# A Consistent Elastoplastic Phase-field Framework for Microstructure Evolution Modeling of High Temperature Materials

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U.S. DEPARTMENT OF ENERGY

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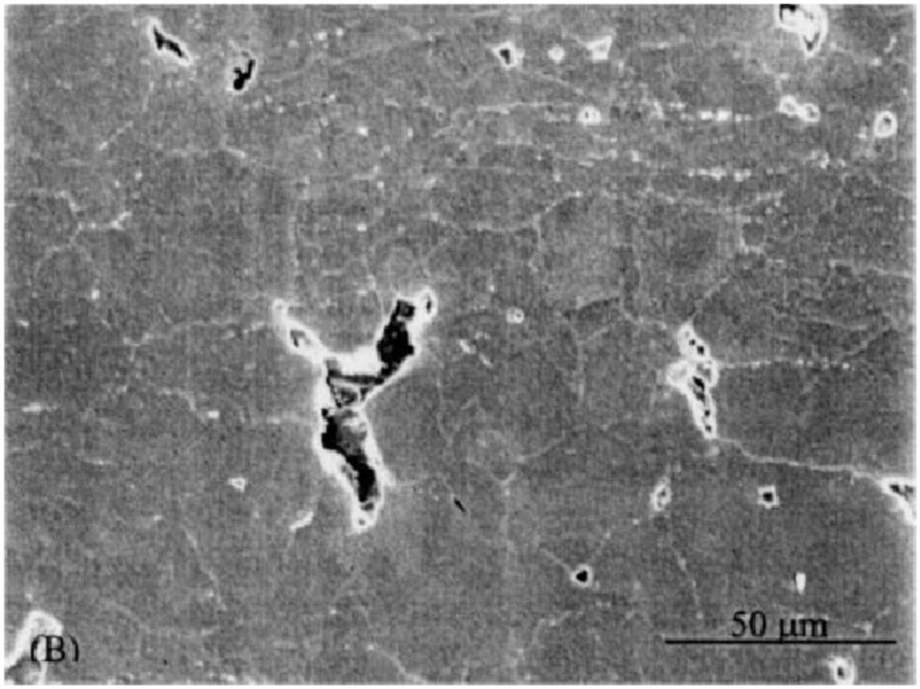
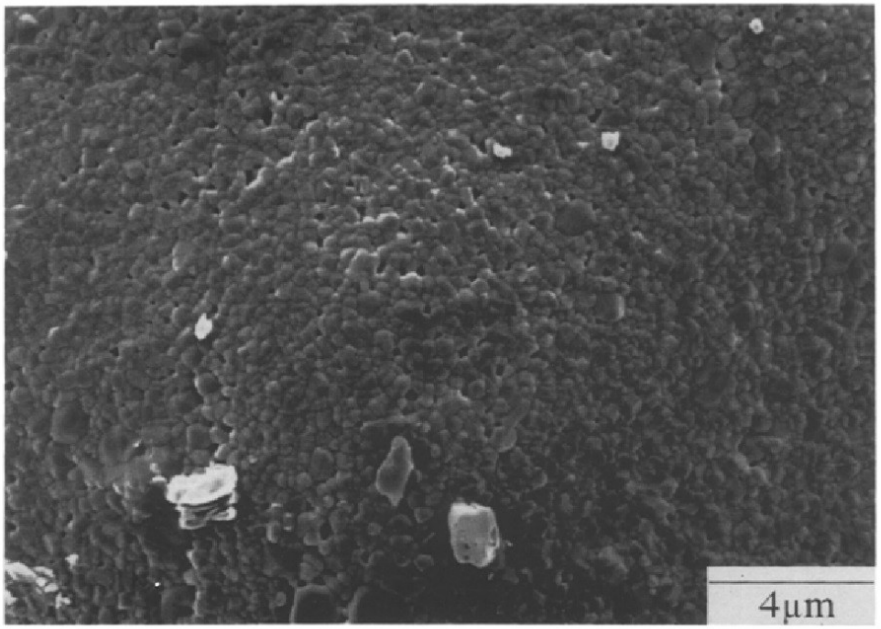
# Coupled Elastoplasticity and Microstructure Evolution: Creep Cavitation




Creep cavitation in stainless steel

SEM micrograph showing creep cavitation in 347 austenitic stainless steel after creep test at 69 Mpa, 750˚C
(Laha K et al, *Metal. Mater. Trans. A* 2005)

