Combined Creep and Fatigue Modeling

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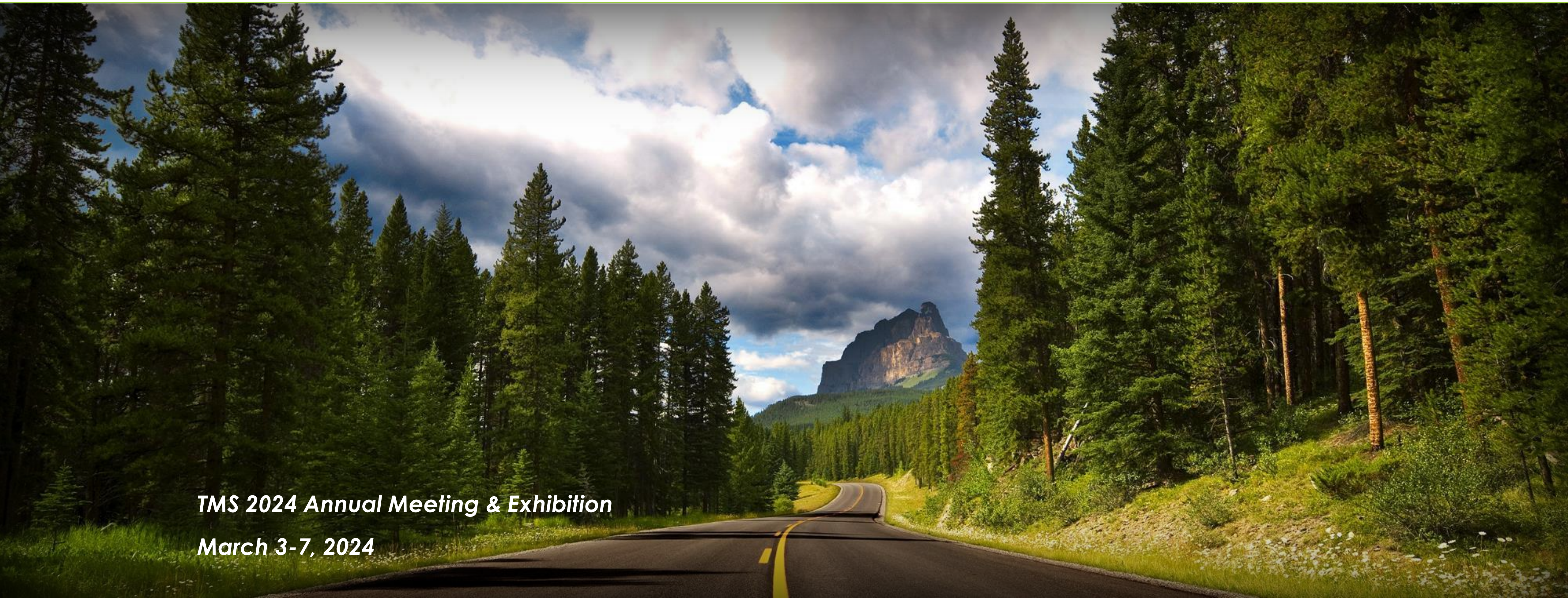

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New market conditions require new tools to address challenges

Penetration of Renewable Energy into the grid

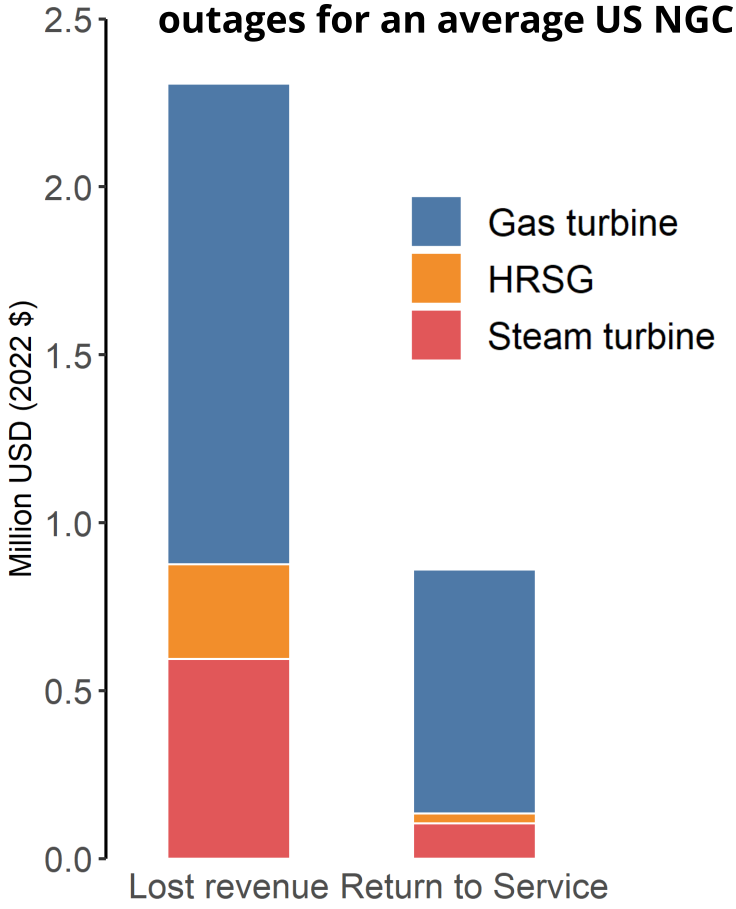
Introduction of RE into the grid and increased cycling is putting **greater strain on components that were not designed to withstand new conditions** resulting in increased fatigue failures

Emergence of hydrogen as a fuel source

Hydrogen **accelerates crack propagation and material failures**, making accurate material and performance life prediction models more critical for quick, effective, and cost-efficient component development

Predictive maintenance for US NGCC plants could be worth $1.2B/yr

Expected economic losses from unplanned outages for an average US NGCC



Adapted from *Grace and Christiansen (2013)*

Across 546 operational NGCCs **unplanned outages likely cost operators $1.6B**

At the plant level, this can mean **3-10% of total revenue lost**

A system that avoids 90% of NGCC lost revenues could likely be valued at **$200K/plant/year**

Current modeling produces limited picture of material degradation

Predictive capability of current modeling is limited and typically relies on wide range of empirical data that is oversimplified with few direct links to underlying mechanisms

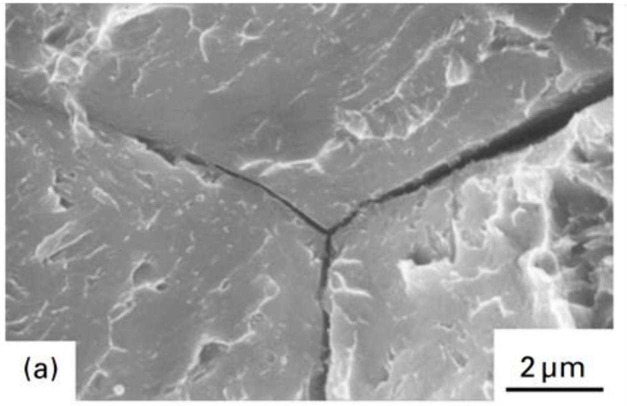
Barrier in understanding time dependent material degradation with respect to changes in microstructure

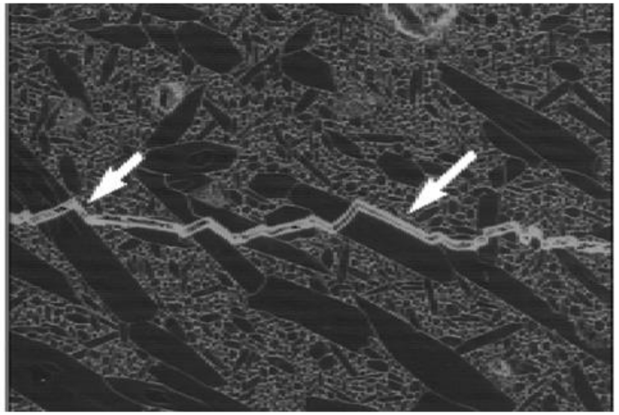
Models do not have combined creep and fatigue modeling together, increasing room for error and taking more time overall

Historical data becoming less relevant for prediction as load following/increased cycling/VRE increases flexible operations

Why Microstructure-Based Modeling?

Intergranular crack paths





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

- Materials performance/life is strongly influenced by the underlying microstructure such as pores, precipitates, grains, etc.
- The microstructure also controls the <u>**rare events**</u> of initiation of micro-cracks, their propagation, interaction, and eventual failure.

<u>Microstructure-based modeling is essential for accurately predicting materials life</u>

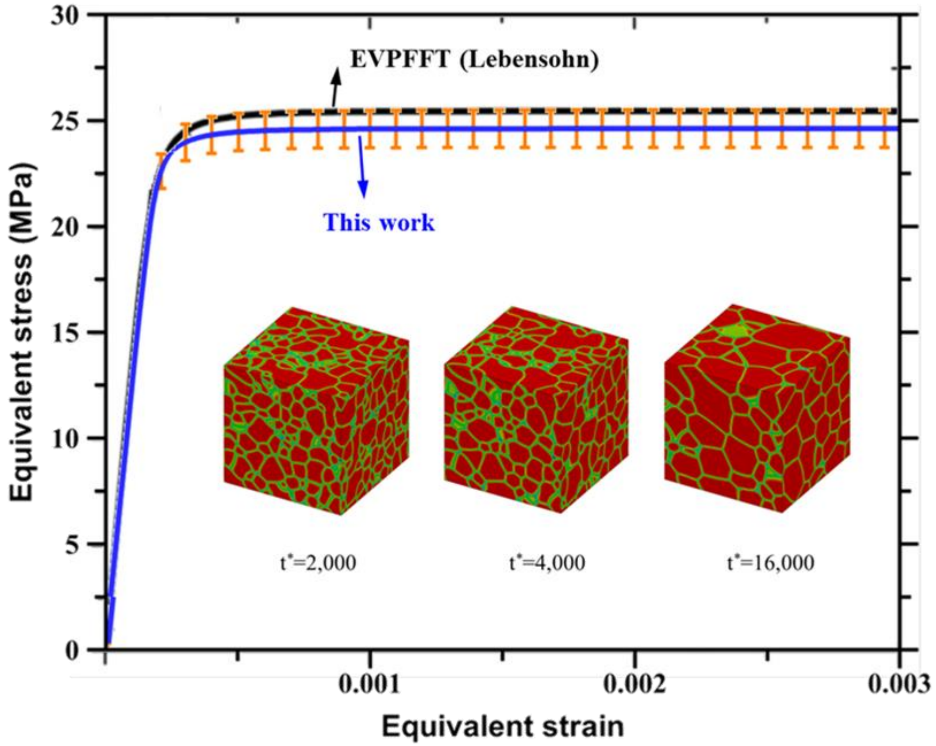
State-of-the-art: Creep & Fatigue Modeling

Existing creep/fatigue models are largely phenomenological. They often rely on a wide range of empirical parameters with few direct links to the underlying mechanisms at the microstructure level.

Microstructure evolution under service conditions is largely ignored in these existing models. There might be some parameters such as volume fraction of certain phases and mean precipitate size/distribution in the models, however, *complex microstructure morphology and heterogeneity are generally not considered*. As such, the direct coupling between microstructure evolution and creep/fatigue is missing.

NETL Approach: Take advantage of the well-recognized microstructure evolution modeling capability by phase-field approach and combine it with creep/fatigue modeling capabilities in a *unified* phase-field modeling framework. Our focus is on microstructure-based & integrated creep & fatigue modeling.

- EY17: Developed an isotropic (J2) plasticity modeling capability under a unified phase-field modeling framework
- EY19: Further developed a crystal plasticity modeling capability.

