Advanced Alloy Development Field Work Proposal Task 16: Design Tool for Creep-Resistant Materials and Low Cycle Fatigue Modeling

Microstructure-Based Creep and Fatigue Modeling

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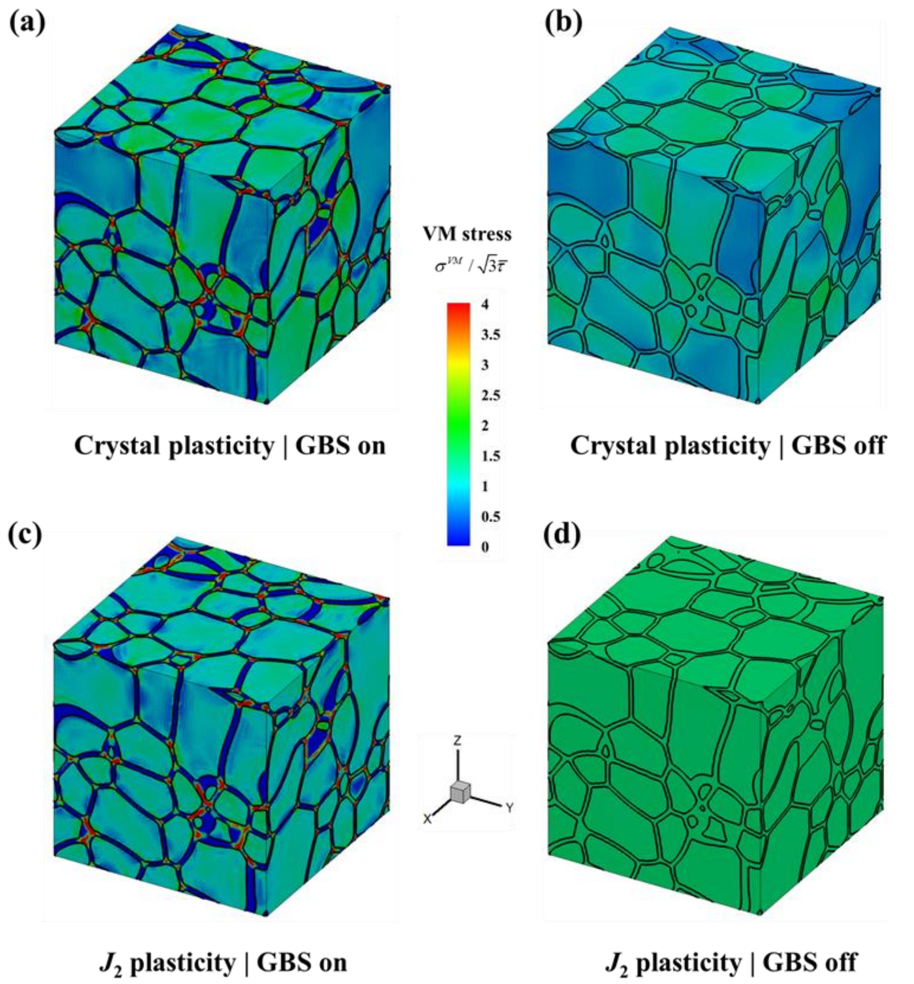
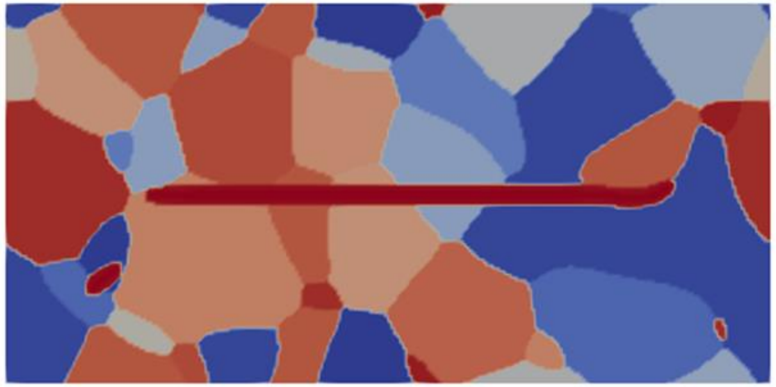
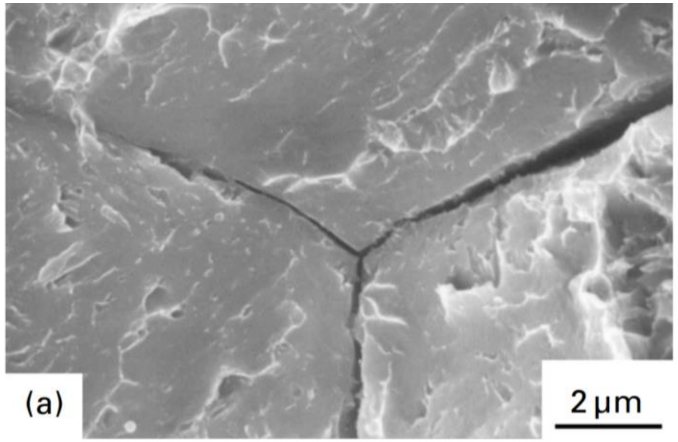
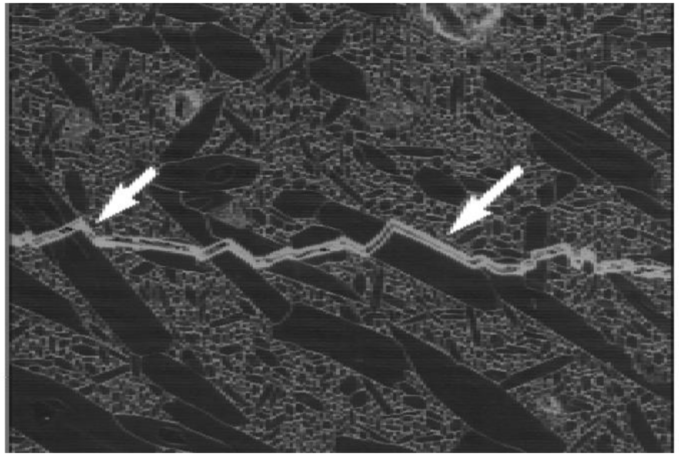




Background: Creep & Fatigue Modeling

Intergranular crack paths





Existing creep/fatigue models are largely phenomenological without explicitly incorporating microstructural effects.

NETL's focus is on **<u>microstructure-based</u>** predictive models that couple creep and fatigue.

Acta Metall., 20, Overview No. 74, 2639–2661, 1988 J. Amer. Ceram. Soc. 81 (11) (1998) 2831

Why Microstructure-Based Modeling is Essential?

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- Materials life is strongly influenced by the underlying microstructure such as pores, precipitates, grains, grain boundaries, etc.

- The shape, size, spatial distribution of these microstructure features control the <u>rare events</u> of initiation of micro-cracks, their propagation, interaction, and eventual failure of the material.

Outline

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Modeling Capabilities of Crack Growth and Fatigue

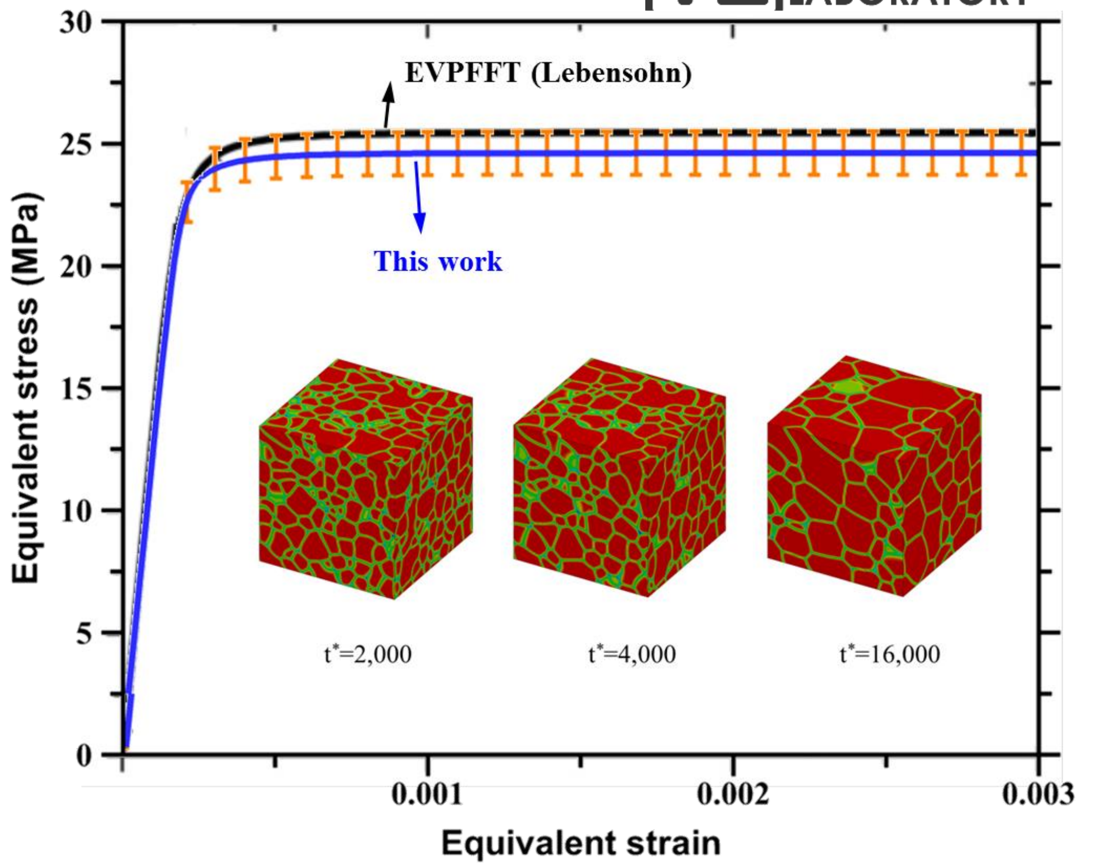
- Modeling of Crack Growth in Single Crystals and Polycrystals
- Modeling of Low Cycle Fatigue
- Modeling of High Cycle Fatigue

Modeling Capability of Large Deformation and Its Application to Creep Damage Modeling of Void Growth

Modeling of Coupled Grain Growth, Crystal Plasticity, and Grain Boundary Sliding under Creep in EY19

This past effort provided a solid foundation for microstructure-based creep modeling capability

Crack growth modeling is incorporated into this modeling framework leading to a unified modeling capability targeting <u>integrated microstructure-based creep & fatigue modeling</u>



Crystal plasticity phase-field simulation of stress-strain curve of a polycrystalline copper

Cheng, Wen, Hawk, *International Journal of Plasticity*, 2019

Phase-field Model for Ductile Fracture in Polycrystals

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A phase-field model is built, considering grain structures, plastic strain, and cracks.

$$F = \int_{\Omega} [f_{\text{grain}} + f_{\text{grad}} + f_{\text{elas}} + f_{\text{frac}}] d\Omega$$

