Design Tool for Creep-Resistant Materials and Low Cycle Fatigue Modeling

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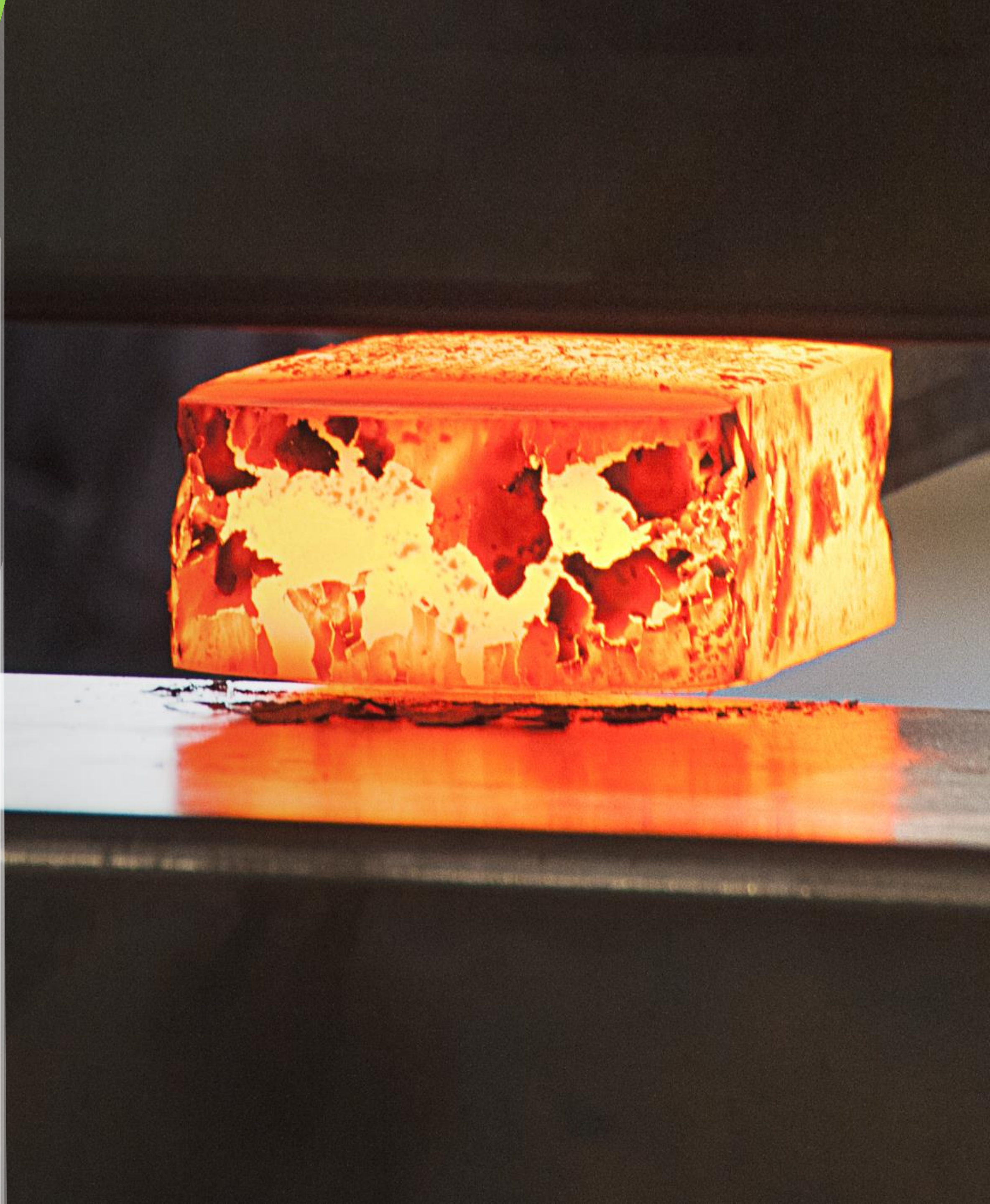
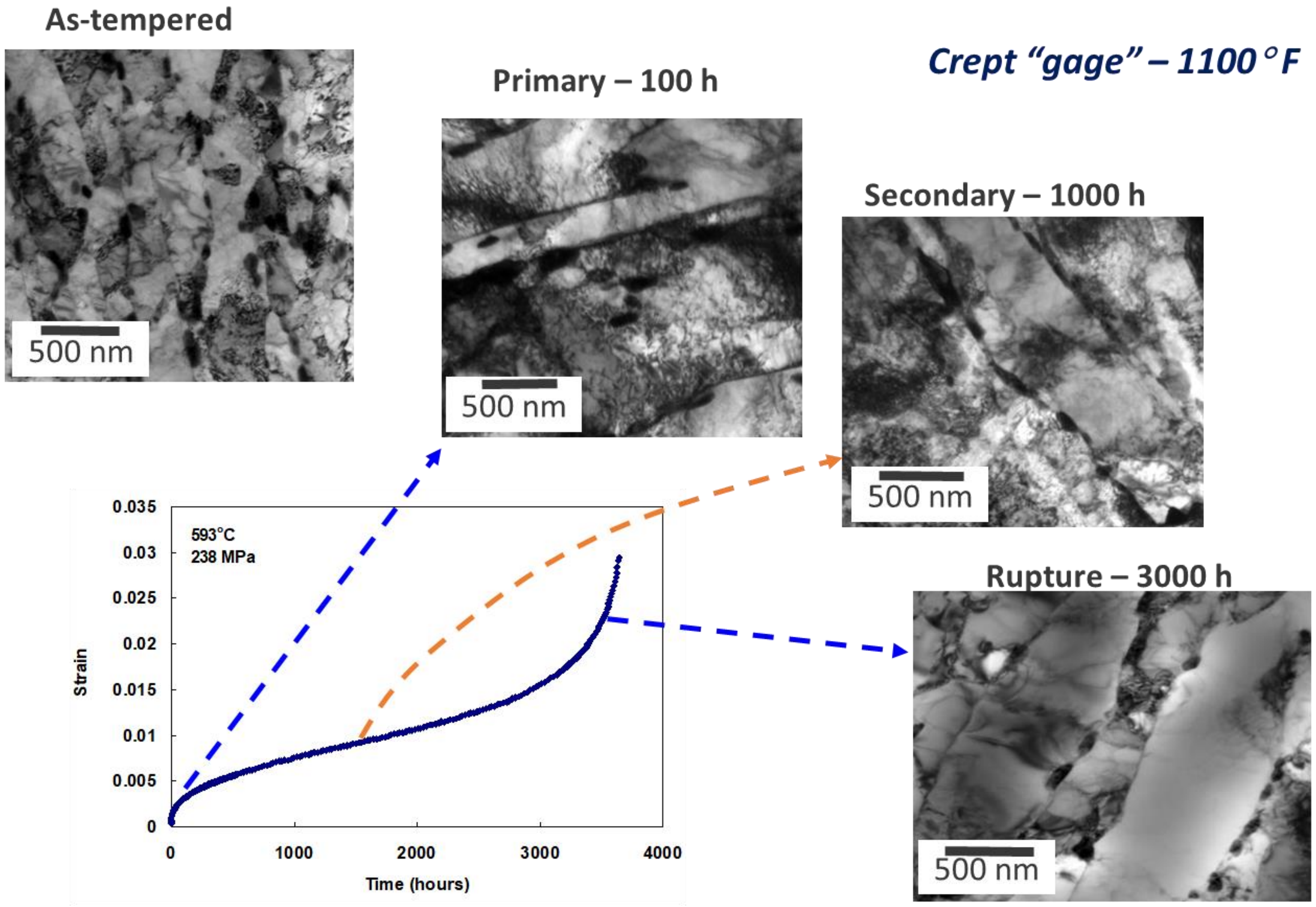