# Coupled Elastoplasticity and Microstructure Evolution: Oxidation

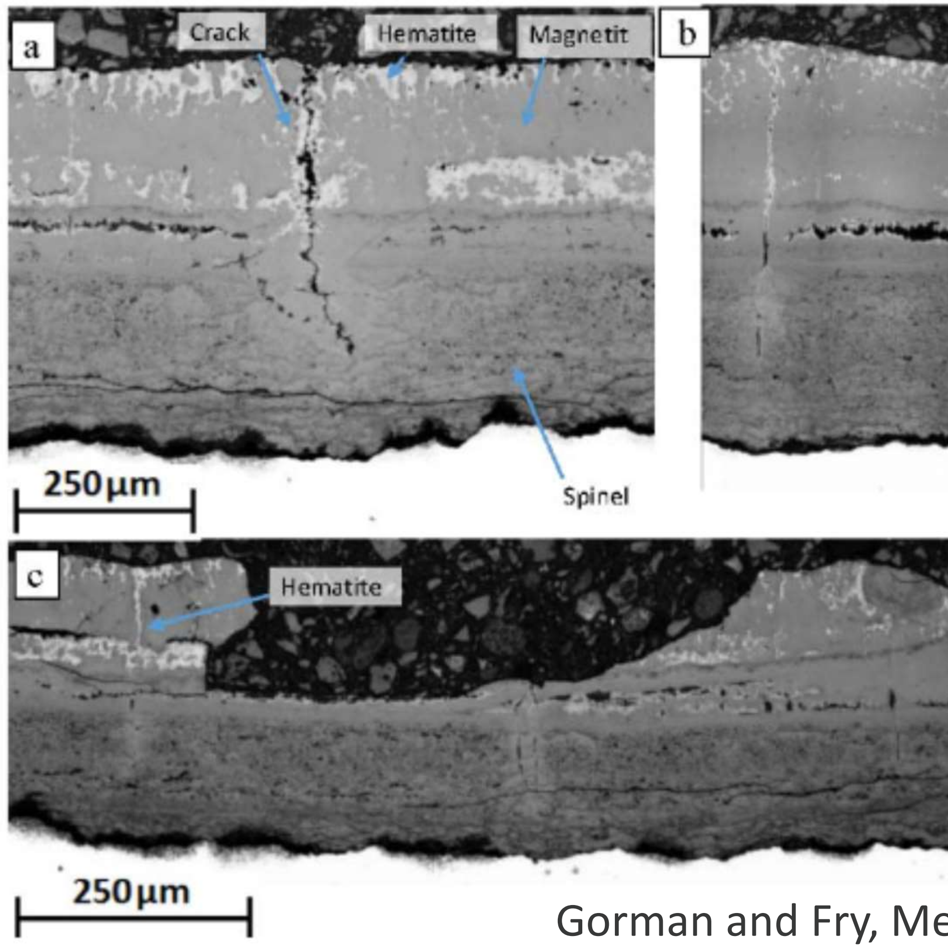



SEM secondary electron image of alpha-$Al_2O_3$ formed on $Y_2O_3$ dispersed $Fe_3Al$ after oxidation for 100hr at 1200˚C (Pint BA, *Oxid. Met.* 1997)

Voids form due to growth stress of oxide scales during oxidation

# Coupled Elastoplasticity and Microstructure Evolution: Spallation

## Boiler Tubing



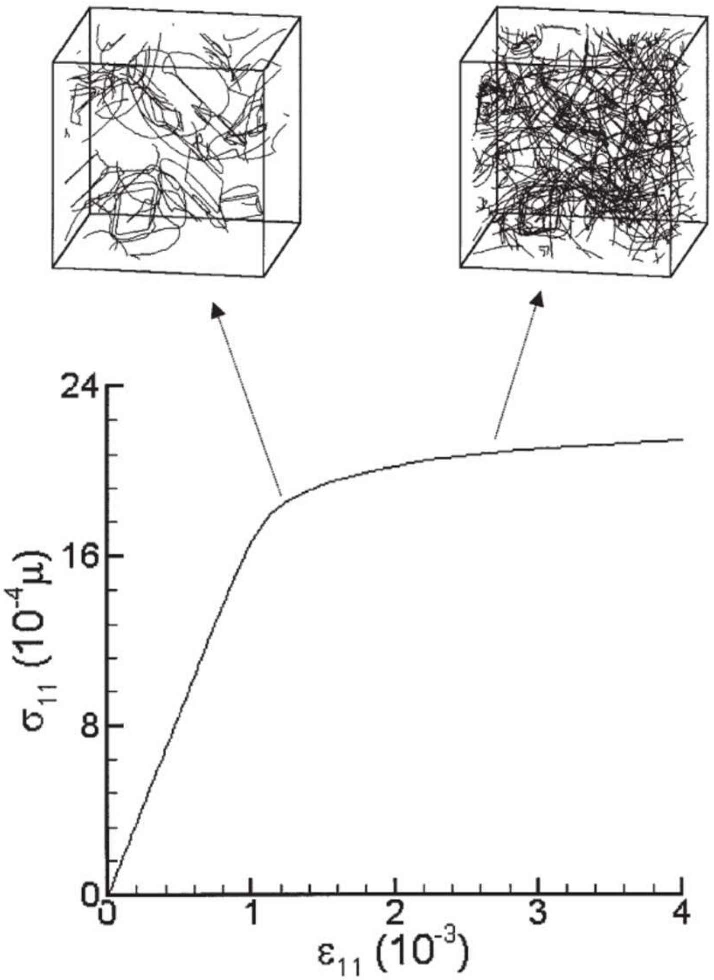

Gorman and Fry, Metals, 2016

Micrographs of T91 Ferritic exposed in plant for 91 kh in the temperature range 500-650C at elevated pressure showing (a,b) through thickness cracking and © region of spalled oxide.

# Outline

- Existing mesoscale phase-field models involving plasticity: a brief survey
- A mesoscale phase-field framework for plasticity
- Simulation results
  - ❖Elastoplastic inclusion problems as compared to analytical solutions
  - ❖Macroscopic anisotropic hardening and Bauschinger effect
  - ❖Polycrystal plasticity and sliding grain boundaries
  - ❖Computational efficiency of the phase-field model
- Summary

# Phase-field models involving plasticity - Dislocation level




(Wang et al., J. Appl. Phys. 2001)

Computationally expensive, not suitable for coupling with microstructure evolution such as oxidation modeling

# Phase-field models involving plasticity - Classical plasticity theories

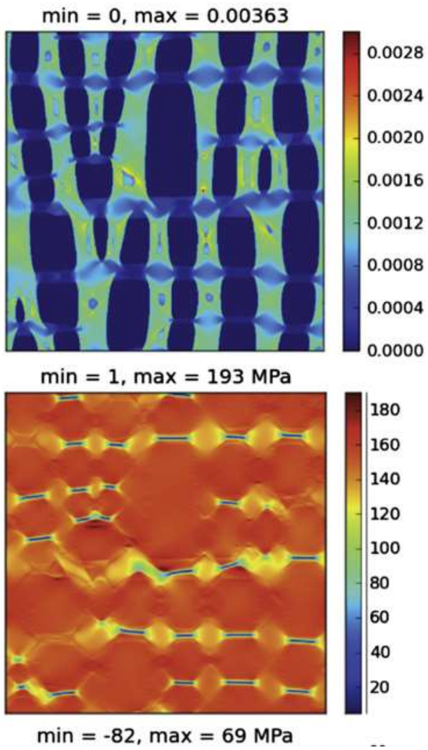
$$\varepsilon = \varepsilon^{el} + \varepsilon^{0} + \varepsilon^{pl}$$

Convex dissipation potential :
(Lemaitre and Chaboche, 1990)

$$\Omega(\sigma, X, R) = \int_V \tilde{\Omega}(\sigma, X, R)\, dV$$

- The postulated convex dissipation potential, if explicitly given, does **not** have a clear connection to the free energy assumed in the phase-field formulation
- Plastic flow is loosely coupled with microstructure evolution through total strain.