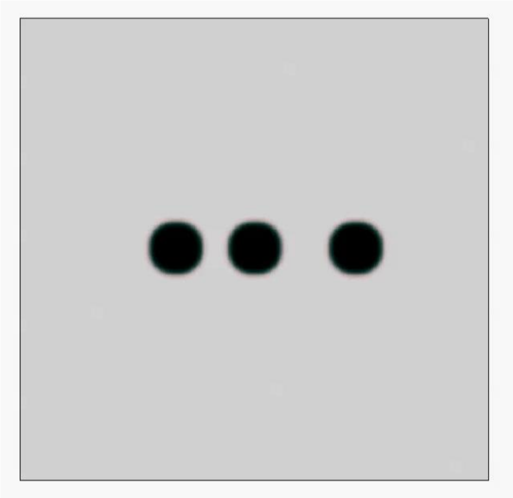


Crystal plasticity phase-field simulation of stress-strain curve of a polycrystalline copper

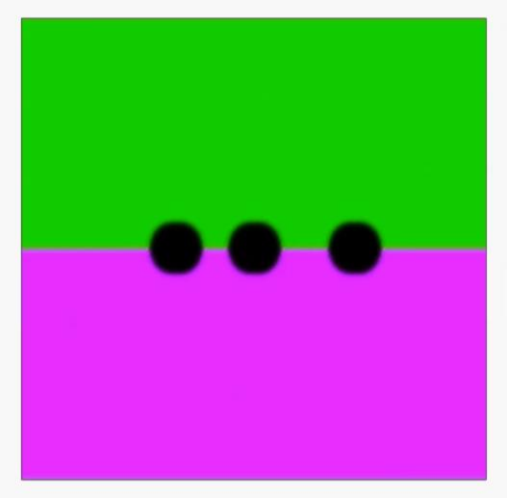
This laid a solid foundation for microstructure-based creep & fatigue modeling

Cheng et al., *International Journal of Plasticity*, 2019

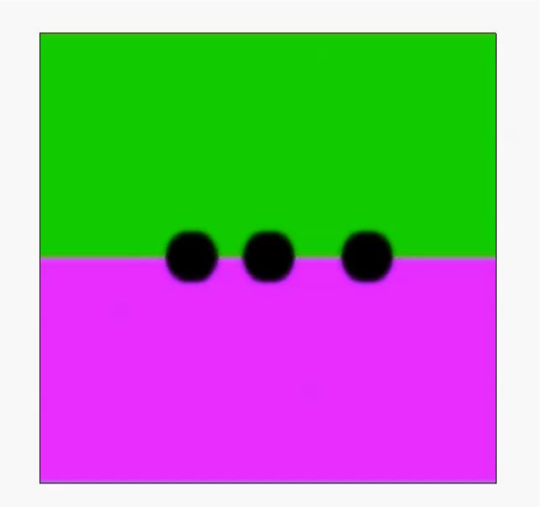
Simulated Void Growth and Coalescence under Unidirectional Tension in the Vertical Direction



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



(b) Pure diffusion



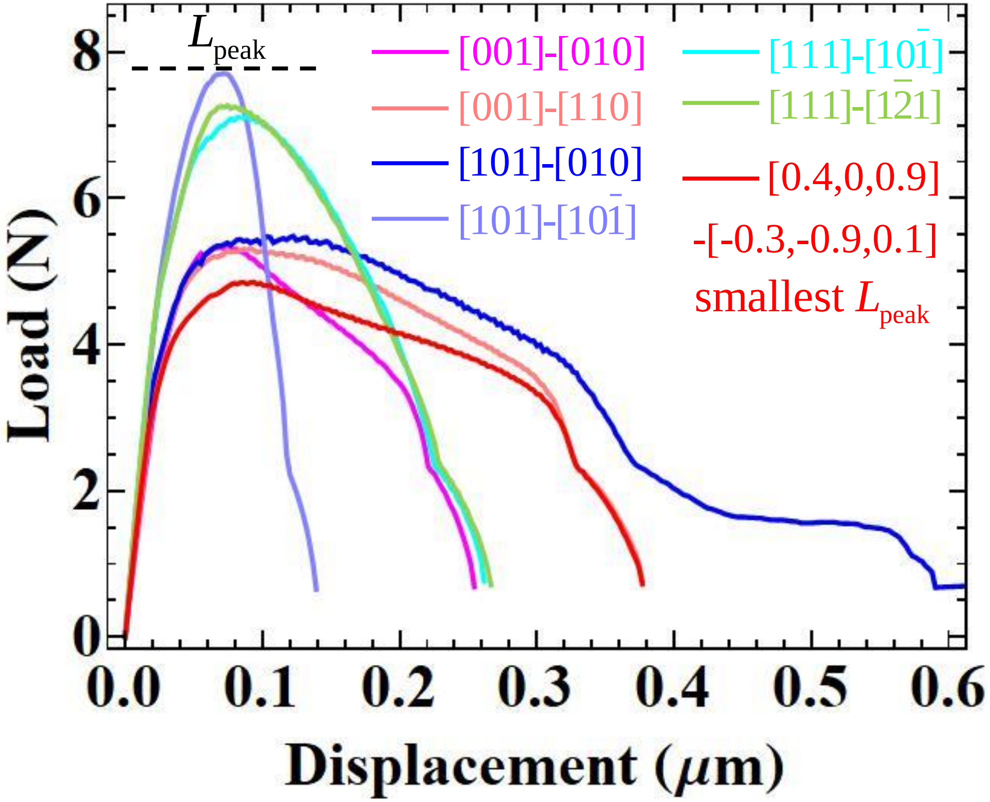
(c) Diffusion-plasticity coupling

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

Cheng and Wen, *Computer Methods in Applied Mechanics and Engineering* (2022)401:115608

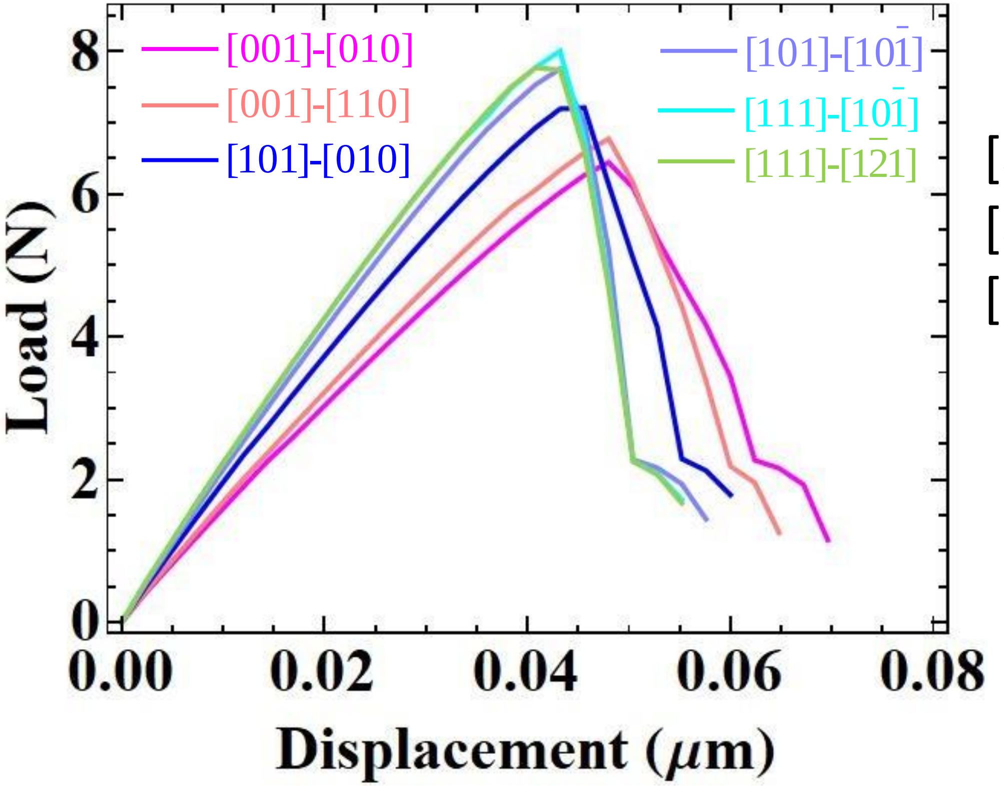
Anisotropy of Crack Growth in Ductile and Brittle Single Crystals – Ongoing

Ductile fracture (pure copper)



Crystal plasticity and elastic tensor anisotropy

Brittle fracture (switch off plasticity)



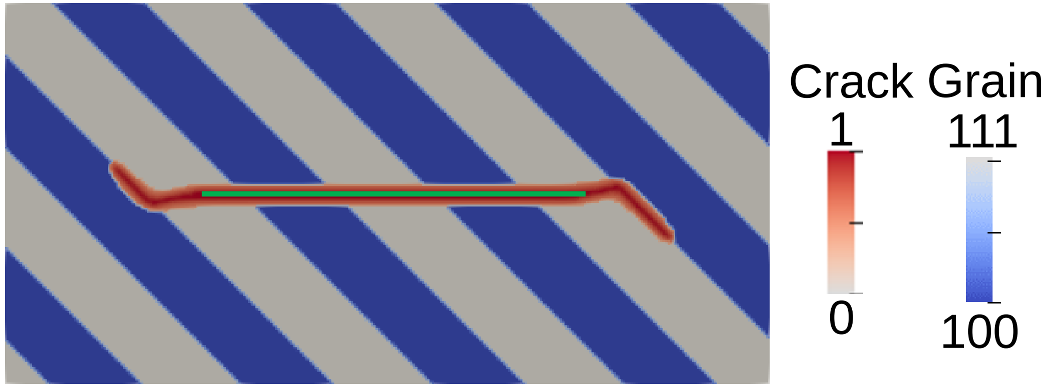
Elastic tensor anisotropy

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

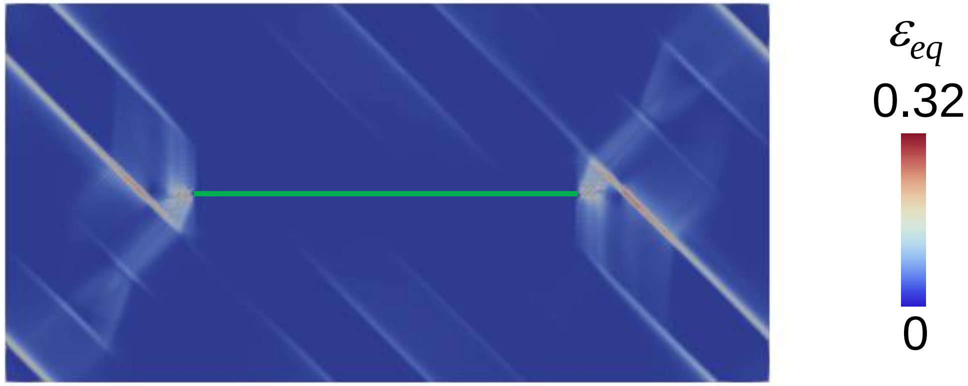
The anisotropy of crack growth is mainly contributed from the anisotropy of crystal plasticity