Background: Creep & Fatigue Modeling



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

NETL's focus is on **microstructure-based** predictive models that couple creep, fatigue, and environmental effects.

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

Some New Modeling Capabilities Established during EY19-EY20

- Modeling of Coupled Grain Growth, Crystal Plasticity, and Grain Boundary Sliding
- Modeling of Coherency Loss of Precipitates

Ongoing Efforts

- Modeling of Low Cycle Fatigue
- Modeling of Crack Growth in Single Crystals and Polycrystals
- Modeling of Internal to External Oxidation Transition

EY21 & Future Work

Modeling of Coupled Grain Growth, Crystal Plasticity, and Grain Boundary Sliding (GBS)

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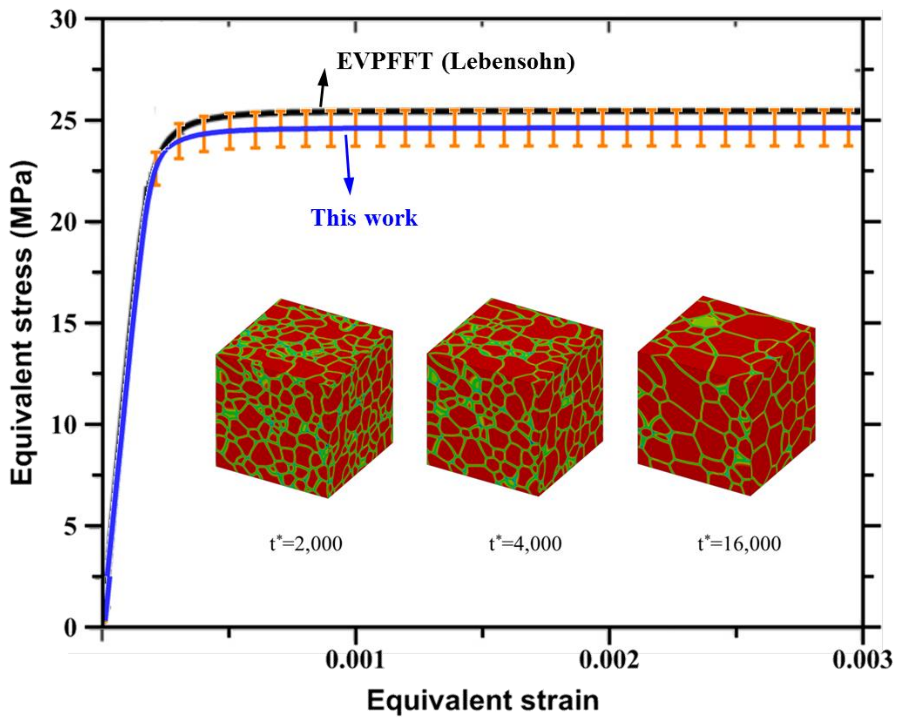
Why we care?

