QuesTek®
INNOVATIONS LLC

Using digital twins to accelerate qualification and certification of fatigue critical components

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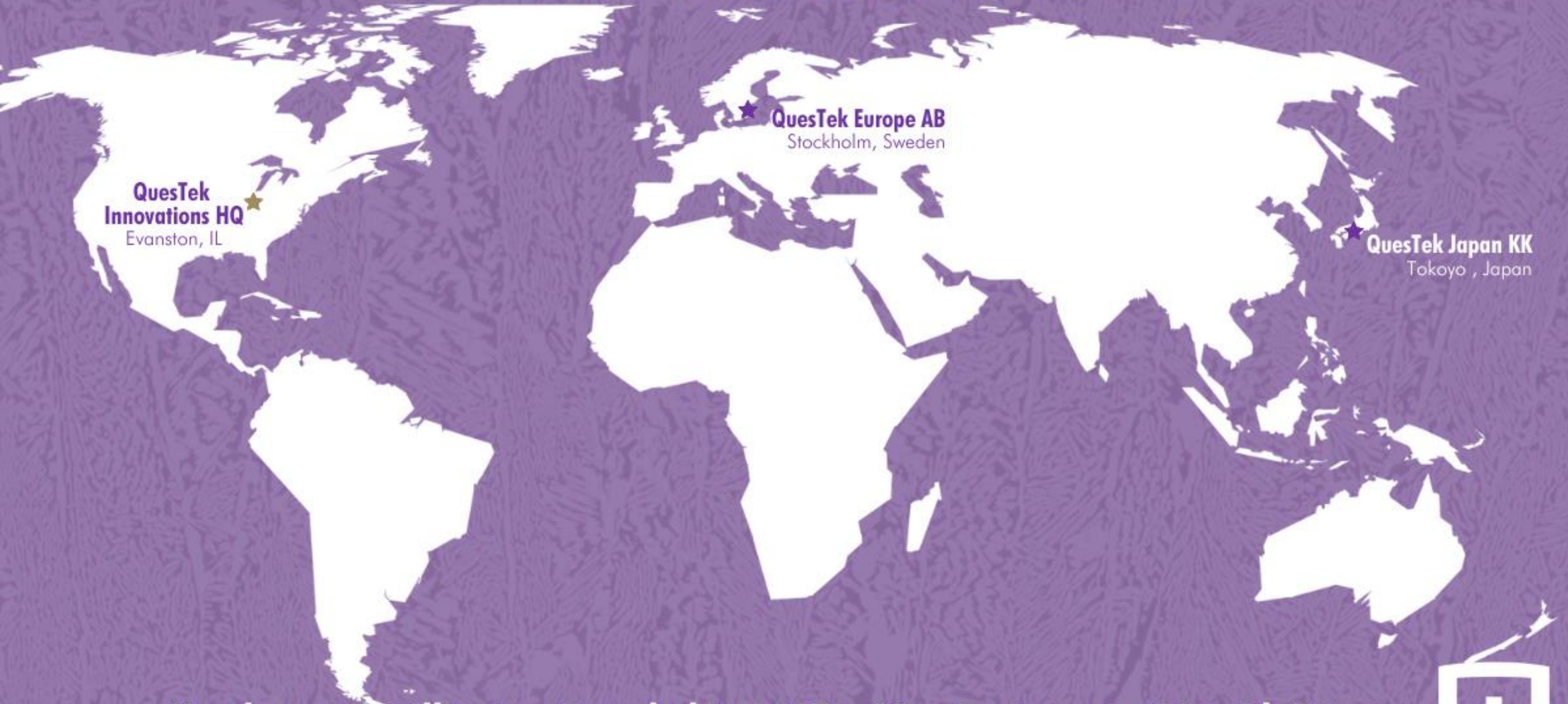
ICAF

Empowering innovators by resolving materials challenges

CORPORATE PROFILE



Headquarters: Illinois • Founded in 1997 • 25+ Engineers • 20+ Ph.D.'s

QUESTEK EXPERIENCE

32
Patents issued and pending

400+
SBIR/STTR Projects awarded

200+
Corporate Engagements

First flight approved “Cyber Steel”

CLIENT SUCCESS: HIGH-PERFORMANCE ALLOYS

> ***"From clean sheet alloy design to flight, this ICME-based program demonstrates the goals set by the 2011 Materials Genome Initiative."***

NIST Report (2018)

Ferrium ® M54 ® Hookshank

Novel Materials improve existing products

DARPA AIM Accelerated Insertion of Materials NAVAIR QuesTek Innovations LLC

MOTIVATION

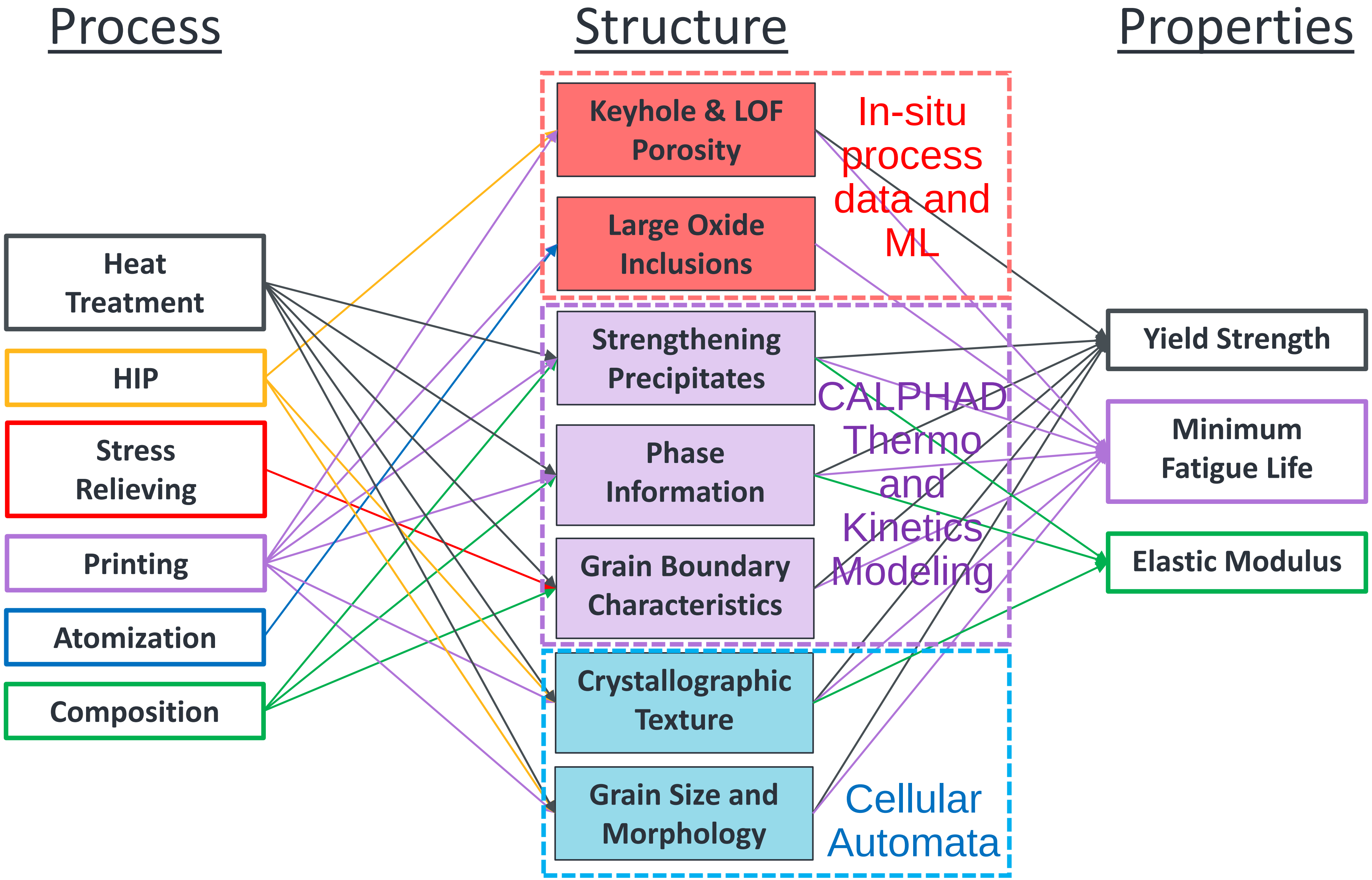
IMPROVE RELIABILITY AND REDUCE COST/TIME FOR QUALIFICATION OF FATIGUE CRITICAL ADDITIVELY MANUFACTURED ALLOYS