Example:




(Cottura et al. *J. Mech. Phys. Solids,* 2012)

# Phase-field modeling of plasticity

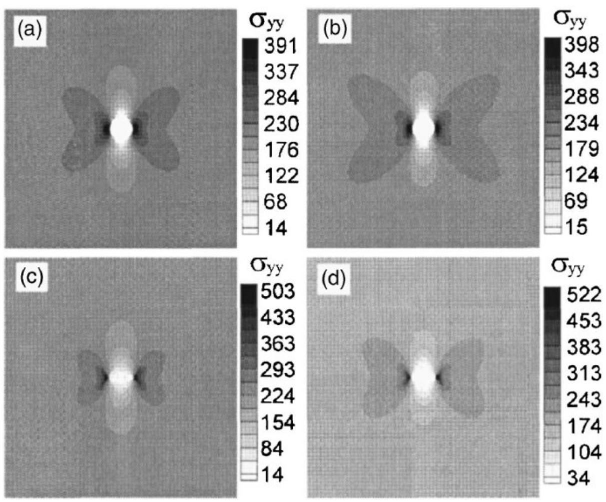
*In any phase-field models, a free energy functional for the whole material system is defined*

*The microstructural evolution is governed by kinetic equations derived from the free energy functional through variational principles.*

**Why can't plastic deformation be derived from the same free energy functional for the sake of self-consistency?**

# Phase field modeling of plasticity

## Continuum (coarse-grain) level




**Guo, Shi, and Ma, *Appl. Phys. Lett.*, 2005**, reiterated/revised by Yamanaka 2008, Yeddu 2012

There have been attempts along this line with the first by Prof. Shi's group from Hong Kong.

- Only elastic-perfectly-plastic constitutive relations were considered, i.e. without any strain hardening.
- **Plastic strain is solved by minimizing shear strain energy alone**.

Can the plastic strain be solved by minimizing the total free energy functional instead?

# Formulating elasto-viscoplasticity in a consistent phase-field framework

- Khachaturian's Micro-elasticity Theory

$$E^{el}=\frac{1}{2}\int_V C_{ijkl}\varepsilon_{ij}^0(\mathbf{r})\varepsilon_{kl}^0(\mathbf{r})d^3r+\frac{V}{2}C_{ijkl}\bar{\varepsilon}_{ij}\bar{\varepsilon}_{kl}-\bar{\varepsilon}_{ij}\int_V C_{ijkl}\varepsilon_{kl}^0(\mathbf{r})d^3r$$
$$-\frac{1}{2}⨍\frac{d^3k}{(2\pi)^3}n_i\tilde{\sigma}_{ij}^0(\mathbf{k})\Omega_{jk}(\mathbf{n})\tilde{\sigma}_{kl}^0(\mathbf{k})^*n_l\ ,$$

→ Total Strain Energy (not shear part alone)

- Imposing Incompressibility Constraint: Lagrange multiplier

$$\mathcal{L}=E^{el}-\int_V\lambda^V(\mathbf{r})\varepsilon_{kk}^p(\mathbf{r})d^3r\ ,$$

- Thermodynamic Equilibrium Condition under constraint:

$$\begin{cases}\dfrac{\delta\mathcal{L}}{\delta\varepsilon_{ij}^p(\mathbf{r})}=\dfrac{\delta E^{el}}{\delta\varepsilon_{ij}^p(\mathbf{r})}-\lambda^V(\mathbf{r})\delta_{ij}=0\,; \\ \dfrac{\delta\mathcal{L}}{\delta\lambda^V}=\varepsilon_{kk}^p(\mathbf{r})=0\,. \end{cases}$$

→ Variational Principles



Cheng, Wen and Hawk, *Int. J. Plasticity*, 2017

# Formulating elasto-viscoplasticity in a consistent phase-field framework

- Thermodynamic equilibrium state of viscoplasticity

$$\sigma_{ij}(\mathbf{r}) - \sigma_{kk}(\mathbf{r})\delta_{ij}/3 = 0$$

- zero deviatoric stress

- Lagrange multiplier solved to be hydrostatic pressure

$$\lambda^V(\mathbf{r}) = \frac{1}{3} tr\left(\frac{\delta E^{el}}{\delta \varepsilon_{ij}^p(\mathbf{r})}\right) = -\frac{1}{3}\sigma_{kk}(\mathbf{r}) = p(\mathbf{r}) \Longrightarrow \left.\frac{\delta \mathcal{L}}{\delta \varepsilon_{ij}^p(\mathbf{r})}\right|_{eq} = -\sigma'_{ij}(\mathbf{r})\Big|_{eq} = 0\,.$$

- Time-dependent Ginzburg-Landau equation

$$\frac{\partial \varepsilon_{ij}^p}{\partial t} = -K_{ijkl}\frac{\delta \mathcal{L}}{\delta \varepsilon_{kl}^p(\mathbf{r})} \Longrightarrow \begin{cases} \dfrac{\partial \varepsilon_{ij}^p}{\partial t} = \dfrac{3}{2}\left(\dfrac{J_2(\mathbf{r})}{\Lambda^*}\right)^{N*} \dfrac{\sigma'_{ij}}{J_2(\mathbf{r})} & \text{Odqvist's law} \\ d\varepsilon_{ij} = \dfrac{1}{E}[(1+\nu)d\sigma_{ij} - \nu\delta_{ij}d\sigma_{kk}] + (\sigma_{ij} - \dfrac{1}{3}\sigma_{kk}\delta_{ij})d\Lambda & \text{Prandtl-Reuss} \end{cases}$$

