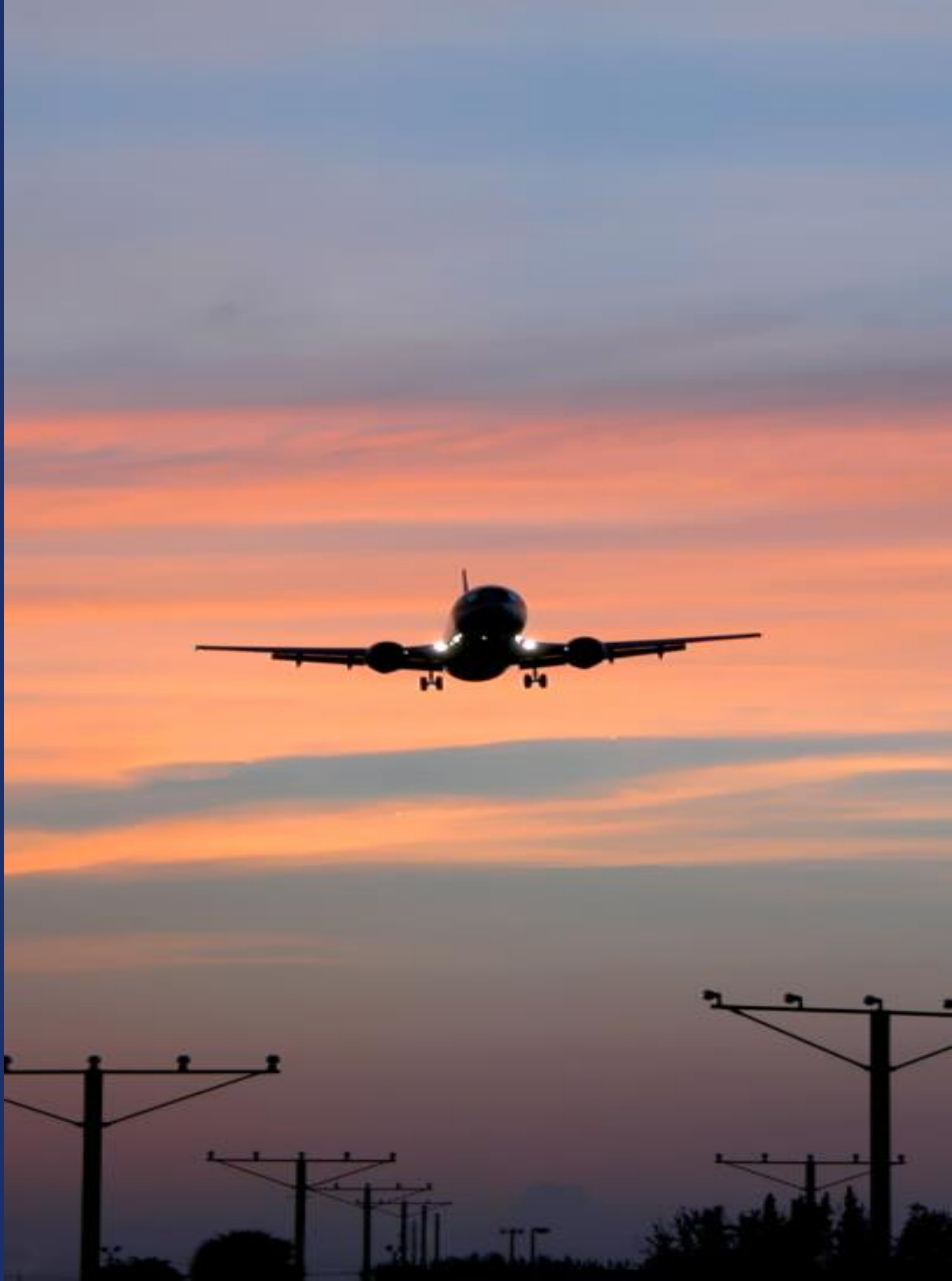
Computational Materials-informed Qualification and Certification of Process-Intensive Metallic Materials



Presented by

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and

Dr. Andrew R. Kitahara

Materials Engineer, Staff
Analytical Mechanics Associates

Outline

- Computational Materials for Qualification and Certification (CM4QC) Steering Group and Roadmap
- Work of the Computational Materials-informed Qualification and Certification Research Group

Input from the Aviation Community

NASA/CR-2018-219771

Vision 2040: A Roadmap for Integrated, Multiscale Modeling and Simulation of Materials and Systems

Xuan Liu and David Furrer
Pratt & Whitney, East Hartford, Connecticut

Jared Kosters and Jack Holmes
Nexight Group, Silver Spring, Maryland

March 2018

NASA/TM-2019-220428

ARMD Workshop on Materials and Methods for Rapid Manufacturing for Commercial and Urban Aviation

Jonathan B. Ransom, Edward H. Glaessgen, and Brian J. Jensen
Langley Research Center, Hampton, Virginia

November 2019

NASA/TM-2021-15175

NASA / NIST / FAA Technical Interchange Meeting on Computational Materials Approaches for Qualification by Analysis for Aerospace Applications

Edward H. Glaessgen
Langley Research Center, Hampton, Virginia

Lyle E. Levine, Paul W. Witherell, and M. Alkan Donmez
National Institute of Standards and Technology, Gaithersburg, Maryland

Michael Gorelik
Federal Aviation Administration, Scottsdale, Arizona

Nathan A. Ashmore
Boeing Research and Technology, St. Louis, Missouri

Richard R. Barto
Lockheed Martin Advanced Technology Laboratories, Cherry Hill, New Jersey

Corbett C. Battaile
Sandia National Laboratory, Albuquerque, New Mexico

Harry R. Millwater
University of Texas at San Antonio, San Antonio, Texas

Gerard J. Nanni
Bell, Fort Worth, Texas

Anthony D. Rollett
Carnegie Mellon University, Pittsburgh, Pennsylvania

Edwin J. Schwalbach
Air Force Research Laboratory, Dayton, Ohio

Vasisht Venkatesh
Pratt and Whitney, East Hartford, Connecticut

May 2021

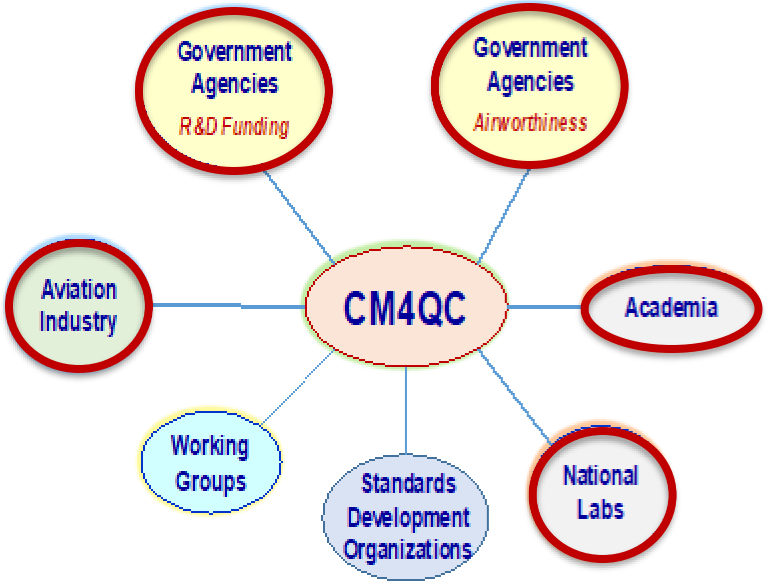
CM4QC Steering Group
Computational Materials for Qualification and Certification

Formed through a NASA-FAA collaboration
Members: 10 industry, 8 government orgs, 8 universities/labs

Primary goals
- Provide coordination for and focus to investments m… d development of computational materials-ba… e metallic materials
- Identify key considerations an… s / certifying authorities' acceptance of CM met… ical PIM parts

Operation
- High TRL… timeline a…
- Mid TRL: S… and transition of Research t…
- Low TRL: De… ent of required computational materials & measurement capabilities

Not "certification by analysis"
…Computational Materials-Informed Q&C
→ CM4QC is a paradigm change



Expected initial outcome –
Multi-year implementation plan

Steering Group Membership

Government

National Aeronautics and Space Administration*

Federal Aviation Administration*

National Institute of Standards and Technology*

Sandia National Laboratory*

U.S. Air Force Research Laboratory

U.S. Army Aviation Command

U.S. Navy Air Systems Command

Oak Ridge National Laboratory

Industry

BAE Systems Inc*

The Boeing Company*

Lockheed-Martin

Raytheon / Pratt & Whitney

General Electric Aviation

Spirit Aerosystems

Honeywell Aerospace

Southwest Research Institute

Northrop-Grumman Corp

Textron Aviation

Academia

Univ Texas San Antonio*

Carnegie Mellon Univ.*

Vanderbilt Univ.

Pennsylvania State Univ.

Northwestern Univ.