Outline

- Digital Twin for material PSP system
- Accelerated Insertion of Materials (AIM)
- Multi-Stage Fatigue
- Microstructure Sensitive Fatigue Modeling
- ICMD® Software demo

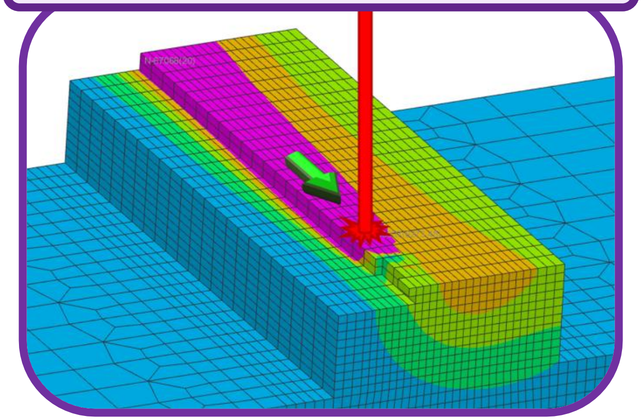
Digital Twin for material PSP system

PROCESS-STRUCTURE-PROPERTY MAP

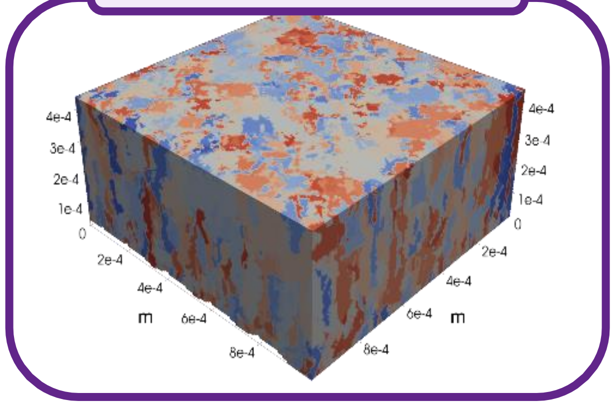


PROCESS-STRUCTURE-PROPERTY MODELING

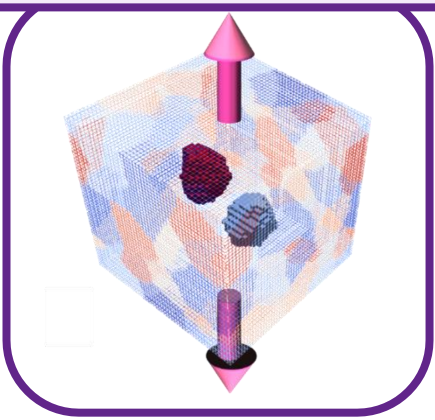
AM Process Simulation



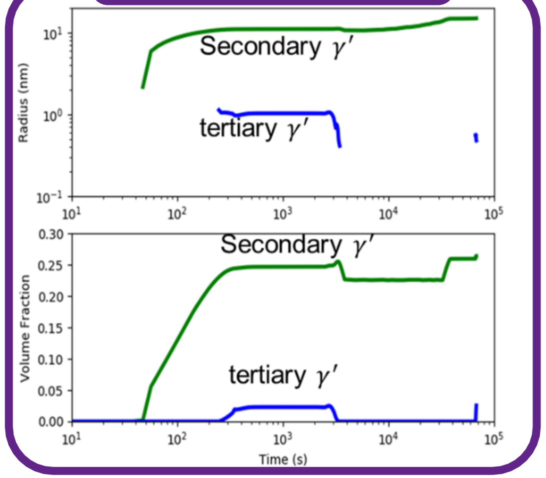
Grain Structure



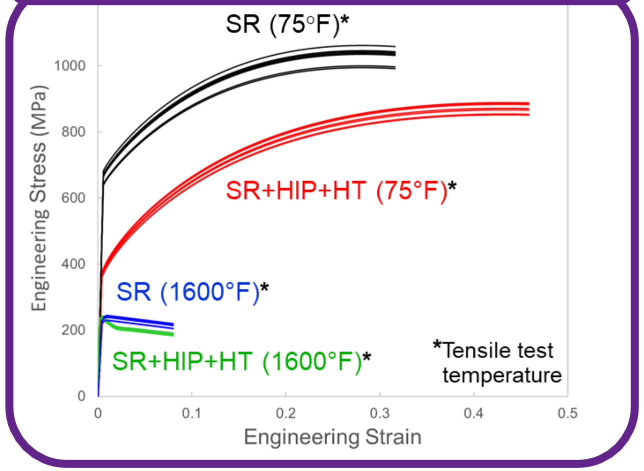
Crystal Plasticity Fatigue



CALPHAD



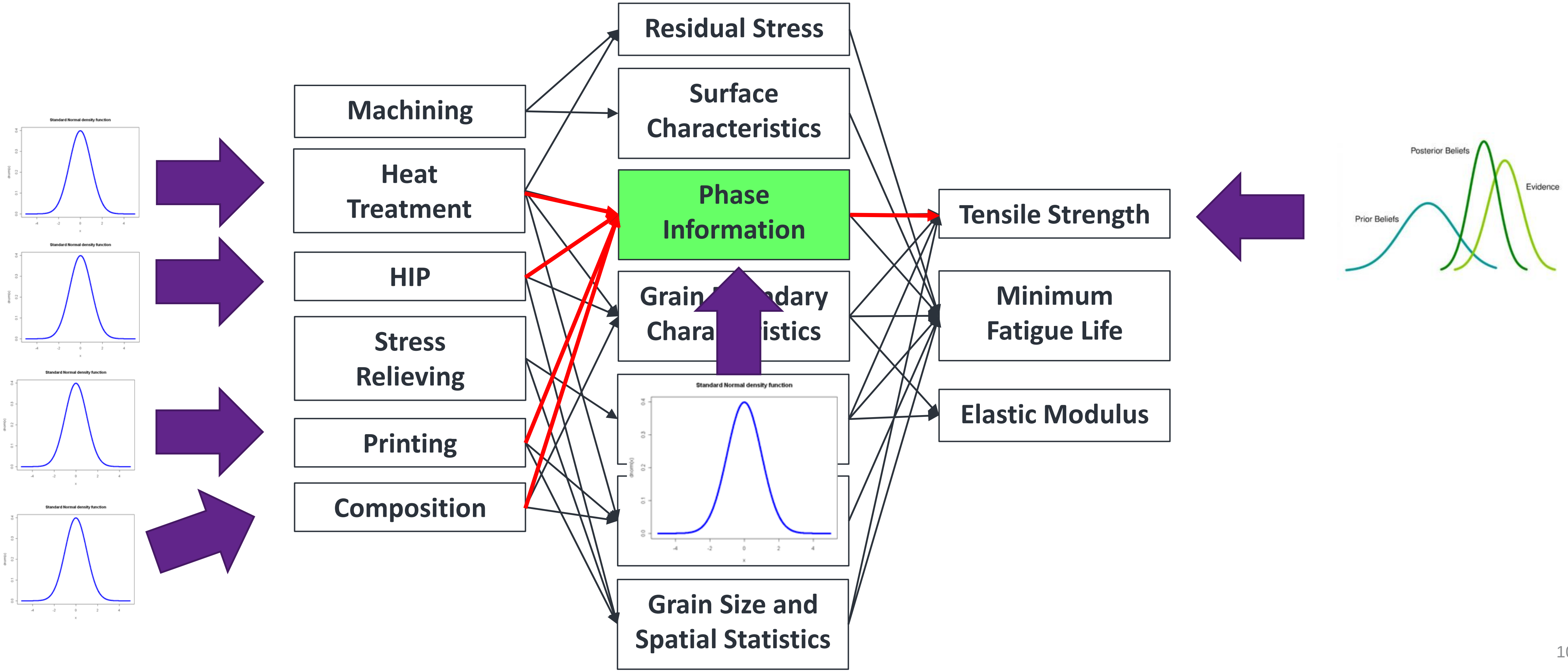
Strength and Ductility



Accelerated Insertion of Materials

ACCELERATED INSERTION OF MATERIALS (AIM)