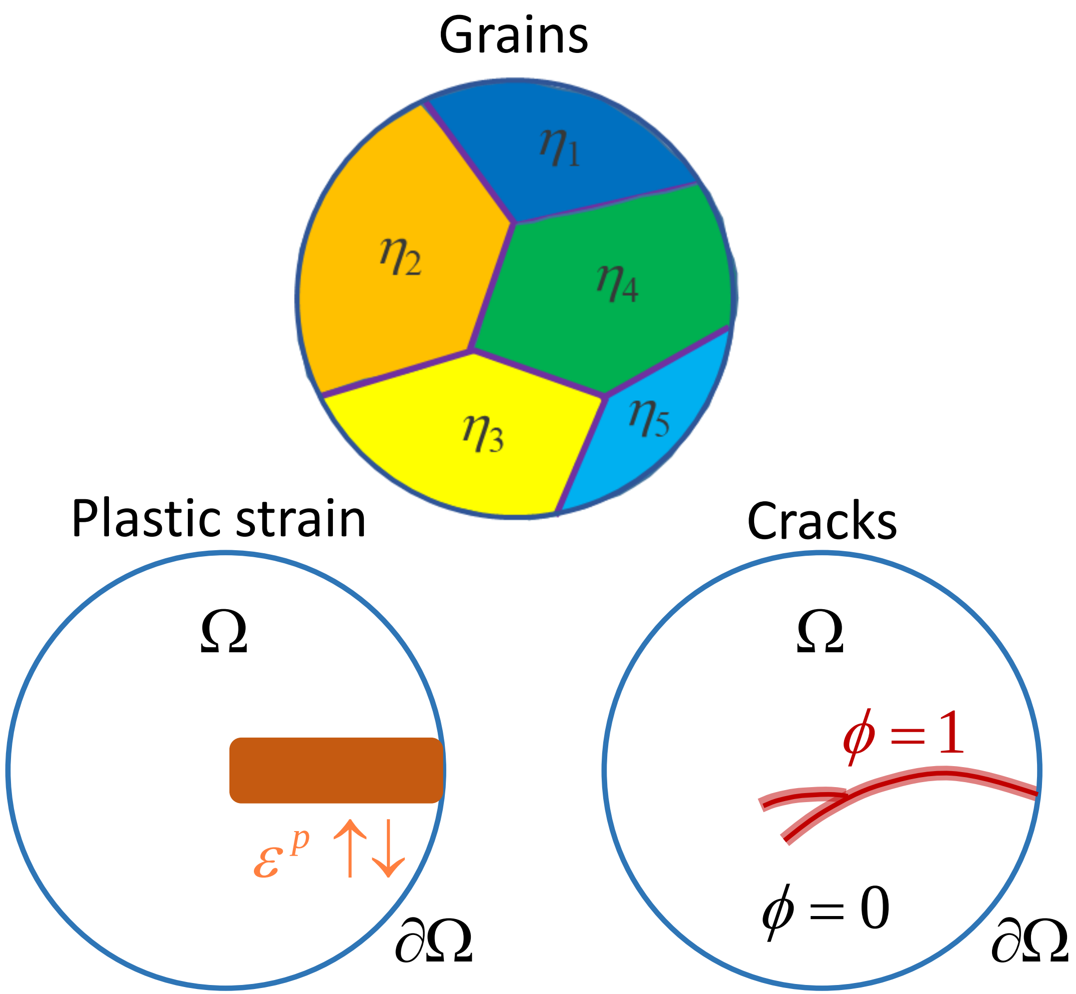
f_{grain} : bulk energy for grain order parameters

f_{grad} : gradient energy for grain order parameters

f_{elas} : elastic energy

f_{frac} : fracture energy

Crystal plasticity is employed within grain interiors accommodated by J_2 plasticity at grain boundaries



Phase-field Model for Ductile Fracture in Polycrystals

Crack order parameter ϕ for diffuse interfaces

$\phi = 1$ fully damage $\quad\quad$ $\phi = 0$ intact

Fracture energy $\quad f_{\mathrm{frac}} = G_C(\eta_g, \boldsymbol{\varepsilon}^p, H^{elas})\left(\frac{\phi^2}{2l_0} + \frac{l_0}{2}\frac{\partial \phi}{\partial x_i}\frac{\partial \phi}{\partial x_i}\right)$

Grain-dependent fracture toughness $\quad G_C(\eta_g) = \sum_g y(\eta_g) G_C^{\mathrm{in}(g)} + [1 - \sum_g y(\eta_g)] G_C^{\mathrm{GB}}$

Elastic energy $\quad f_{elas} = \frac{1}{2} c_{ijkl}^{eff}(\eta_g, \phi)(\varepsilon_{ij} - \varepsilon_{ij}^p)(\varepsilon_{kl} - \varepsilon_{kl}^p)$

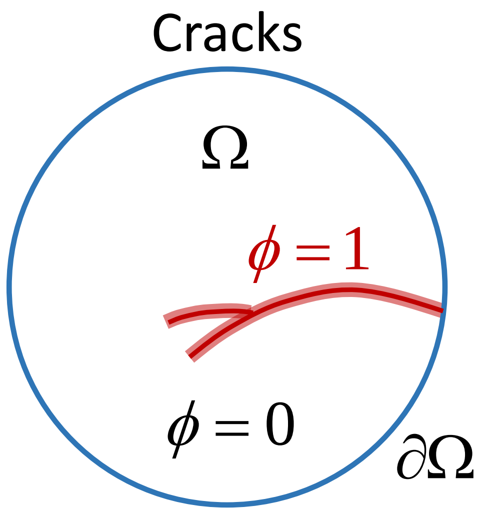
Elastic tensor is a function of grain structure

$$c_{ijkl}(\eta_g) = \sum_g y(\eta_g) c_{ijkl}^{(g)} + [1 - \sum_g y(\eta_g)] c_{ijkl}^{(\mathrm{GB})}$$

Grain interior $\quad$ Grain boundary

Effective elastic tensor is a function of cracks and grain structure

$$c_{ijkl}^{eff}(\eta_g, \phi) = (1-\phi)^2 c_{ijkl}(\eta_g)$$



$\boldsymbol{\varepsilon}^{p}$: equivalent plastic strain

H^{elas}: damage from stress cycling

$y(\eta_g)$: interpolation function

Anisotropy of Crack Growth in Ductile Single Crystals

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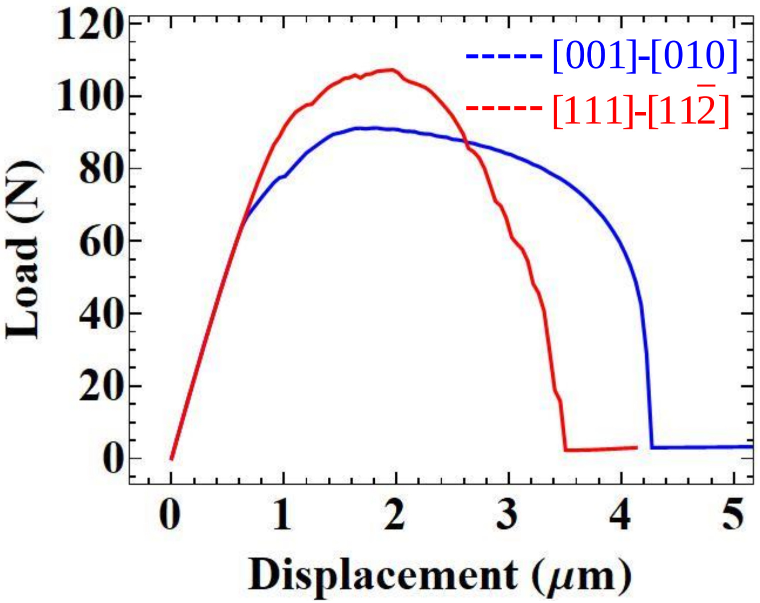
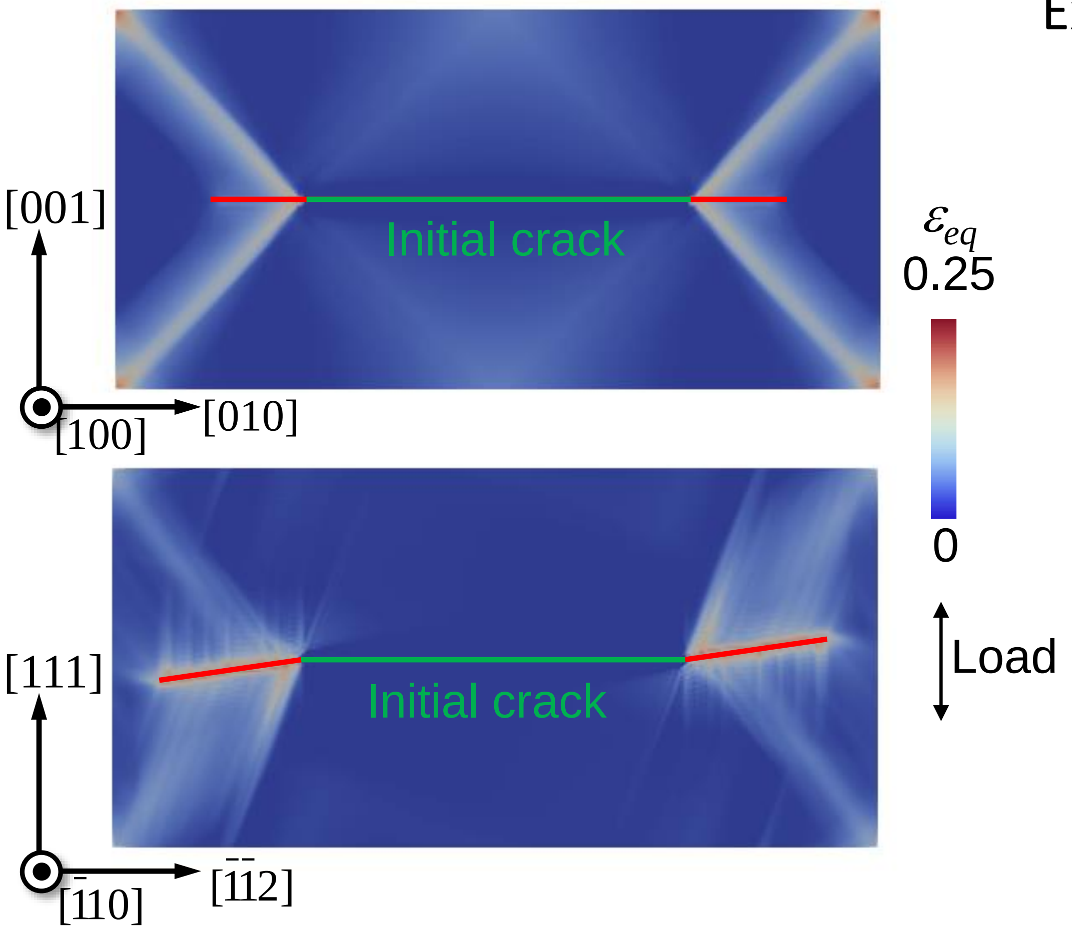
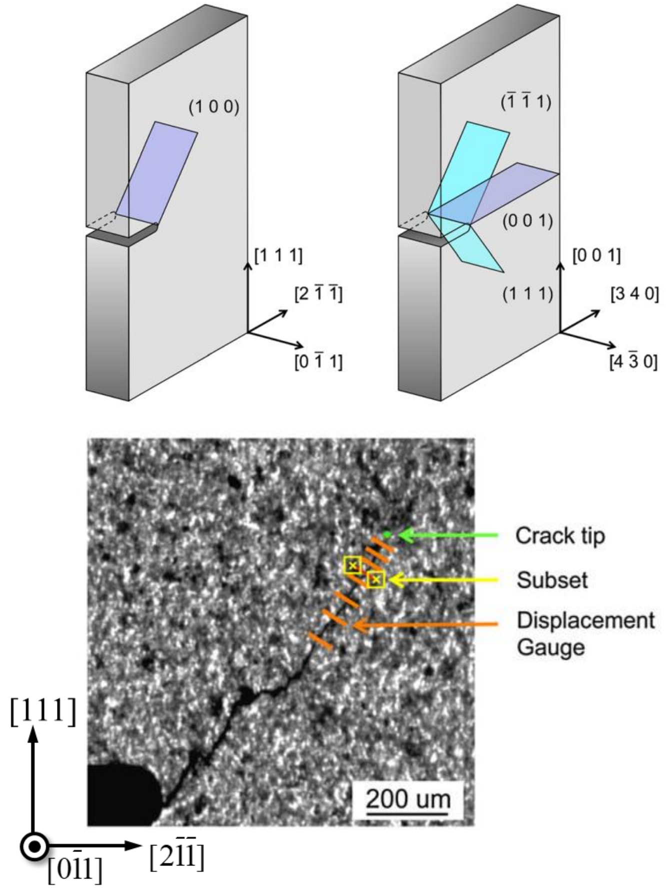
Load-displacement curves



