Phase-Field Modeling of Microstructure Evolution Coupled with Plasticity, Interfacial Sliding and Coherency Loss

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Materials applied at high temperatures may undergo microstructure evolution coupled with plastic deformation and interfacial sliding. For example, grain boundary sliding (GBS) is an important mechanism of creep and creep damage in polycrystalline alloys. In addition, for precipitation hardened materials during aging (Ostwald ripening) when coherent precipitates grow bigger and bigger they gradually lose coherency to release elastic energy. The incoherent interfaces are considered to behave similar to sliding grain boundaries. In the literature, there yet lacks a modeling tool that is able to capture the coupled kinetic process of plasticity, interfacial sliding and microstructure evolution. By extending our recently published diffuse-interface crystal plasticity model (*Int. J. Plas.* 114, 106-125, 2019), a general crystal plasticity multi-phase-field framework (CP-MPF) is developed that can incorporate microstructure evolution, crystal plasticity, interfacial sliding and coherency loss under a unified thermodynamic potential. This CP-MPF framework, incorporated with multicomponent diffusion, is validated against several literature results. The simulation results demonstrate Ostwald ripening in different situations for precipitates with (a) no eigenstrain (where classical Lifshitz-Slyozov-Wagner theory applies); (b) eigenstrain and coherent interface (c) eigenstrain and incoherent interface (d) eigenstrain and spontaneous coherency loss.

APPROACH

Crystal Plasticity Multi-Phase-Field modeling (CP-MPF)

Total free energy $F = \int \left(f^{chem} + f^{elas} + f^{int} + f^{pena} \right) dV$

Elastic energy $f^{elas}(\{\boldsymbol{\eta}\}, \boldsymbol{\varepsilon}^p)$ (Khachaturyan, 1983)

Interfacial energy $f^{int}(\{\boldsymbol{\eta}\}, \boldsymbol{\varepsilon}^p) = m_0 \left[\sum_{\alpha=1..M} \sum_{i=1}^{N^\alpha} \left(\frac{\eta_{\alpha i}^4}{4} - \frac{\eta_{\alpha i}^2}{2} + \frac{\chi}{2} \sum_{\beta=1..M} \sum_{j=1;\beta j \neq \alpha i}^{N^\beta} \eta_{\alpha i}^2 \eta_{\beta j}^2 \right) + \frac{1}{4} \right]$

$+ \sum_{\alpha=1..M} \sum_{i=1}^{N^\alpha} \frac{\kappa_\alpha}{2} |\nabla \eta_{\alpha i}|^2 + \psi\left(\varepsilon_{ij}^p\right)$ (Moelans N, *Acta Mater.* 2011)

Chemical energy $f^{chem}(\{\eta_p\}, \{x_k\}) = \sum_{\alpha=1..M} g_\alpha(\boldsymbol{\eta}) G^\alpha(T, \{X_k\})$ $\quad g_\alpha(\boldsymbol{\eta}) = \frac{\sum_{i=1}^{P_\alpha} \eta_{\alpha i}^2}{\sum_\rho \sum_{i=1}^{P_\rho} \eta_{\rho i}^2}$

(linked to CALPHAD database)

KKS treatment
$$\begin{cases} X_k = \sum_{\alpha=1}^{M} g_\alpha(\boldsymbol{\eta}) X_k^\alpha \\ \frac{\partial G_m^\alpha}{\partial X_k^\alpha} = \frac{\partial G_m^\beta}{\partial X_k^\beta} = \ldots = \frac{\partial G_m^M}{\partial X_k^M} \end{cases}$$ (Kim S. *et al.*, *Phys. Rev. E* 1999)

- Time-dependent Ginzburg-Landau (TDGL) equation

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

$$\begin{cases} L_{ijkl}^{(A)} = \frac{3\dot{\gamma}_0^a}{2J_2} \left(\frac{J_2}{\Lambda^*} \right)^{N^*} \delta_{ik}\delta_{jl}[1 - \sum_g y(\eta_g)] \\ L_{ijkl}^{(\alpha;g)} = \dot{\gamma}_0^c \frac{1}{\tau^{(\alpha;g)}} \left| \frac{\tau^{(\alpha;g)}}{s^{(\alpha;g)}} \right|^{1/m} sign(\tau^{(\alpha;g)}) \delta_{ik}\delta_{jl} y(\eta_g) \end{cases}$$