Process Structure Properties



AIM APPLIED TO TENSILE STRENGTH OF AM IN718+

Mechanistic Property Models → Property Predictions (TYS, UTS, RT-1000°F) → Design Allowables Forecasting

$$\sigma_{yield} = \sigma_{yield}\left(D_{gr};\ f_{\gamma};f_{\gamma'_p};f_{\delta};f_{\gamma'_s};r;\gamma_{APB}\right)$$

$$= f_{\gamma+\gamma'_s}\sigma_{\gamma+\gamma'_s} + f_{\gamma_{p'}}\sigma_{\gamma_{p'}} + f_{\delta}\sigma_{\delta}$$

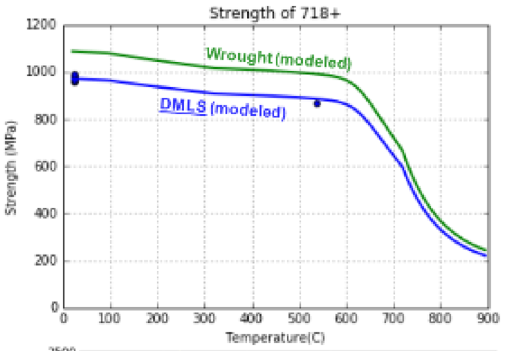
$$\sigma^{\gamma'_p} = \sigma_0^{Ni_3Al} + \Delta\sigma^{SS}(C_i)$$

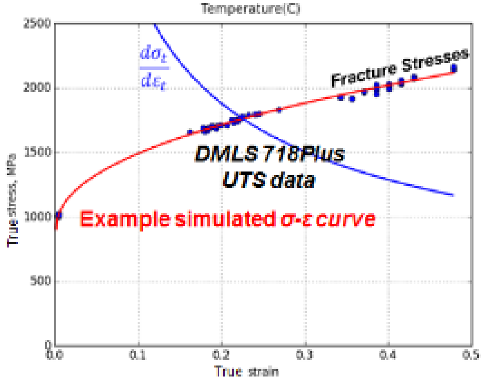
Strengthening in primary γ' due to base strength of Ni_3Al and solid solution strengthening

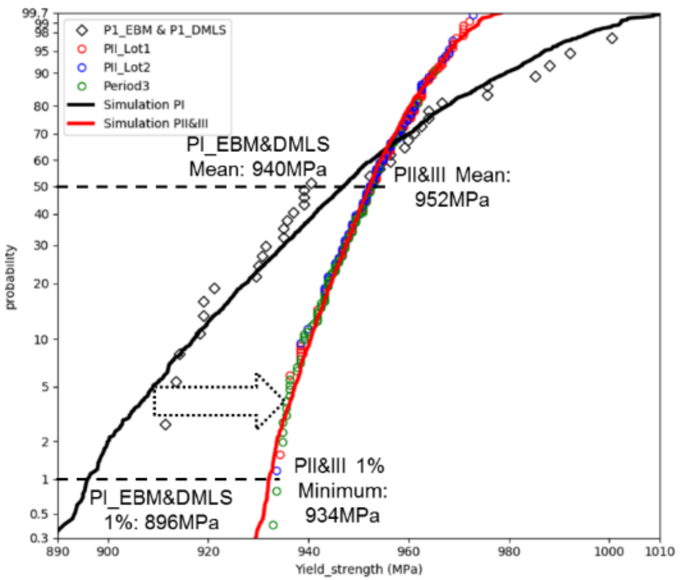
Strength of δ phase extracted from YS of soln. treated material

$$\sigma^{(\gamma+\gamma'_s)} = \sigma^{HP}(D_{gr}) + \sigma^{SS}(C_i) + \sigma^{Precip}(f_{\gamma'_s};r;\gamma_{APB})$$

Strengthening in γ matrix includes grain size, solid solution and secondary γ' precipitate strengthening



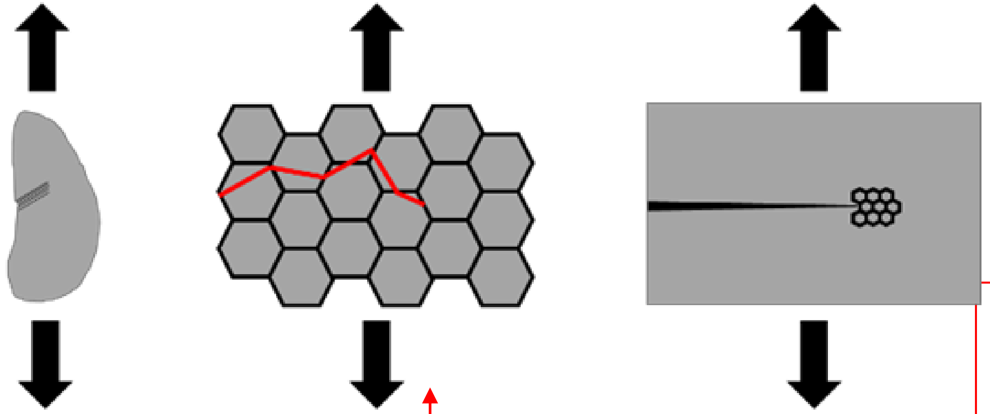




Modeling-informed heat treatment optimization resulted in mean YS improvement from 940 to 952 MPa and 1% min. YS improvement from 896 to 934 MPa

Multi-Stage Fatigue

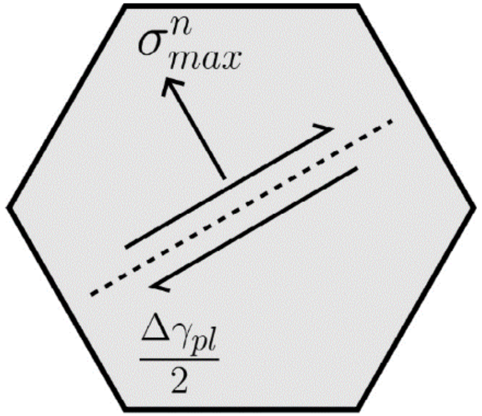
MULTI-STAGE FATIGUE



Incubation occurs at persistent slip bands or pre-existing defects at the sub grain scale

Microstructurally small cracks grow through several grains, being slowed by grain boundaries and meandering to the path of least resistance

Physically long cracks begin once the plastic zone at the crack tip becomes appreciably larger than grains, resulting in an averaging effect such that crack follows linear elastic fracture mechanics



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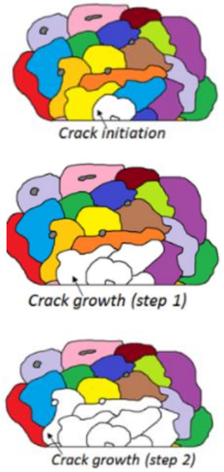