Crack paths from simulations



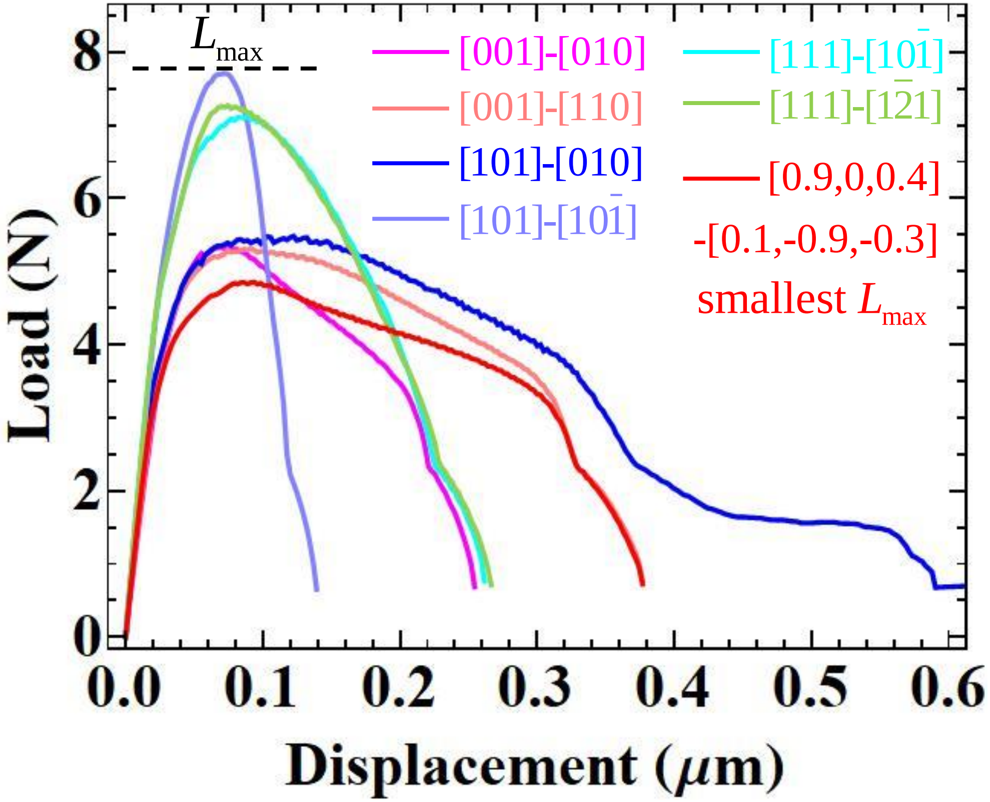
Experimental observations



Crystal plasticity leads to a change from pure Mode-I cracking to mixed-mode cracking

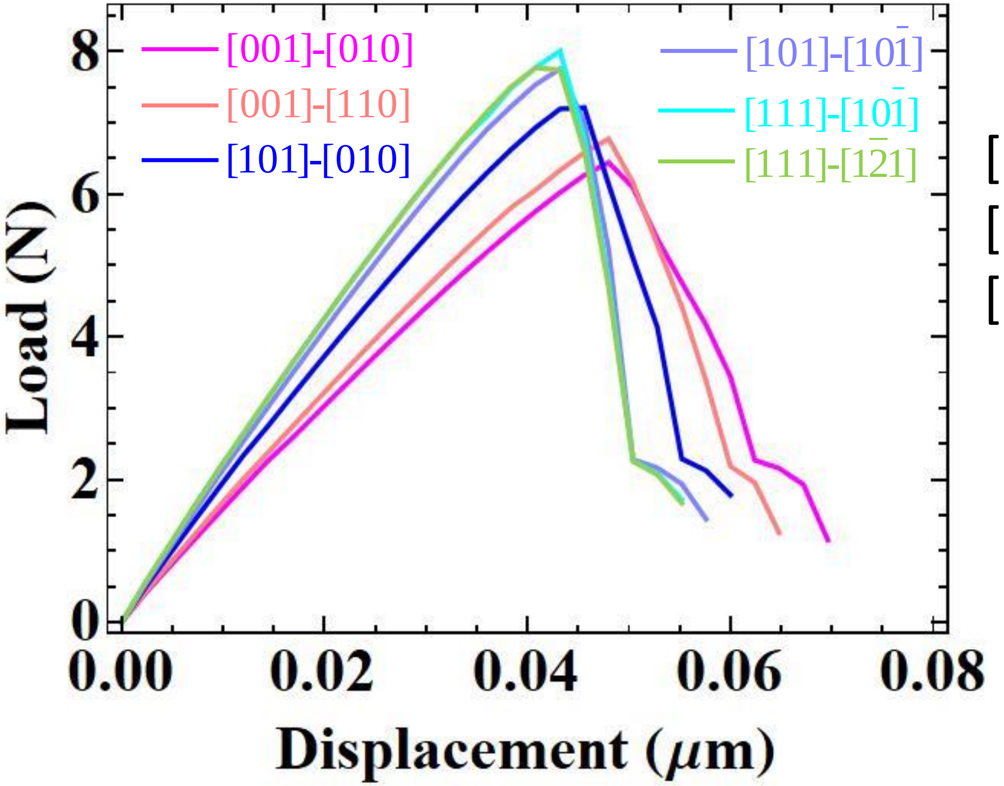
Anisotropy of Crack Growth in Ductile and Brittle Single Crystals

Ductile fracture (pure copper)



Crystal plasticity and elastic tensor anisotropy

Brittle fracture (switch off plasticity)



Elastic tensor anisotropy

[abc]-[def]: orientation
[abc]: elongation axis,
[def]: compression axis

The anisotropy of crack growth is mainly contributed from the anisotropy of crystal plasticity

High Throughput Phase-field Simulations on Ductile Single Crystals

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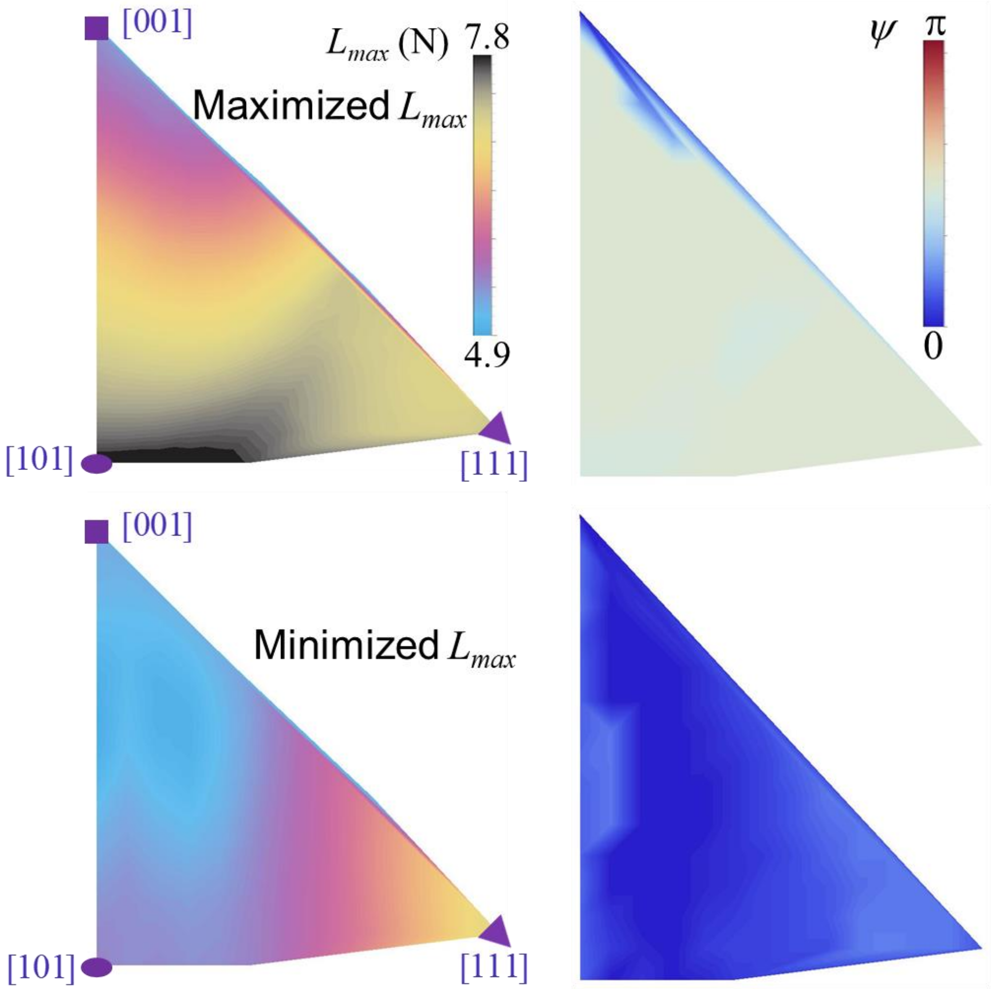
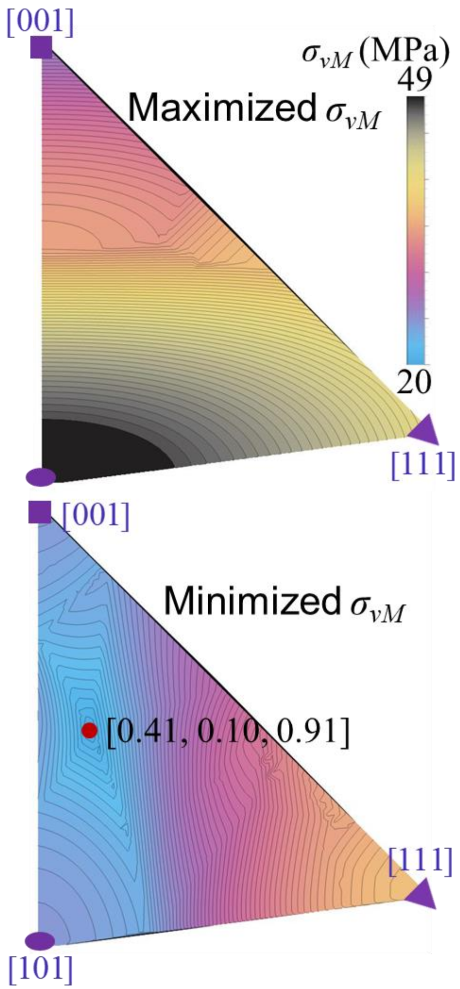
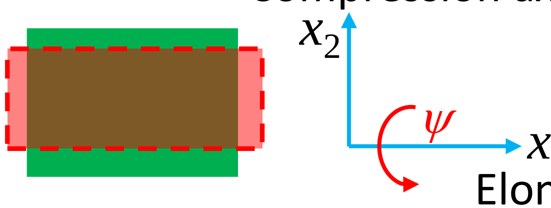
Phase-field simulations