Simulations of Crack Growth in Ductile Polycrystals

Crack growth in bicrystals

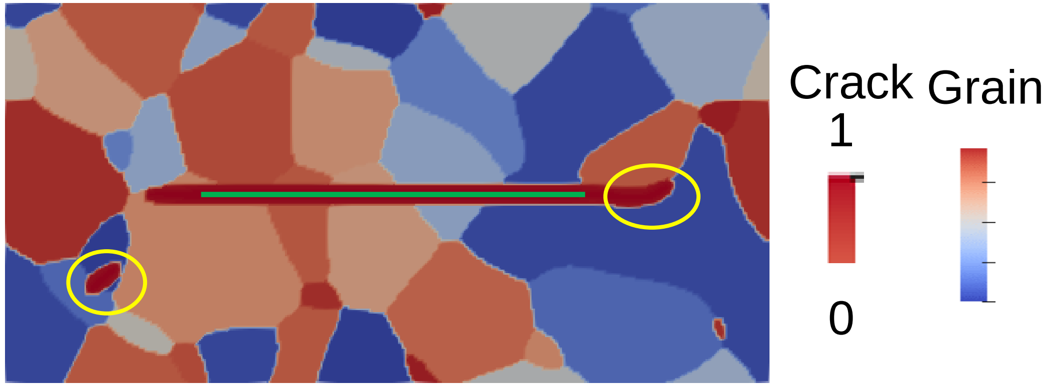


Equivalent plastic strain

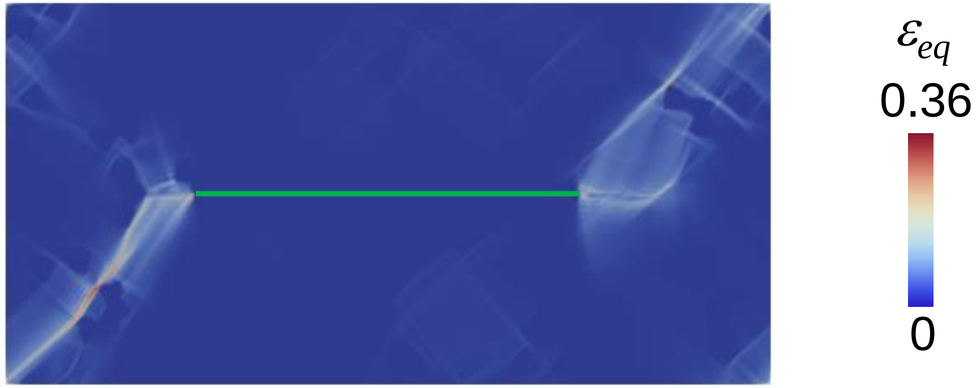


— Pre-damaged region

Crack growth in polycrystals



Equivalent plastic strain



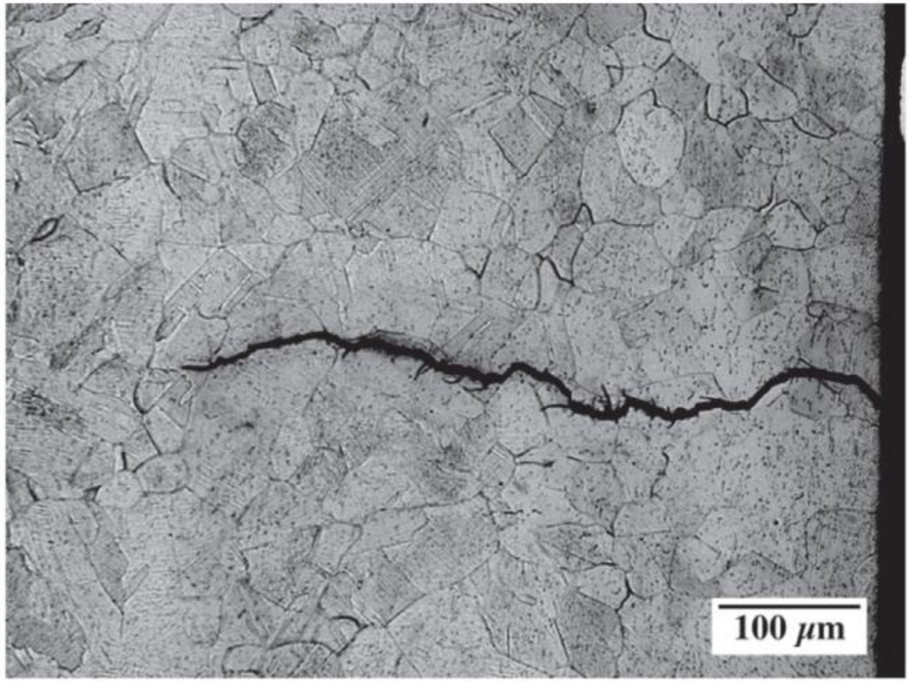
— Pre-damaged region

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

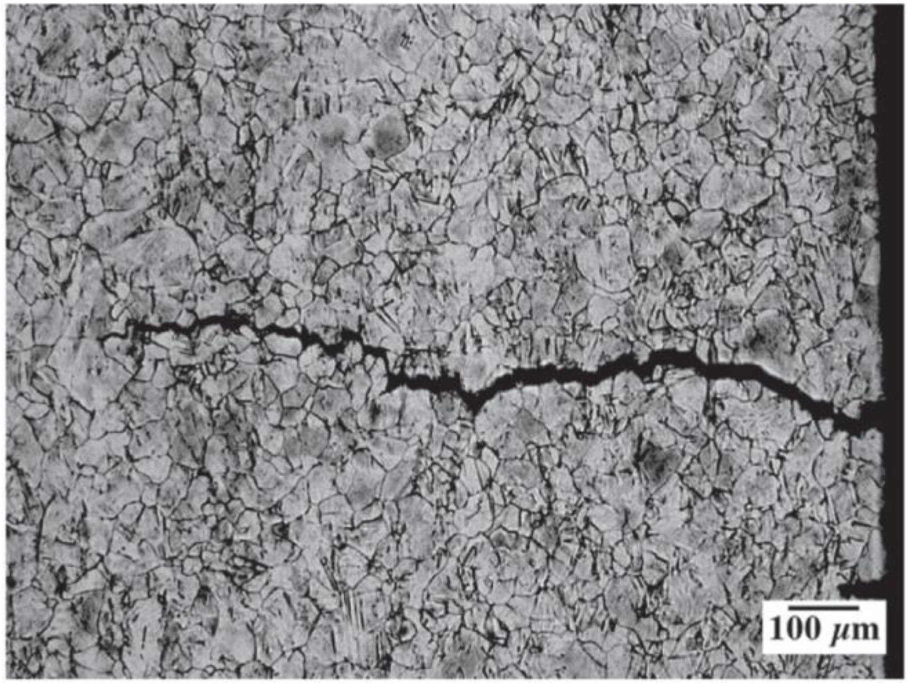
Xue et al., *npj Computational Materials*. 2022

Crack Growth under Fatigue and Creep

Transgranular cracking under pure fatigue



Intergranular cracking under creep-fatigue

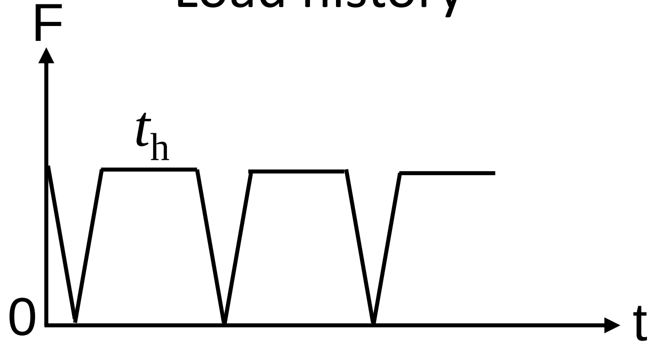


Porter et al., International Journal of Fatigue. 2019;124:205-16.

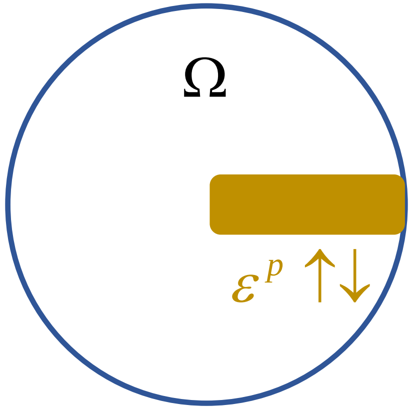
Crack growth rate is a key factor for both creep and fatigue

Phase-field Model for Crack Growth under Creep-fatigue

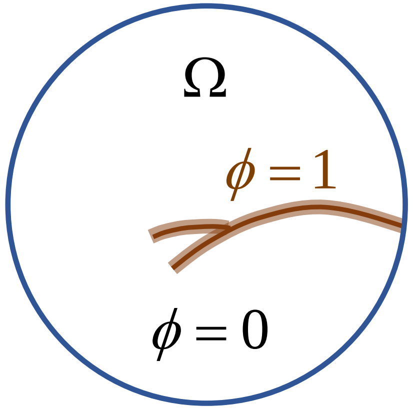
Load history



Plastic strain



Cracks



Cyclic plasticity is considered

Key features of the model:

- Employ diffuse interfaces for crack surfaces to avoid numerical remeshing
- Consider load history explicitly
- Consider the damages from fatigue, creep, and their interaction
- Could be used to predict crack paths and materials life under fatigue and/or creep

Xue et al., *npj Computational Materials*. 2022

Xue et al., *in preparation* 2024

Phase-field Model for Crack Growth under Fatigue and Creep

Total energy $$F = \int_{\Omega} [\, f_{\text{elas}} + f_{\text{frac}} \,] d\Omega$$

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

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

H^{elas}: elastic damage

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

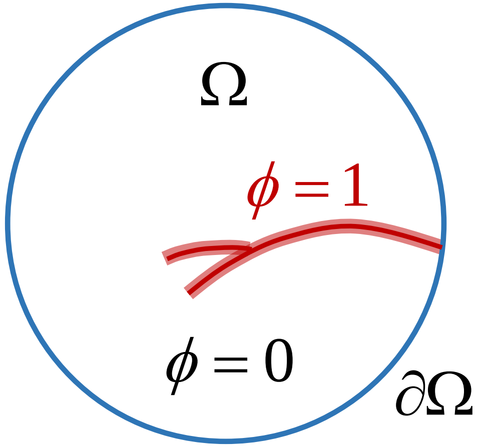
Effective elastic tensor is a function of the crack order parameter

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

Plastic strain due to yield $$\frac{\partial \varepsilon_{ij}^{\text{p}}}{\partial t^*} = L_{ijkl}^{\text{yield}} \sigma'_{kl} \quad L_{ijkl}^{\text{yield}} = \begin{cases} 0, J_2 \le \sigma_{\text{Y}}^0 + R \\ L_y \delta_{ik} \delta_{jl}, J_2 > \sigma_{\text{Y}}^0 + R \end{cases}$$

Plastic strain due to creep $$\frac{\partial \varepsilon_{ij}^{\text{p}}}{\partial t} = L_{ijkl}^{\text{creep}} \sigma'_{kl} \quad L_{ijkl}^{\text{creep}} = A_{\text{cr}} \exp\left(-\frac{Q_{\text{cr}}}{RT}\right)\left(\frac{J_2}{\sigma_{\text{Y}}^0 + R}\right)^{N^*} \frac{\delta_{ik}\delta_{jl}}{J_2}$$