*CM4QC Leadership Team

Highlights from the CM4QC Roadmap

Maturation of computational materials approaches in qualification and certification for metal additive manufacturing (as an example of process-intensive materials) in aviation

Produced by the Computational Materials for Qualification and Certification (CM4QC) Steering Group

The purpose of this group is not to establish Federal policy, but to enable a free-ranging discussion of emerging issues. Participants have provided non-consensus, non-voting advice, informational background, and technical and administrative assistance.

Outline

- CM4QC Steering Group and Roadmap
- Work of the Computational Materials-informed Qualification and Certification Research Group

Computational Materials-informed Qualification and Certification Research Group

NASA and On-site Contractors

Sang-Hyon Chu[1]
Erik L. Frankforter[1]
Andrew R. Kitahara[2]
Patrick E. Leser[1]
John Andrew Newman[1]
Joshua D. Pribe[2]
Brodan Richter[1]
Peter W. Spaeth[1]
David W. Wagner[1]
George R. Weber[1]
Vesselin Yamakov[2]
Saikumar Yeratapally[3]
Joseph N. Zalameda[1]

Adjuncts and Students

Evan B. Adcock
Claire E. Borden
Eric R. Burke[1]
Devin E. Burns[1]
Jared S. Fell[1]
Ariel Gluck
Brian T. Gockel
Erick R. Ramirez
Sierra Stevenson
Seth T. Strayer

[1] National Aeronautics and Space Administration, Langley Research Center, Hampton, VA 23681
[2] Analytical Mechanics Associates, Hampton, VA 23666
[3] Science and Technology Corporation, Hampton, VA 23666

The Valley of Death

Mid Technology Readiness Level

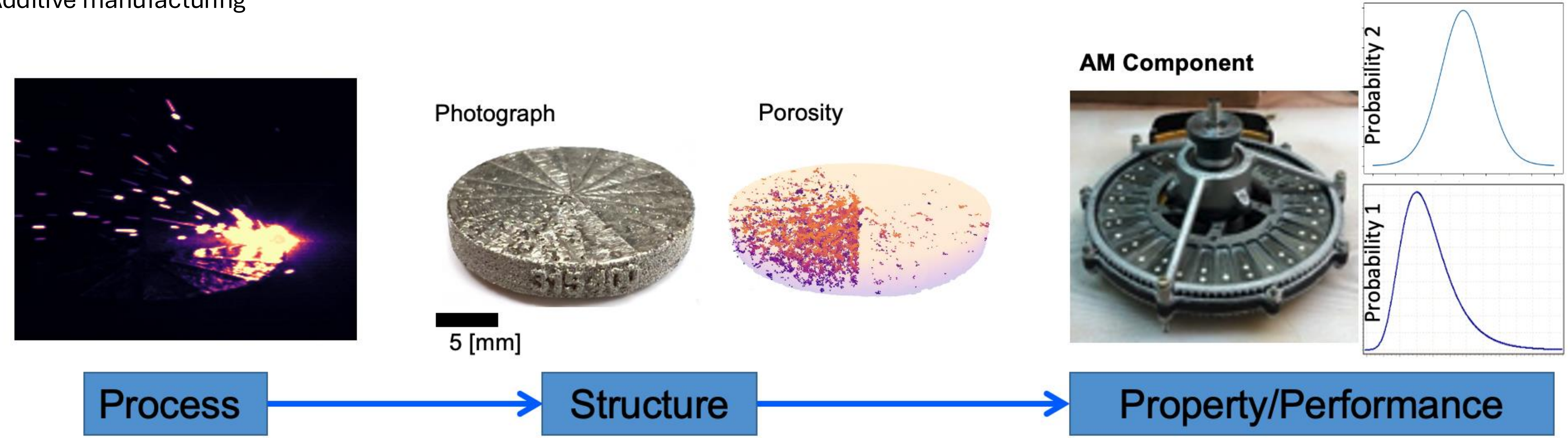
The place where low TRL capabilities & technologies go to die

A Few (Rhetorical) Questions

- What is the gap between the State-of-the-Art and the State-of-Practice?
- How much foundational research is funded and published every year?
- How much of it languishes for decades, trapped in journal papers?
- Which components of this work (by NASA, others) can/should be matured as the foundation for new solutions for flight?

Computational Materials-Informed Qualification and Certification of Additively Manufactured Flight Hardware

Q&C: Qualification and certification
AM: Additive manufacturing



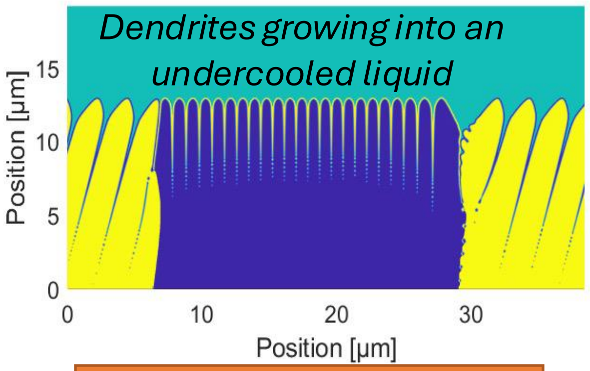
Small deviations in processing parameters may result in large differences in performance
Current approaches for Q&C of metallic materials (including AM) are entirely based on test data

Goal is to <u>change the paradigm for Q&C</u>: Develop a computational materials-informed ecosystem for quantifying sources of variability in fatigue performance of additively manufactured metallic materials through integrated multi-scale, multi-physics simulation, characterization and monitoring

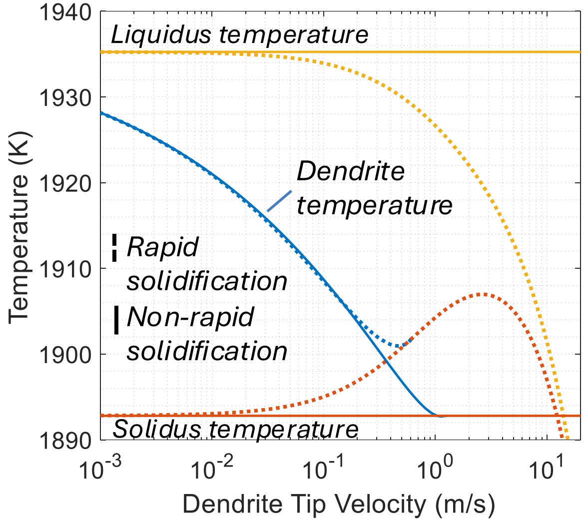
Grain-scale Process-Structure Modeling

Grain-scale Prediction of Microstructure Evolution

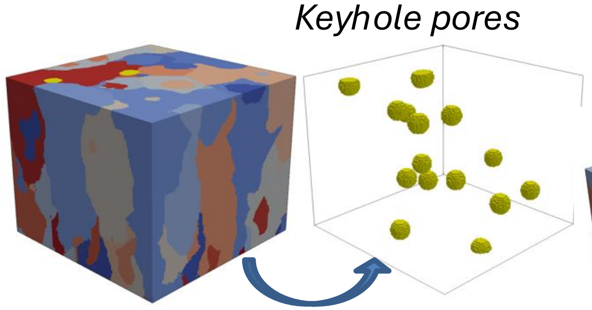
Analytical modeling of dendritic growth



Phase-field modeling of dendritic growth (input to Monte Carlo simulation)