Analytical method



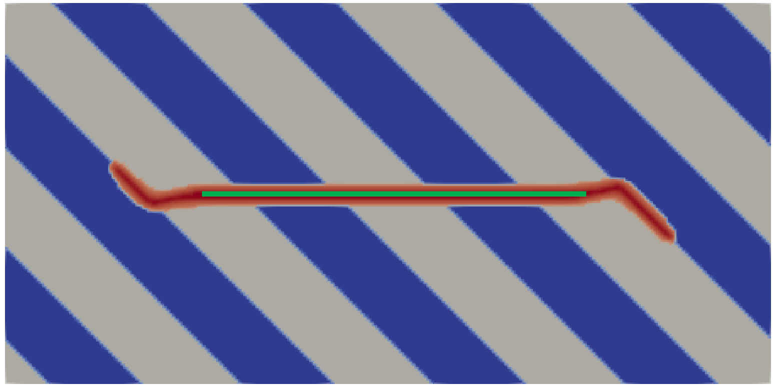


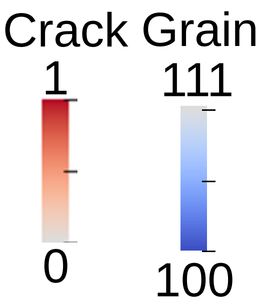
Results (left) are from 3,441 simulations, considering elastic stiffness tensor anisotropy

L_{max} obtains its maximum along [101]-[$10\bar{1}$] and its minimum along [0.9,0,0.4]-[0.1,-0.9,-0.3]

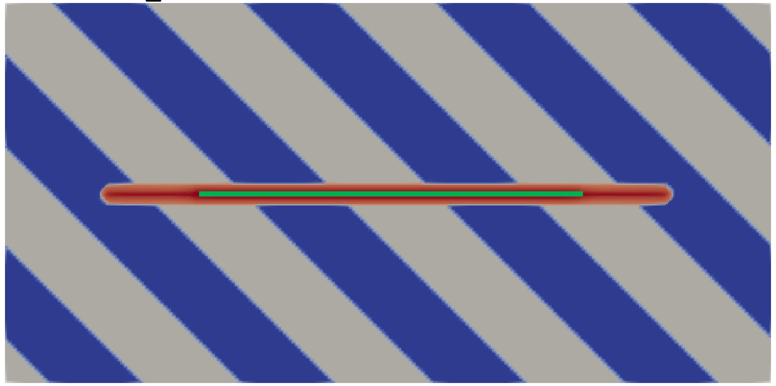
Simulations of Crack Growth in Ductile Bicrystals

Using crystal plasticity within each grain



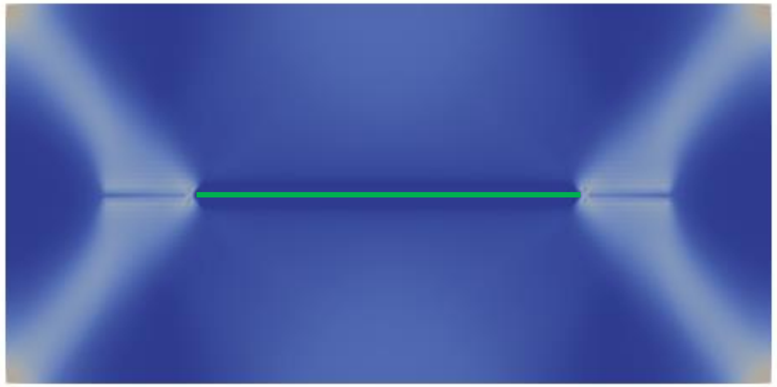


Using J_2 plasticity within each grain



Equivalent plastic strain

Equivalent plastic strain



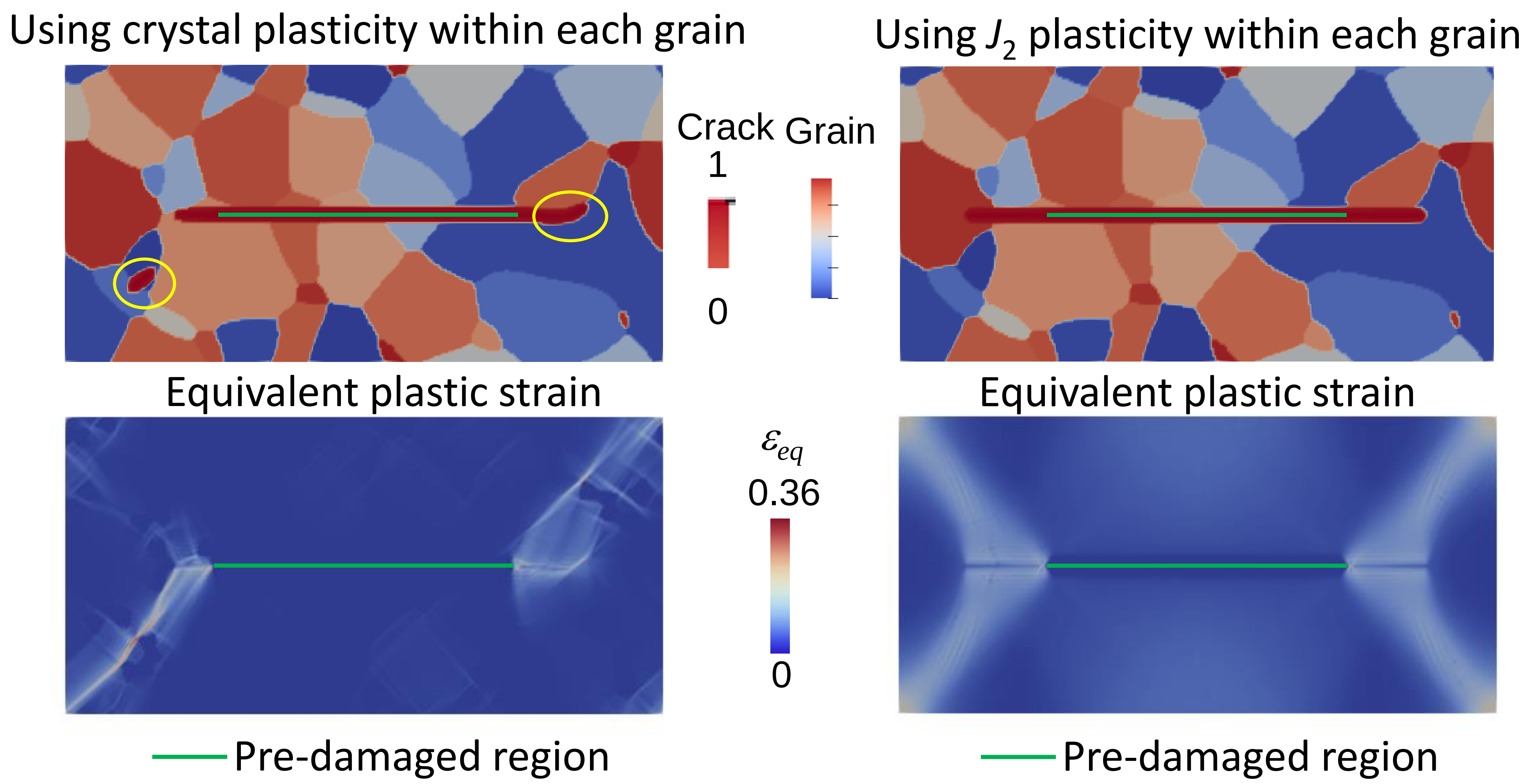
— Pre-damaged region

— Pre-damaged region

The crack deflects into grain boundaries, caused by significant plastic strain at grain boundaries

Xue, Cheng, Lei, and Wen, *npj Computational Materials*. 2022

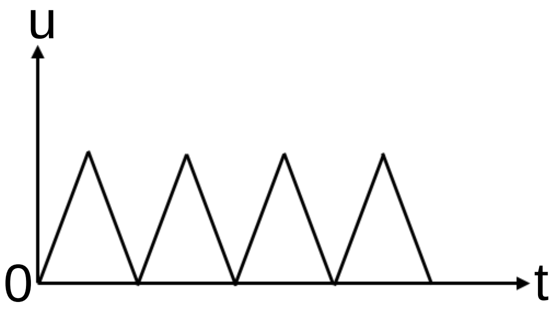
Simulations of Crack Growth in Ductile Polycrystals

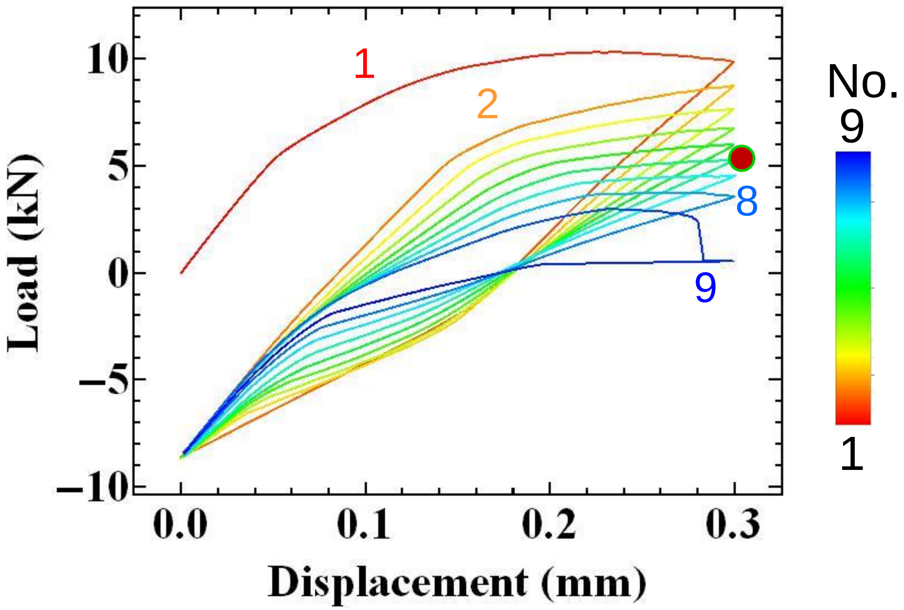


Cracks grow and nucleate at grain boundaries due to heterogeneous plastic strain distribution

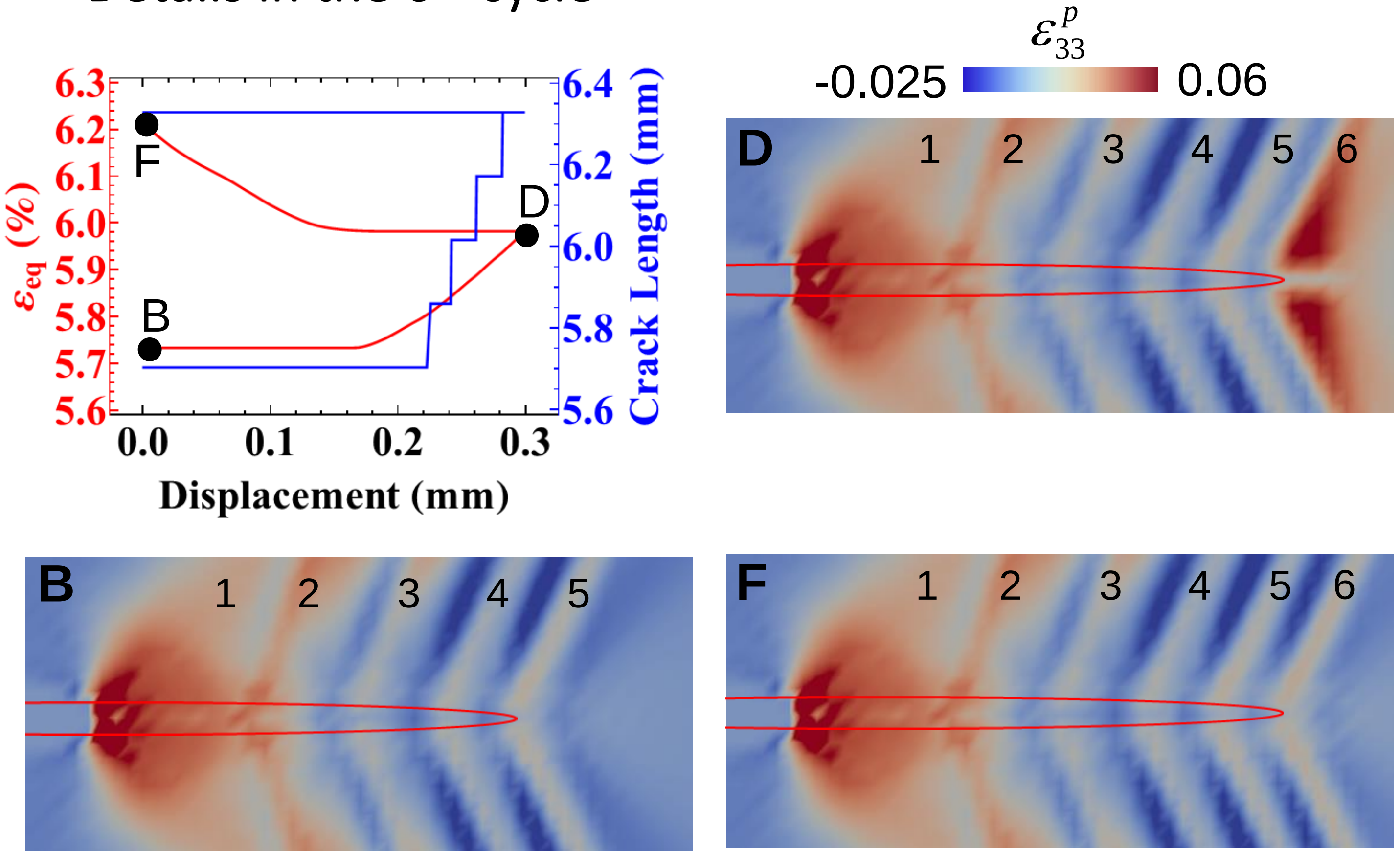
Crack Growth under Low Cycle Fatigue (LCF)