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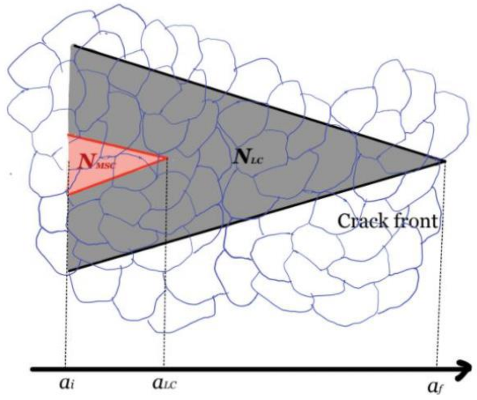

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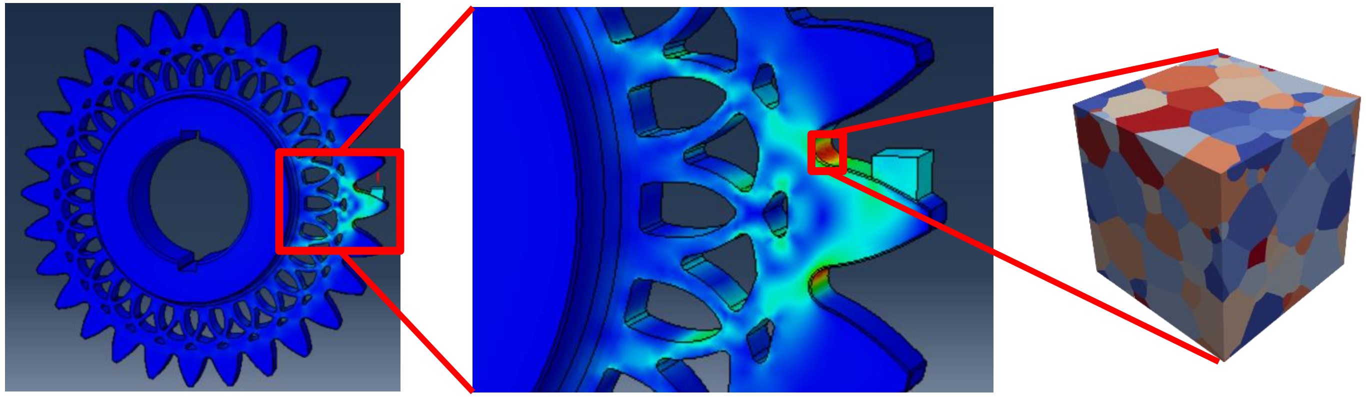
MULTI-STAGE FATIGUE

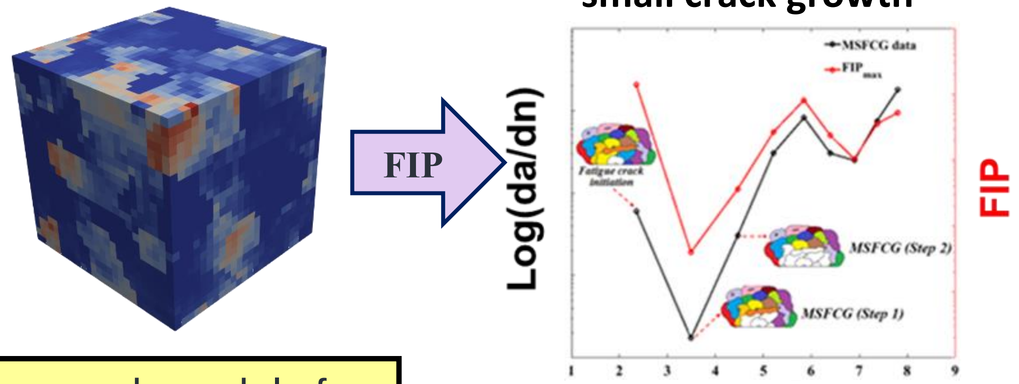
1. Identify key stress hot spots from component scale loading conditions

2. Apply microstructure sensitive fatigue modeling framework at mesoscale to predict component life

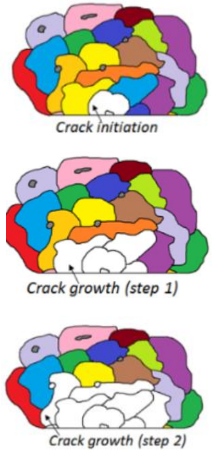


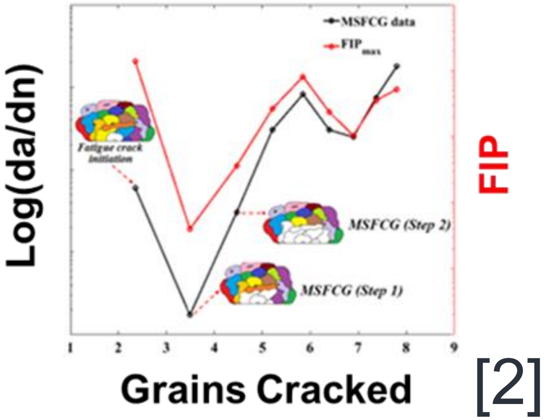
Localized plastic strain

Microstructurally small crack growth



3. Combine microstructurally small crack and long crack models for full component life in high or low cycle fatigue





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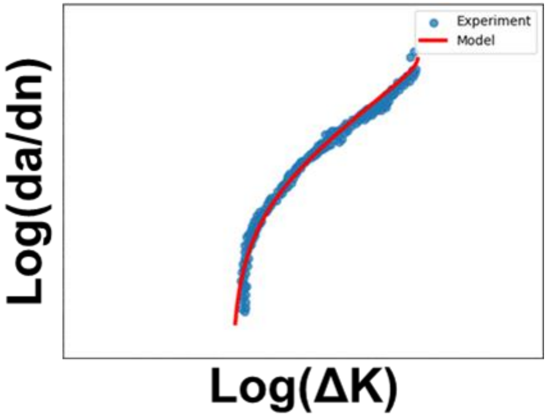