Cracks



t^* : Numerical time

σ'_{kl} : Deviatoric stress

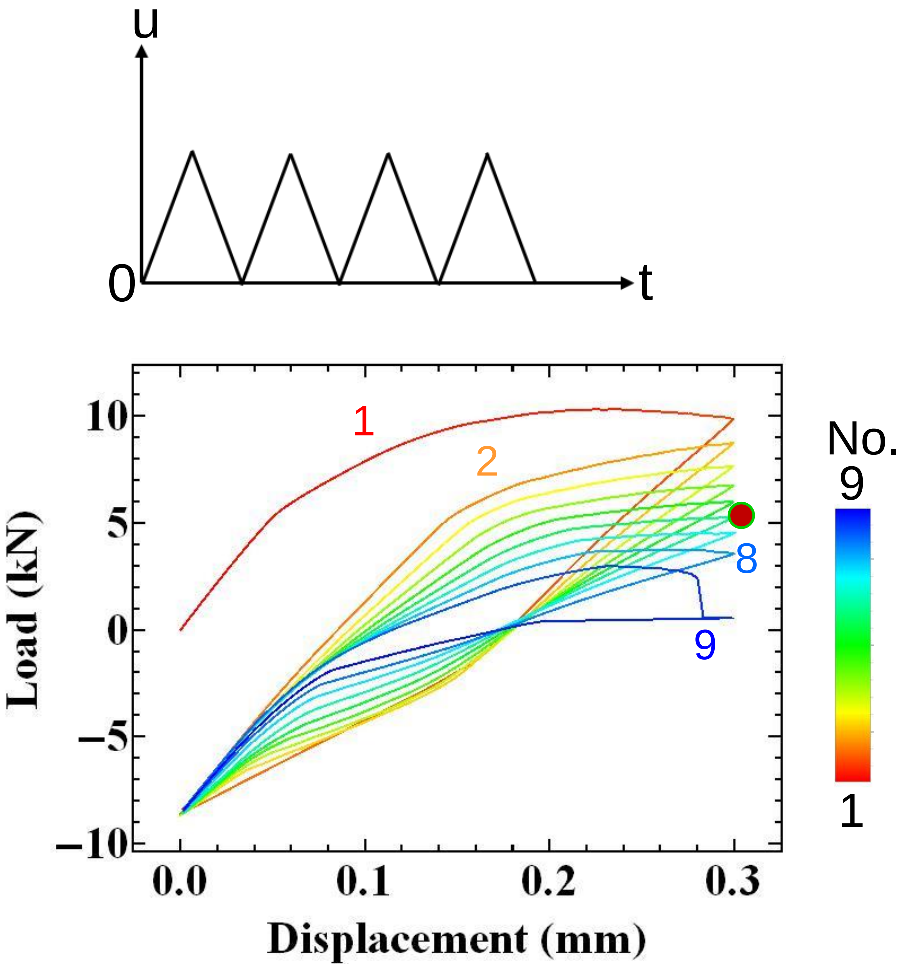
J_2 : Second invariant of stress tensor

Xue et al., *npj Computational Materials*. 2022

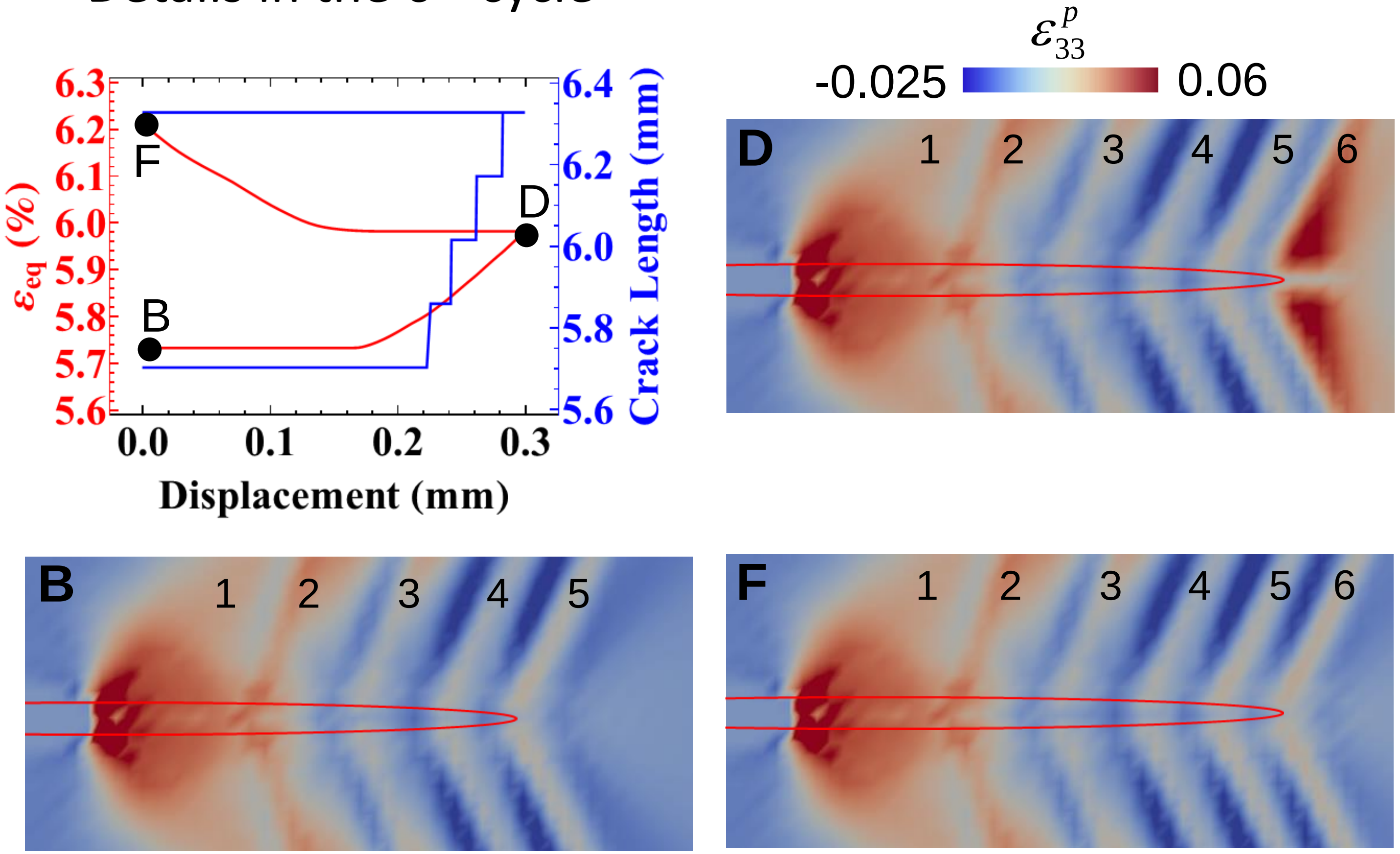
Xue et al., *in preparation* 2024

Crack Growth under Low Cycle Fatigue

Displacement evolution



Details in the 6th cycle



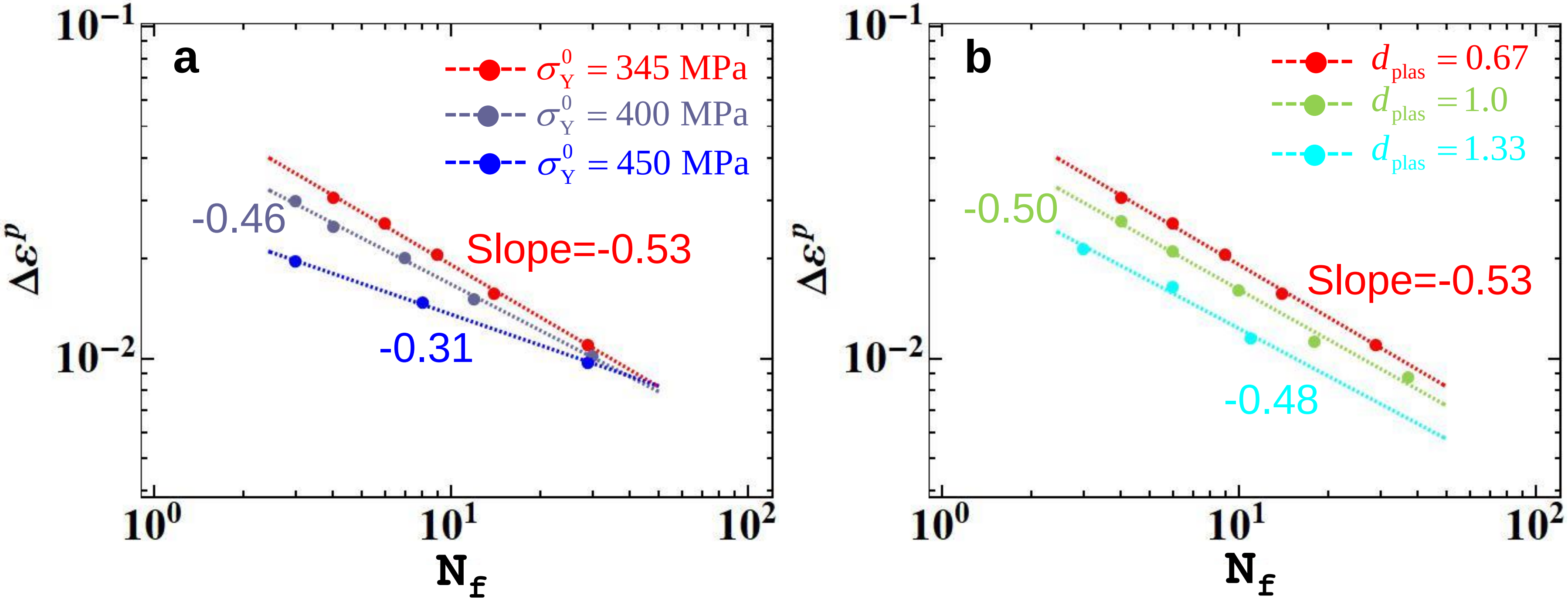
Each cycle produces one stripe in the plastic strain distribution, possible origin of fatigue striation

Xue et al., *npj Computational Materials*. 2022

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 coefficient



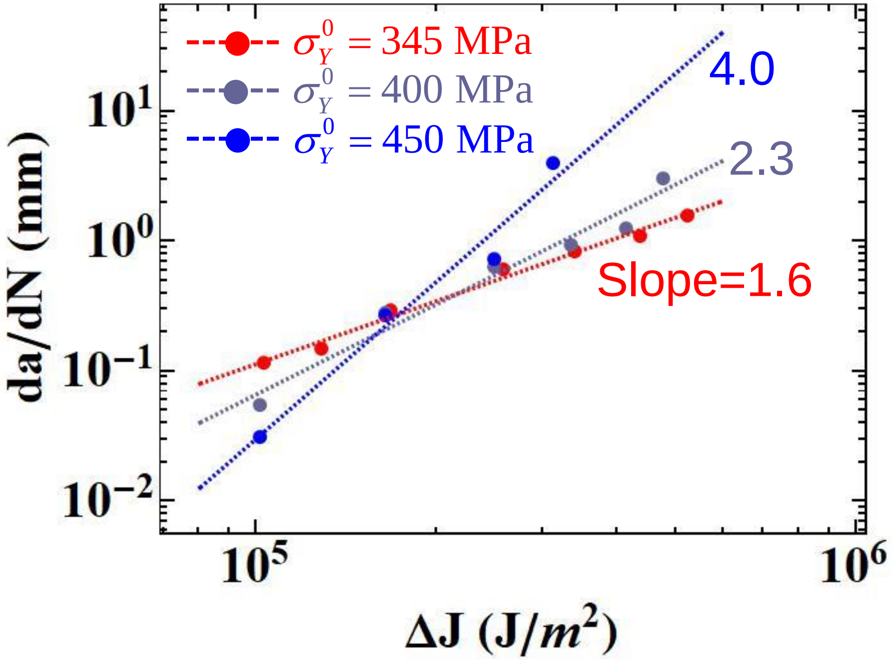
Larger yield strength and larger d_{plas} lead to shorter fatigue life and smaller slope of the fitted line

Xue et al., *npj Computational Materials*. 2022

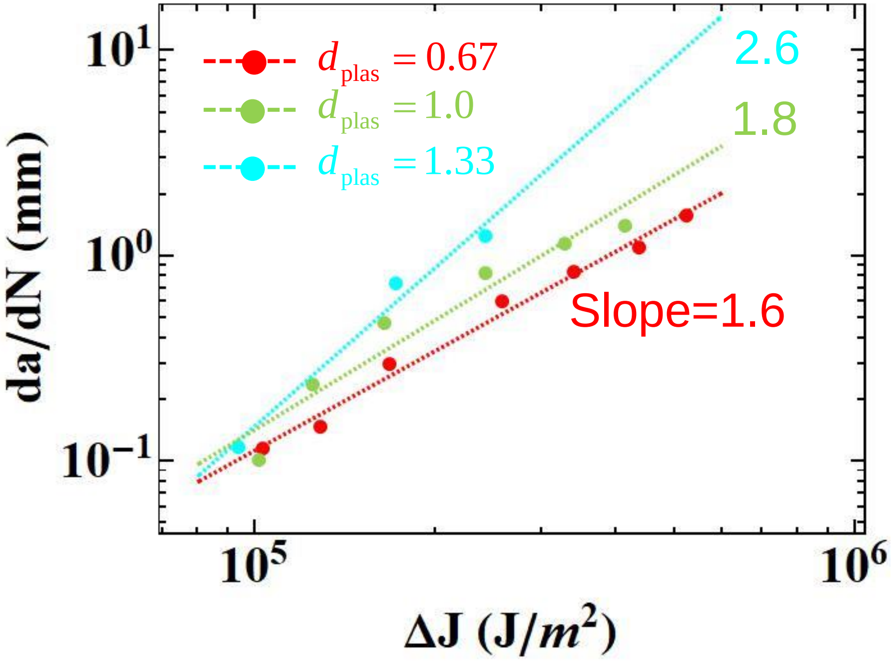
Crack Growth Rate vs ΔJ under Low Cycle Fatigue

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

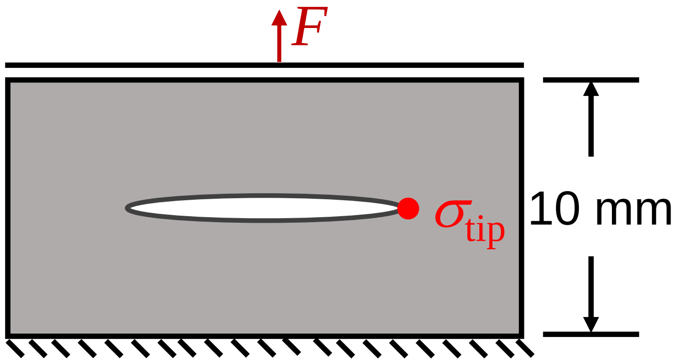
Larger yield strength leads to larger slope and crossovers between two fitted lines are observed.

Larger d_{plas} leads to faster crack growth and larger exponent of the growth law.