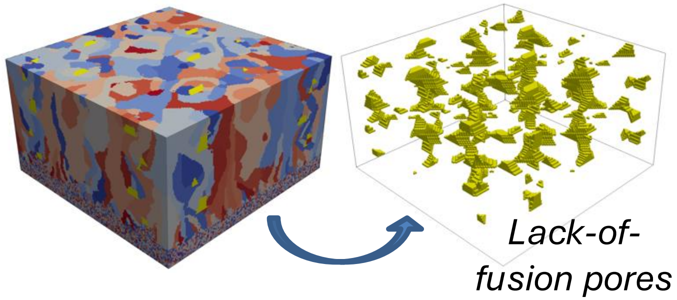


Defect modeling



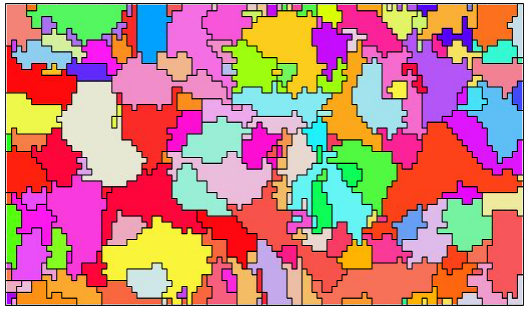
(Stochastic) Keyhole modeling

(Geometric) Lack-of-fusion modeling

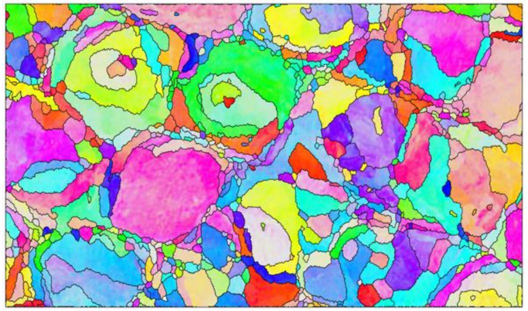


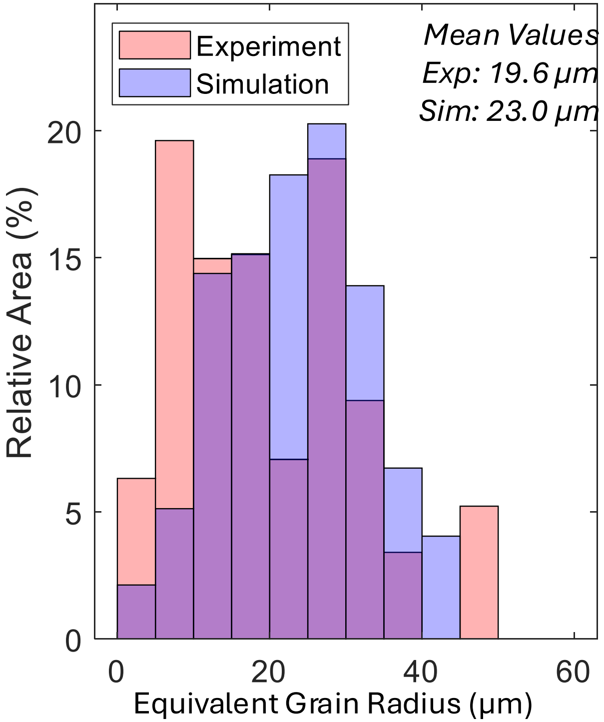
Simulation vs. Experiment

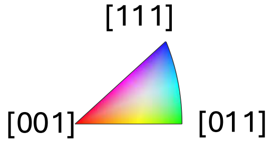
Simulated Microstructure



Experimental Microstructure







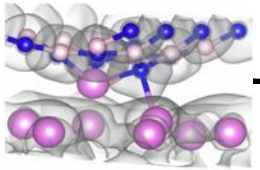
Observations:

- Calibrated microstructure evolution models can accurately capture simulate grain morphology
- Enables studying how process parameters affect resulting structure
- Provides a hand-off for structure-property-performance simulations

POC: Brodan Richter

Physically Informed Neural Networks (PINN) Atomistic Simulations

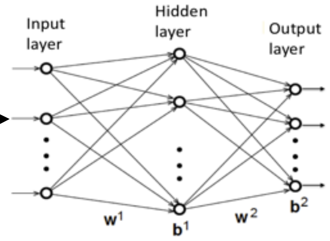
Large scale atomistic simulations with quantum mechanics accuracy: machine learning and empirical potentials



Atomic environment

$$\begin{pmatrix} G_1 \\ G_2 \\ \vdots \\ G_n \end{pmatrix}$$

Structure coefficients



Neural Network (NN)

$$\begin{pmatrix} A_i \\ \alpha_{ij} \\ B_i \\ \beta_{ij} \\ \vdots \end{pmatrix}$$

Custom pot. parameters

Bond Order Potential (BOP)

$$\frac{1}{2}\sum_{j\neq i}\left[e^{A_i-\alpha_{ij}r_{ij}} - S_{ij}b_{ij}e^{B_i-\beta_{ij}r_{ij}}\right]f_c(r_{ij}) = E_i$$

NN customizable potential energy function

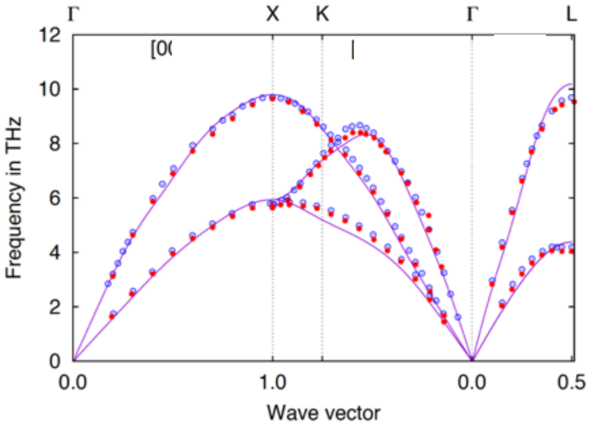
Retains the physics of the atomic interactions

$$\hat{H}|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$$

Contains the "knowledge" of the QM calculations

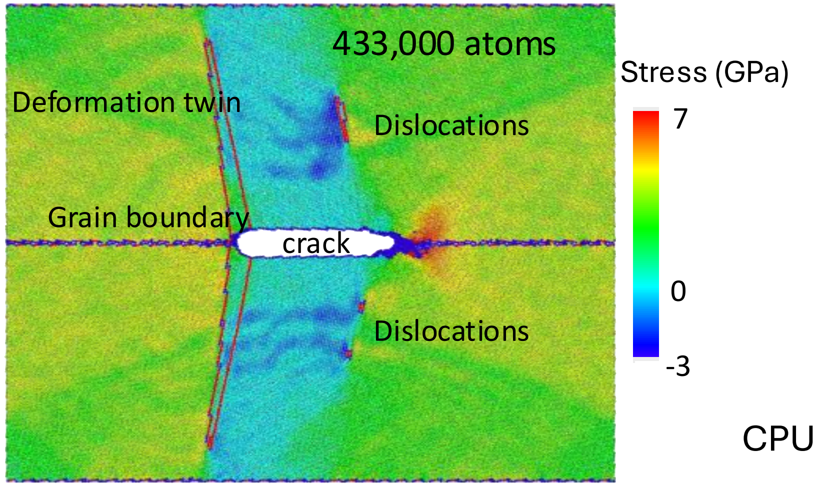
Accuracy: PINN ~1% of DFT

Phonon spectrum

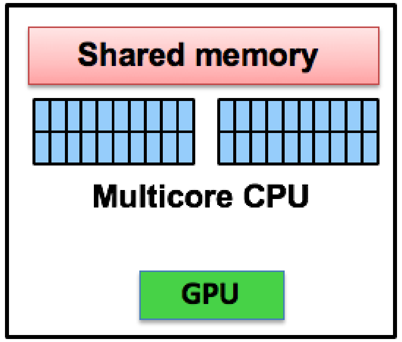


Quantum mechanics-based Density Functional Theory (DFT) calculations are used to train a NN

Fracture simulation with DFT precision: central crack nucleation in Al



Computing: optimized for multicore processors with graphic (GPU) accelerators



427,330 atoms
40 Skylake cpus + 4 V100 GPU
CPU time for 12,000 integration steps: 14 cpu hours

Speed: PINN ≫ DFT

t (s) 100 Steps	PINN 16 cores	DFT 32 nodes
N=500 atoms	35 s	46,688 s
N=72,000	528 s	13.5 years*

*Extrapolation

POC: Vesselin Yamakov

G. P. Purja Pun, et al., *Physical Review Materials*, 4 (2020) 113807.

Crystal Plasticity Framework and Applications

$$F = F^e F^p$$ elastic-plastic

$$L^p = \sum_{\alpha}^{N_{ss}} \dot{\gamma}_\alpha (s_\alpha \otimes m_\alpha)$$ slip rule

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \frac{\tau_\alpha}{g} \left| \frac{\tau_\alpha}{g} \right|^{\frac{1}{m}-1}$$

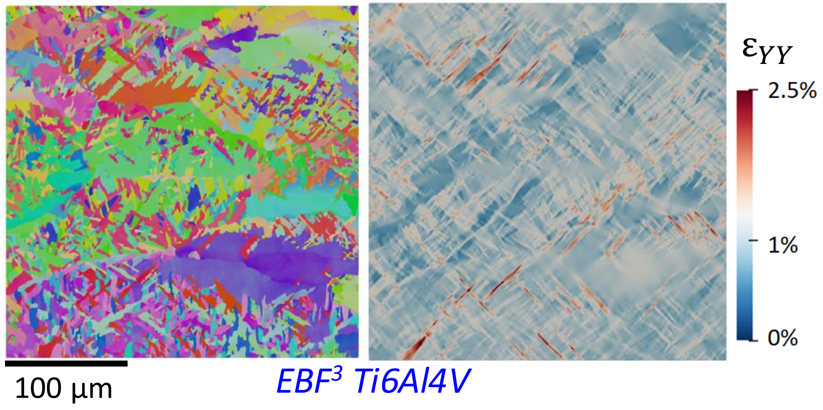
$$\dot{g} = G_0 \left(\frac{g_s - g}{g_s - g_0} \right) \dot{\gamma}_t$$ Voce-Kocks hardening

