Phase-Field Model Development for Plasticity/Creep

Youhai Wen[a], Tianle Cheng[a,b], Jeffrey A. Hawk[a], David E. Alman[a]

[a] National Energy Technology Laboratory, 1450 Queen Avenue SW, Albany, OR 97321, USA

[b] Leidos Research Support Team, 626 Cochrans Mill Rd, P.O. Box 10940, Pittsburgh, PA 15236-0940, USA

INTRODUCTION

Components in fossil energy (FE) power generation devices are often subject to high temperatures for hundreds of thousands of hours. Consequently, creep is a major concern for design of alloy toward more efficient FE applications. Common creep models are, unfortunately, largely empirical in nature. Physics-based phase-field modeling has attracted increasing interests for its capability of modeling the kinetics of materials at microscale. In the literature, there has been models that attempt to couple phase-field modeling with (classical) plasticity or crystal viscoplasticity. These models normally directly invoke the plasticity theories. However, they lack a unified thermodynamic potential that governs both plastic flow and microstructure evolution. Here we develop a thermodynamically consistent crystal plasticity phase-field framework in which the plastic strain is taken as a phase-field variable subject to the time-dependent Ginzburg-Landau equation. This way, the plasticity is fully coupled with microstructure evolution through a common free energy functional. In addition, in this modeling framework, J_2 plasticity can coexist with crystal plasticity. Such a feature is utilized to model grain boundary sliding (GBS), which is also an important mechanism for creep. In the GBS model, the grain boundary region behaves more of J_2 plasticity and the bulk crystal constrained to the crystallographic slip systems (crystal plasticity). The modeling results are carefully validated against analytical solutions, finite element solutions (M. Ashby *et al.*) and the FFT-EVP algorithm (R. Lebensohn *et al*).

APPROACH

Formulating J_2 plasticity and crystal plasticity in a unified Ginzburg-Landau framework

- Phase-field microelasticity theory (PFME) (Khachaturyan 1983)

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

- Imposing constraints: Lagrange multiplier

$$\mathcal{L} = F - \int_V \lambda^V \varepsilon^{p(A)}_{kk} dV - \sum_g\sum_\alpha\int_V \lambda^{S(\alpha;g)}_{ij}\left(\varepsilon^{p(\alpha;g)}_{ij} - \varepsilon^{p(\alpha;g)}_{kl} m^{(\alpha;g)}_{kl} m^{(\alpha;g)}_{ij}\right)dV$$

- Condition of thermodynamic equilibrium under constraint:

$\sigma_{ij}'(\mathbf{r}) = 0$ **Zero deviatoric stress: Isotropic (J_2) plasticity**

$\sigma'_{kl}\, m^{(\alpha;g)}_{kl} m^{(\alpha;g)}_{ij} = 0$ **Zero resolved shear stress: Crystal plasticity**

- Lagrange multipliers solved to be hydrostatic pressure & negative stress

$$\lambda^V(\mathbf{r}) = -\frac{1}{3}\sigma_{kk}(\mathbf{r}) = p(\mathbf{r}) \qquad \lambda^{S(\alpha;g)}_{ij}(\mathbf{r}) = -\sigma_{ij}(\mathbf{r})$$

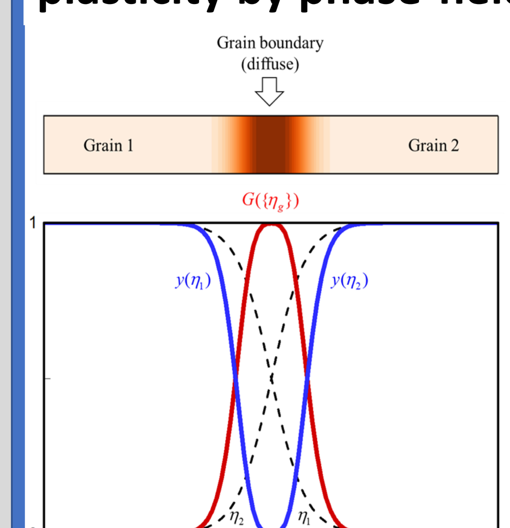
- Time-dependent Ginzburg-Landau (TDGL) equation