Xue et al., *npj Computational Materials*. 2022

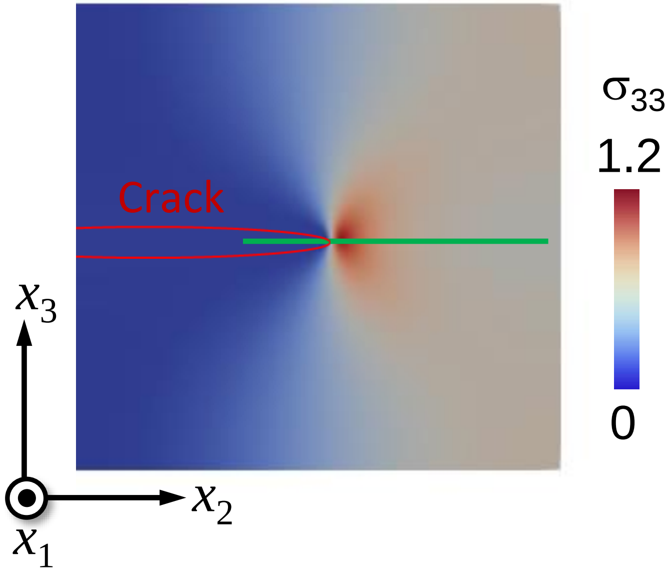
Initial Condition and Load Condition for HCF and Creep

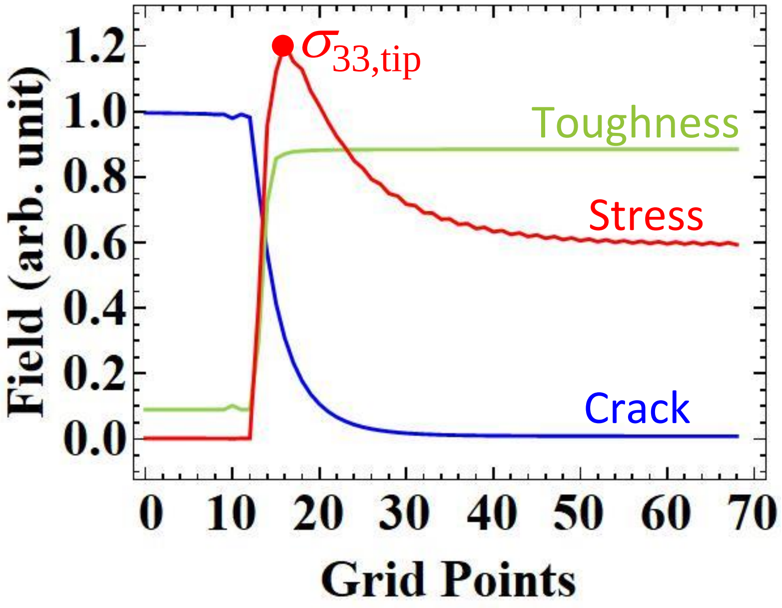
Initial Condition



An initial crack is added to simulate quasi-static crack growth

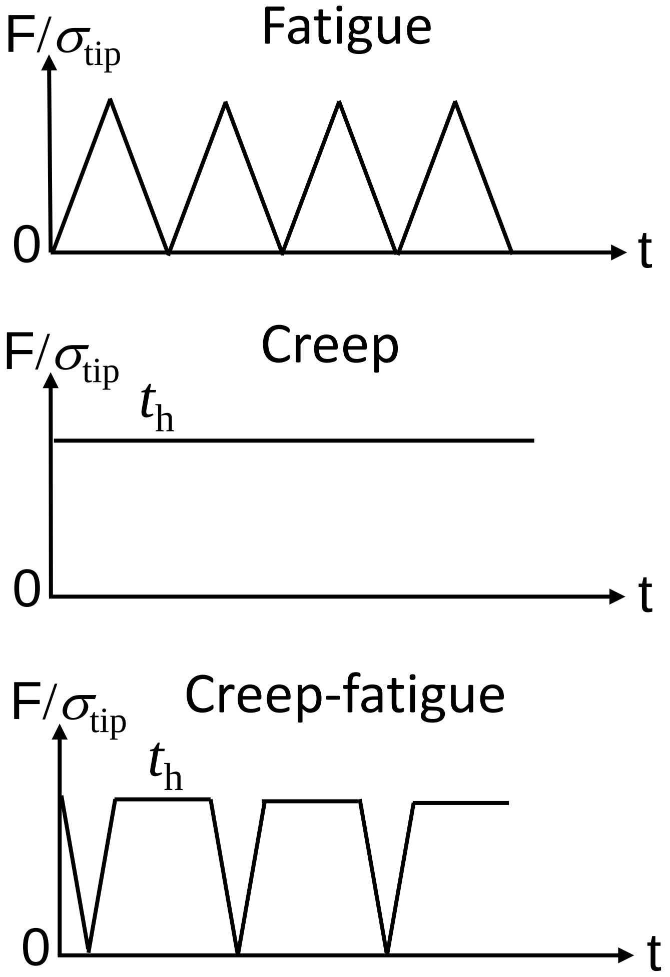
Stress distribution





Crack tip stress is available in the model

Load Condition



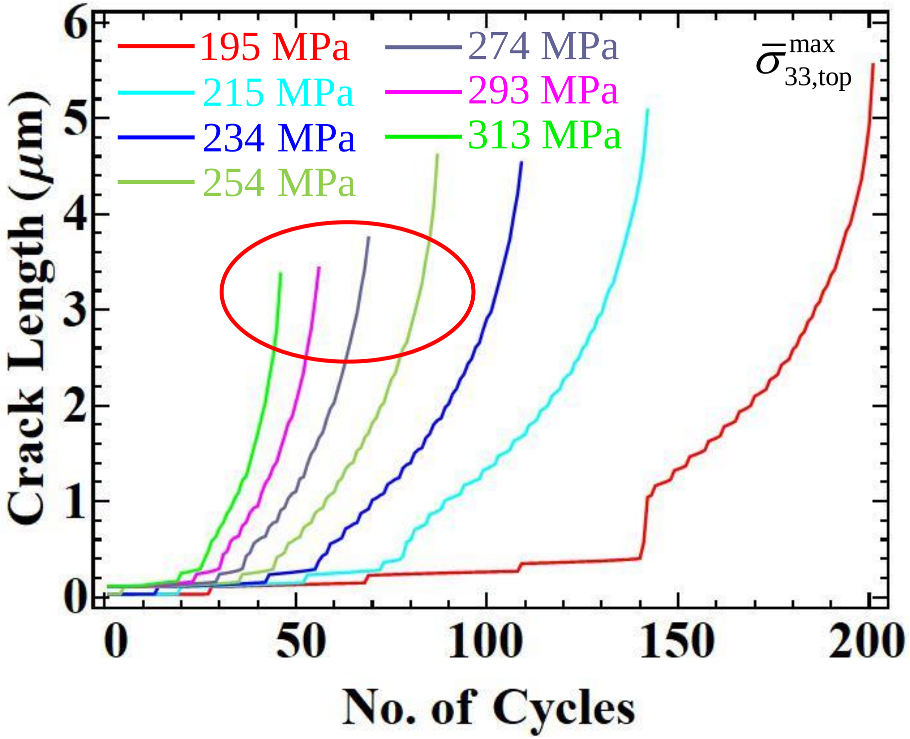
Stress Controlled Condition vs ΔK Controlled Condition

Paris Law: $\frac{da}{dN} = C(\Delta K)^n$ $K = \sigma_{\text{remote}} \sqrt{\pi a}\, f(a/W)$

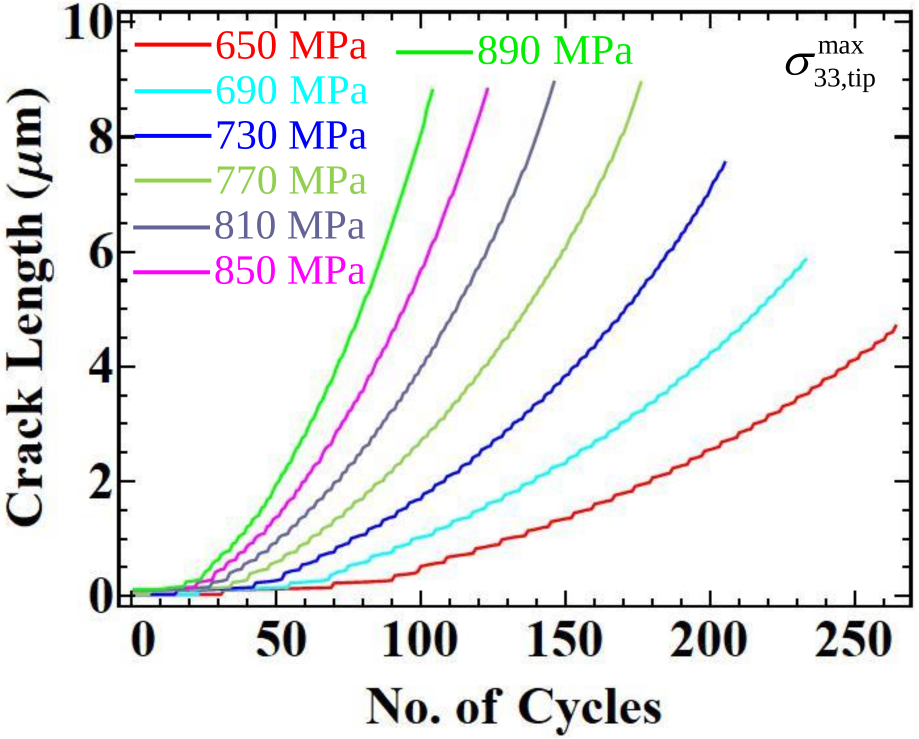
Stress intensity factor K describes the stress magnitude ahead of the crack tip.

In addition to controlling $\Delta\sigma_{\text{remote}}$, we can also control $\Delta\sigma_{\text{tip}}$ during each cycle

$\Delta\sigma_{\text{remote}}$ controlled



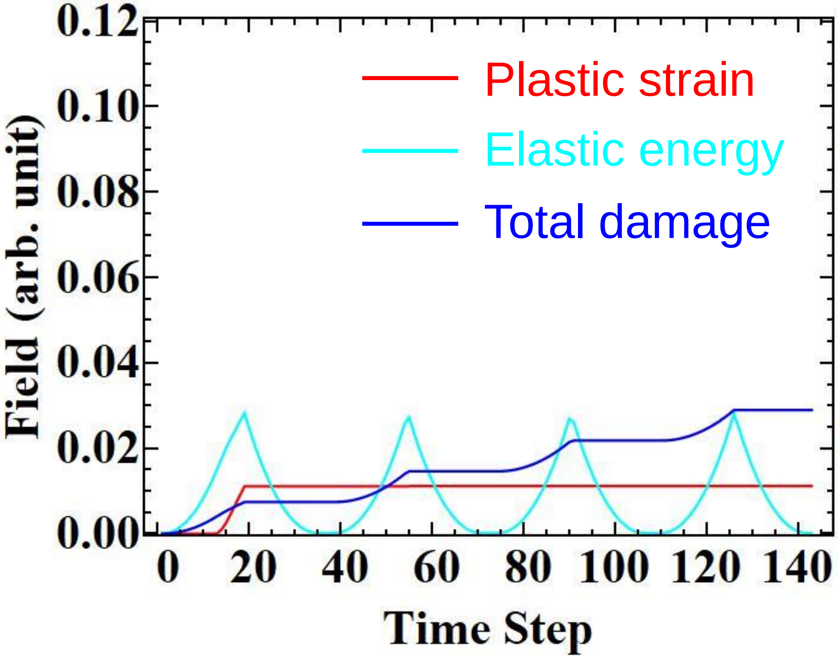
ΔK controlled



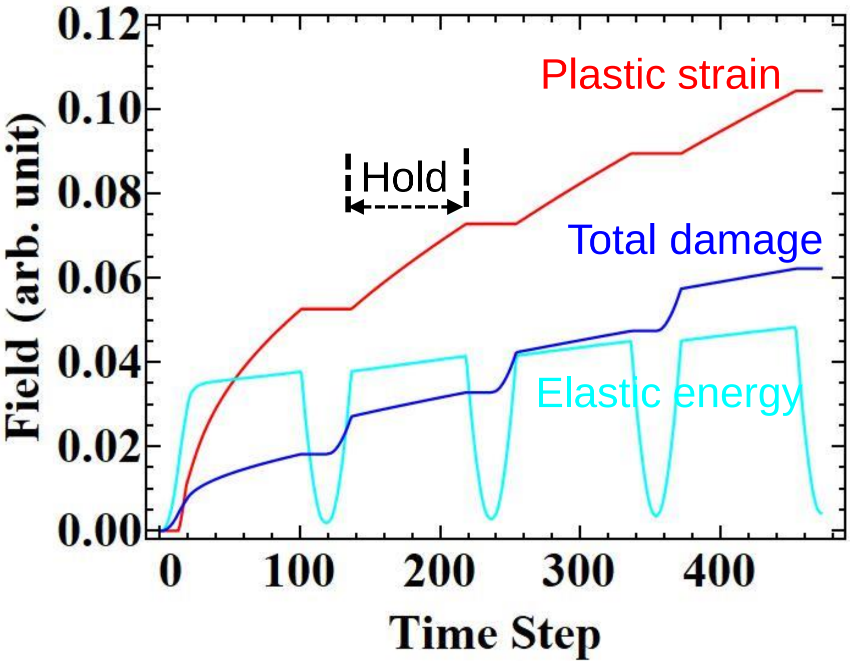
Damage Evolution during the Stress-controlled Condition

Plastic, elastic, and total damage ahead of the crack tip is analyzed from the simulation results