- Crystal plasticity addresses the intrinsic anisotropic nature of plastic deformation in creep and low cycle fatigue modeling
- GBS plays a significant role in creep rate for polycrystal alloys as well as in creep damage and crack initiation

State-of-the-art

Crystal plasticity finite element (CPFE) is the common approach with the following shortcomings:

1) GBS is NOT incorporated
2) Not coupled with microstructure evolution modeling
3) High computational cost



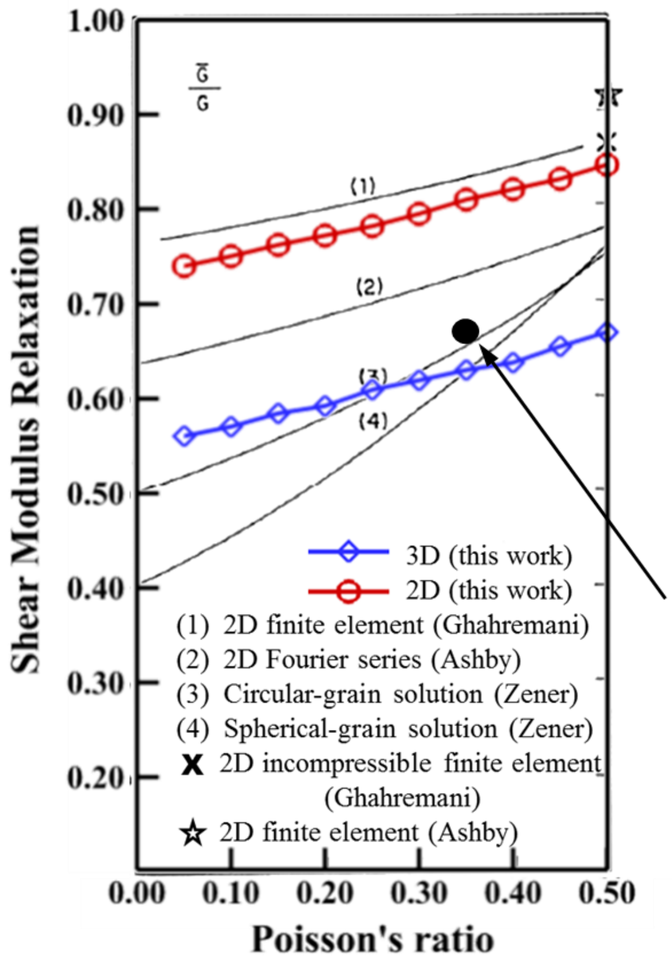
Crystal plasticity phase-field simulation of stress-strain curve of a polycrystalline copper

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

Modeling of Coupled Grain Growth, Crystal Plasticity, and Grain Boundary Sliding

Accomplishments

- Developed a crystal plasticity phase-field modeling framework which combines J_2 and crystal plasticity to integrate shear deformation in each slip system together with grain boundary sliding;
- Validated the phase-field crystal plasticity and grain boundary sliding model against literature results



Validation against literature results regarding the effect of GBS on shear modulus of a polycrystal

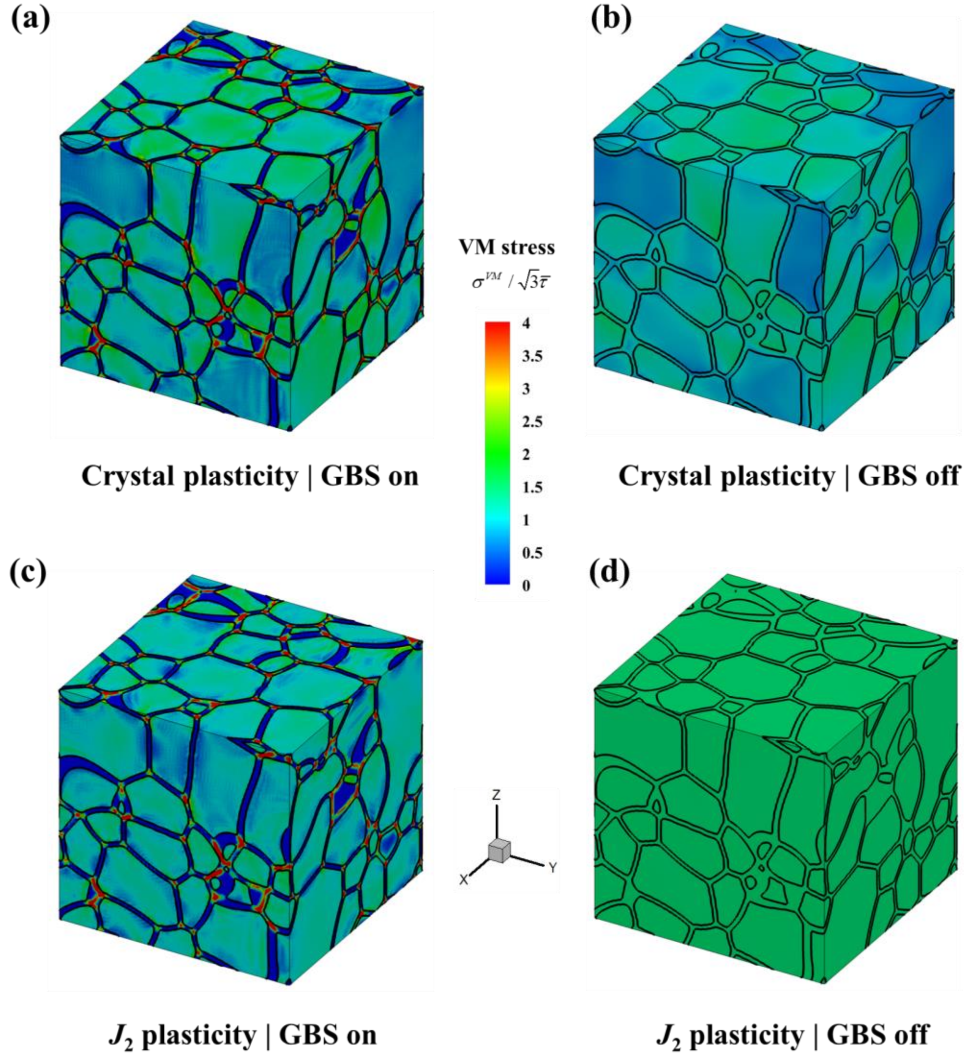
- Experiment for aluminium (Ke et al., Phys. Rev. 1947)

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

Modeling of Coupled Grain Growth, Crystal Plasticity, and Grain Boundary Sliding

Impact

- This model lays a solid foundation for integrating crystal plasticity and GBS with microstructure evolution simulation, which is essential for microstructure-based creep and fatigue modeling
- The fast Fourier-transform based algorithm is highly efficient, which is also a practical advantage for creep and fatigue simulations that are normally time-consuming.