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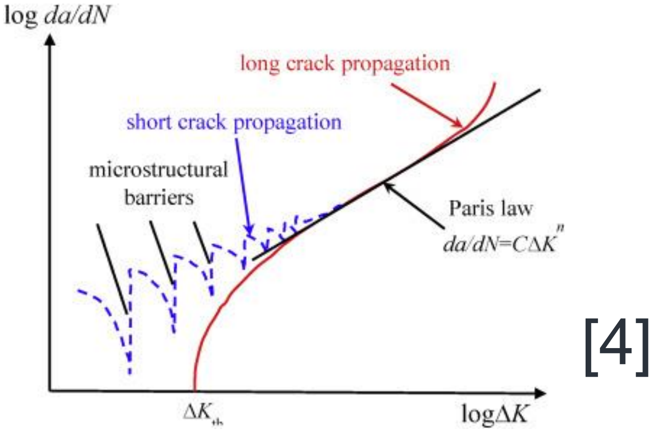
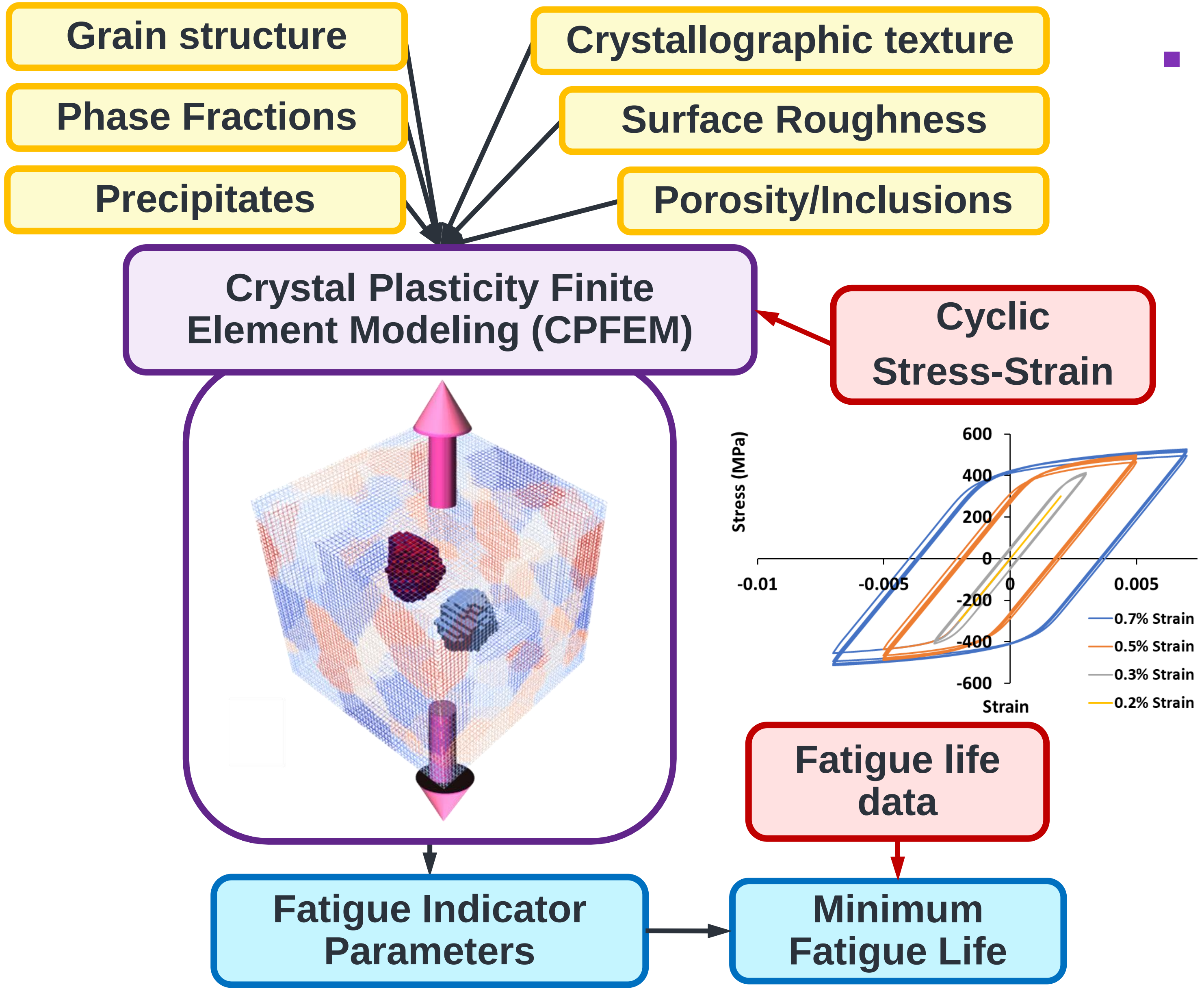


Microstructurally small cracks - CPFEM **Physically long cracks – Modified-NASGRO** **Full Fatigue Life**

Micro-Structure Sensitive Fatigue Crack Initiation

FATIGUE CRACK INITIATION MODEL



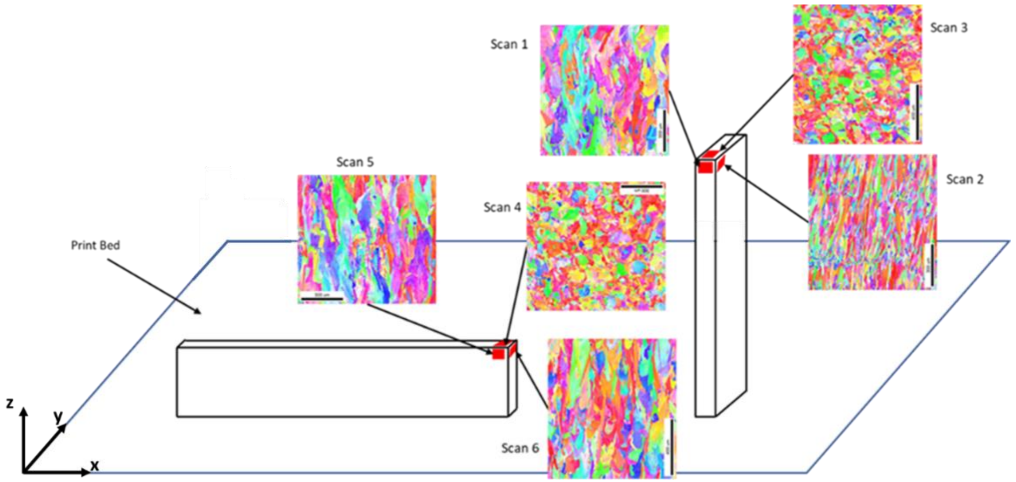
- **Crystal Plasticity Fatigue Modeling**
  - **Simulates:**
    - Crack Initiation and MSC Growth
    - Low- and High-Cycle Fatigue
  - **Used For:**
    - Minimum Fatigue Life
    - Component-scale Performance
  - **Calibrated with:**
    - Cyclic (10) stress-strain data
      - 2 Strain Ratios (R=-1, 0.1)
      - 2 Orientations
    - VHCF Fatigue life data

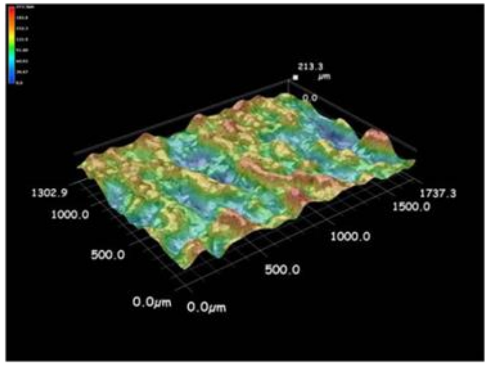
CHARACTERIZATION AND DIGITAL TWIN

EBSD
- Grain size
- Volume fractions
- Crystallographic Texture

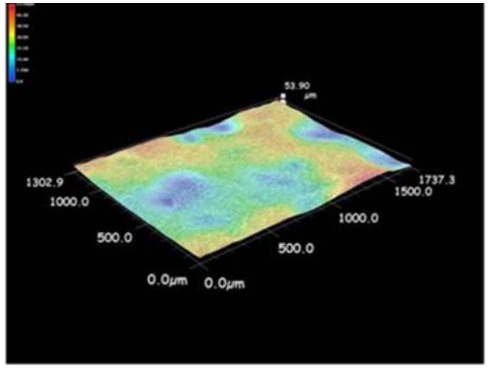
Coherence Scanning Interferometer-based 3D Surface Analysis
- As-built surface roughness
- Post-processed surface roughness

SEM
- Porosity statistics (pre- and post-HIP)
- Inclusion statistics and chemistry (From EDS)