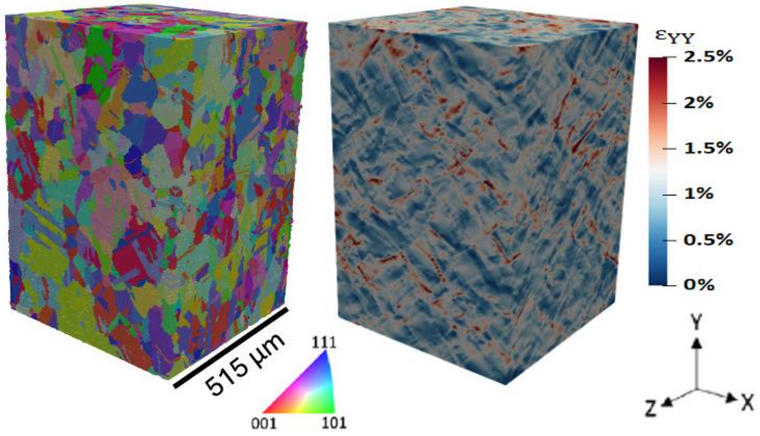
$$\dot{\gamma}_t = \sum_{\alpha}^{N_{ss}} |\dot{\gamma}_\alpha|$$

$$g_s = (g_0 + g_s^*) |\dot{\gamma}_t|^\omega$$

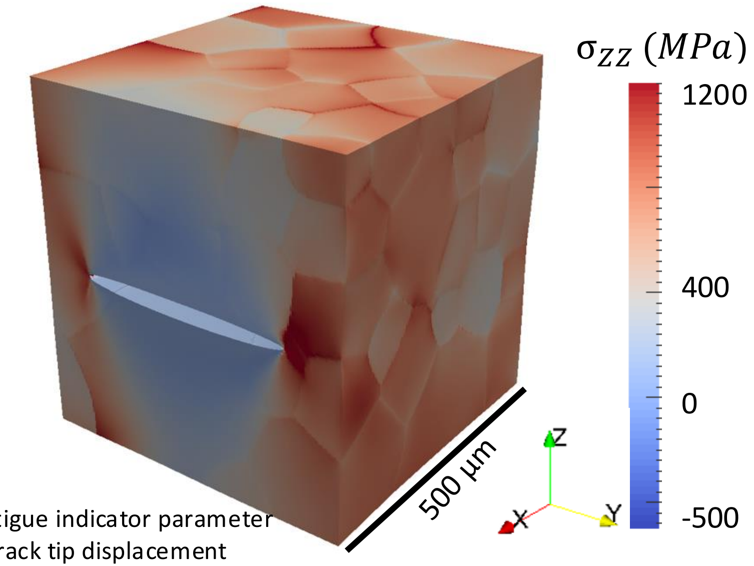
- *F is deformation gradient*
- *F^e, F^p are elastic and plastic portion of F, respectively*
- *L^p is the velocity gradient; $\dot{\gamma}_0$ is the reference slip rate*
- *$\dot{\gamma}^\alpha$ is the slip rate along slip system α*
- *$\dot{\gamma}_t$ is the absolute sum of slip rate on all slip systems*
- *g is the slip resistance*
- *m is the shear rate sensitivity parameter*
- *τ^α is the resolved shear stress acting on slip system α*
- *$\dot{g}$ is the rate of hardening; G_0 is hardening coefficient*
- *N_{ss} represents the number of slip systems*
- *ω is saturation rate exponent*
- *g_s^* is normalized reference saturation hardness*

Example application 1: Study structure-property relations in AM materials



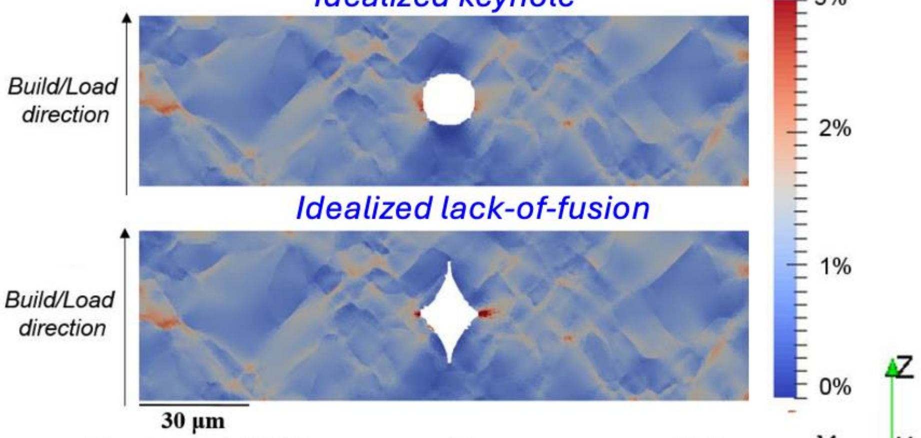


Example application 2: Study CTD/FIP relation using explicit cracks



FIP: fatigue indicator parameter
CTD: crack tip displacement

Example application 3: Strain localization near pores

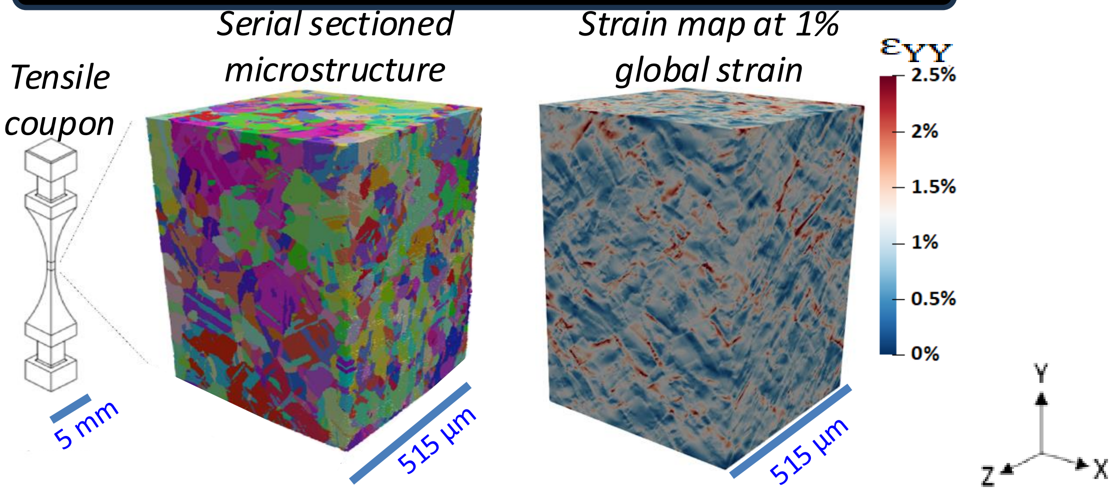


Nodes: 4.5E6
Applied strain: 1%
Processors: 400
Simulation time: ~14 hours

Microstructure Generation

Microstructure models from characterization

Method 1: Use characterization data directly

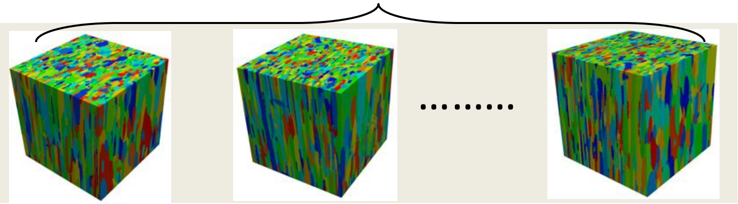


Method 2: Generate statistically equivalent microstructures based on characterization data

EBSD/XCT/HEDM/Serial sectioned microstructure → Statistics (grain size/shape/grain boundary character/texture etc.,)

↓

Statistically equivalent microstructures

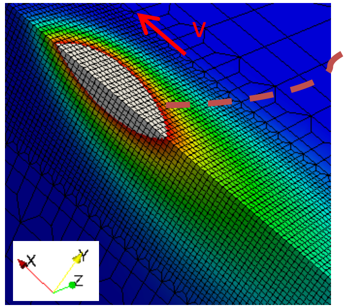


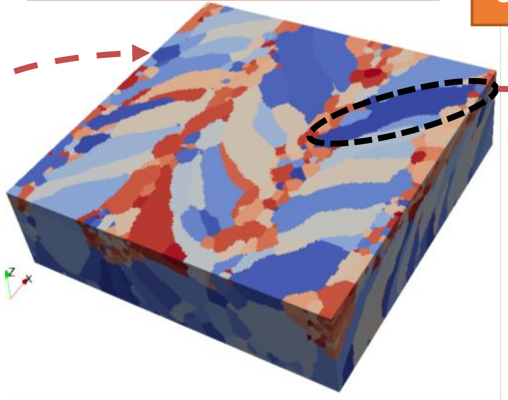
Process-specific 3D microstructure

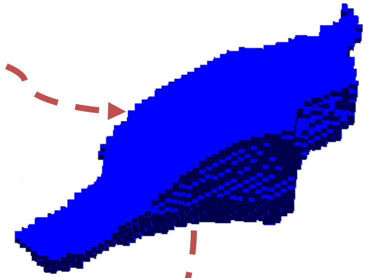
Finite Element Thermal Analysis

AM process simulation SPPARKS[1]

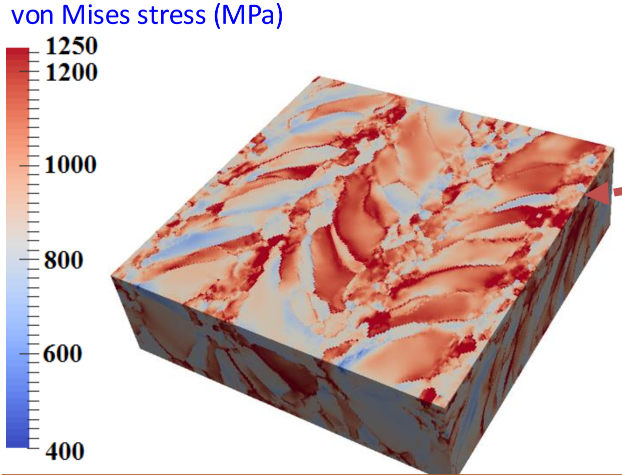
Use Output from SPPARKS and generate .stl files of grains using DREAM. 3D[2]