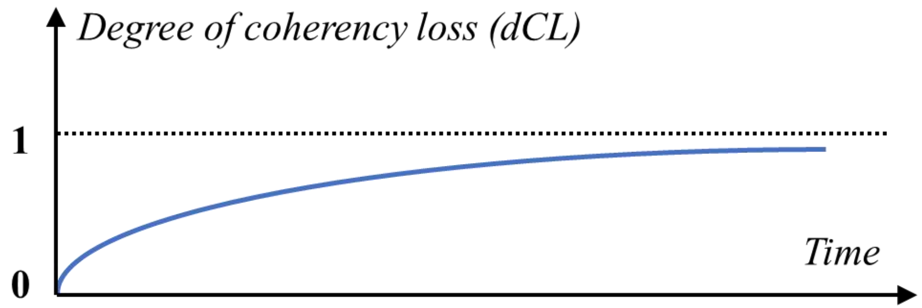


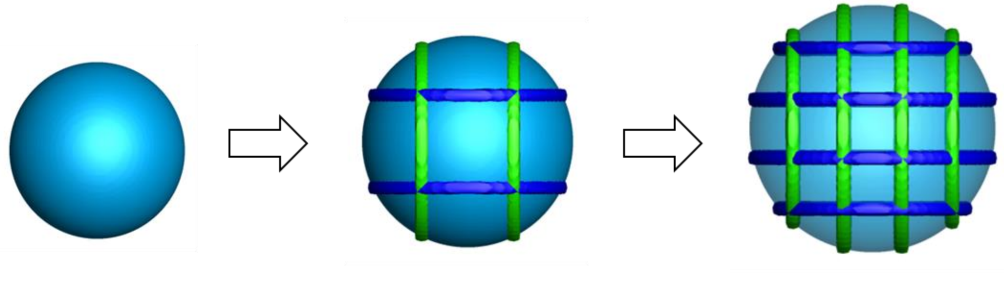
Modeling of Coherency Loss of Precipitates

Why we care?

- Interfacial coherency plays an important role for the mechanical performance and performance degradation of various precipitation-hardened alloys over aging and creep
- Change of coherence state also affects rate of microstructure evolution and thus yield strength and creep rate
- Incoherent precipitates are often weak spots in an alloy for nucleation of undesired phases and crack initiation

Coherency loss is a continuous process





(a) Coherent (b) Start to lose coherency (c) Semi-coherent

Cheng and Wen, *npj Computational Materials*. 2021

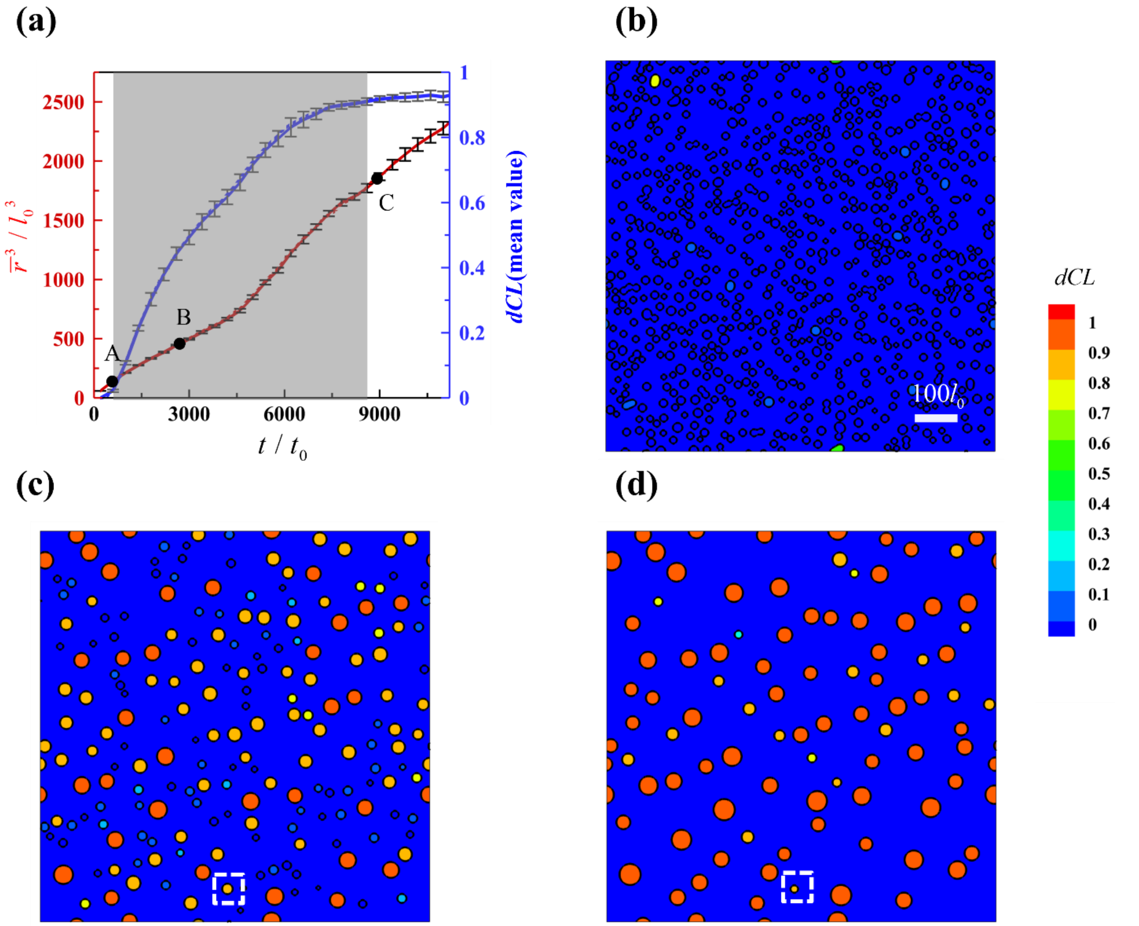
Modeling of Coherency Loss of Precipitates

