' size is expected to be smaller than that during static exposure.**

# Summary

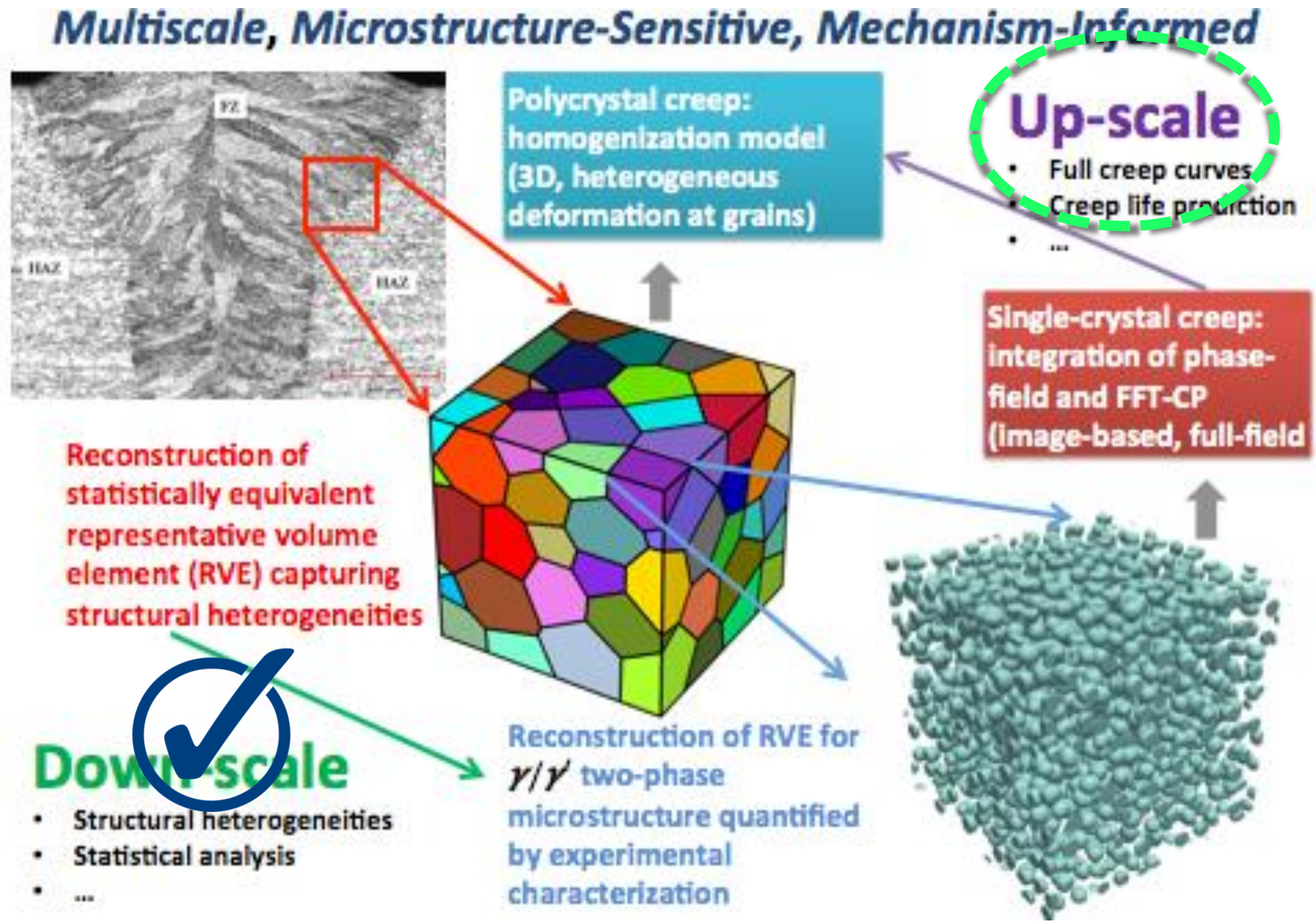
- **An integrated full-field creep model for single crystal Ni-base superalloys has been developed**

 γ' evolution can accelerate creep

 Plasticity can stabilize wavy γ/γ' Interface

 Plasticity can stabilize small γ' particles in alloys like H282 and lead to a smaller average particle size