As-Printed



Surface Finished

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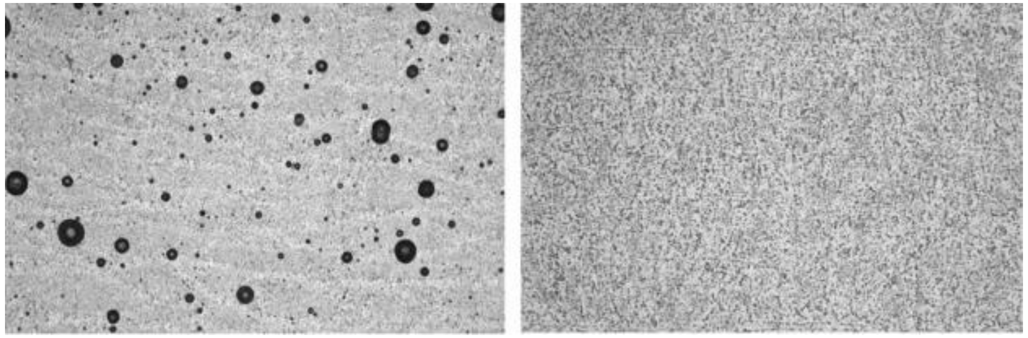
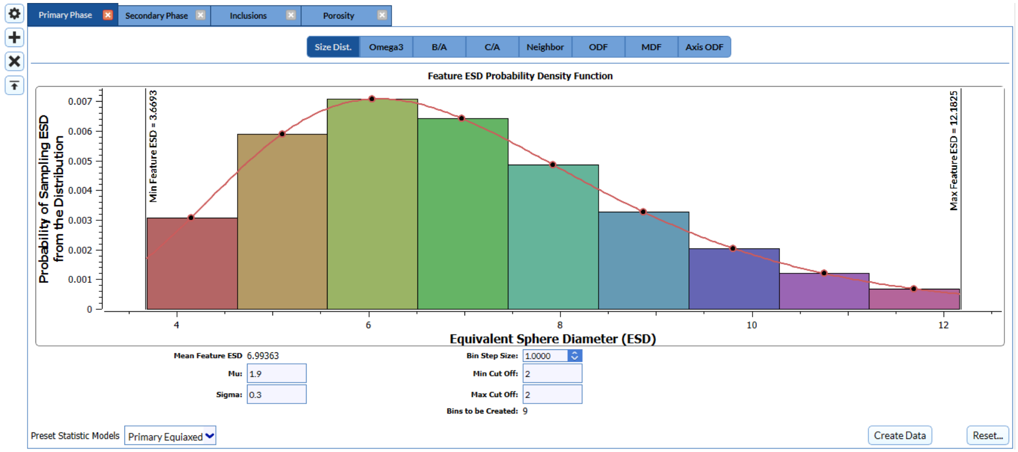
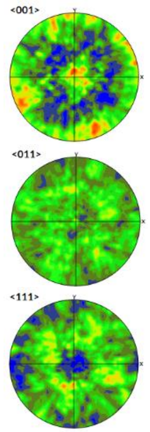


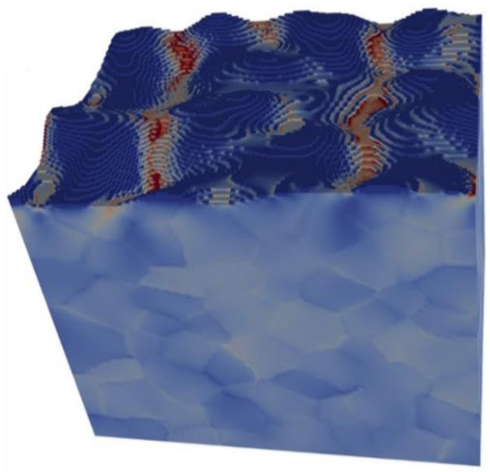
CHARACTERIZATION AND DIGITAL TWIN

- Generate digital microstructures with appropriate grain morphology, phases, and crystallographic texture

- Add surface roughness, porosity/inclusions to digital microstructures







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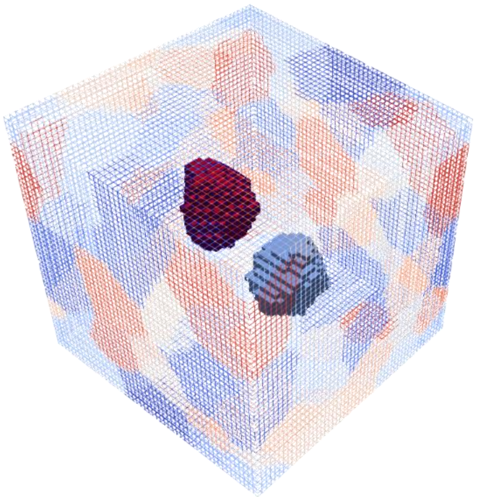
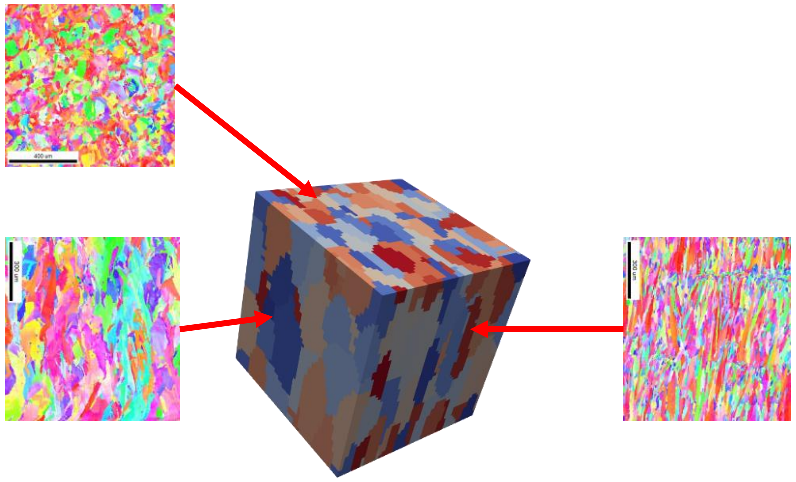
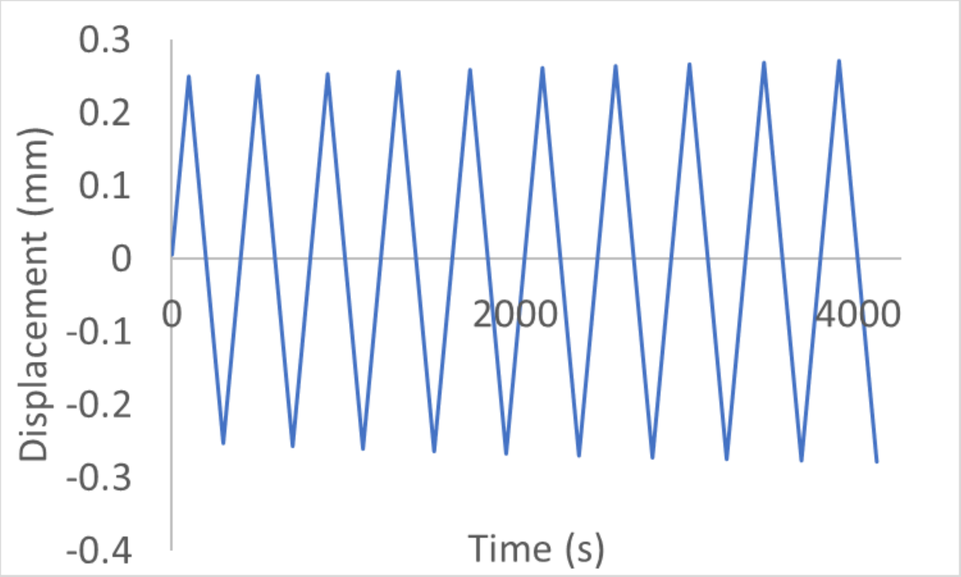
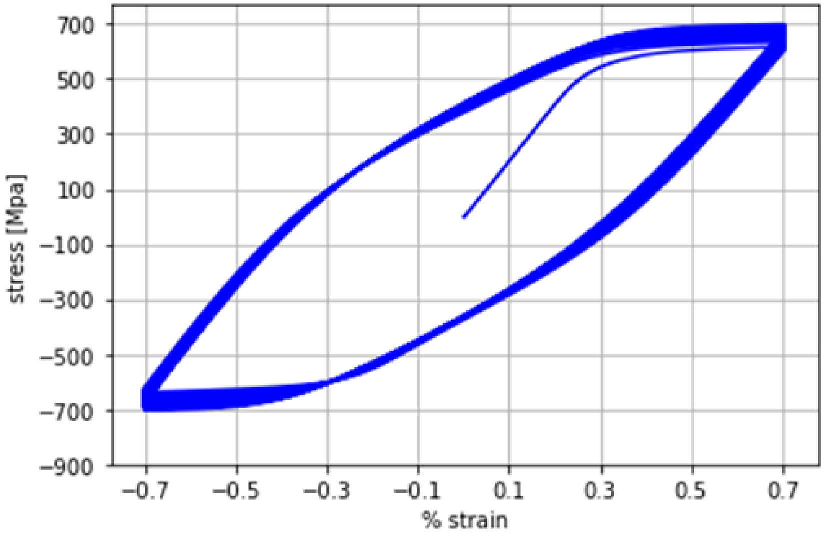