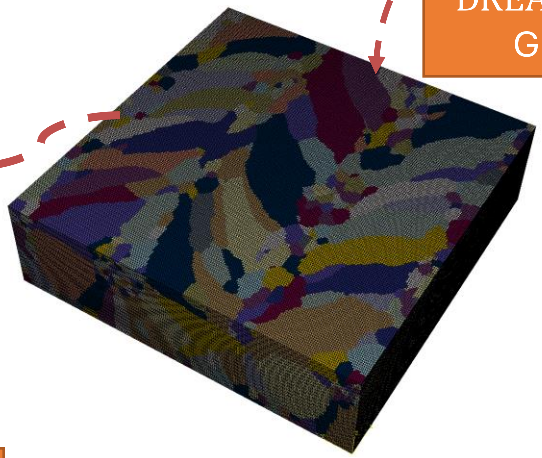






DREAM. 3D[3]/ Gmsh





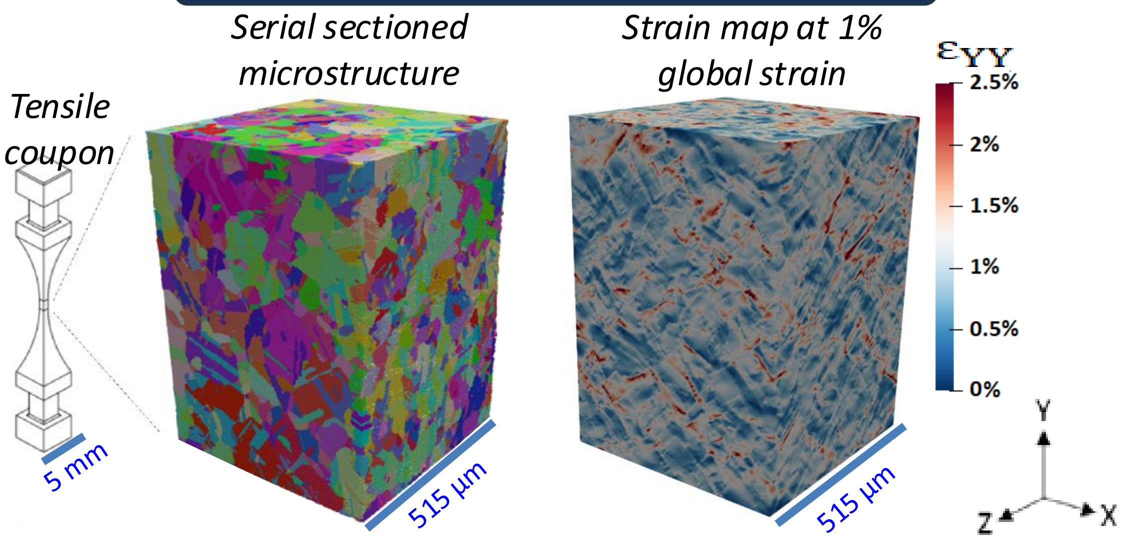
Use ScIFEN[3] to solve for heterogeneous stress/strain fields

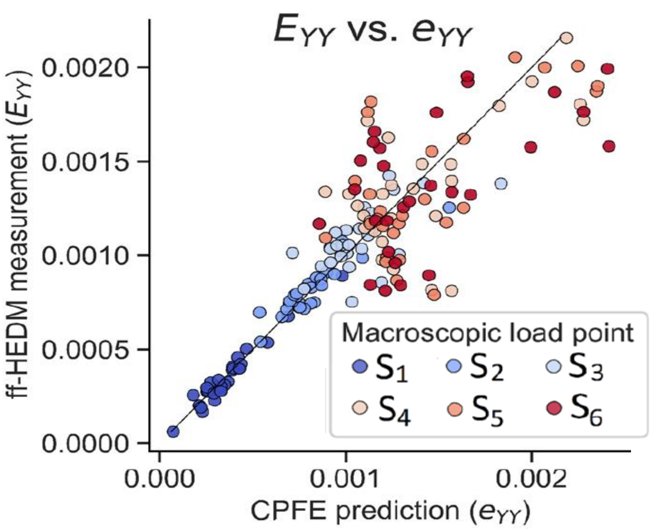
[1]SPPARKS: spparks.sandia.gov
[2]DREAM.3D: dream3d.bluequartz.net
[3]ScIFEN: https://software.nasa.gov/software/LAR-18720-1

POCs: Sai Yeratapally / George Weber

CP Simulation Validation Efforts

AFRL AM Modeling Challenge (2020)

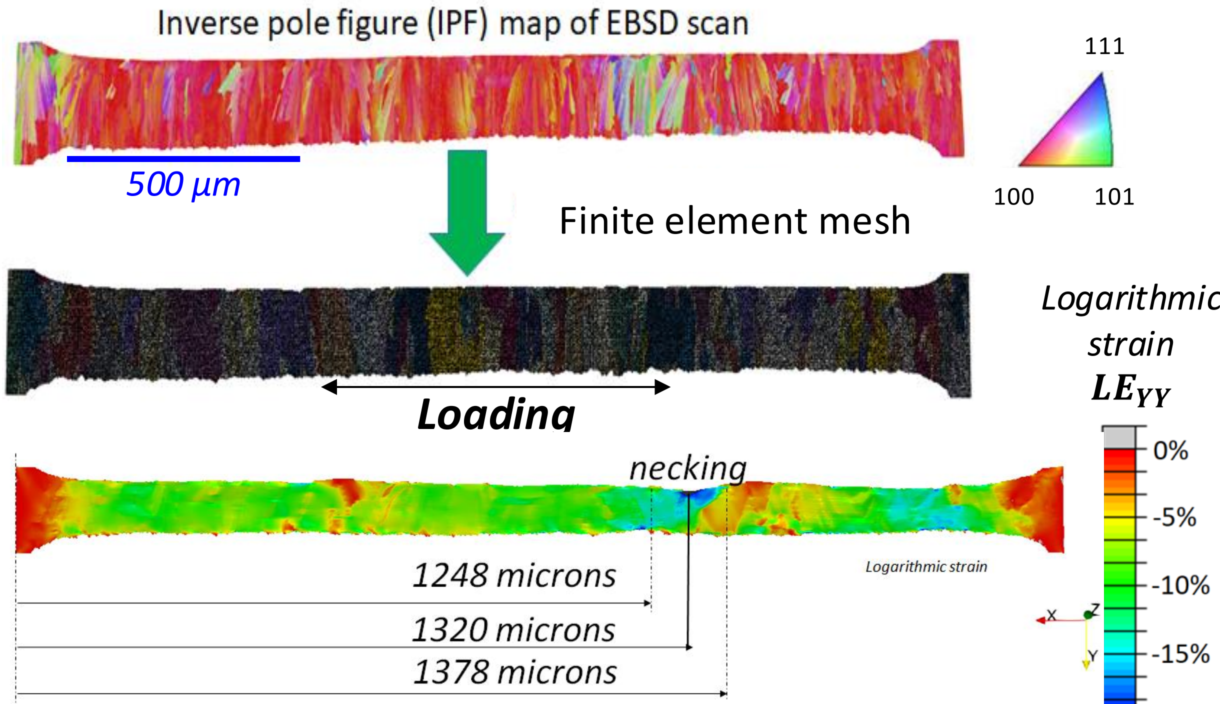




Observations:

- CPFE predictions show good agreement with HEDM measurements for grain-average elastic strains in elastic regime
- Discrepancies observed in plastic regime
- Percentage error in elastic modulus is ~ 1.5%

NIST AM-Bench Modeling Challenge (2022)

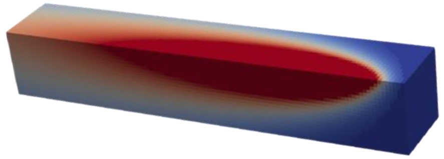


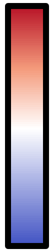
Observations:

- Percentage error in predicted elastic modulus is ~ 40%
  - Measured elastic modulus: 102 GPa
  - Predicted elastic modulus: 141 GPa
- High prediction errors observed across all participating teams
- Sources of discrepancy
  - Lack of full 3D microstructure (only 2D EBSD data was given)
  - Potential error in C_{ij} values (borrowed from literature)

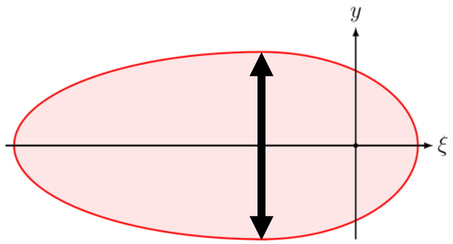
Process-Structure-Property Simulations with Uncertainty Quantification