# Simulation results vs analytical solutions

## 1. Elasto-plastic inclusion problem: elastic/perfectly-plastic matrix

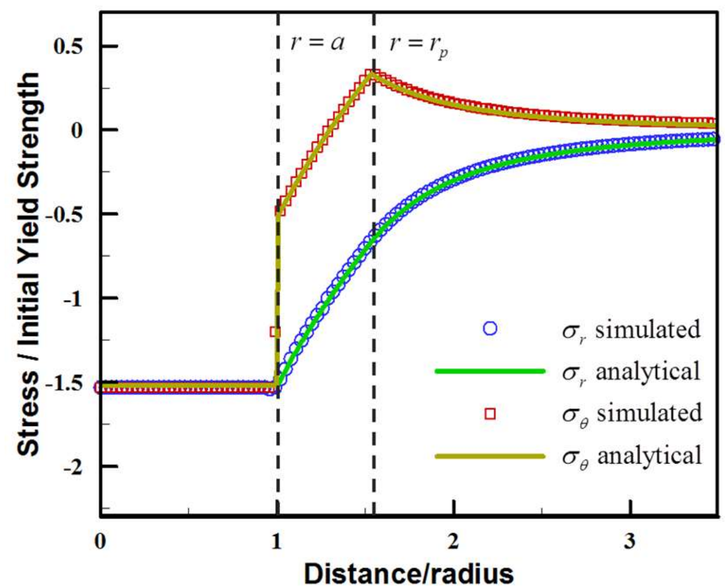
Radial and tangential stress distribution

$$\begin{cases} \sigma_r = \sigma_\theta = \sigma_I, \;\; 0 \le r \le a; \\ \sigma_r = \sigma_\theta - \sigma_Y^0 = \sigma_I + 2\sigma_Y^0 \ln\left(\frac{r}{a}\right), a \le r \le r_p; \\ \sigma_r = -2\sigma_\theta = -\frac{2\sigma_Y^0}{3}\left(\frac{r_p}{r}\right)^3, \;\; r_p \le r < \infty, \end{cases}$$

Size of plastic zone:

$$r_p = \left(\frac{6\mu\alpha\varepsilon}{\sigma_Y^0}\right)^{1/3} a$$

Analytical solution by (Lee, Earmme, Aaronson, and Russell, *Metal. Trans. A* 1980)




Simulated distributions of stress components in radius direction as compared to analytical solution; matrix being elasto-perfectly-plastic

# Simulation results vs analytical solutions

## 2. Elasto-plastic inclusion problem: linear elastic-plastic matrix

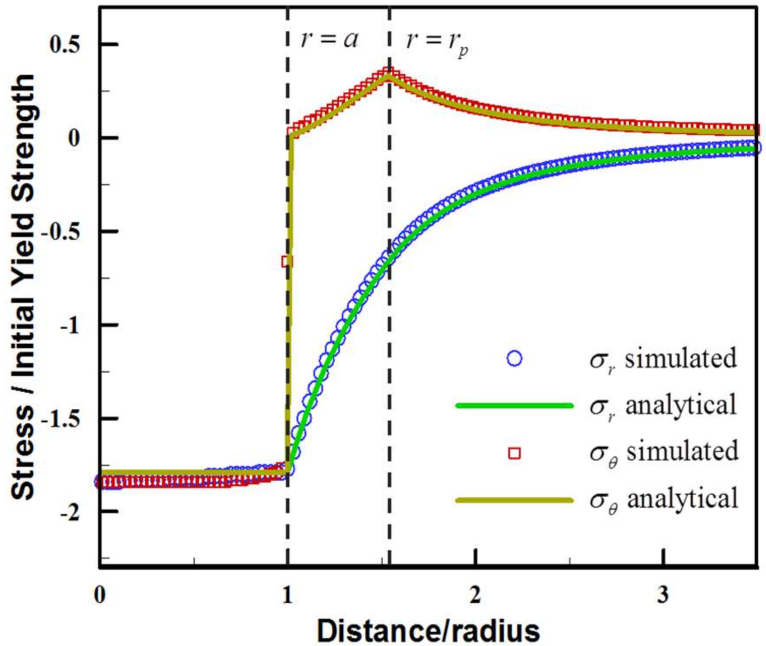
Radial and tangential stress distribution

$$\begin{cases} \sigma_r = \sigma_\theta = \sigma_I, \; 0 \le r \le a; \\ \sigma_r = \dfrac{2\sigma_Y^0}{3}\left[3\ln\left(\dfrac{r}{r_p}\right) - 2\phi(1-\nu)\left(\dfrac{r_p}{r}\right)^3 - 1\right], a \le r \le r_p; \\ \sigma_\theta = \dfrac{2\sigma_Y^0}{3}\left[3\ln\left(\dfrac{r}{r_p}\right) + \phi(1-\nu)\left(\dfrac{r_p}{r}\right)^3 + \dfrac{1}{2}\right], a \le r \le r_p; \\ \sigma_r = -2\sigma_\theta = -\dfrac{2\sigma_Y^0}{3}\left(\dfrac{r_p}{r}\right)^3, \; r_p \le r < \infty, \end{cases}$$

Size of plastic zone:

$$r_p = \left(\frac{6\mu\alpha\varepsilon}{\sigma_Y^0}\right)^{1/3} a$$

Analytical solution by (Earmme, Johnson, Lee, *Metal. Trans. A* 1981)