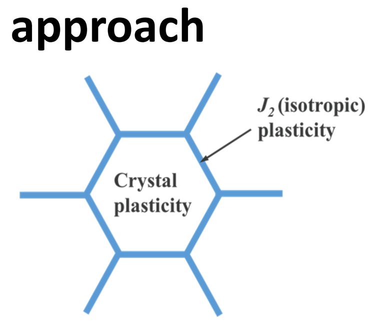
$$\frac{\partial\varepsilon^p_{ij}}{\partial t} = \frac{\partial}{\partial t}\left(\varepsilon^{p(A)}_{ij} + \sum_{g=1}^{N}\sum_{\alpha=1}^{S_g}\varepsilon^{p(\alpha;g)}_{ij}\right) = -L_{ijkl}^{(A)}\frac{\delta\mathcal{L}}{\delta\varepsilon^{p(A)}_{kl}} - \sum_g\sum_\alpha L_{ijkl}^{(\alpha;g)}\frac{\delta\mathcal{L}}{\delta\varepsilon^{p(\alpha;g)}_{kl}}$$

$$\begin{cases} L_{ijkl}^{(A)} = \dfrac{3\dot{\gamma}^a_0}{2J_2}\left(\dfrac{J_2}{\Lambda^*}\right)^{N^*}\delta_{ik}\delta_{jl}[1-\sum_g y(\eta_g)] \\ L_{ijkl}^{(\alpha;g)} = \dot{\gamma}^c_0\dfrac{1}{\tau^{(\alpha;g)}}\left|\dfrac{\tau^{(\alpha;g)}}{s^{(\alpha;g)}}\right|^{1/m} sign(\tau^{(\alpha;g)})\delta_{ik}\delta_{jl}y(\eta_g) \end{cases}$$

$$\Rightarrow \begin{cases} \dfrac{\partial\varepsilon^p_{ij}}{\partial t} = \dfrac{3}{2}\left(\dfrac{J_2(\mathbf{r})}{\Lambda^*}\right)^{N^*}\dfrac{\sigma'_{ij}}{J_2(\mathbf{r})} & \text{Odqvist's law } (J_2 \text{ plasticity}) \\ \dfrac{\partial\varepsilon^{p(\alpha)}_{ij}}{\partial t} = \dot{\gamma}_0\left|\dfrac{\tau^{(\alpha)}}{s^{(\alpha)}}\right|^{1/m} sign(\tau^{(\alpha)})m^{(\alpha)}_{ij} & \text{Asaro \& Needleman (crystal plasticity)} \end{cases}$$

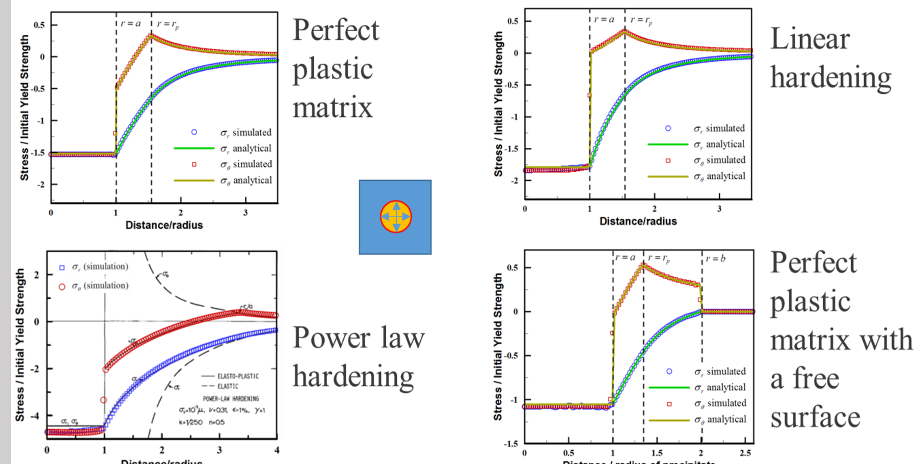
Defining the diffuse interface as J_2 plasticity and bulk region as crystal plasticity by phase-field approach



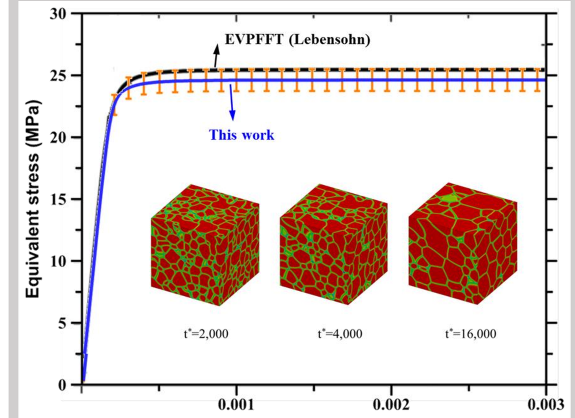


- Shape function to specify the phase fraction of "J_2 phase" and "Crystal plasticity phase"
- J_2 region can be toggled off