Pure fatigue



Creep-fatigue

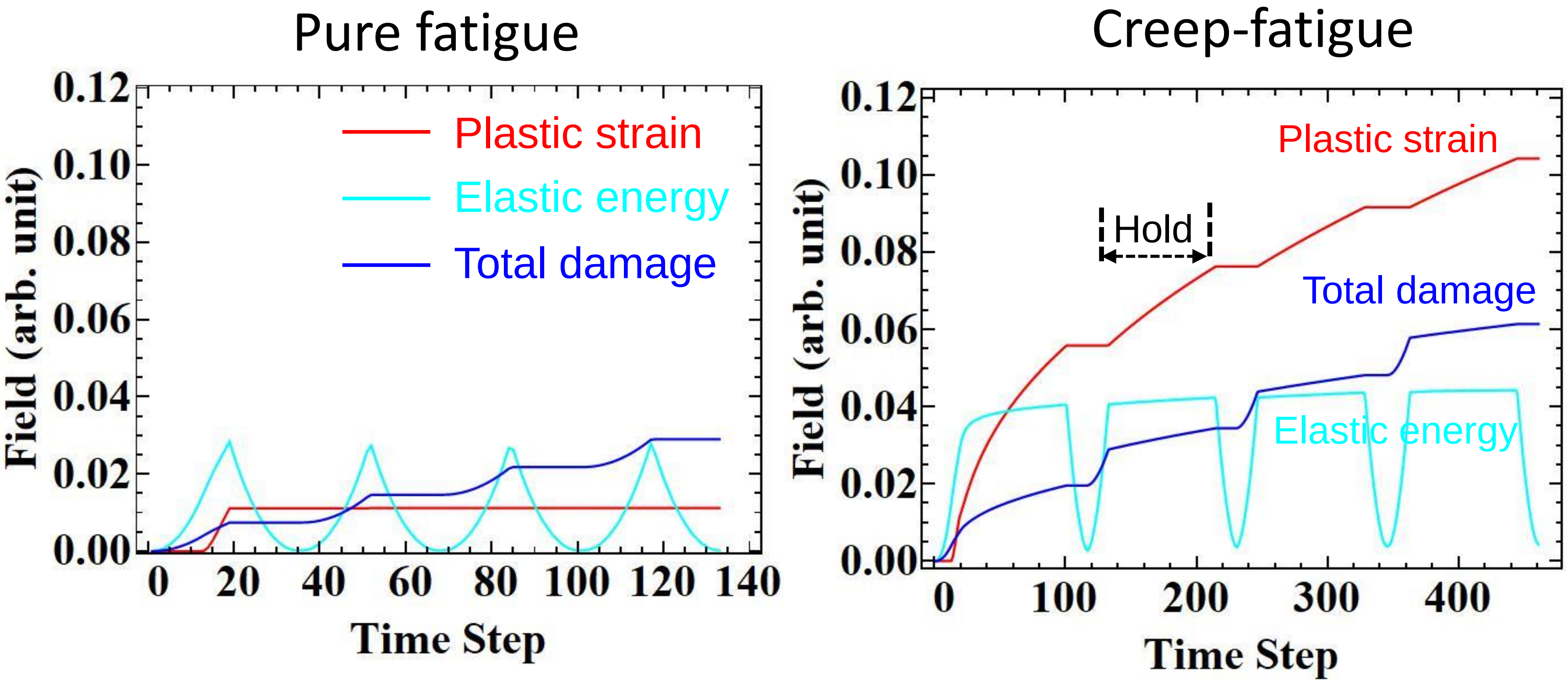


After several cycles, creep increases the stresses ahead of the crack tip

Xue et al., *in preparation* 2024

Damage Evolution during the ΔK-controlled Condition

Plastic, elastic, and total damage ahead of the crack tip is analyzed from the simulation results



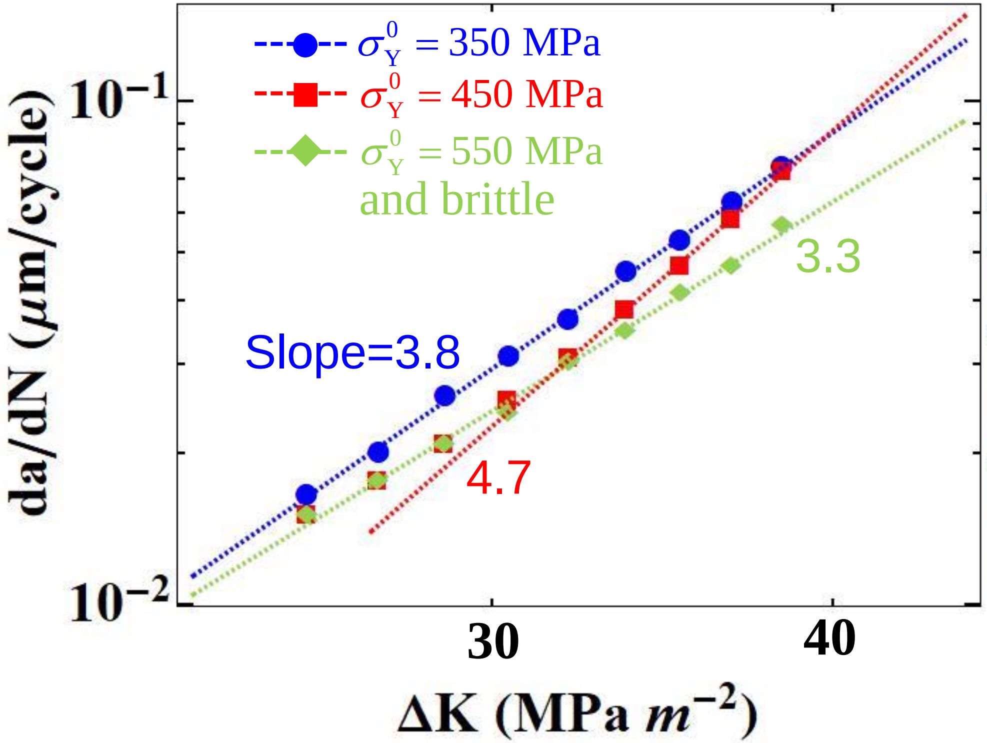
The crack tip stress is almost a constant after several cycles

Xue et al., *in preparation* 2024

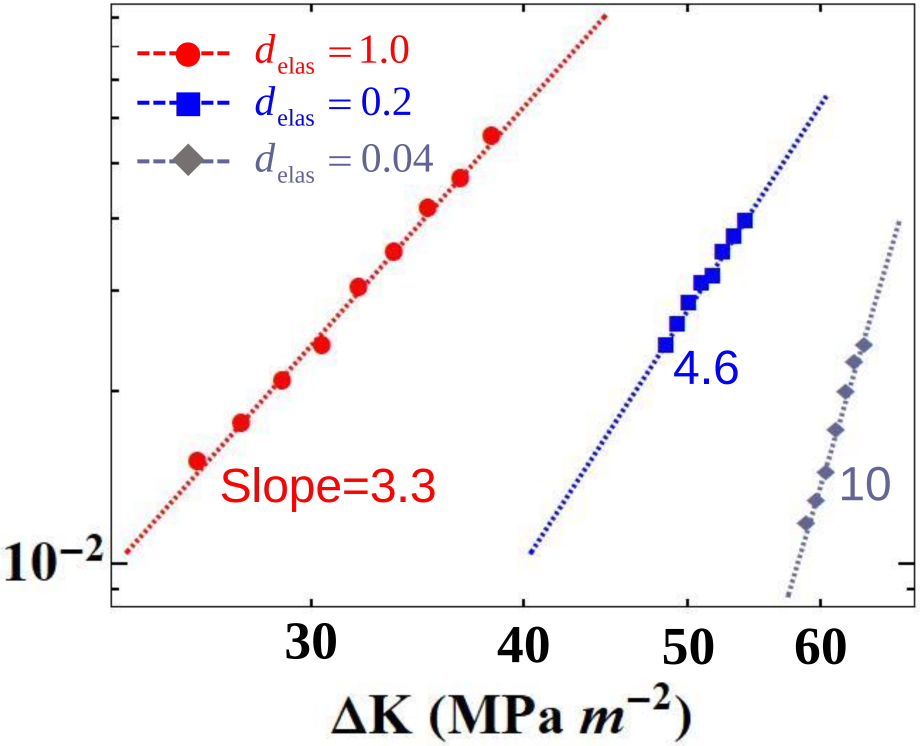
Crack Growth under Fatigue at Low Temperatures

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

Ductile materials



Brittle materials



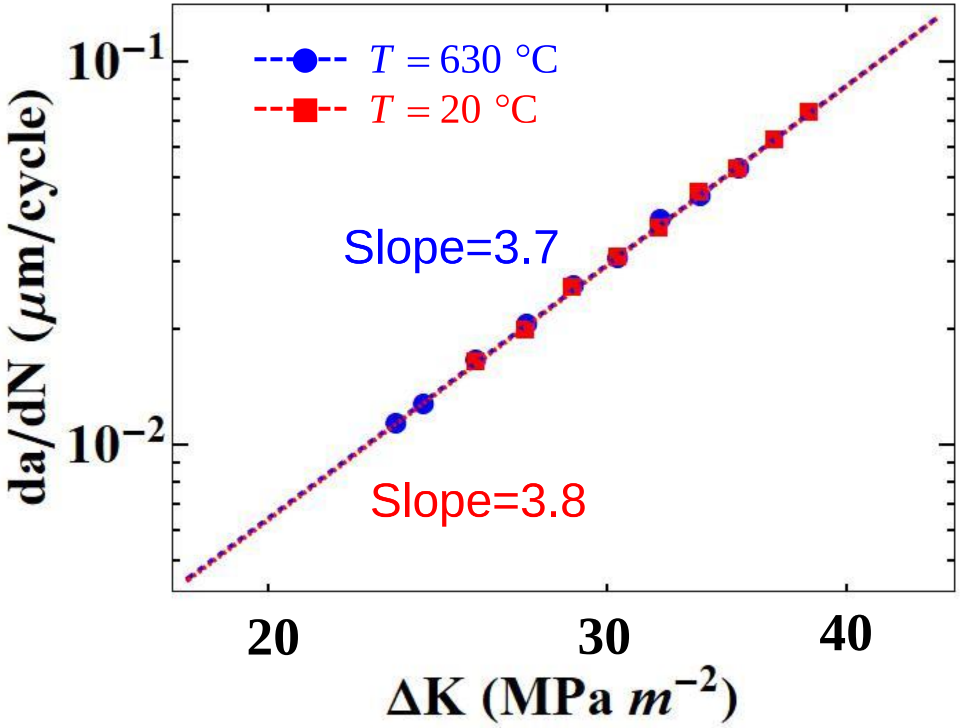
Known Paris exponents
2~4 for ductile materials
n>10 for brittle materials

The degradation due to elastic damage in brittle materials is slower than that in ductile materials