State-of-the-art

- Most existing models treat precipitates as either coherent or incoherent, without capturing the process of coherency loss or coupling coherency loss with microstructure evolution

Accomplishments

- Developed an efficient phase-field model that builds in the mechanism of coherency loss coupled with microstructure evolution



Simulated coarsening (Ostwald ripening) accompanied by coherency loss

Cheng and Wen, *npj Computational Materials*. 2021

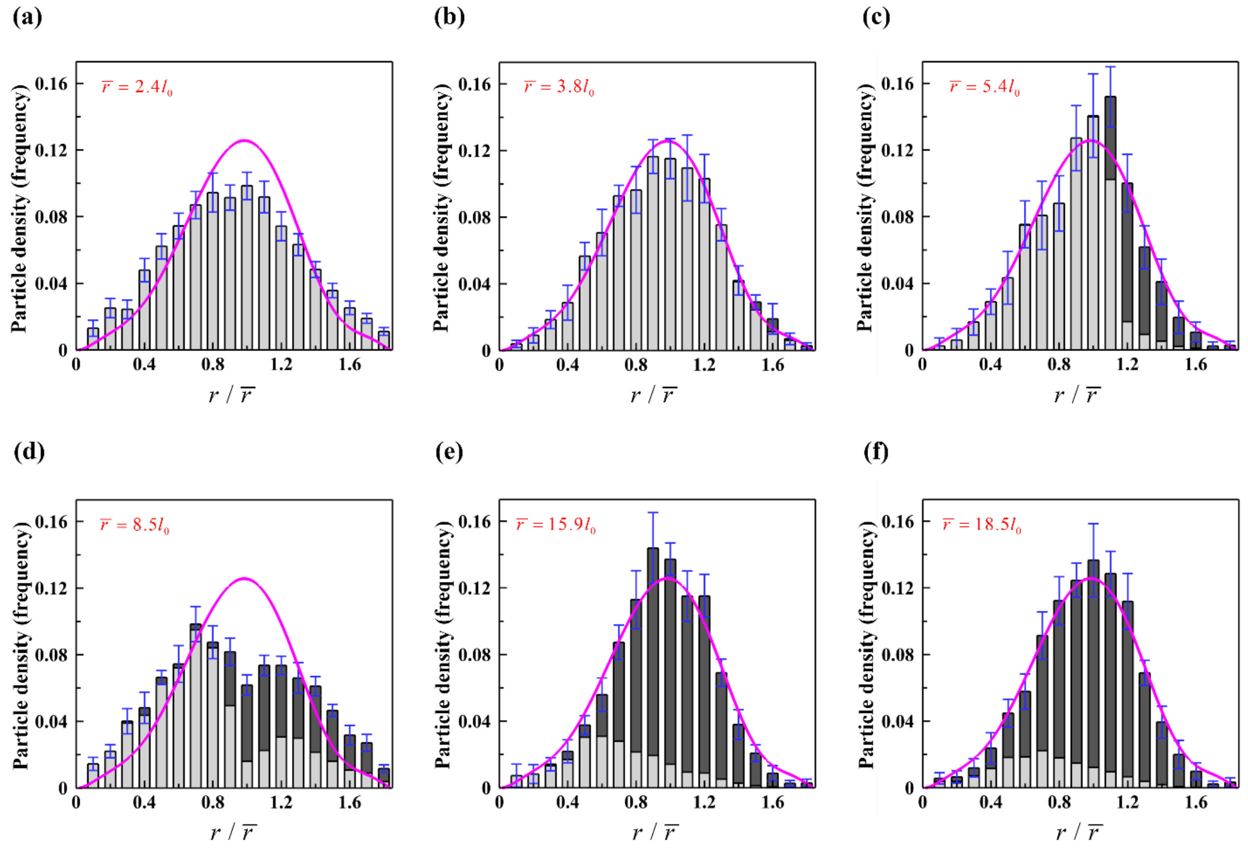
Modeling of Coherency Loss of Precipitates

Accomplishments (continued)

- Revealed the mechanism for change of coarsening rate and particle size distribution by coherency loss

Impact

- This model makes it practical to perform large-scale simulation of aging with spontaneous coherency loss in precipitation-hardened alloys, linking to macroscopic mechanical performance of the alloy