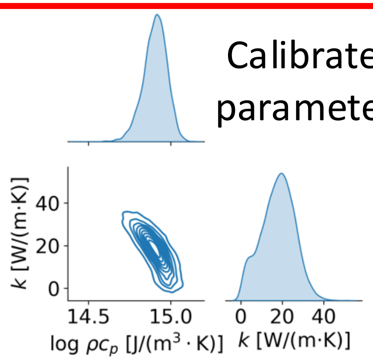
1. Thermal model: melt pool, temperature field





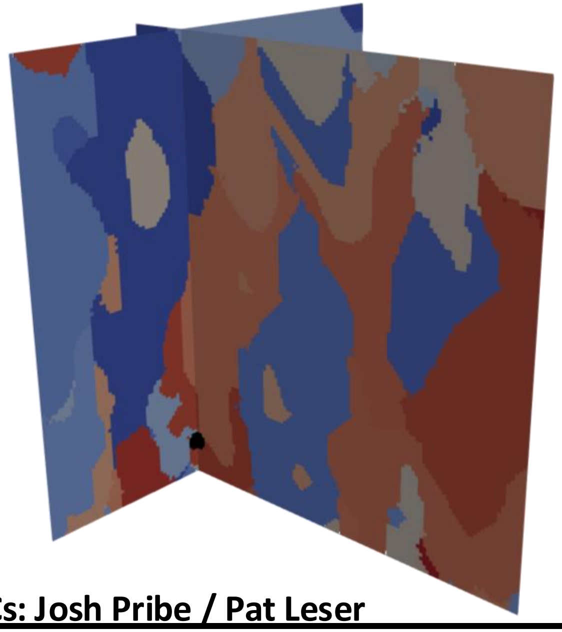
Probabilistic calibration



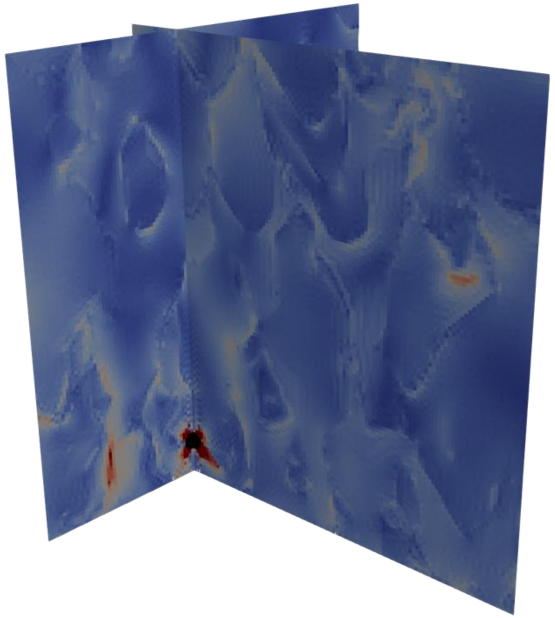


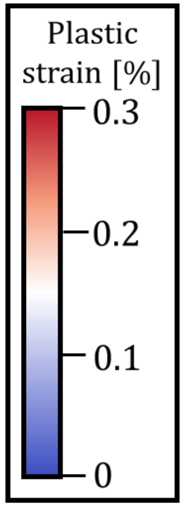
Repeat simulations

2. Process-structure model: solidification, texture, defects

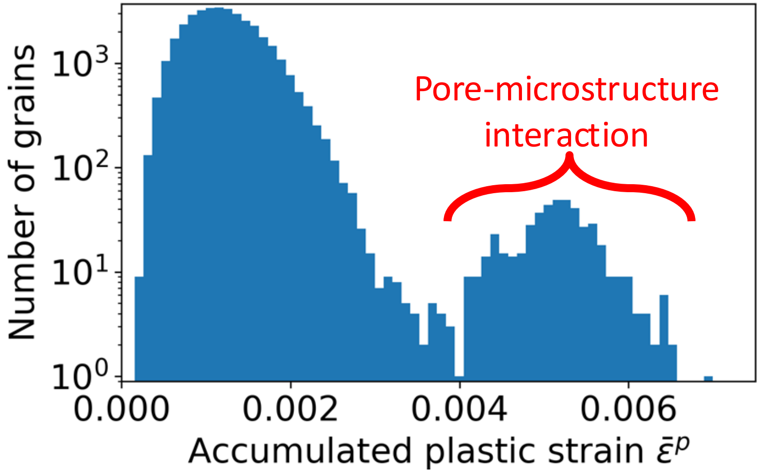


3. Structure-property model: stress and strain fields, fatigue indicator parameters





Fatigue indicator parameter statistics and extreme values



POCs: Josh Pribe / Pat Leser

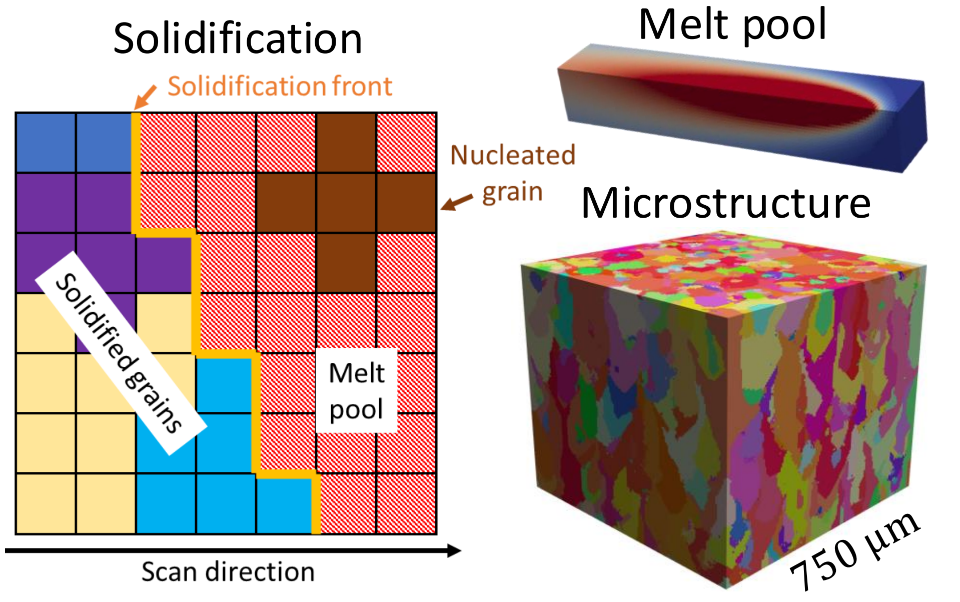
Global Sensitivity Analysis

Identifying inputs that need further calibration and process conditions that need tighter control using global sensitivity analysis of process-structure model

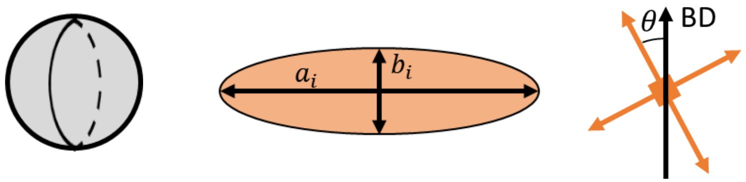
Uncertain inputs

Material properties, process conditions

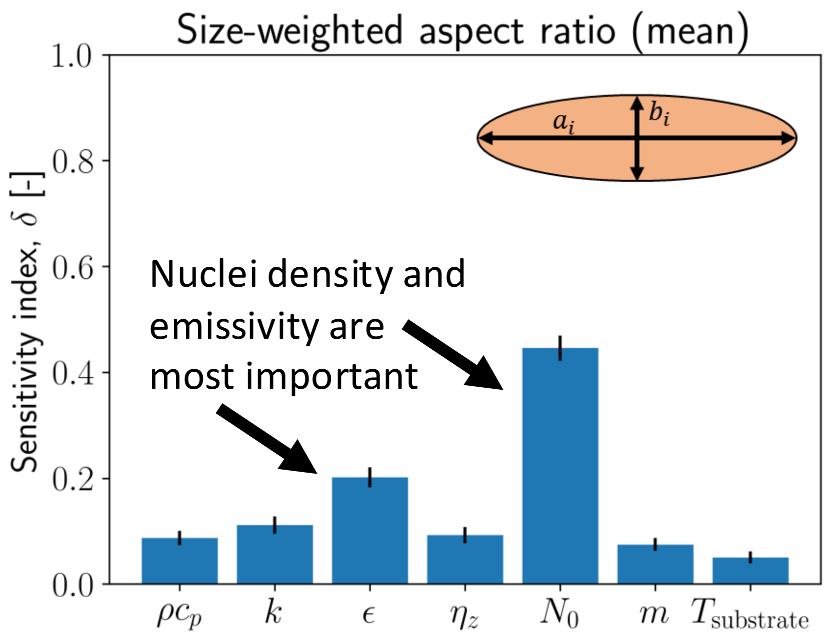
Thermal and process-structure simulations



Microstructure quantities of interest



Sensitivity indices



Configurable Architecture Additive Testbed (CAAT)