Displacement evolution





Details in the 6th cycle

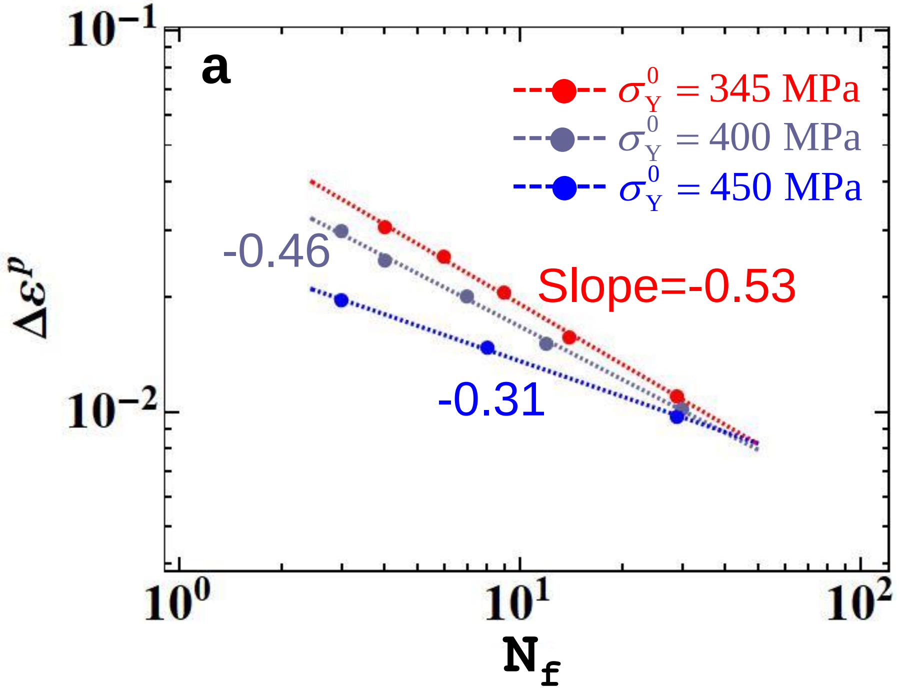


Each cycle produces one stripe in the plastic strain distribution, possible origin of fatigue striation

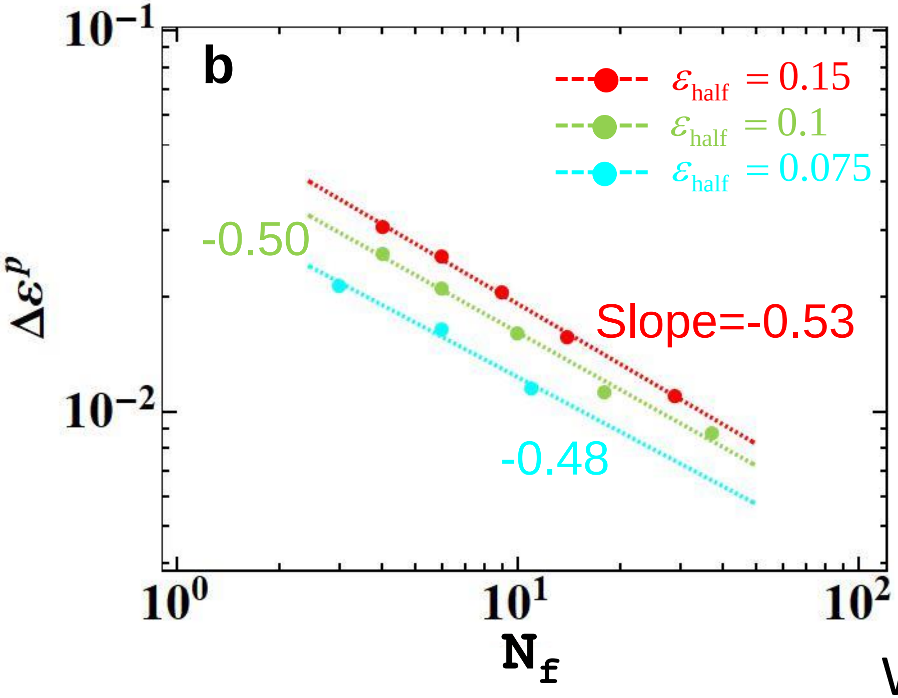
Plastic Strain vs Cycle Number to Failure: Coffin–Manson Relation

Coffin–Manson relation: $\Delta\varepsilon^{\mathrm{p}} = \alpha_{\mathrm{f}} N_{\mathrm{f}}^{\beta}$

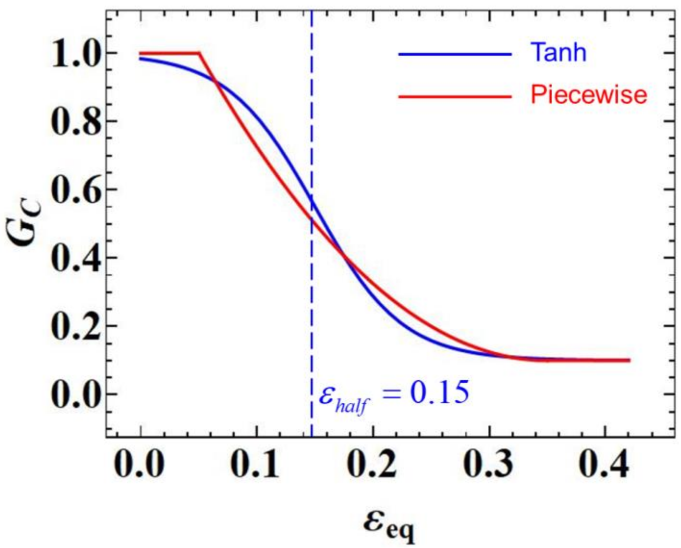
Influence of yield strength



Influence of plastic degradation rate



Fracture toughness vs ε_{eq}



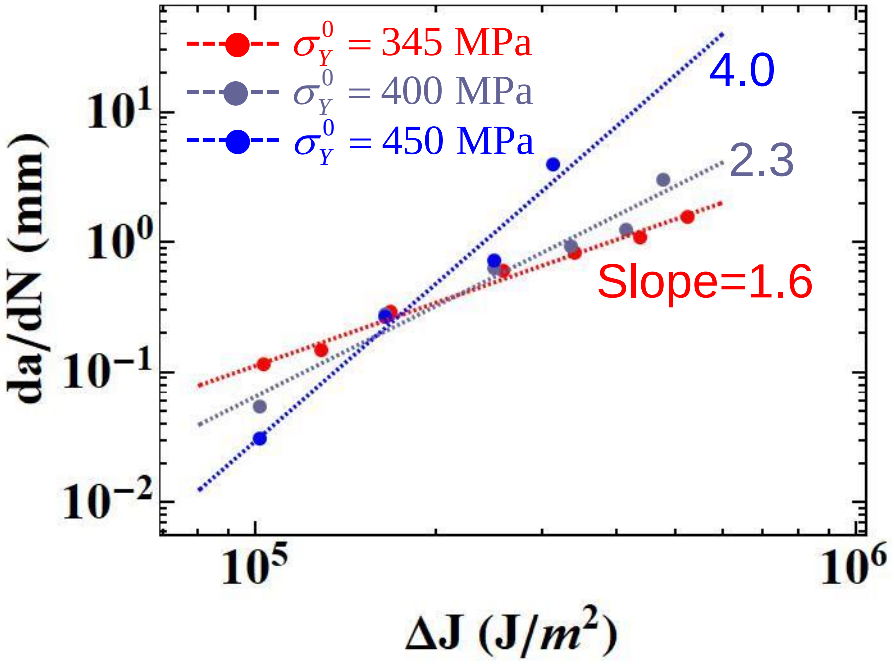
When $\varepsilon_{eq} = \varepsilon_{half}$, G_C is degraded to the half of its initial value

Larger yield strength and smaller ε_{half} lead to shorter fatigue life and smaller slope of the fitted line

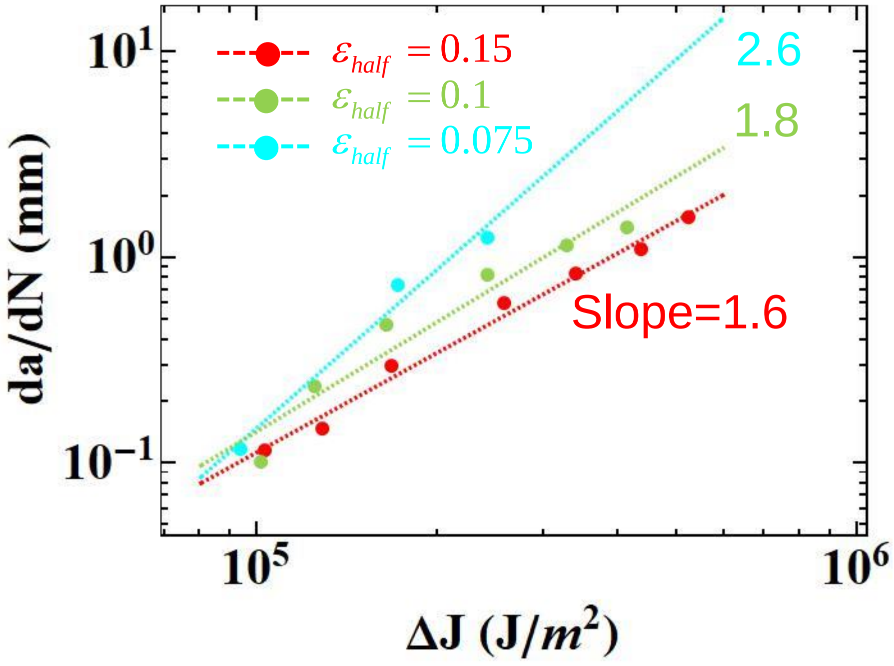
Crack Growth Rate vs ΔJ under Low Cycle Fatigue (LCF)

Crack growth rate for LCF $\frac{da}{dN} \sim (\Delta J)^n$

Influence of yield strength



Influence of plastic degradation rate



$$\Delta J = \int_\Gamma (W n_1 - n_j \Delta\sigma_{jk} \frac{\partial \Delta u_k}{\partial x}) ds$$