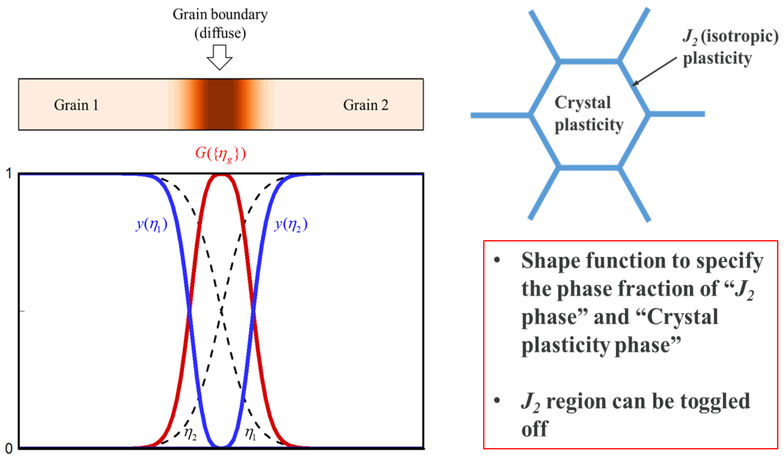
$$\begin{cases} \frac{\partial \varepsilon_{ij}^p}{\partial t} = \frac{3}{2} \left(\frac{J_2(\mathbf{r})}{\Lambda^*} \right)^{N^*} \frac{\sigma'_{ij}}{J_2(\mathbf{r})} \\ \frac{\partial \varepsilon_{ij}^{p(\alpha)}}{\partial t} = \dot{\gamma}_0 \left| \frac{\tau^{(\alpha)}}{s^{(\alpha)}} \right|^{1/m} sign(\tau^{(\alpha)}) m_{ij}^{(\alpha)} \end{cases}$$ Odqvist's law (J_2 plasticity)

Asaro & Needleman (crystal plasticity)

- Governing equation for microstructure evolution and multicomponent diffusion

$$\begin{cases} \frac{\partial \eta_i}{\partial t} = -K^\eta \frac{\delta L}{\delta \eta_i} \\ \frac{\partial X_k}{\partial t} = \nabla \cdot M_k \left(\nabla \frac{\delta L}{\delta X_k} \right) \end{cases}$$ TDGL; Cahn-Hilliard

Defining interfacial region as J_2 plasticity and bulk region as crystal plasticity via special shape functions



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

Rank (r)	Shape function $y = h^{(r)}(\phi)$
1	$y = \phi^2(3 - 2\phi)$
2	$y = \phi^3(10 - 15\phi + 6\phi^2)$
3	$y = \phi^4(35 - 84\phi + 70\phi^2 - 20\phi^3)$

$y(\eta) = h^{(r)}[\phi(\eta)]$, $\phi = \eta^p$,

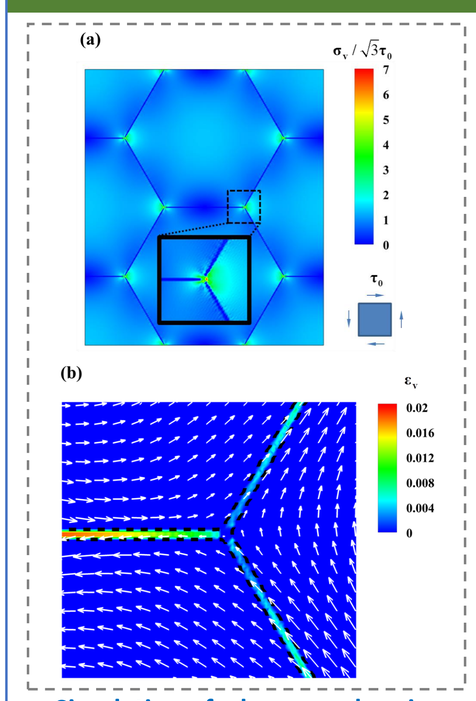
where p is an even number.