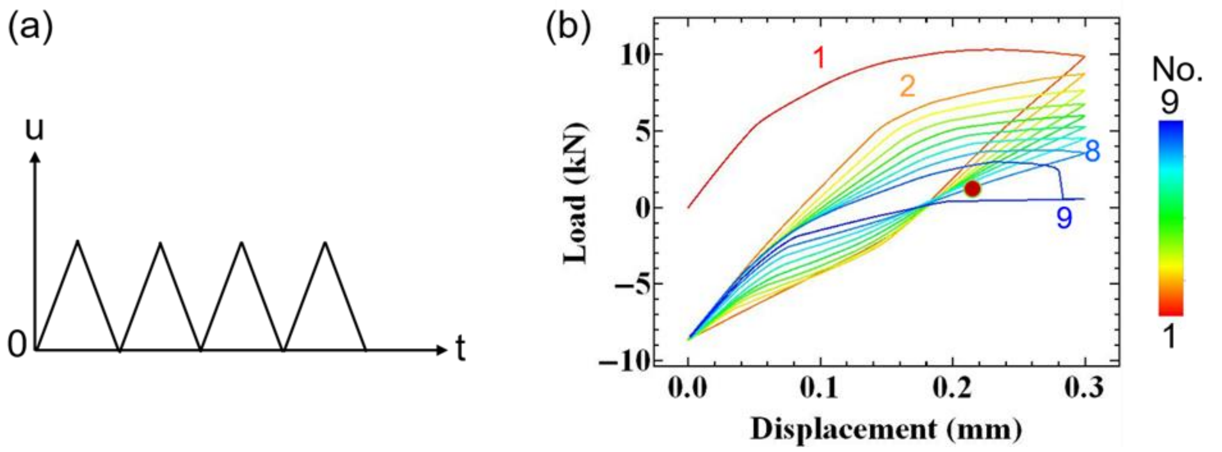


Simulated particle size distribution during coarsening accompanied by coherency loss (in agreement with experiment of Iwamura 2004

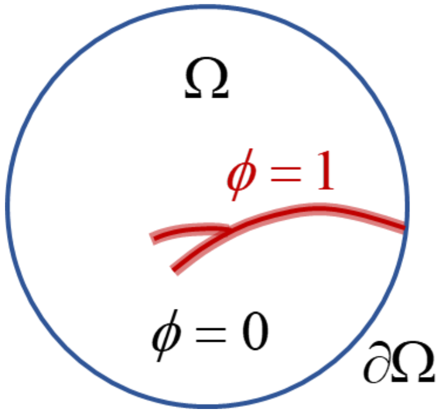
Cheng and Wen, *npj Computational Materials*. 2021

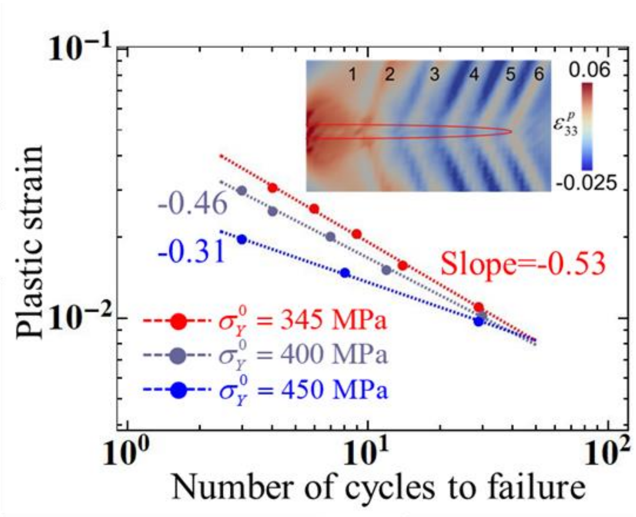
Ongoing Effort: Modeling of Low Cycle Fatigue

- Developed a phase-field model to simulate the simultaneous evolution of complex crack patterns and plastic strain in ductile materials.
- The model is employed to study LCF. Without *a priori* assumption, the simulated fatigue life and plastic strain relationship agrees with the Coffin-Manson relation.
- Our model predicts the LCF life dependence on the material parameters, such as yield strength. This work will be further expanded to include HCF.