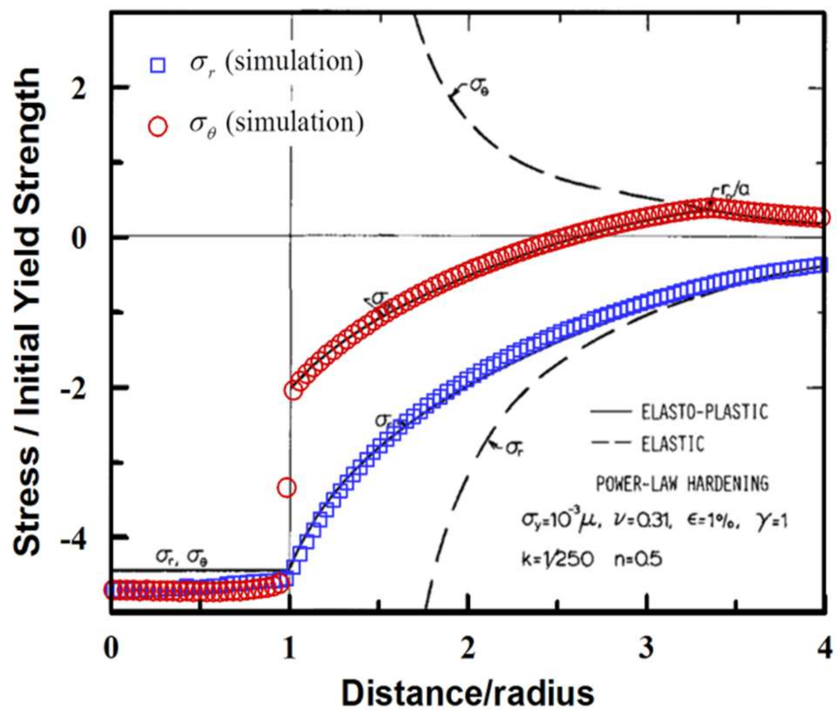

Simulated distributions of stress components in radius direction as compared to analytical solution; matrix being elasto-plastic with linear hardening

## Simulation results vs analytical solutions

### 3. Elasto-plastic inclusion problem: elastic-plastic matrix with power-law hardening

Analytical solution NOT available!

Phase-field simulation compared to numerical solutions
(Earmme, Johnson, Lee, *Metal. Trans. A* 1981)



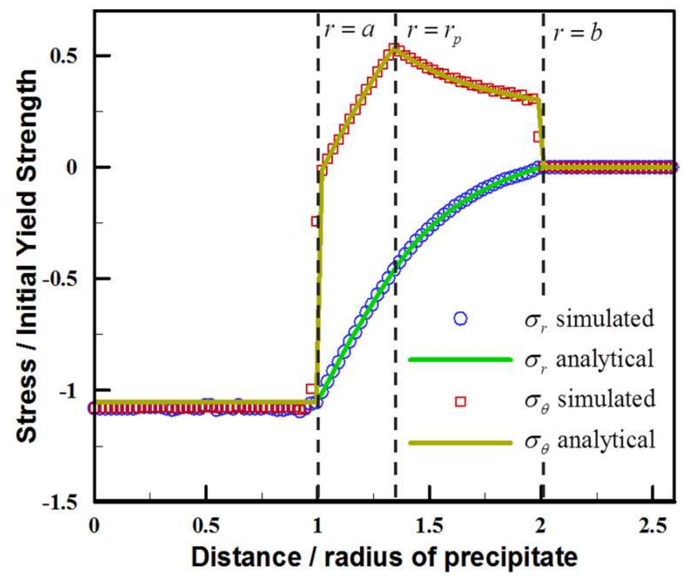

Simulated distributions of stress components in radius direction as compared to analytical solution; matrix being elasto-plastic with power-law hardening

## Simulation results vs analytical solutions

# 4. Elasto-plastic inclusion problem: elastic/perfectly-plastic matrix with a free surface

Radial and tangential stress distribution

$$
\begin{cases}
\sigma_r = \sigma_\theta = \sigma_I, \; 0 \le r \le a; \\
\sigma_r = \sigma_\theta - \sigma_Y^0 = \sigma_I + 2\sigma_Y^0 \ln\left(\dfrac{r}{a}\right), a \le r \le r_p; \\
\sigma_r = 4\mu\alpha\varepsilon a^3 \left(\dfrac{1}{b^3} - \dfrac{1}{r^3}\right), \; r_p \le r \le b; \\
\sigma_\theta = 4\mu\alpha\varepsilon a^3 \left(\dfrac{1}{b^3} + \dfrac{1}{2r^3}\right), \; r_p \le r \le b,
\end{cases}
$$




**Analytical solution developed in this work**

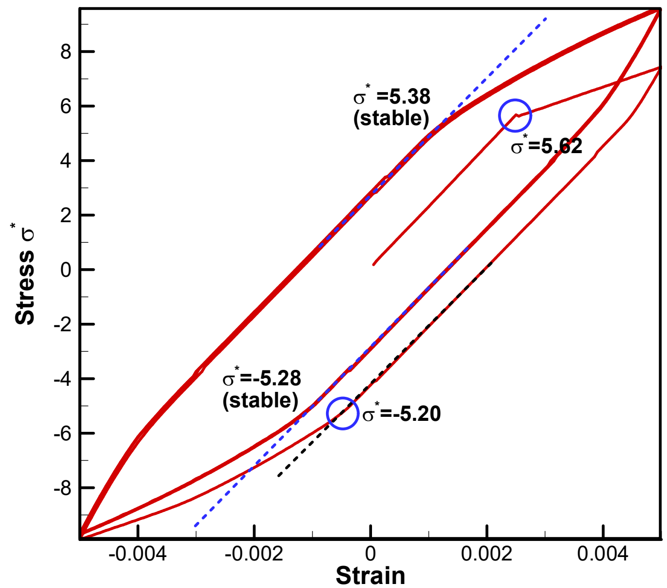
Simulated distributions of stress components in radius direction as compared to analytical solution; matrix being elasto-perfectly-plastic with a free surface