MODEL CALIBRATION

- Conduct cyclic tensile/compressive tests on coupons in Z (build) direction and XY (orthogonal) direction for ~10 cycles
- Alternatively yield strength and modulus of elasticity can be predicted using mechanistic models to calibrate CPFEM model

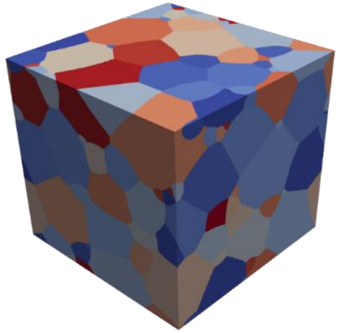


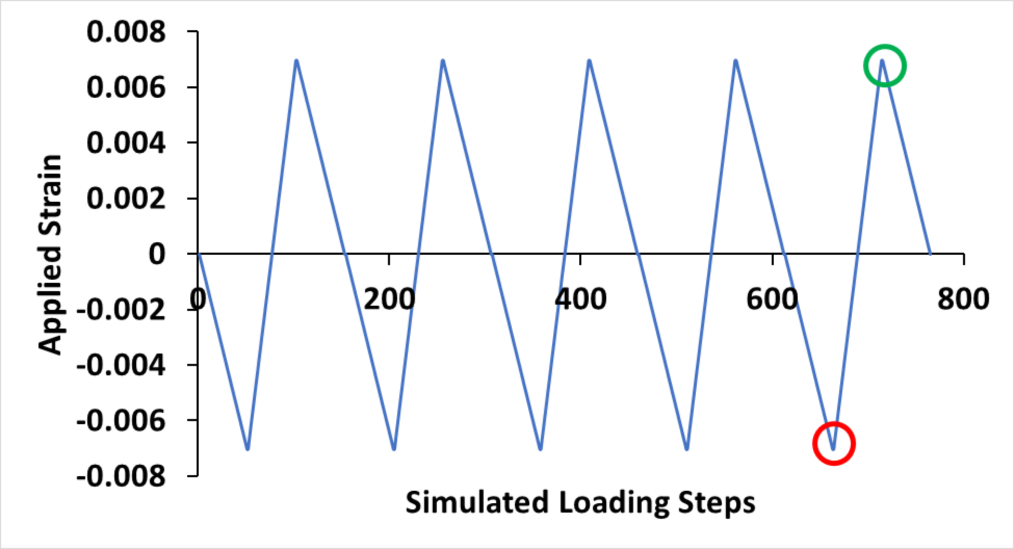


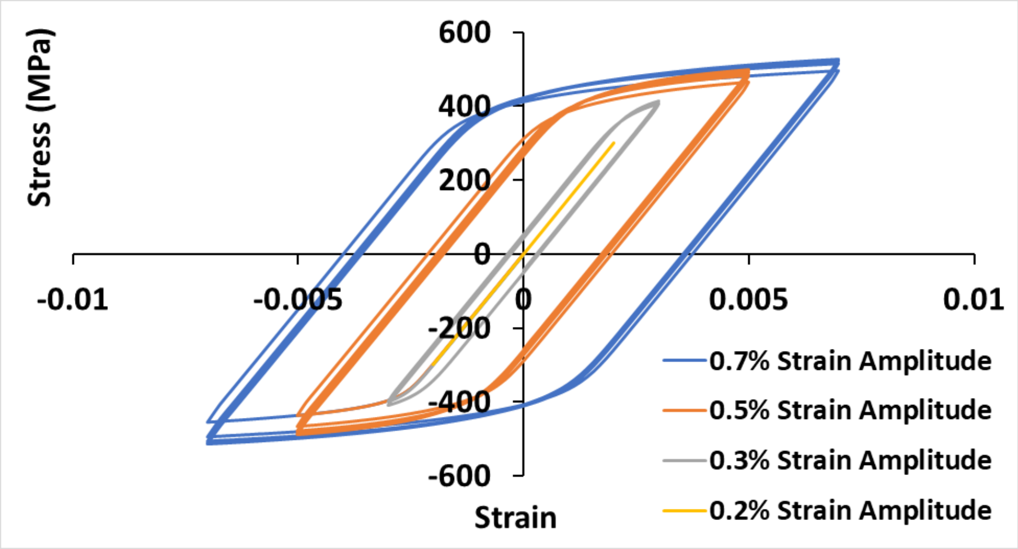
FATIGUE INDICATOR PARAMETERS

- Fatigue indicator parameters are a surrogate measure of driving forces for fatigue crack initiation and microstructurally small crack growth

$$FIP_{FS} = \frac{\Delta \bar{\gamma}^{p}_{\max}}{2}\left[1 + k\frac{\bar{\sigma}^{n}_{\max}}{\sigma_y}\right]$$