# Next Steps



Multiscale, Microstructure-Sensitive, Mechanism-Informed
FZ
HAZ
HAZ
Polycrystal creep: homogenization model (3D, heterogeneous deformation at grains)
Up-scale
• Full creep curves
• Creep life prediction
• ...
Single-crystal creep: integration of phase-field and FFT-CP (image-based, full-field
Reconstruction of statistically equivalent representative volume element (RVE) capturing structural heterogeneities
Down-scale
• Structural heterogeneities
• Statistical analysis
• ...
Reconstruction of RVE for $\gamma/\gamma'$ two-phase microstructure quantified by experimental characterization

# Thank you for listening!

# FFT-CP Model for γ/γ' superalloys

In the analytic expression of inter-particle spacing, cubic array is assumed

$$\lambda_p = 1.6 r_p \left[ \sqrt{\frac{\pi}{4 f_p}} - 1 \right]$$

***Experimentally identified dislocation-precipitate interaction features in alloys like HA282:***

- **Full matrix dislocations** serve as the dominant plasticity carriers

- Depends only on $f_p$ and average $r_p$
- Still missing microstructural inhomogeneity.

**Our solution**:
Introduce the *location-dependent* nearest-neighbor (NN) distance $d_{\mathrm{NN}}(\mathbf{x})$ to measure the *local* "channel width", which will lead to spatially variation of Orowan strength.

**For Orowan loop, the critical stress is:**

$$\tau_{\mathrm{Oro}} = \frac{0.84\mu b}{2\pi(1-\nu)^{1/2}} \frac{\ln(R_0/r_0)}{\lambda_p}$$

Where
- $\mu$ - shear modulus, $\nu$ – Poisson's ratio
- $b$ – Burgers vector magnitude
- $R_0$ and $r_0$ - outer and inner cutoff radius
- $\lambda_p$ - inter-particle spacing

**For climb/bypass, a Dyson's model yields:**

$$\dot{\gamma}^{\alpha} = \rho_{\mathrm{es}}^{\alpha} f_p \frac{\lambda_p}{r_p} c_{\mathrm{jog}} D_s \sinh\left(\frac{\tau_{\mathrm{eff}} b^2 \lambda_p}{k_B T}\right)$$

Where
- $\rho_{\mathrm{es}}$ - escaped dislocation density
- $c_{\mathrm{jog}}$ – dislocation line jog density
- $f_p$ - particle volume fraction
- $r_p$ - particle radius
- $D_s$ - volume diffusivity

# At tensile conditions:

## Orowan-type ($\dot{\gamma} = \rho v b$) kinetic equation:

$$\dot{\gamma}^\alpha = \begin{cases} 0, & |\tau^\alpha| \le \tau^\alpha_{\text{pass}} \\ \dot{\gamma}^\alpha_0 \exp\left[-\frac{Q_{\text{slip}}}{k_B T}\right] \sinh\left[\frac{|\tau^\alpha| - \tau^\alpha_{\text{pass}} - \tau^\alpha_{\text{oro}}}{\tau^\alpha_{\text{cut}}}\right] \text{sign}(\tau^\alpha), & |\tau^\alpha| > \tau^\alpha_{\text{pass}} \end{cases}$$

**Our solution**: $\tau^\alpha_{\text{oro}}$ accounts for the slip resistance due to dispersed $\gamma'$ particles

# At creep conditions:

## Climb/bypass kinetic equation:

$$\dot{\gamma}^\alpha = \rho^\alpha_{\text{es}} f_p \left(\frac{\lambda_p}{r_p}\right) c_{\text{jog}} D_s \sinh\left(\frac{\tau_{\text{eff}} b^2 \lambda_p}{k_B T}\right)$$

**Our modification:**

- Location-dependent $\lambda_p$ using NN scheme is used.
- Escaped dislocations: $\rho^\alpha_{\text{es}} = \rho^\alpha_M * \eta$, where $\eta$ is the reaction rate of dislocations climbed and by-passed the particle for any given time.
- $\tau_{\text{eff}} = \tau_{\text{app}} - \tau_{\text{pass}} - \tau_{\text{back}}$ where the additional back stress $\tau_{\text{back}}$ due to the climb is a modification to Dyson's model.
- Same full-field dislocation evolution equations as in tensile condition are used.