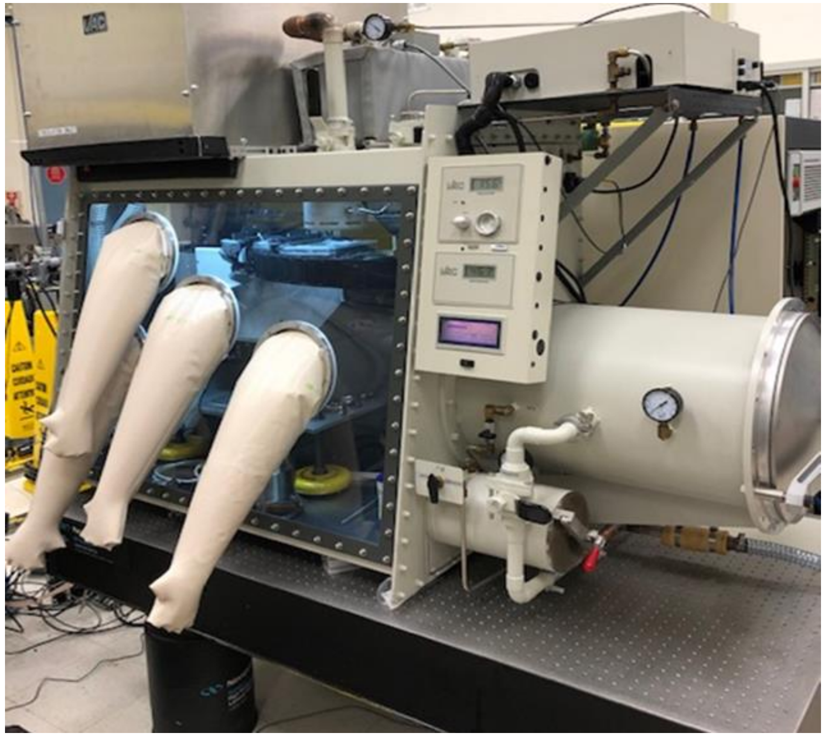
Configurable architecture AM testbed including in-situ non-destructive evaluation (NDE) for build quality assessment, informing qualification / certification models, processing condition measurements, and comparison to post build inspections with data fusion

Approach: Achieve high-fidelity understanding and measurements of process to structure relationships so that quality of build assessments can be informed in industry relevant conditions
Establish: the Configurable Architecture Additive Testbed (CAAT) Lab

The CAAT lab studies the LPBF additive manufacturing using:

1) CAAT process capabilities:
    1) Max power: 700W
    2) Max speed: 2.5 m/s
    3) Minimum spot-size: 35 µm
2) Suite of in-situ process monitoring: Fully registered
3) In-situ monitoring to calculate, calibrate, and validate process metrics at the part scale
4) Connection with higher fidelity models
    1) thermal measures integrate with microstructure models

The CAAT lab is well suited to develop in-situ NDE based on the P-S-P models for LPBF additive manufacturing

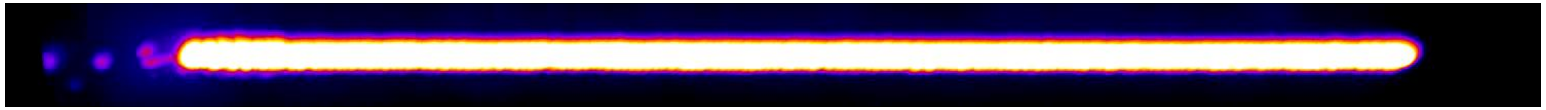


POC: Joe Zalameda

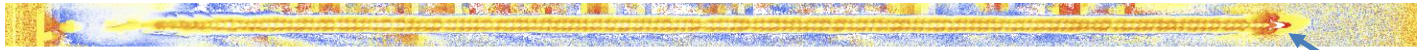
In-situ NDE for Metal Additive Manufacturing[1]

Near Infrared 750 nm Band Imagery Reconstructed to Follow Build Path[2]

Near Infrared 750 nm Band Imagery Reconstructed for NDE Inspection



In-situ NDE Inspection Image using Principal Component Analysis



Defect Area

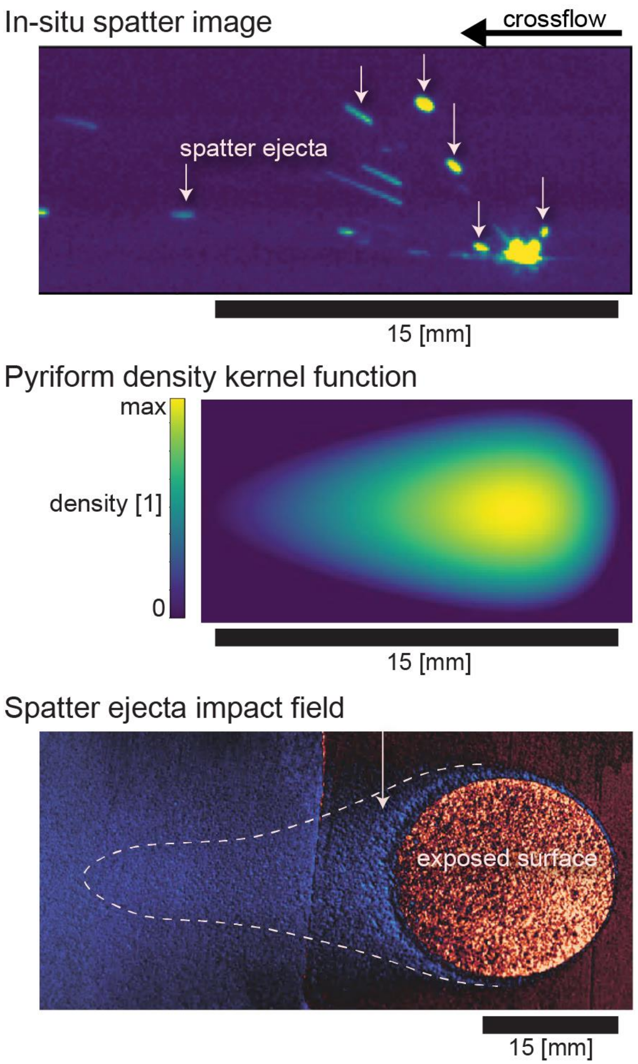
X-ray CT Validation of Detected Damage

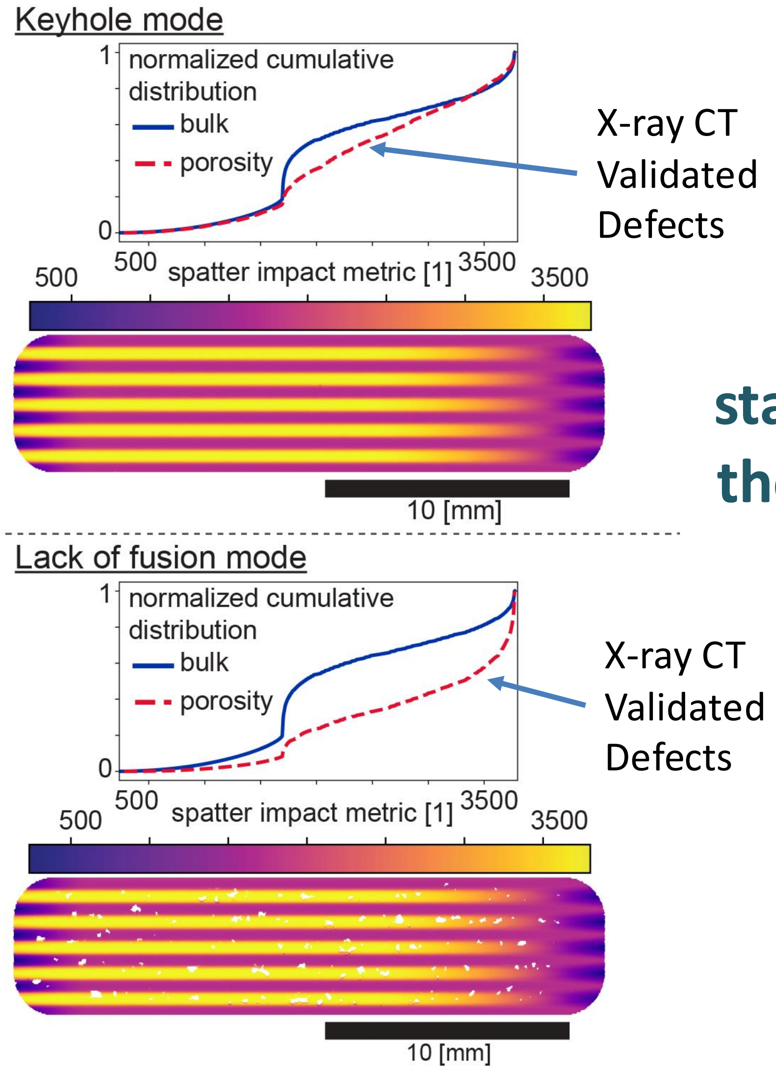
- Use Co-axial to the Laser Thermal Imaging to Monitor Temperature
- ⇩
- Reconstruct Thermal Imagery to Follow the Laser Build Path and Obtain Layer by Layer Temperature
- ⇩
- Process the Layer Temperature Responses for Changes in Transient Cool Down to Detect Defects

[1] NASA US Patent 11.027.332, "In-situ Characterization and Inspection of Additive Manufacturing Deposits using Transient Infrared Thermography"

[2] Joseph N. Zalameda, Samuel J. A. Hocker, Peter W. Spaeth, Brandon Widener, "Near-infrared in-situ measurements for the detection of keyhole porosity in autogenous Ti-6Al-4V welds," Proc. SPIE 13047, Thermosense: Thermal Infrared Applications XLVI, 130470X (7 June 2024); https://doi.org/10.1117/12.3014612.