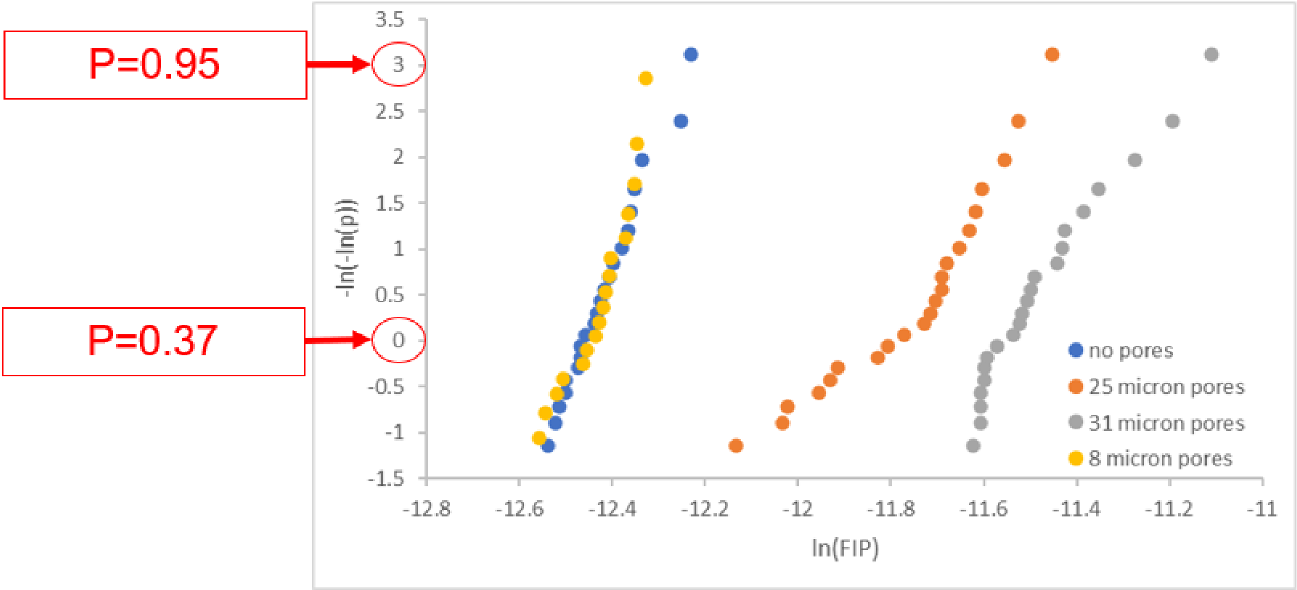




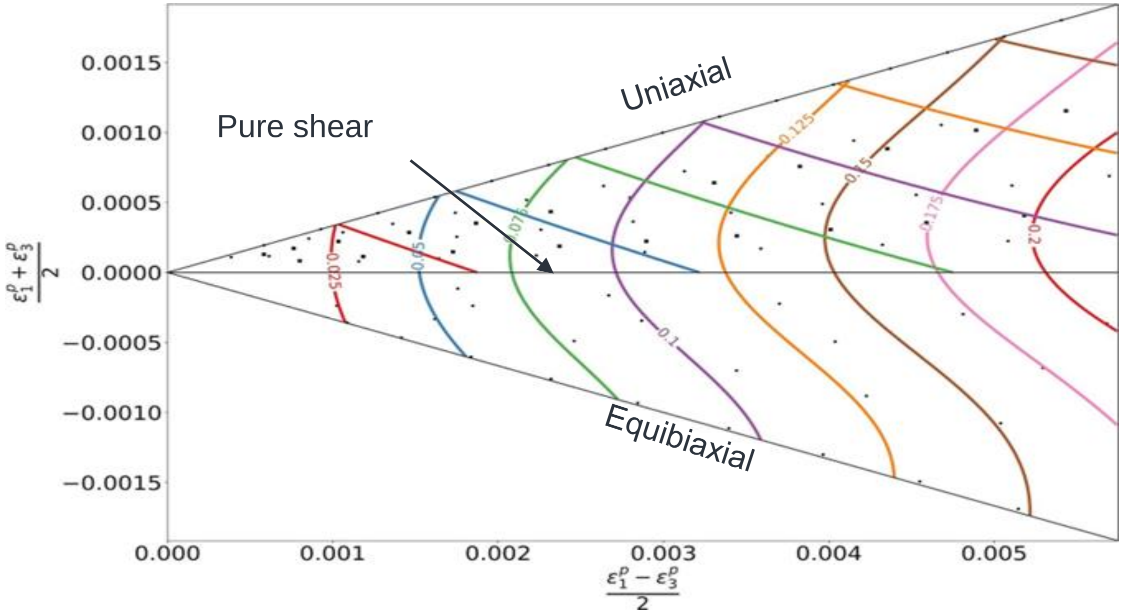


FIP ANALYSIS USE CASES

- Example 1 – Study of effect of maximum pore size on fatigue performance in AM Ti64 can be used to determine critical pore size
- Example 2 – iso-FIP contour showing fatigue performance in complex strain states can be used for topological optimization of fatigue critical components



HIP optimization for HCF life



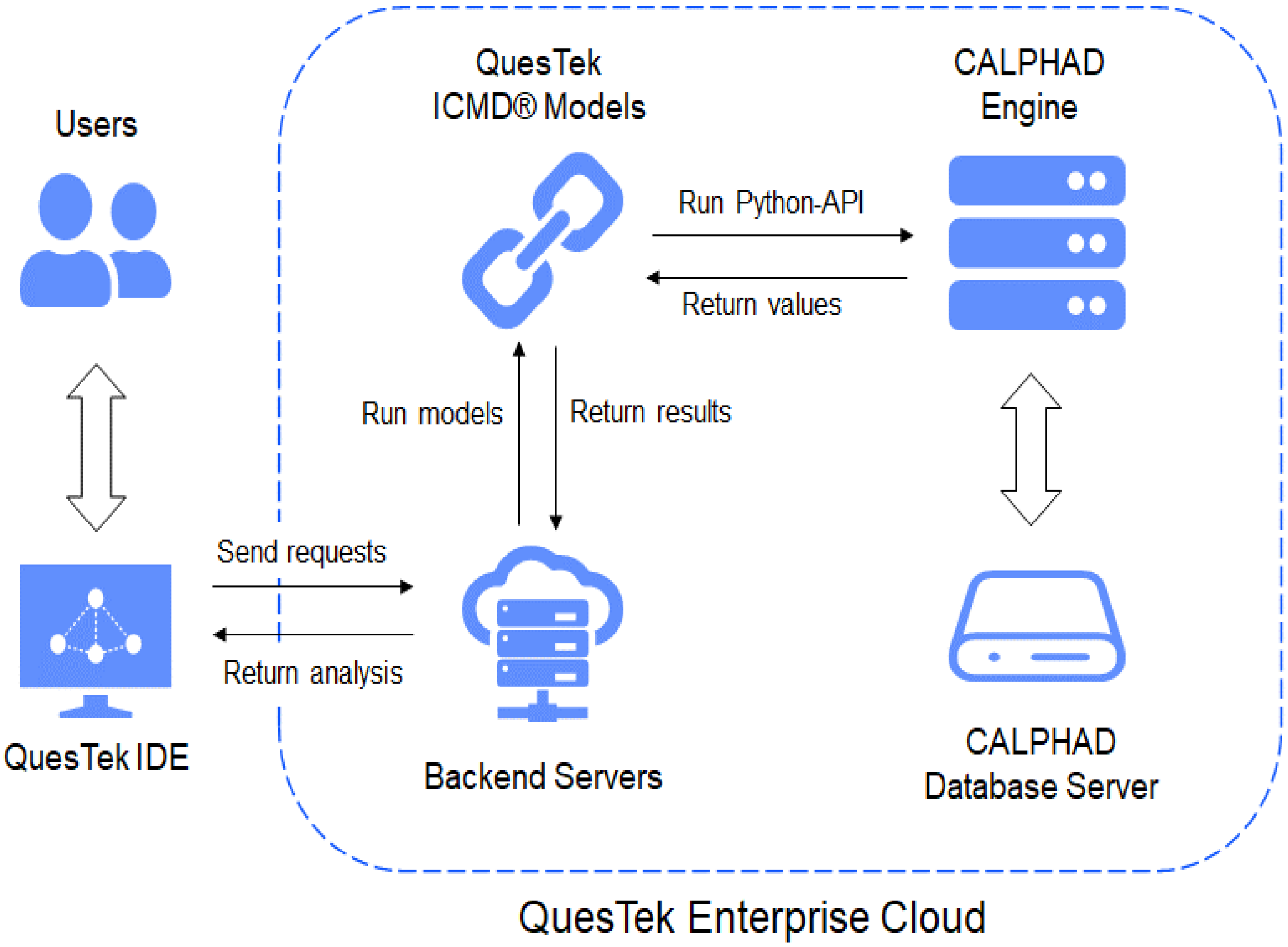
Fatigue sensitive TopOp

Yaghoobi, Mohammadreza, Krzysztof S. Stopka, Aaditya Lakshmanan, Veera Sundararaghavan, John E. Allison, and David L. McDowell. "PRISMS-Fatigue computational framework for fatigue analysis in polycrystalline metals and alloys." *npj Computational Materials* 7, no. 1 (2021): 38.

ICMD® Software Platform

ICMD® PLATFORM

- **Productizing our proven library of software, databases, models, and analytics: ICMD®**
- **Platform toolkits:**
  - **Alloy Design**
  - **Alloy Qualification**
  - **CALPHAD ('24)**
  - **Fatigue Simulation ('24)**
  - **Additive Simulation ('24)**
- **Packaged as a SaaS offering via web-accessible cloud-based Integrated Digital Environment**
- **Licensing and subscription availability next month!**



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4. Chowdhury, P., and H. Sehitoglu. "Mechanisms of fatigue crack growth–a critical digest of theoretical developments." Fatigue & Fracture of Engineering Materials & Structures 39, no. 6 (2016): 652-674.
5. http://pencerw.com/feed/2016/11/29/ebm-and-chemical-surface-finishing
6. Stopka, Krzysztof S., Mohammadreza Yaghoobi, John E. Allison, and David L. McDowell. "Microstructure-Sensitive modeling of surface roughness and notch effects on extreme value fatigue response." *International Journal of Fatigue* 166 (2023): 107295.

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