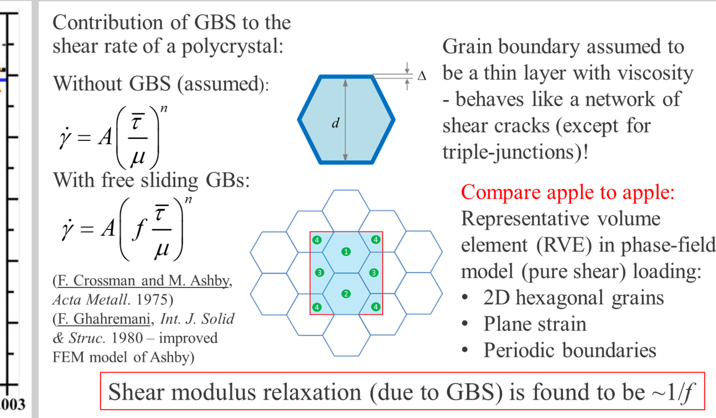
RESULTS



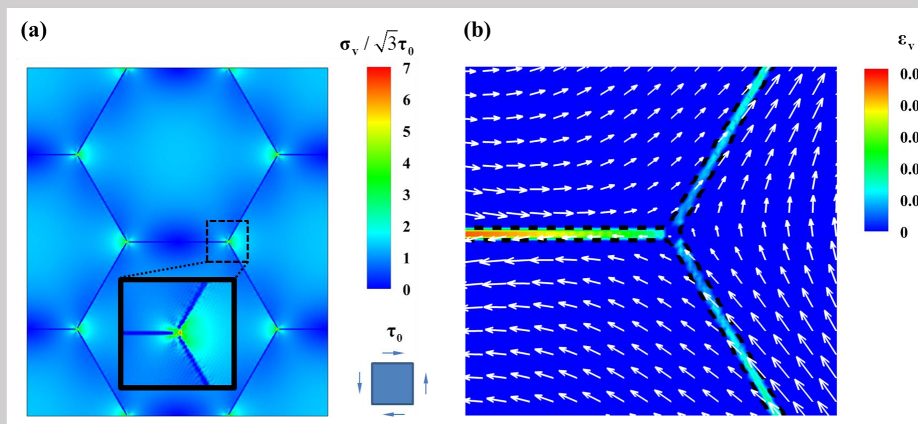
J_2 plasticity validation with analytical solutions



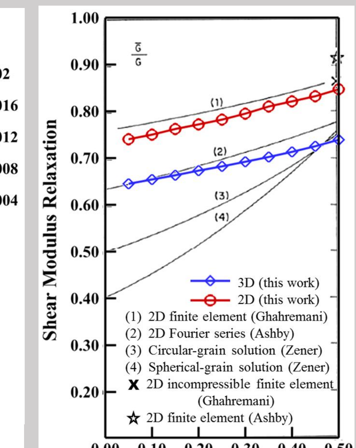
Crystal plasticity against the FFT-EVP



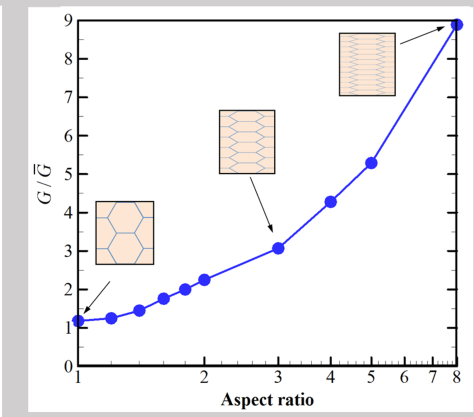
Simulation of GBS -- an important deformation mechanism for creep