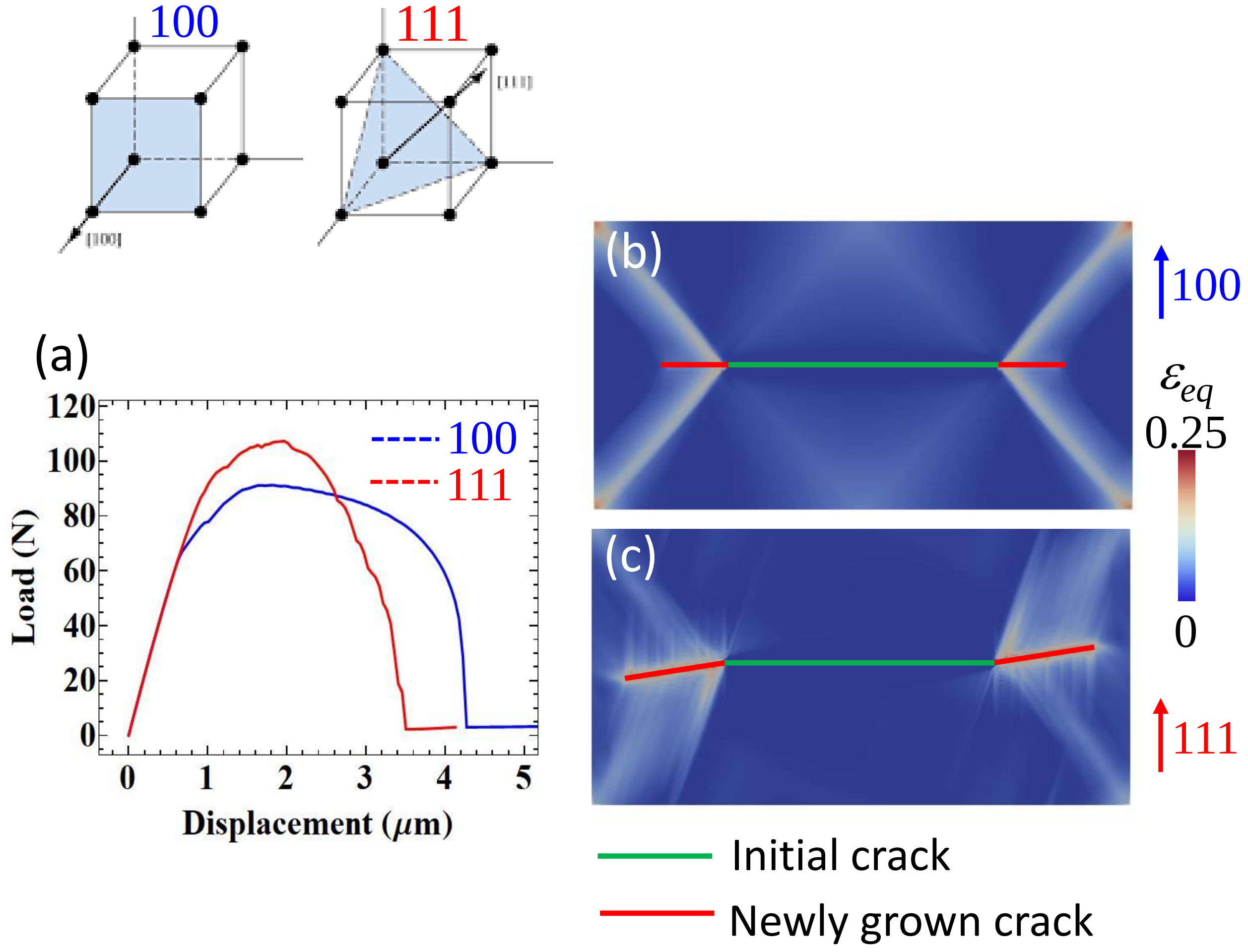
Displacement and load evolution under cyclic loads





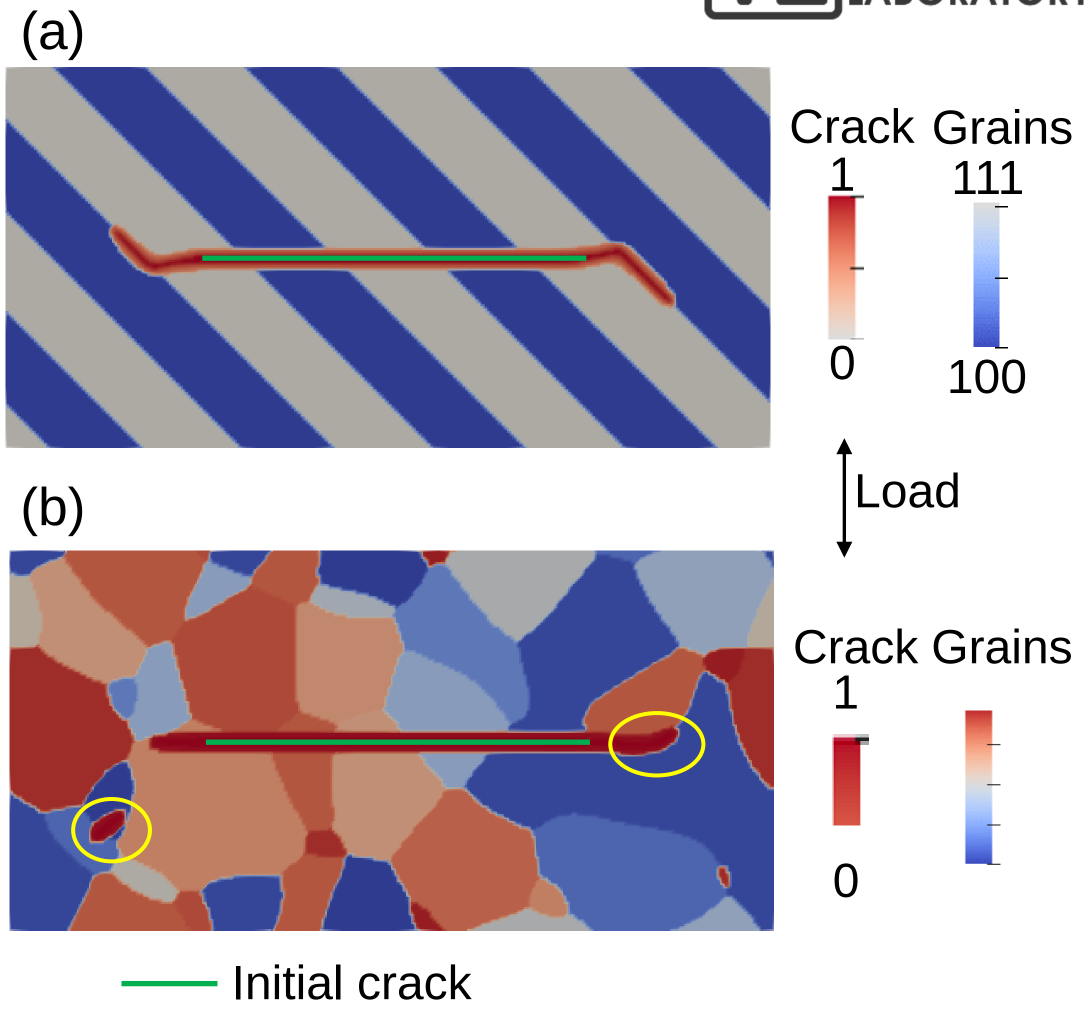
Ongoing Effort: Modeling of Crack Growth in Single Crystals

- Developed a fracture-crystal-plasticity phase-field model to describe the coupled evolution of cracks and plastic strain in single crystals.
- The model is employed to study crack growth with load applied to different directions of a single crystal. Our simulations predict the orientation-dependent plastic flow and crack paths.
- A systematic study of the orientation dependence may provide guidance for the design and application of nickel-base single crystal superalloys.