Γ : Integral path

W : Elastic energy density

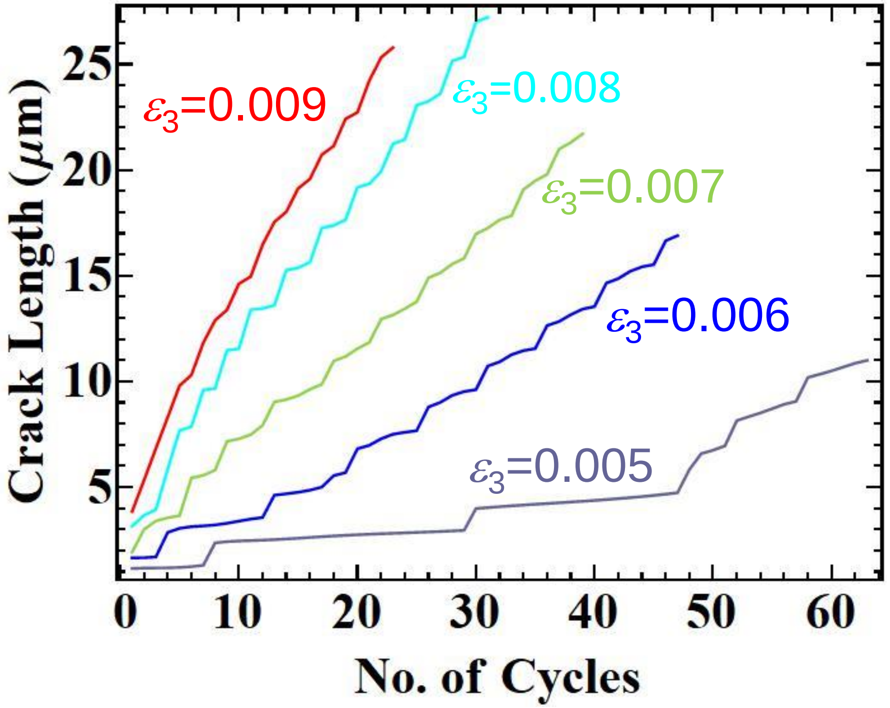
n_j : Normal to the path

Larger yield strength leads to larger slope and crossovers between two fitted lines are observed.

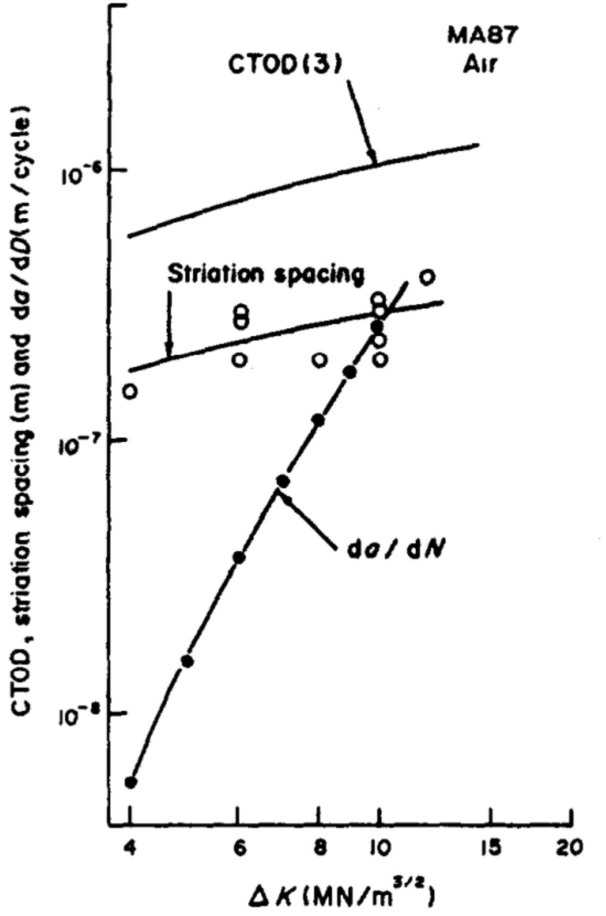
Smaller $\varepsilon_{\text{half}}$ leads to faster crack growth and larger exponent of the growth law.

Intermittent Crack Growth under High Cycle Fatigue (HCF)

Phase-field simulations



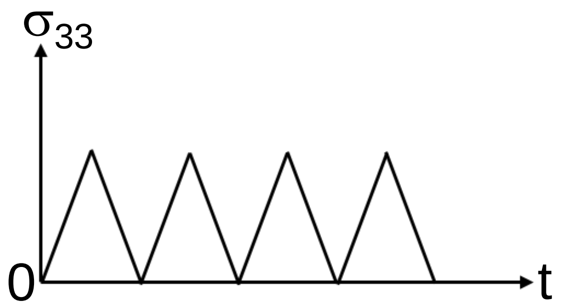
Experimental observations



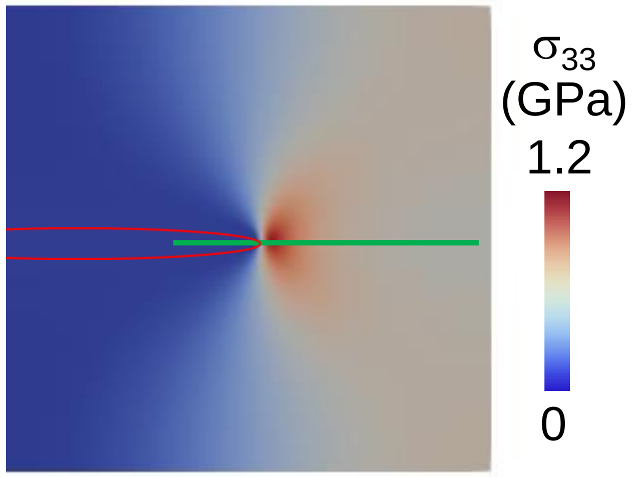
Crack growth is intermittent, and the cycle number for each growth period decreases with increasing ε_3

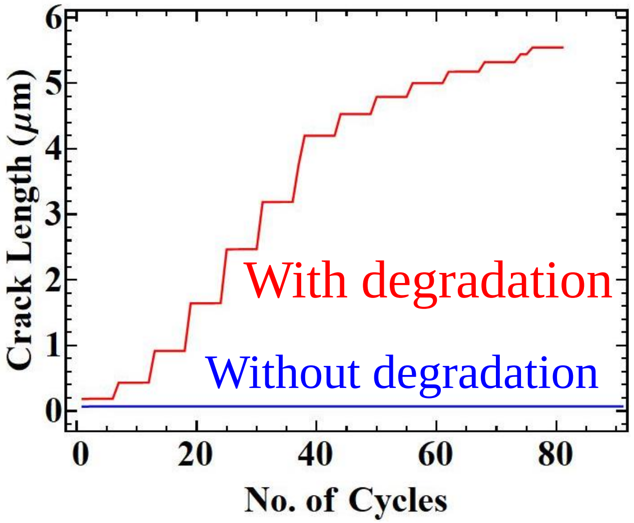
Intermittent Crack Growth under High Cycle Fatigue (HCF)

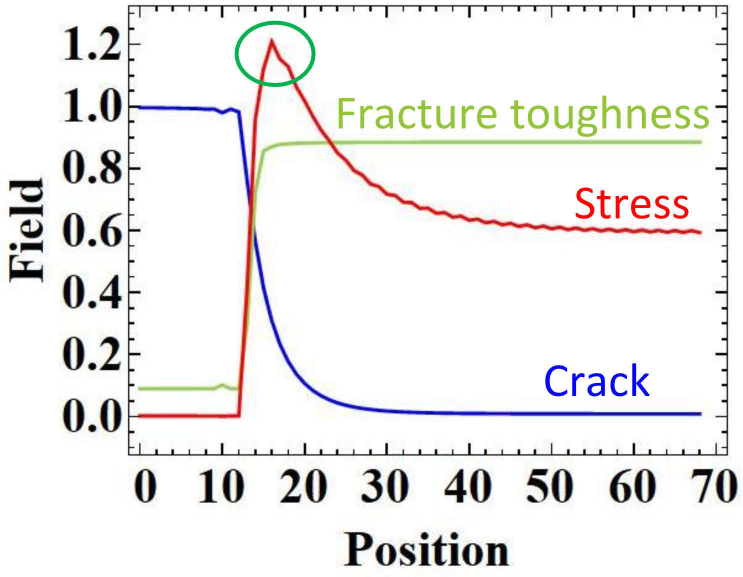
Stress evolution



Peak stress distribution







Fracture energy

$$f_{\text{frac}} = G_C(\eta, \boldsymbol{\varepsilon}^p, H^{elas})\left(\frac{\phi^2}{2l_0} + \frac{l_0}{2}\frac{\partial\phi}{\partial x_i}\frac{\partial\phi}{\partial x_i}\right)$$

H^{elas}: damage from stress cycling

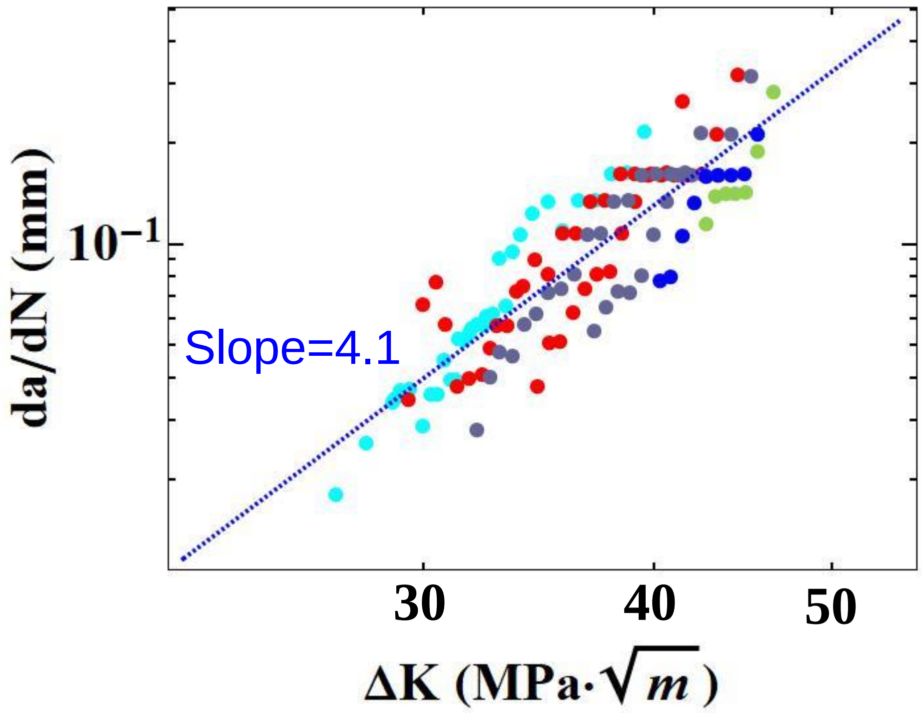
Fracture toughness G_C is degraded under stress cycling