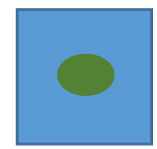
# Ongoing Efforts

**Anisotropic hardening in the 'constitutive relation'?**

- Anisotropic hardening is caused by heterogeneous plastic deformation
- Explicit modeling of the microstructural heterogeneity can lead to macroscopic anisotropic hardening behavior
- Direct application of kinematic hardening is not useful in phase field modeling because the heterogeneity is not captured – the local stress is important in PFM

Simulation of cyclic loading of a dual-phase composite with different isotropic hardening in each phase – macroscopic kinematic hardening shown

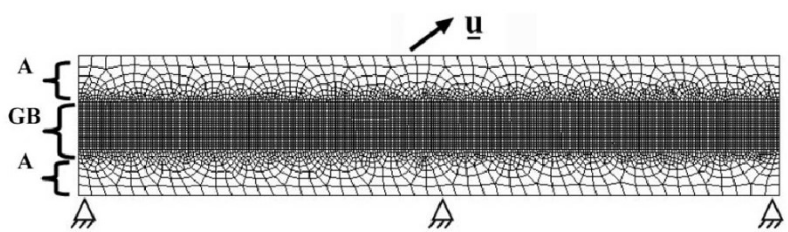


# Sharp interface models for polycrystal plasticity: Accommodation of grain boundary sliding?

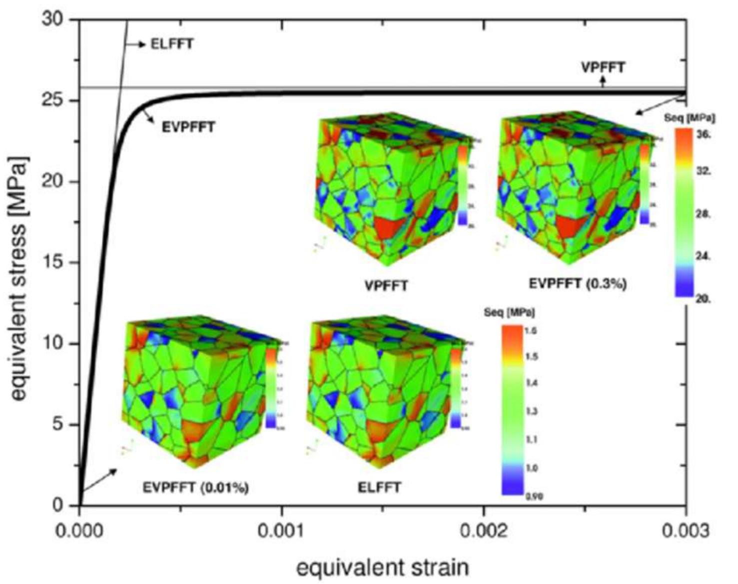
**Grain boundary sliding:**
**Important deformation mechanism for polycrystals at elevated temperatures with relatively**
**(a) low stress or,**
**(b) Low strain rate loading**

## Finite element models:




(Wei YJ and Anand L, *Acta Mater.* 2006)

## FFT-EVP:




(Lebensohn RA *et al.*, *Int. J. Plast.* 2012)

**Diffuse-interface model to accommodate GBS?**

# Simulation of grain boundary sliding

### Contribution of grain boundary sliding (GBS) to the shear rate of polycrystals

Without GBS (assumed):

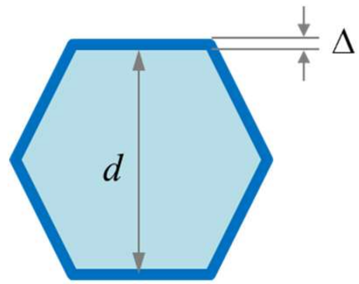
$$\dot{\gamma} = A\left(\frac{\overline{\tau}}{\mu}\right)^n$$

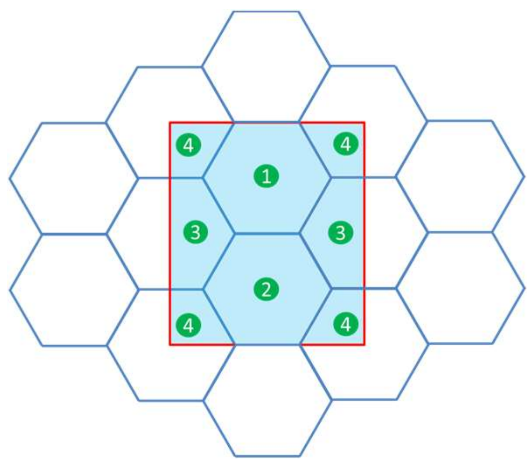
With free sliding GBs:

$$\dot{\gamma} = A\left(f\,\frac{\overline{\tau}}{\mu}\right)^n$$

$$\boxed{f = 1.2 \pm 0.12}$$

(F. Crossman and M. Ashby, *Acta Metall.* 1975)




4 order parameters are required to describe the grains in 2D

- Grain boundary assumed to be a thin layer with certain viscosity
- Grain interior deform by power-law creep
- In the low-stress (strain-rate) limit grain boundaries behaves like a network of shear cracks!