Xue et al., *in preparation* 2024

Crack Growth under Pure Fatigue at High Temperatures

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

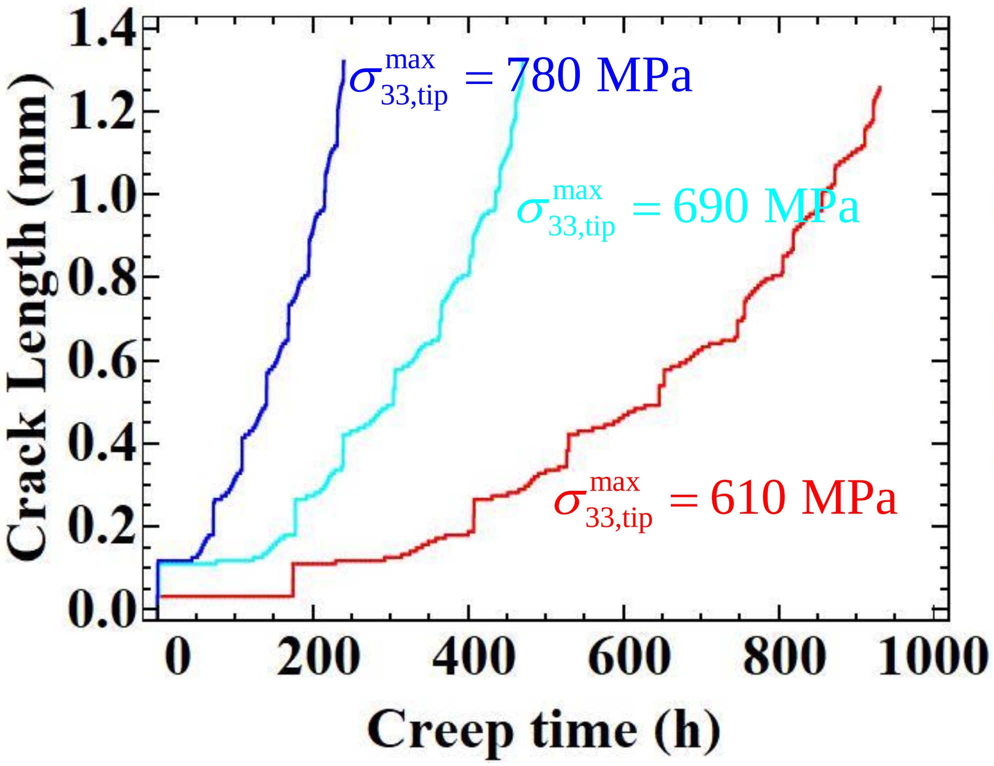


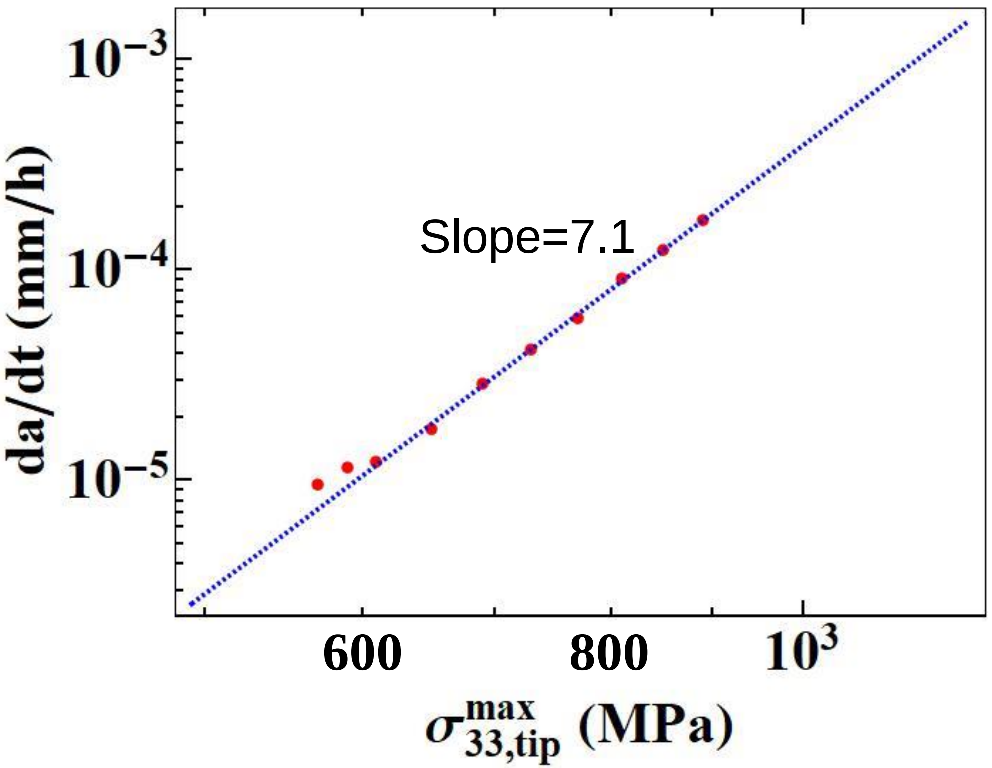
Creep during the loading and unloading period makes minor contributions to the crack growth

Xue et al., *in preparation* 2024

Crack Growth under Creep

$$\frac{da}{dt} = C(K_{\max})^m$$ K: Stress intensity factor



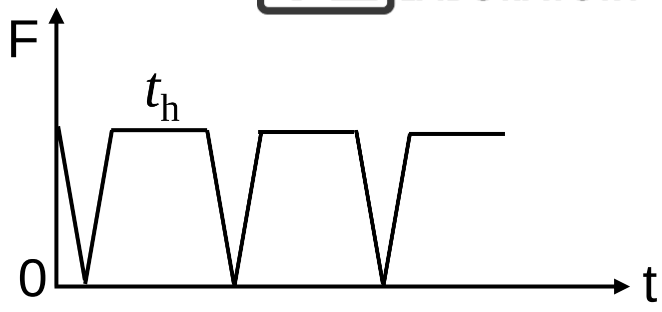


Crack growth rate versus hold stress exhibits power-law behavior under creep

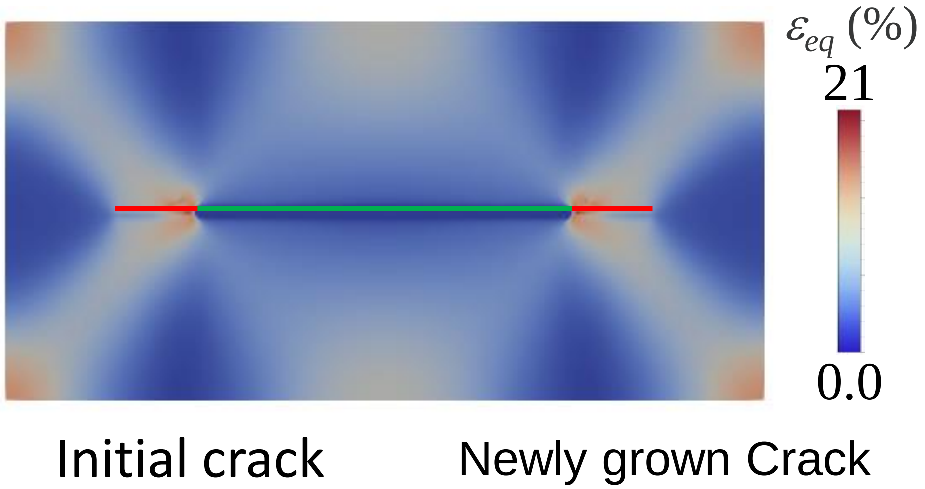
Xue et al., *in preparation* 2024

Crack Growth under Creep-Fatigue

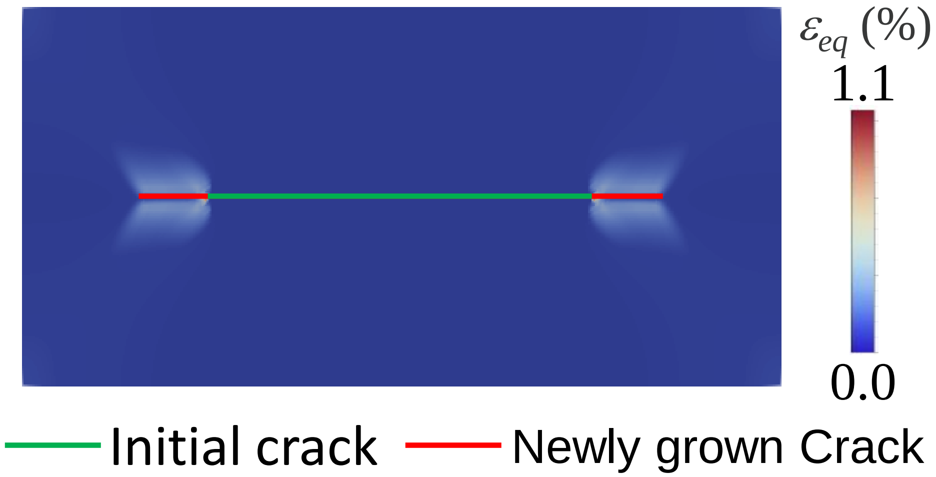
Creep-fatigue: unloading and loading cycle followed by constant stress



Plastic strain under creep-fatigue



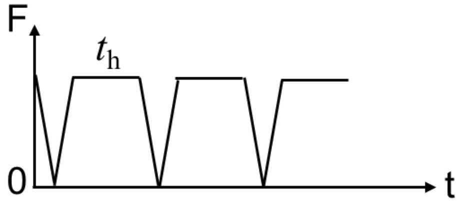
Plastic strain under pure fatigue



Plastic strain is widely distributed under coupled creep-fatigue, in contrast to localized distribution under pure fatigue

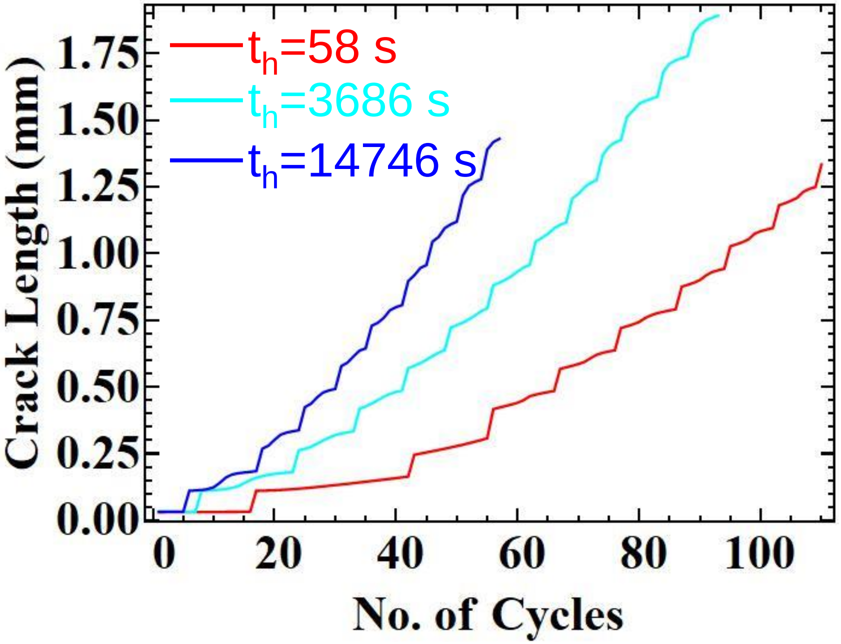
Xue et al., *in preparation* 2024

Crack Growth under Creep-Fatigue

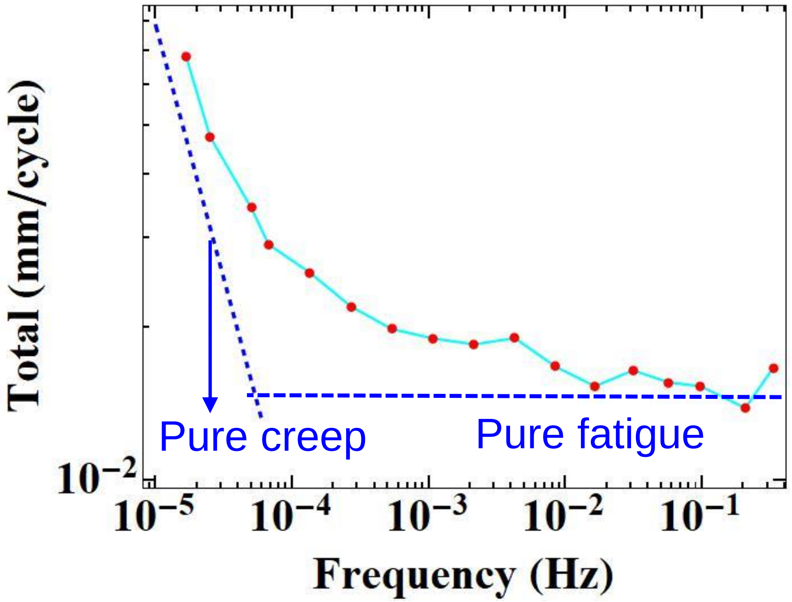


Crack growth rate versus hold time

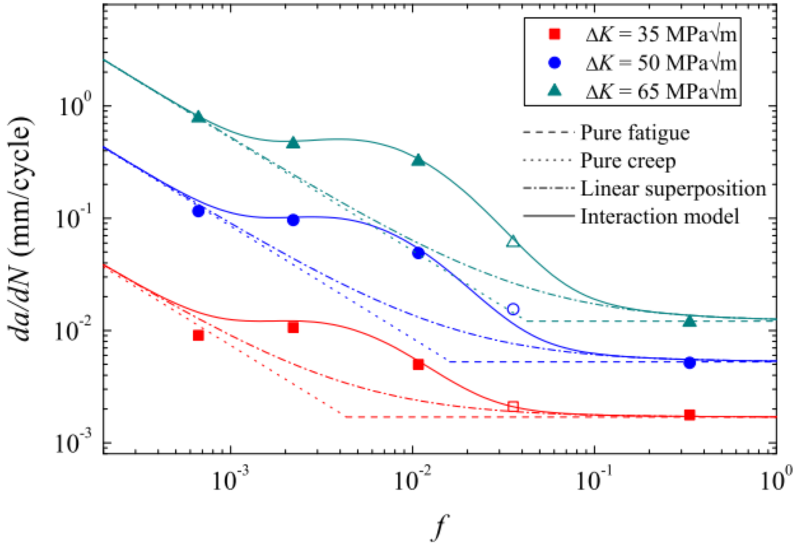
Crack length vs cycle number



Crack growth rate vs frequency



Experiments



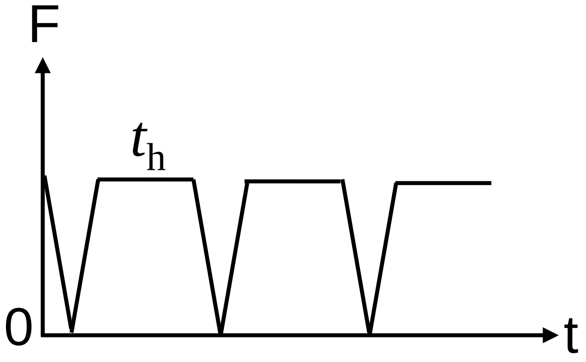
Engineering Fracture Mechanics 124 (2014): 112