Intermittent crack growth is mainly due to stress cycling degradation

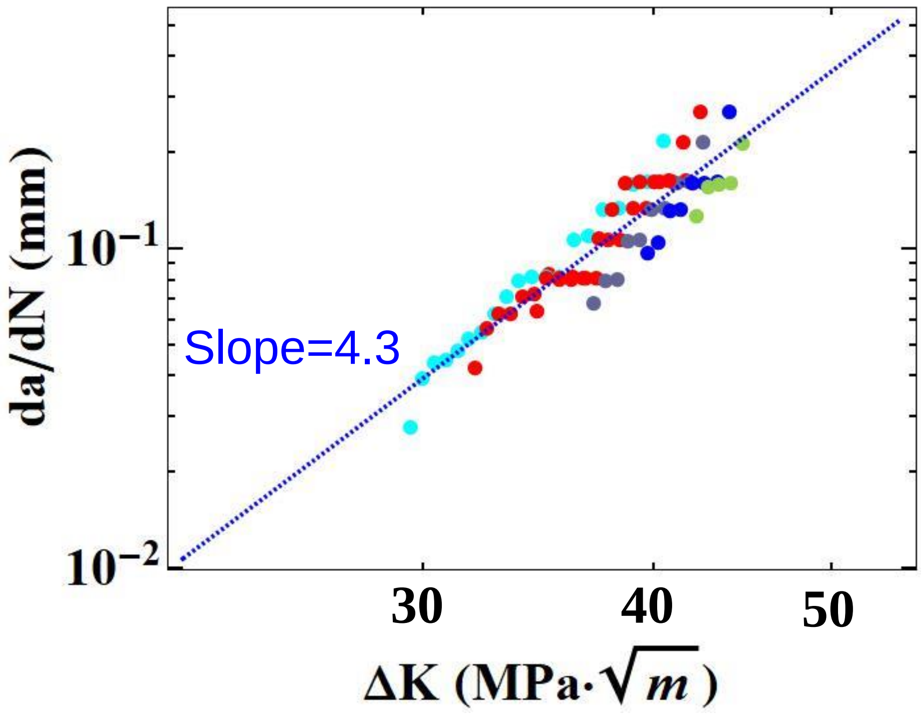
Paris Law under High Cycle Fatigue (HCF)

Paris Law: $\frac{da}{dN} = C(\Delta K)^n$ K: Stress intensity factor

Initial yield strength: 350 MPa



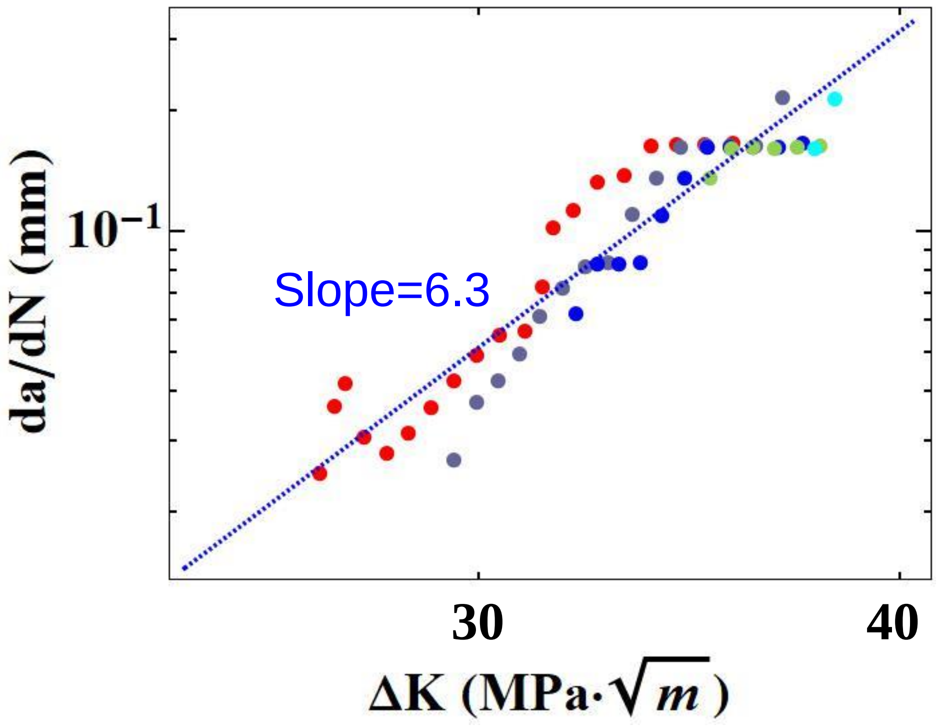
Initial yield strength: 450 MPa



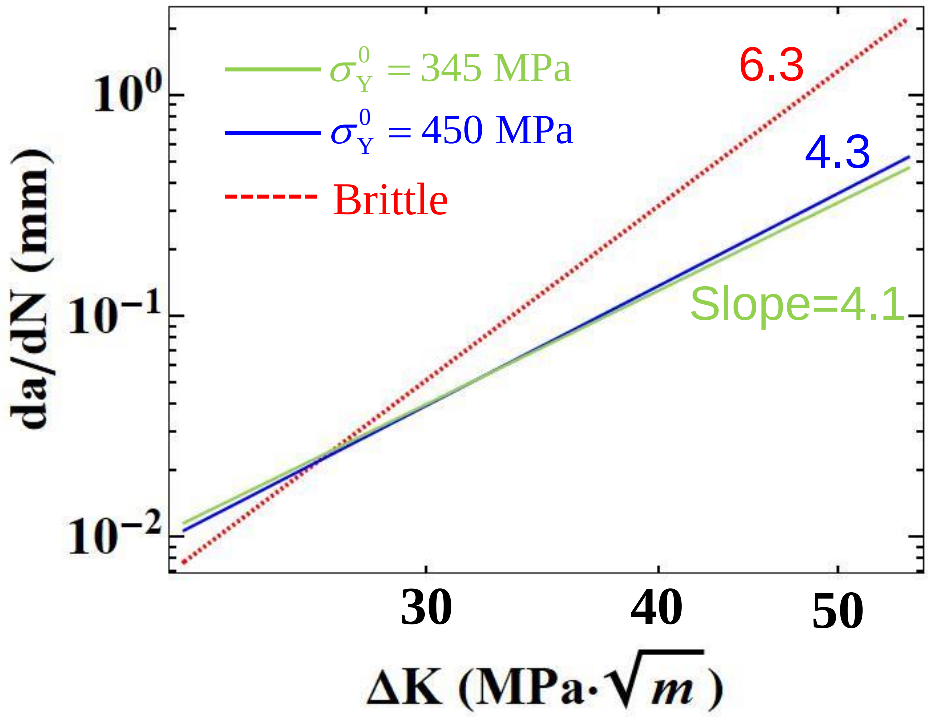
Consistent with experimental Paris exponent (n=2~4 for ductile materials)

Influence of Plasticity on Paris Law under High Cycle Fatigue (HCF)

Brittle materials (switch off plasticity)

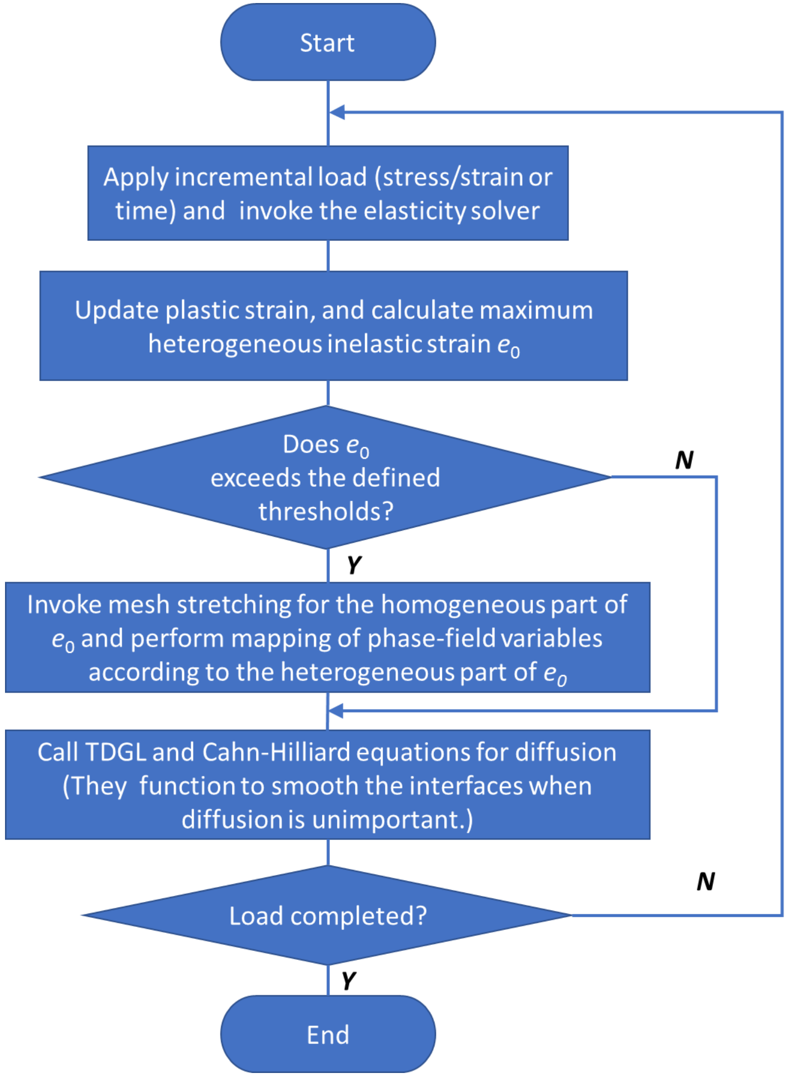


Influence of yield strength



The intersection of the fitted lines indicates that plastic deformation results in faster crack growth under small stress and slower crack growth under large stress

Modeling Capability of Large Deformation and Its Application to Creep Damage Modeling of Void Growth

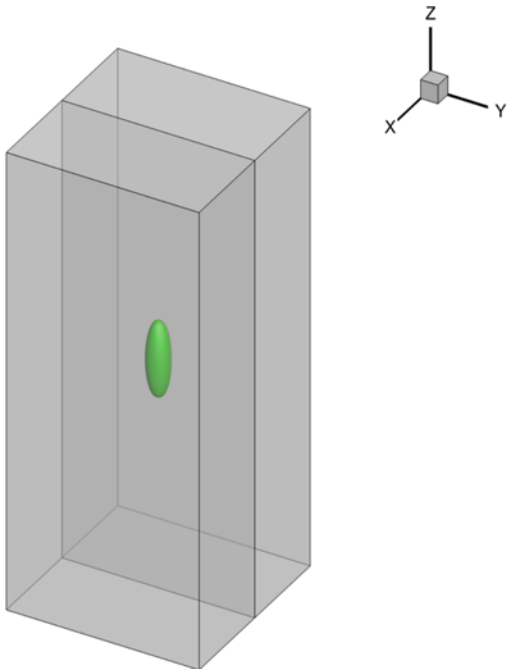


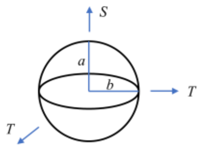
Summary of the model:

- **Multi-phase field method**
- **Kim-Kim-Suzuki (KKS) treatment**
- **IRID to deal with large deformation**
  - **Separation of displacement into homogeneous and heterogeneous parts**
  - **Homogeneous part to be implemented by stretched grid**
  - **Heterogeneous part to be implemented by advection/rotation**