The large p is, the broader the interfacial layer is;

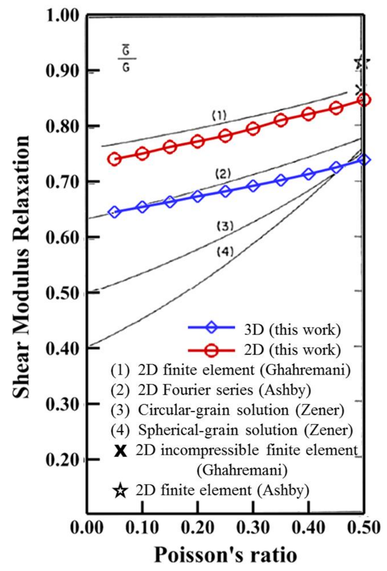
the larger r is, the steeper the shape function is.

"There is substantial room at the phase-field interface." Particularly, the thin-interface phase-field approach (Karma & Rappel 1996; Kim, Kim & Suzuki 1999; Steinbach & Apel 2006, Moelans 2011, *etc.*) allows for more space for defining interfacial properties distinct from the bulk.

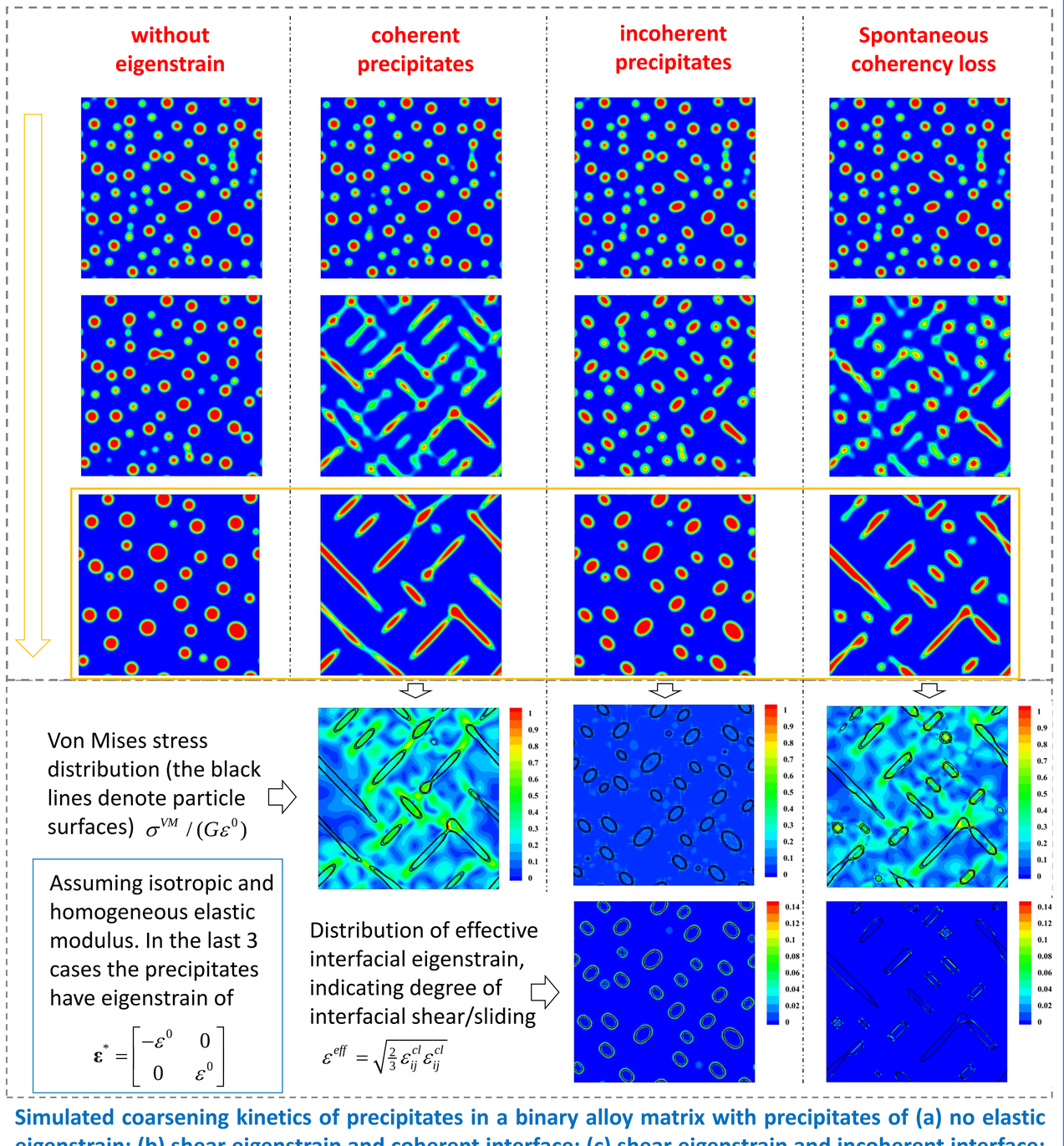
RESULTS



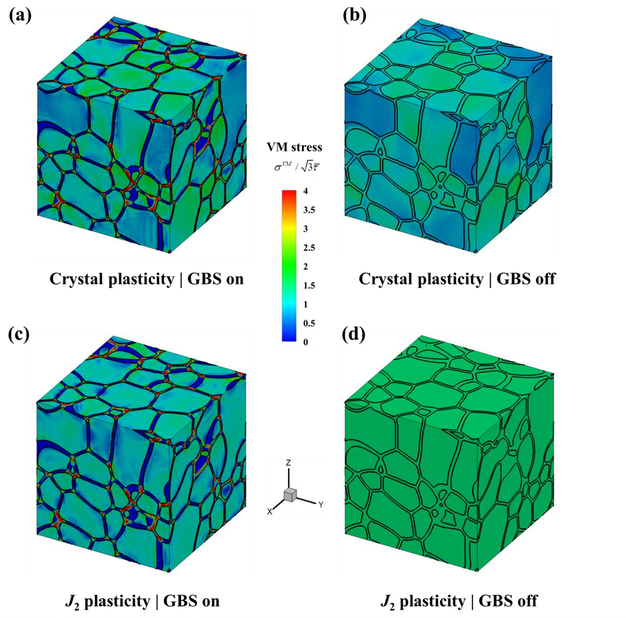
Simulation of a hexagonal-grain polycrystal, with grain boundary sliding, under external shear



Simulated modulus relaxation of a polycrystal with comparison to literature results



Simulated coarsening kinetics of precipitates in a binary alloy matrix with precipitates of (a) no elastic eigenstrain; (b) shear eigenstrain and coherent interface; (c) shear eigenstrain and incoherent interface; (d) shear eigenstrain and spontaneous coherency loss.



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

SUMMARY

- Developed a mesoscale crystal-plasticity multi-phase-field (CP-MPF) framework that can couple J_2 plasticity and crystal plasticity with microstructure evolution and multicomponent diffusion [1,2].
- Grain boundary sliding (GBS) is modeled by assigning J_2 type viscosity to the grain boundary layer, and for 2D simulations, the results agree with the finite element simulations of Ashby (1975) and Ghahremani (1980) [2]; the 3D results show quantitative difference from 2D simulations.
- The coherency loss is modeled by variational approach in which the interfacial eigenstrain is linked to interfacial energy; and such method can capture coherency loss as a continuous process.
- This modeling framework has demonstrated its capability to simulate complex kinetic processes of materials at high temperatures in which microstructure evolution is coupled with multicomponent diffusion, plasticity, interfacial sliding and coherency loss.

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ADDITIONAL REFERENCES

[1] T.-L.Cheng, Y.-H. Wen, and J. A. Hawk, "Modeling Elasto-Viscoplasticity in a consistent phase field framework," International Journal of Plasticity, 96(2017), 242-263

[2] T.-L.Cheng, Y.-H. Wen, and J. A. Hawk, "Diffuse interface approach to modeling crystal plasticity with accommodation of grain boundary sliding," International Journal of Plasticity, 114(2019), 106-125

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