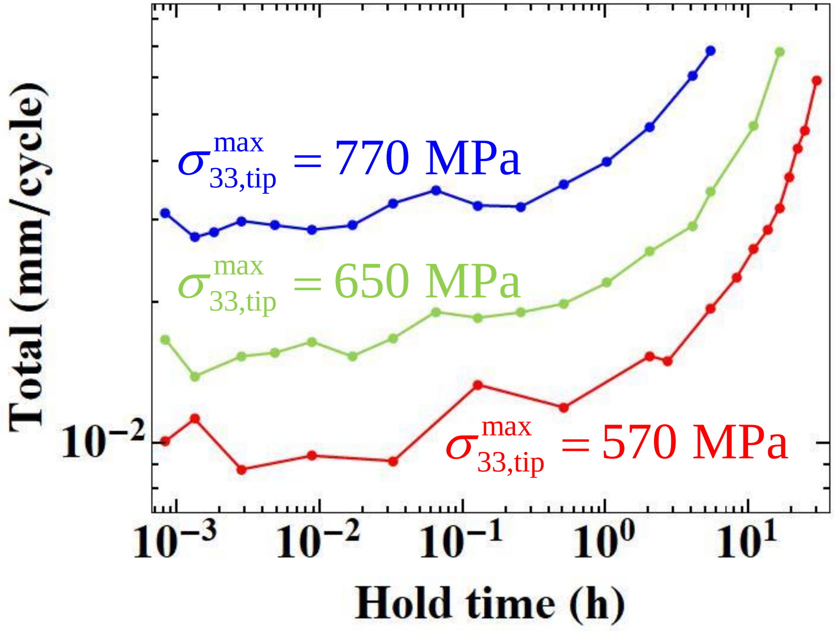
The deviation from the blue dashed lines is caused by the creep-fatigue interaction

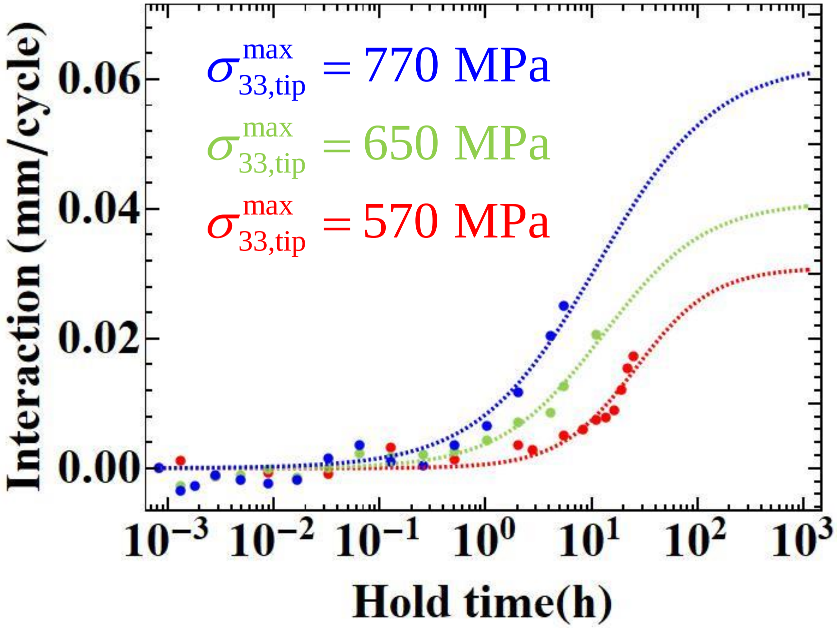
Crack Growth due to Creep-Fatigue Interaction

Total crack growth rate can be divided into three contributions:

$$\left(\frac{da}{dN}\right)_{\text{total}} = \left(\frac{da}{dN}\right)_{\text{fatigue}} + \left(\frac{da}{dN}\right)_{\text{creep}} + \left(\frac{da}{dN}\right)_{\text{interaction}}$$



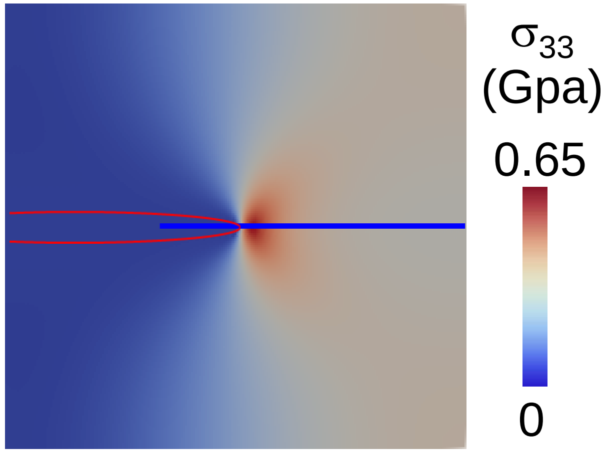

Total crack growth rate


Creep-Fatigue Interaction

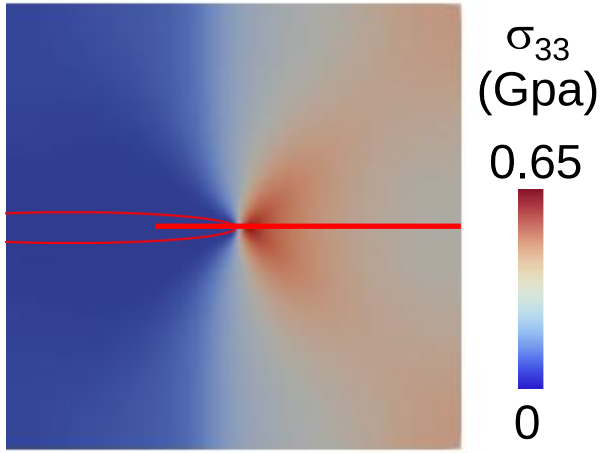
The interaction term can be described by the logistic function of the logarithm of the hold time

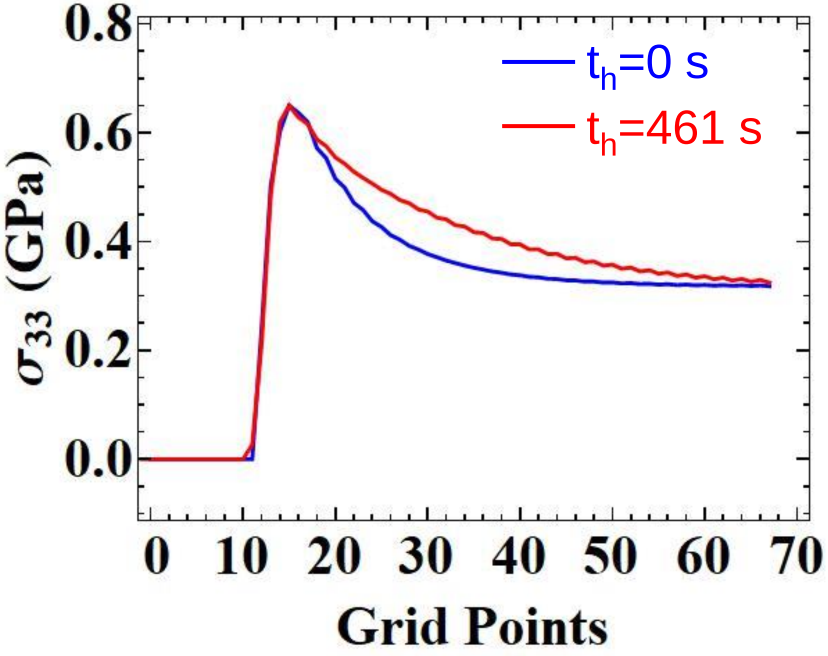
Analysis of the Origin of Creep-fatigue Interaction

Fatigue



Creep-fatigue





High-cycle fatigue

$$\sigma_{ij}(r,\theta) = \frac{K}{\sqrt{2\pi r}} f_{ij}(\theta) + \text{higher order terms}$$

r,θ : polar coordinates

$f_{ij}(\theta)$: dimensionless function

Steady-state creep

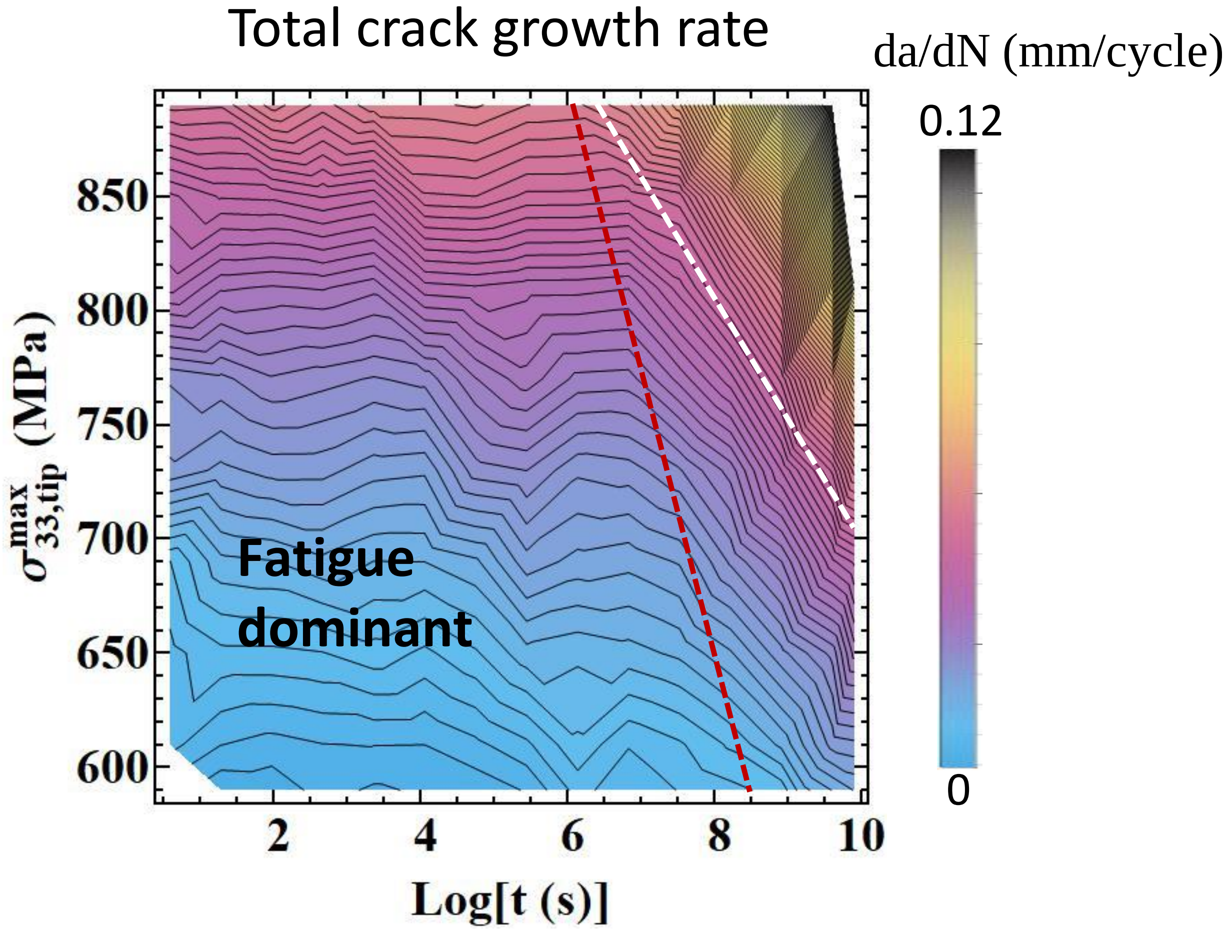
$$\sigma_{ij} = \left(\frac{C^*}{A_{cr} I_n r}\right)^{1/6} \tilde{\sigma}_{ij}(\theta)$$

$\tilde{\sigma}_{ij}(\theta)$: dimensionless function

Anderson, T.L., 2017. Fracture mechanics: fundamentals and applications

The smaller stress gradient ahead of the crack tip under creep-fatigue leads to enhanced elastic damage than that under fatigue

High Throughput Simulations under Creep-Fatigue



In the upper right corner, both creep and fatigue make significant contributions, while in the lower left region, the crack growth is fatigue-dominant

Conclusions

- This work develops a phase-field model that enables simulations of crack growth under fatigue, creep, and coupled creep-fatigue.
- Smaller yield strength is found to result in faster fatigue crack growth in ductile materials. The degradation rate due to elastic damage in brittle materials is found to be smaller than that in ductile materials.
- By comparing the crack growth rates under fatigue, creep, and coupled creep-fatigue, a creep-fatigue interaction term is obtained as a function of hold stress and hold time.
- The creep-fatigue interaction is proposed to be caused by the smaller stress gradient ahead of the crack tip under coupled creep-fatigue, which leads to enhanced elastic damage, compared to the situation under pure fatigue

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