Phase-field approach accommodating large deformation

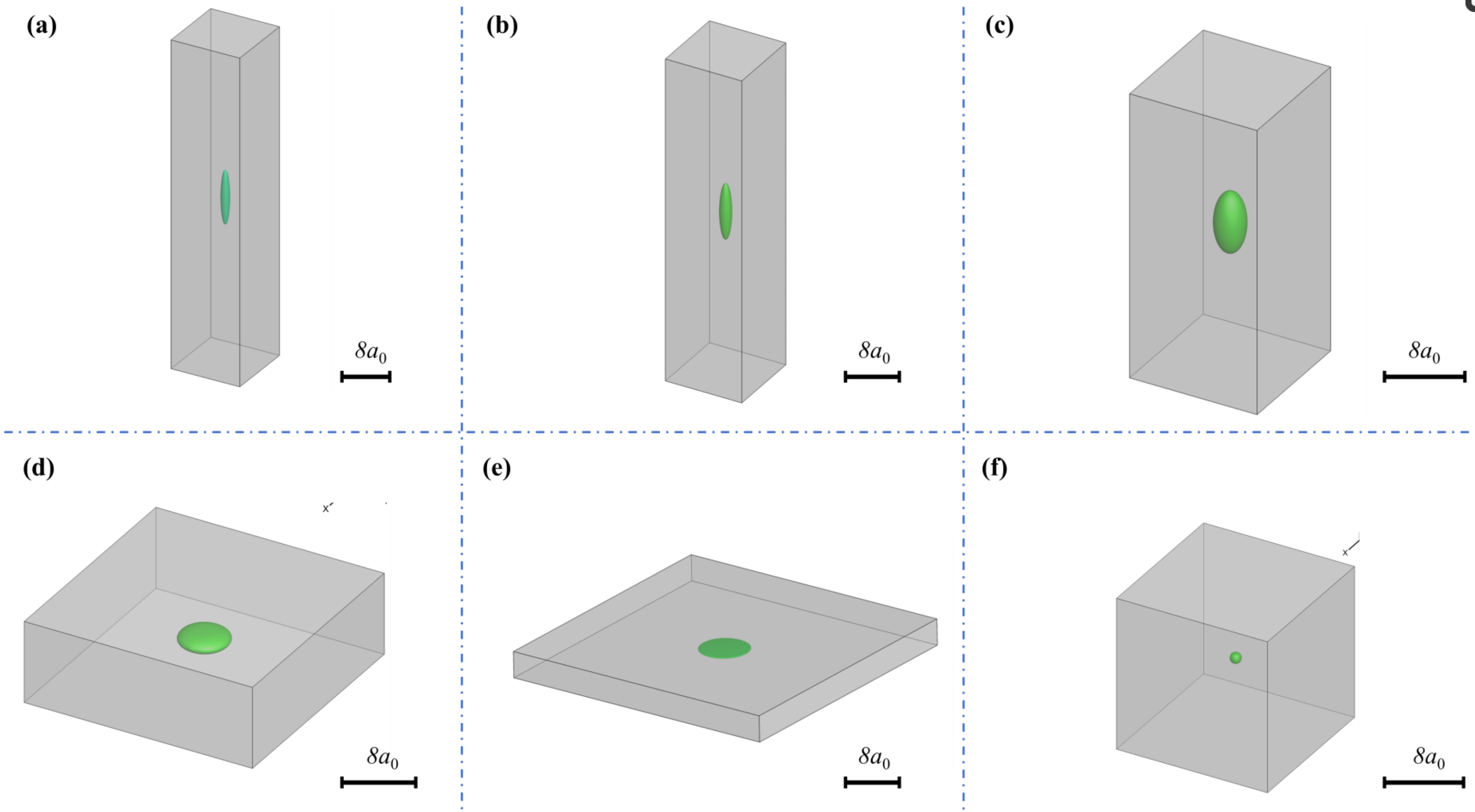
Simulated void growth under linear viscoplasticity



		V/V_0	a/b	a/a_0	b/b_0	*Void shapes*
S=1 T=0	Simulation	**1.24** (when a/a_0=4.0)	↑↑	↑↑	↓↓	Fig (a)
	Asymptotic solution	**1.26**	∞	∞	0	Needle
S>0 S/T=4	Simulation	↑↑	↑↑	↑↑	**0.755** (when a/a_0=4.5)	Fig (b)
	Asymptotic solution	∞	∞	∞	**0.794**	Cylinder
S>0 S/T=1.5	Simulation	↑↑	2.16 (when a/a_0=3.5)	↑↑	↑↑	Fig (c)
	Asymptotic solution	∞	a/b>1	∞	∞	Prolate spheroid
S>0 S/T=0.5	Simulation	↑↑	0.299 (when a/a_0=0.85)	↑↑	↑↑	Fig (d)
	Asymptotic solution	∞	0<a/b<1	∞	∞	Oblate spheroid
S=0 T=1	Simulation	**1.84** (when a/a_0=0.30)	↓↓	↓↓	↑↑	Fig (e)
	Asymptotic solution	**2.36**	0	0	∞	Crack
S<0 S/T=1	Simulation	↓↓	1	↓↓	↓↓	Fig (f)
	Asymptotic solution	0	1	0	0	Point

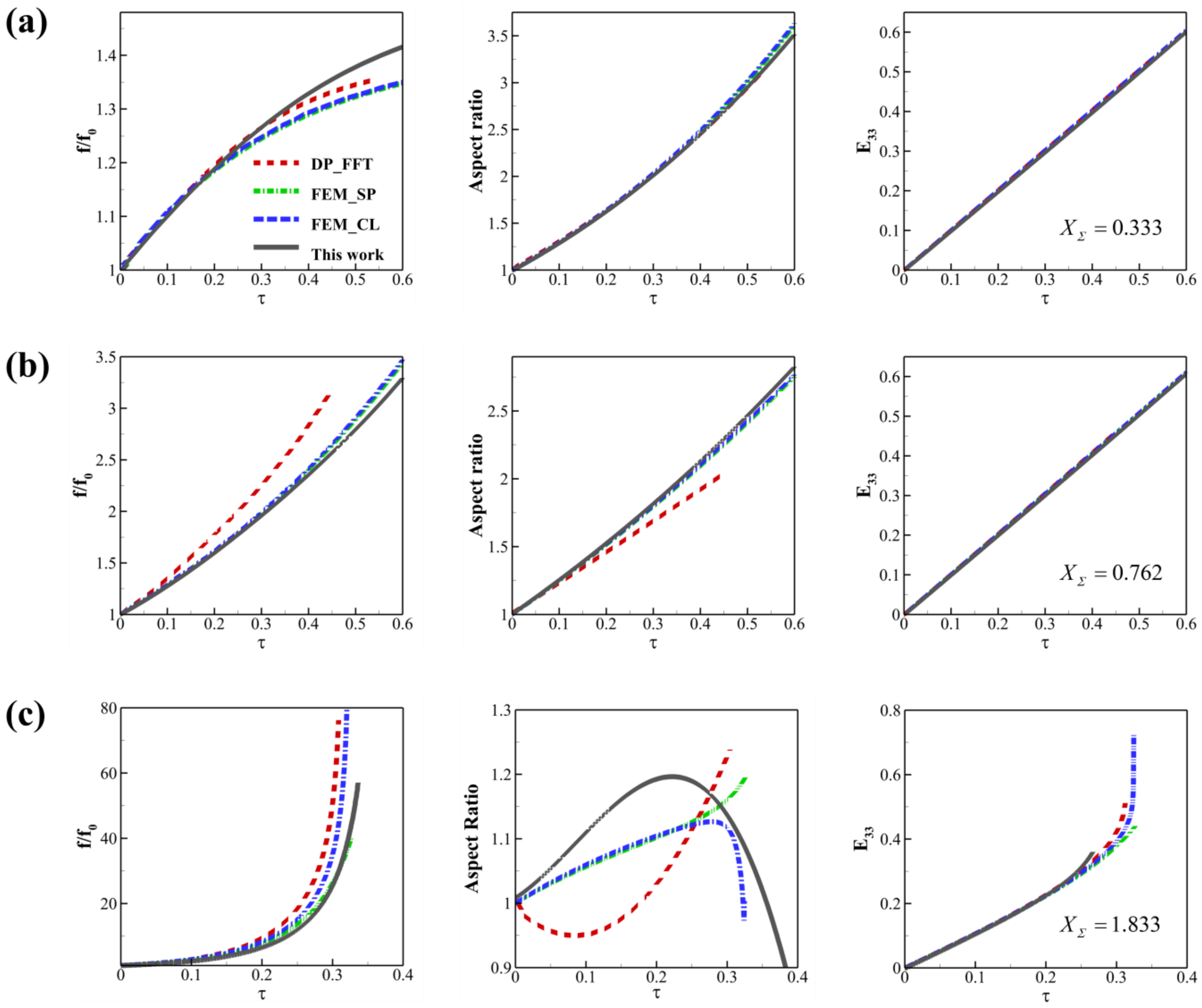
- 3D simulations of a single void under transversely isotropic creep load
- Matrix obeys linear viscoplasticity (power-law creep with n=1)
- In quantitative agreement with the asymptotic solutions of Budiansky 1982

Simulated void growth under linear viscoplasticity



(a_0 is the original void radius)

Simulated void growth under 5-power creep



- DP_FFT: dilatational plasticity – FFT (R. A. Lebensohn et al., Acta Mater. 61, 6918; 2013)

- FEM_SP: FEM with spherical cell
- FEM_CL: FEM with cylindrical cell (M. Gărăjeu, et al., Comp. Meth. Appl. Mech. & Eng. 183, 223; 2000)

- This work: 3D phase-field simulation with the IRID algorithm

$$X_\Sigma = \sigma_m / \sigma^{VM}$$

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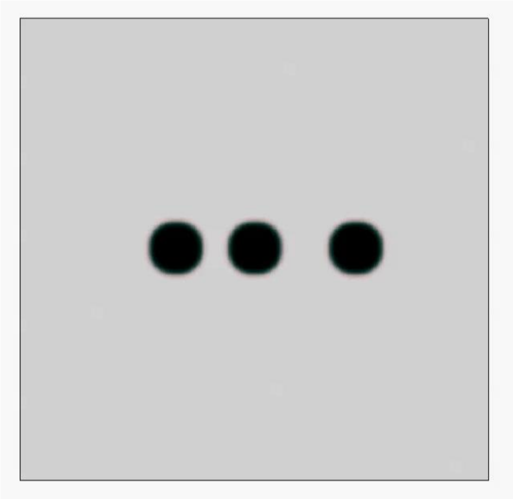
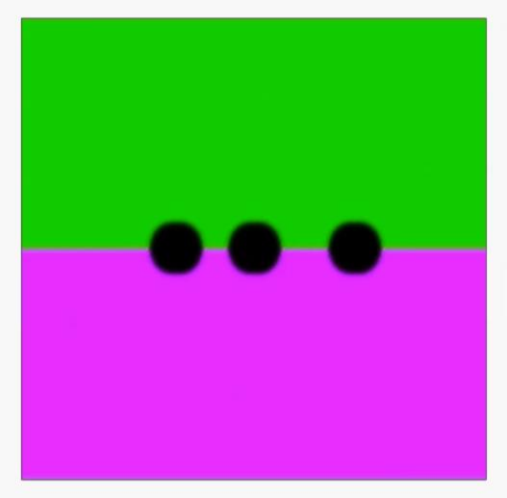
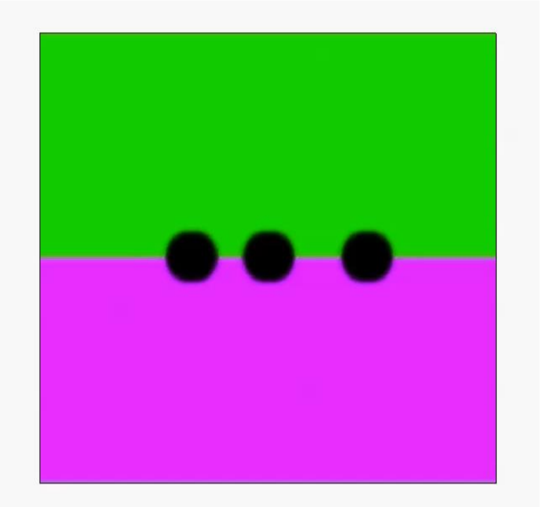
Simulated void growth and coalescence under unidirectional tension in the vertical direction



(a) Pure plasticity under 5-power-law creep



(b) Pure diffusion



(c) Diffusion-plasticity coupling

Void growth and coalescence under coupled diffusion and plasticity can be much faster than under each individual mechanism.

EY22 & Future Work

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EY21	**EY22**	EY23-24
1) Combined LCF & HCF modeling; 2) Creep damage modeling	**1) Combined creep and fatigue modeling addressing hold-time creep-fatigue;** **2) Crack-environment interaction**	A microstructure-based life prediction tool to consider coupling among creep, fatigue, and environmental effects

Progression of NETL Microstructure-based Life Prediction Tool Development

Acknowledgement

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