Representative volume element (RVE) in phase-field model (pure shear) loading:

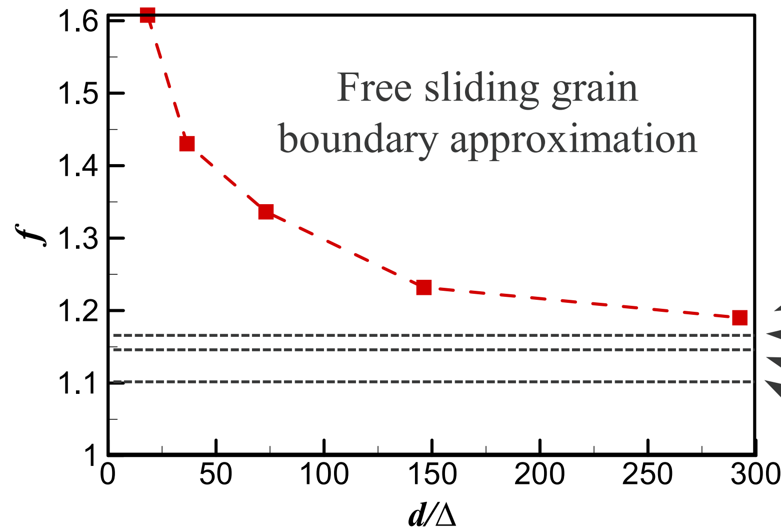
- 2D hexagonal grains
- Plane strain
- Incompressibility
- Periodic boundaries

# Shear of polycrystals by GBS and power-law creep

Diffuse interface (PF)

vs

Sharp interface (FEM)



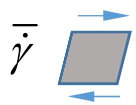

This work (phase field)

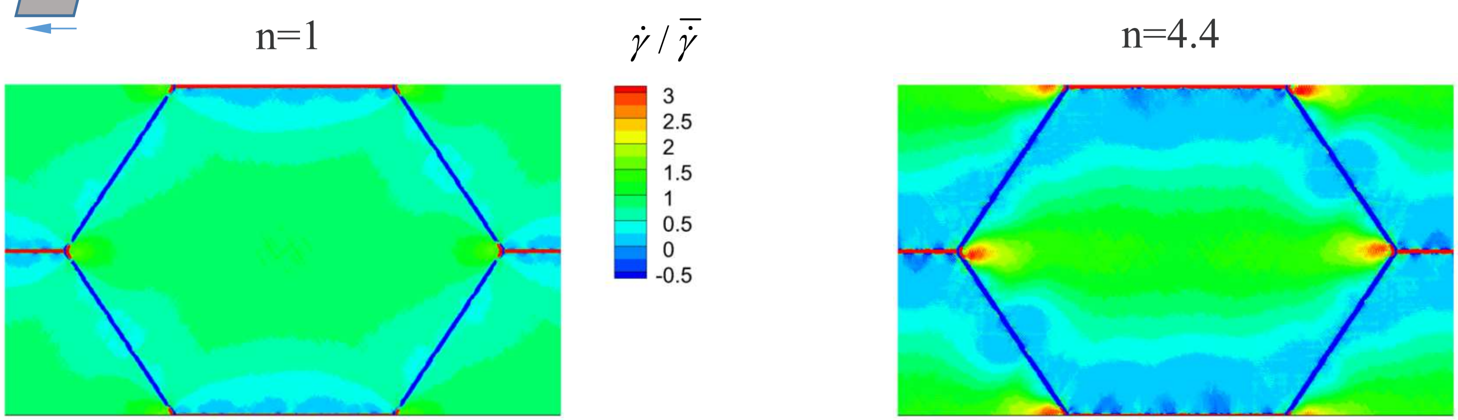
Ghahremani (fine mesh)

Ghahremani (coarse mesh)

Crossman & Ashby

**Does $f$ depend on the texture / grain shape?**

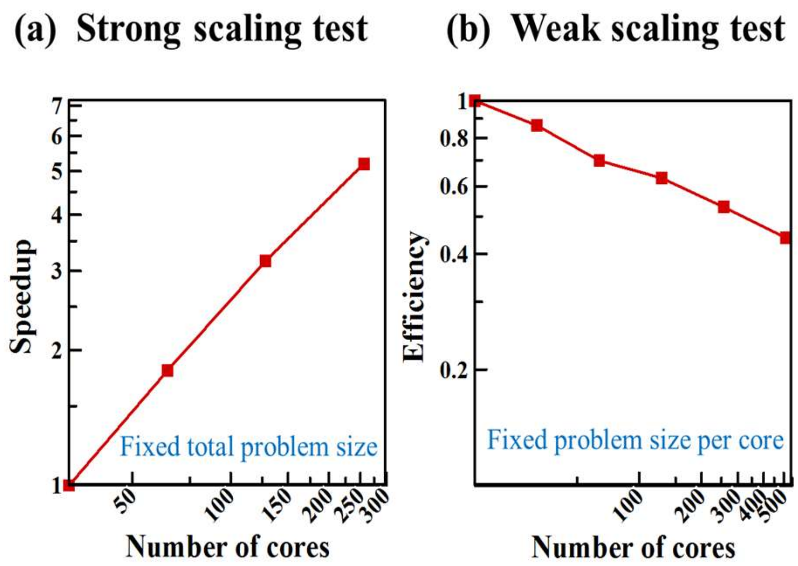



Relatively uniform deformation

More nonuniform deformation

# Efficiency of the phase-field model: parallel scaling test




Strong scaling performance:

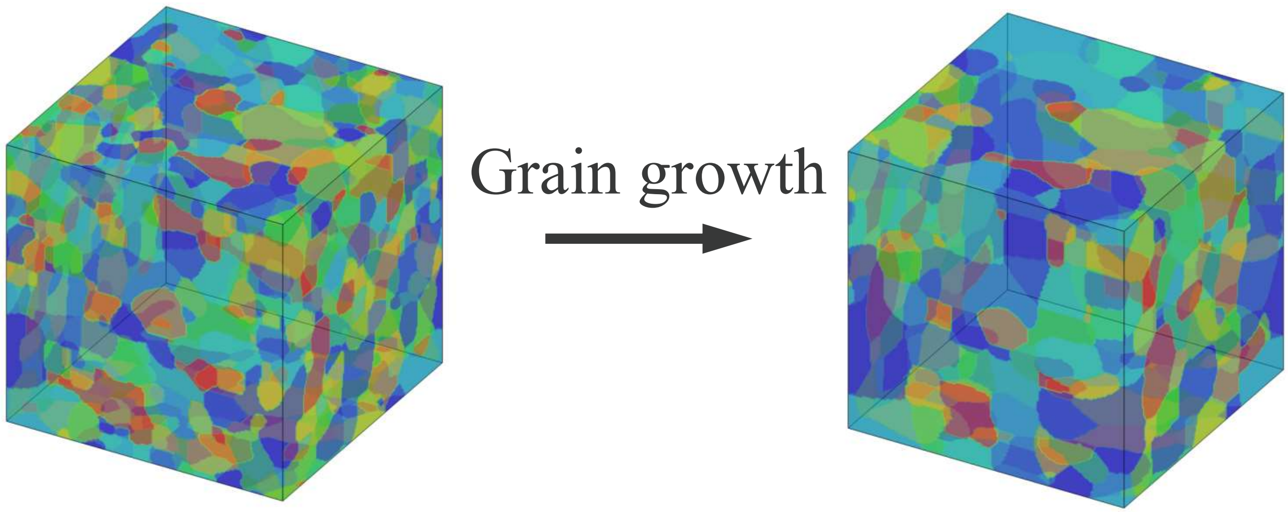
| Number of cores (nodes) | Wall clock time (secs) | Speedup | Efficiency |
|---|---|---|---|
| 32 (2) | 678 | 1 | 100% |
| 64 (4) | 375 | 1.8 | 90% |
| 128 (8) | 215 | 3.16 | 79% |
| 256 (16) | 130 | 5.20 | 65% |