Ongoing Effort: Modeling of Crack Growth in Polycrystals

- Extended the fracture-crystal-plasticity phase-field model to the situation of polycrystals by incorporating the grain structures.
- The model is employed to study crack growth in bicrystals and polycrystals. Our simulations demonstrate the dependence of crack paths on the underlying grain structures.
- Our model may help optimize the fracture toughness and fatigue life by tuning the grain structures such as average grain size and grain boundary orientations.



Crack growth and nucleation at grain boundaries

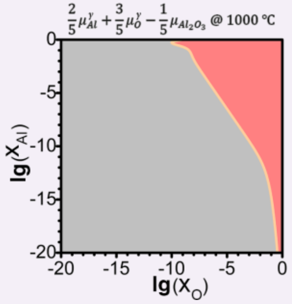
Ongoing XMAT Effort: Modeling of Internal to External Oxidation Transition

Input → **Output**

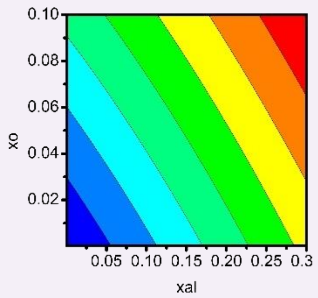
E.g. oxidation in Ni-Al

- Thermodynamic and kinetic databases

Chemical potentials

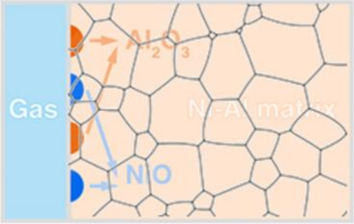


Interdiffusivity



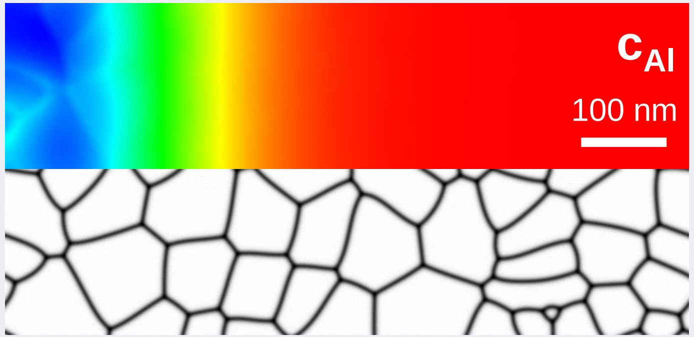
- Parameters: T, composition, p_{O2}, γ, …

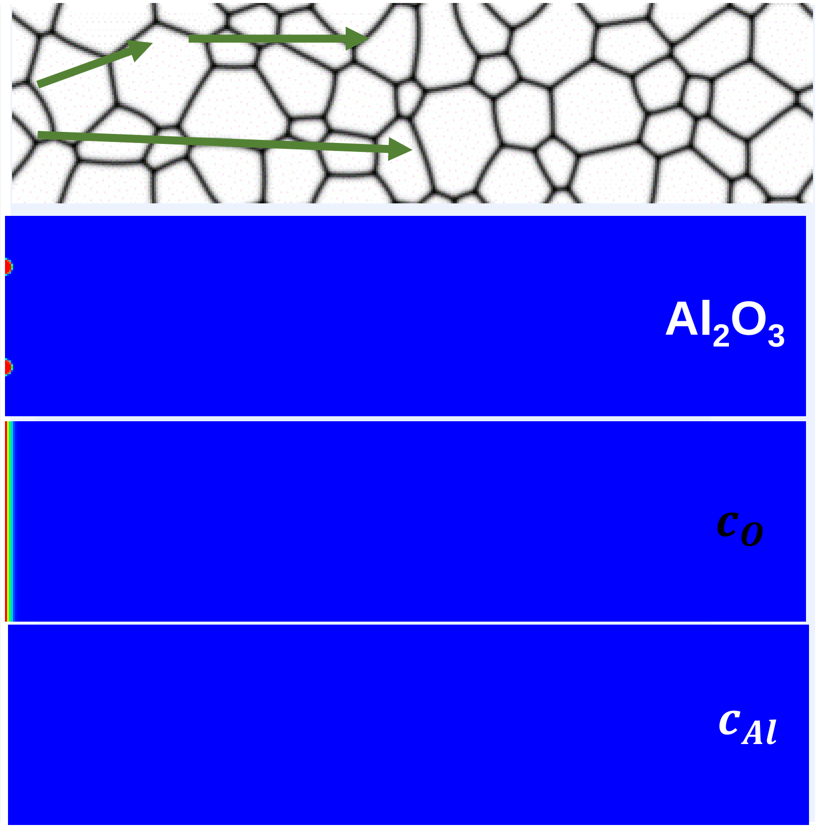
- User defined initial microstructure



- Support concurrent nucleation and growth governed by driving force

- Support coupling with polycrystalline structure





EY21 & Future Work

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

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