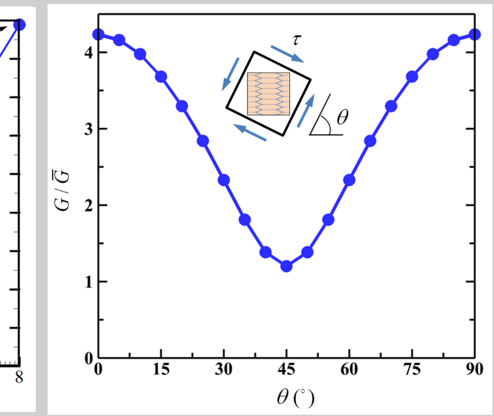
Simulated shear deformation accommodated by GBS in a relaxed hexagonal-grain polycrystalline solid subject to external shear stress



Comparison with literature results

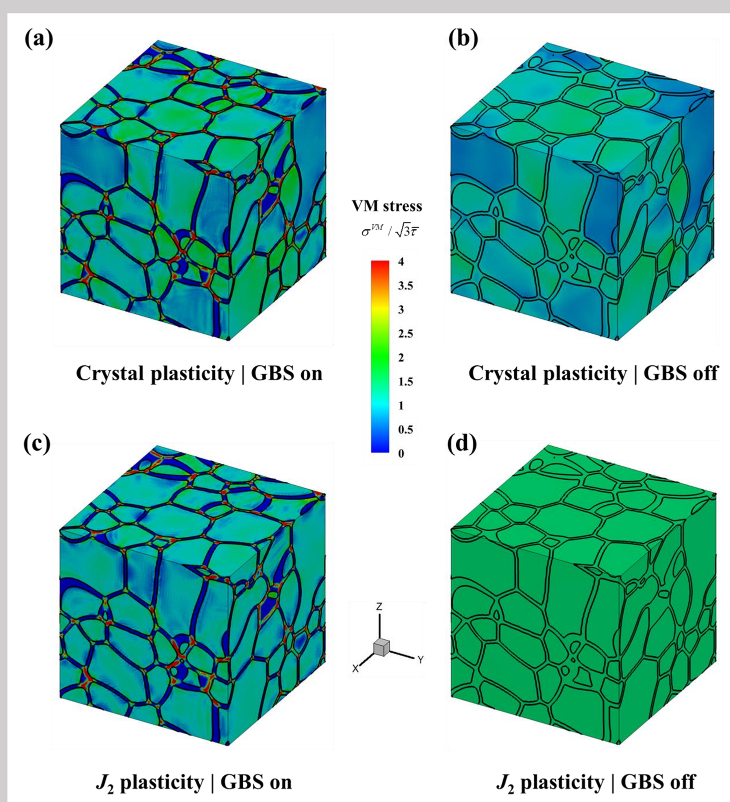


Grain shape effect



Load orientation effect

Simulated grain shape and load orientation effects on the contribution of GBS on modulus relaxation



3D Simulation of plasticity with/without GBS: Crystal plasticity vs J_2 plasticity

SUMMARY

- Developed a thermodynamically consistent crystal-plasticity phase-field framework that can couple plasticity (viscoplasticity) and crystal viscoplasticity with phase transformation and microstructure evolution [1,2].
- Applied this modeling framework to model grain boundary sliding coupled with crystal plasticity, and the results agree with the finite element simulations of Ashby (1975) and Ghahremani (1980) in the limit of free GBS, and conform to the FFT-EVP result of Lebensohn (2012) in the limit of zero GBS [2].
- **Paved the way for developing a physics-based creep model that provides quantitative understanding for the correlation between macroscopic creep performance and underlying mechanisms at microstructure level.**

ACKNOWLEDGEMENTS

This technical effort was performed in support of the DOE-FE & NETL Crosscutting Research Program, Briggs White, NETL Technology Manager, and Regis Conrad, DOE-FE HQ Program Manager. The research was executed through NETL Research & Innovation Center's Advanced Alloy Development FWP.

REFERENCES

[1] Tian-Le Cheng, You-Hai Wen, and Jeffrey A. Hawk, "Modeling Elasto-Viscoplasticity in a consistent phase field framework," International Journal of Plasticity, 96(2017), p. 242

[2] Tian-Le Cheng, You-Hai Wen, and Jeffrey A. Hawk, "Diffuse interface approach to modeling crystal plasticity with accommodation of grain boundary sliding," International Journal of Plasticity, 114(2019), p. 106

NATIONAL ENERGY TECHNOLOGY LABORATORY

2019 Crosscutting Annual Review Meeting
Pittsburgh April 10th, 2019, Pennsylvania

U.S. DEPARTMENT OF ENERGY