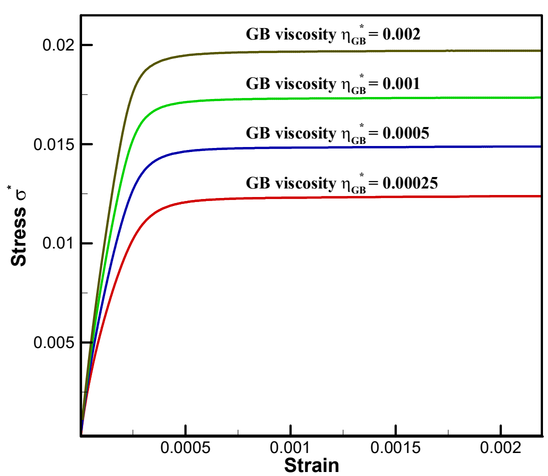
Weak scaling performance:

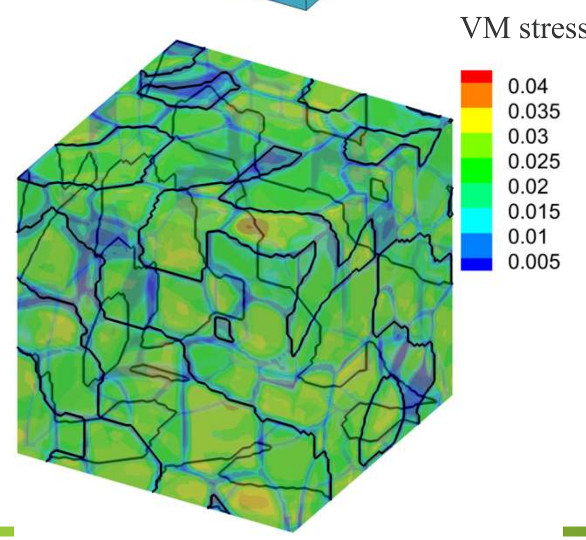
| Number of cores (nodes) | Grid points | Wall clock time (secs) | Efficiency |
|---|---|---|---|
| 16 (1) | 512×256×256 | 262 | 100% |
| 32 (2) | 512×512×256 | 304 | 86% |
| 64 (4) | 512×512×512 | 375 | 70% |
| 128 (8) | 512×512×1024 | 416 | 63% |
| 256 (16) | 512×1024×1024 | 495 | 53% |
| 512 (32) | 1024×1024×1024 | 595 | 44% |

Tested on the Stampede supercomputer at XSEDE: https://www.xsede.org/

# 3D PF simulation with concurrent grain growth / experimentally imported grain structure



# A Consistent Elasto-plastic Phase-field Framework

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Define free energy as a functional of inelastic eigenstrain, non-conserved and conserved order parameters for the whole material system

Non-conserved order parameters: TDGL equation (phases, grains, voids/cracks *etc.*)

Plastic flow rules derived from TDGL type equation as well, including grain boundary sliding

Conserved order parameters: Cahn-Hilliard equation (mass density, composition *etc.*)

$$\frac{\partial \eta_k}{\partial t} = -K_k^{\eta} \frac{\delta F}{\delta \eta_k}$$

$$\frac{\partial \varepsilon_{ij}^{p}}{\partial t} = -K_{ijkl}\left(\eta_k(\mathbf{r})\right) \frac{\delta \mathcal{L}}{\delta \varepsilon_{kl}^{p}}$$

$$\frac{\partial X_k}{\partial t} = \nabla \cdot \left( M \nabla \frac{\delta F}{\delta X_\alpha} \right)$$

$$\boxed{F = E^{el} + E^{chem} + E^{\text{int}} = F\left[ \varepsilon_{ij}^{p}(\mathbf{r}), \{\eta_\alpha(\mathbf{r})\}, \{X_k(\mathbf{r})\} \right]}$$

**A unified free energy functional**

# Summary

- Proposed a novel approach to formulate elasto-viscoplasticity within a consistent phase-field framework by minimizing the total strain energy with constraint – allowing coupling between plastic flow and microstructure evolution modeling through total free energy (rather than through total strain)
- Modeled grain boundary sliding, results in agreement with the classical Crossman-Ashby model
- Good parallel efficiency of the phase-field model is demonstrated
- This work lays a foundation to further couple polycrystal plasticity (including GBS) with void coalescence, crack propagation, grain boundary migration, and phase transformations, within a thermodynamically consistent phase-field framework

# Advanced Alloy Development Task 3
# Computational Materials Modeling

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This work was funded by the Crosscutting Technologies Program at the National Energy Technology Laboratory. The Research was executed through NETL's Research and Innovation Center's Advanced Alloy Development Field Work Proposal.