Spatter and Defects[1]





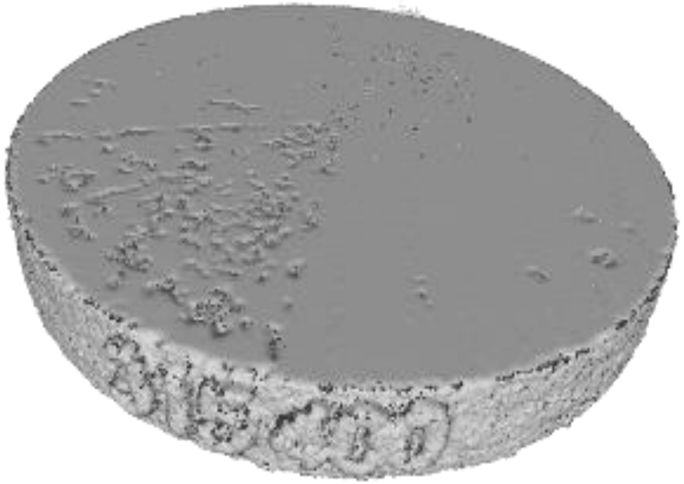
Process defects are statistically correlated with the spatter impact metric.[2]

[1] NASA US Patent Application 18/224,935, "A Method and a Pyriform Process Metric to Predict and Mitigate Spatter- Induced Defects in Powder Bed Fusion-Laser Beam Metals AM"

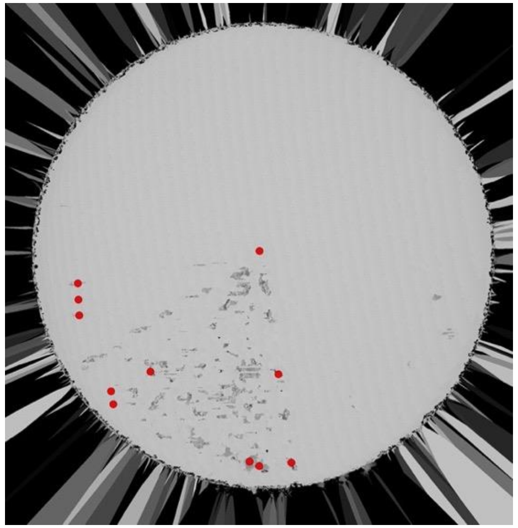
[2] Hocker, Samuel J.A., Andrew R. Kitahara, Brodan Richter, Sang-Hyon Chu, Brandon Widener, Peter W. Spaeth, Joseph N. Zalameda, and Edward H. Glaessgen. "A Novel Additive Manufacturing Process Metric for Predicting Spatter Related Porosity in Laser Powder Bed Fusion." Integrating Materials and Manufacturing Innovation (Nov 2024). https://doi.org/10.1007/s40192-024-00376-0.

Improving X-Ray CT Defect Characterization by Integration with Optical Profilometry

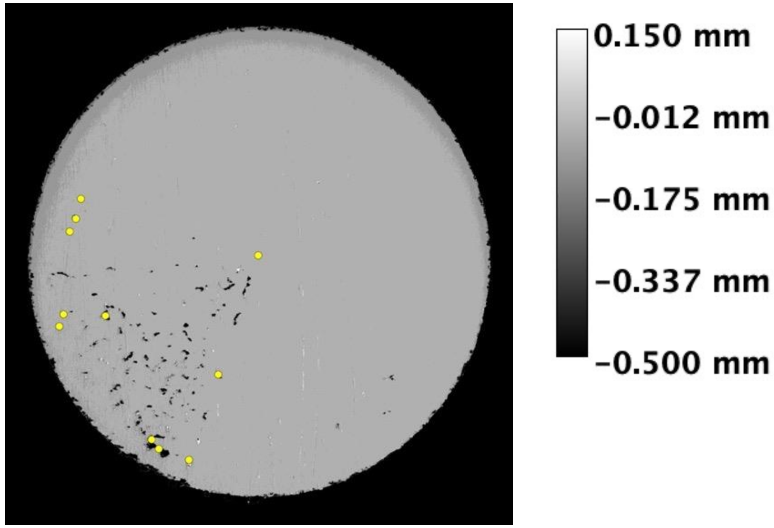
Component surface derived from X-ray CT segmentation



Surface depth estimated from X-ray CT segmentation



Comparison against high resolution surface profilometry



- Improvements to defect detection and metrological accuracy of X-Ray CT for AM metal porosity detection
    - Material agnostic algorithm, may be applied to other material and defect types
- Approach may be used to both characterize and optimize X-Ray CT volumetric defect detection

Patent Pending

E. Frankforter and P. Spaeth: "System and Method of Quantifying and Improving X-Ray Computed Tomography Measurement Accuracy"

X-Ray Computed Tomography (CT) Integration with Optical Profilometry Enables Improved Measurement Accuracy for Additive Manufacturing Porosity Defects

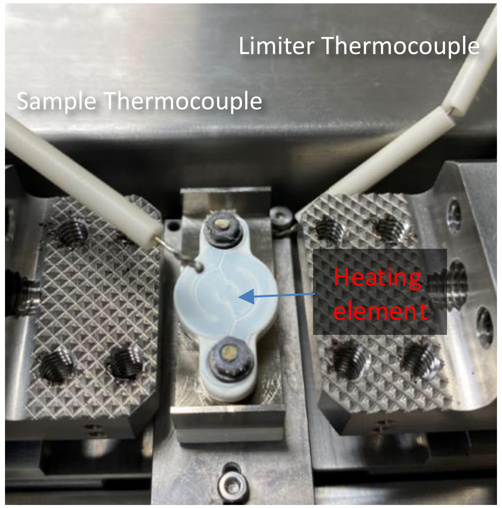
POCs: Peter Spaeth / Erik Frankforter

Testing at Elevated Temperatures

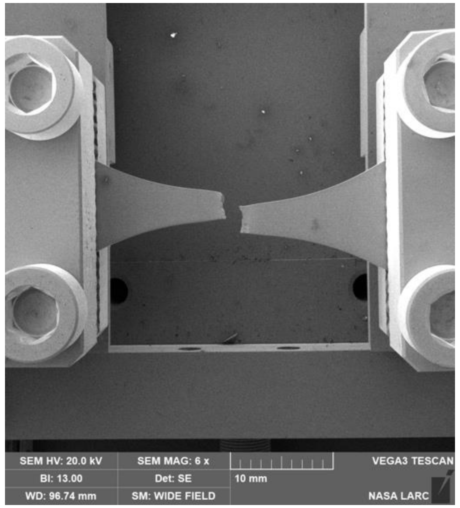
In-situ Mechanical Tests at Elevated Temperatures

High-Temperature Setup for In-Situ Tests

- A significant impact of **operation temperatures** on crack behaviors in Ni-based superalloys
- In-situ load stage system is rated up to 800°C
- **Thermal electron emission** (starting over 500°C) interferes SEM-DIC and EBSD
- Local heating induces thermal expansion in both the sample and the stage, causing vibration and drift of samples during loading
- Solutions to high-temperature in-situ: contact heater, thermal insulation to isolate the other parts, uniform thermal expansion



Heating element for in-situ stage

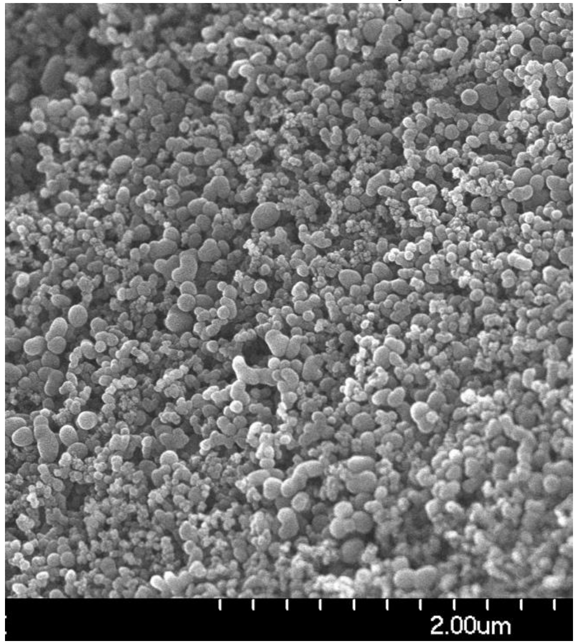


In-situ tensile test under SEM

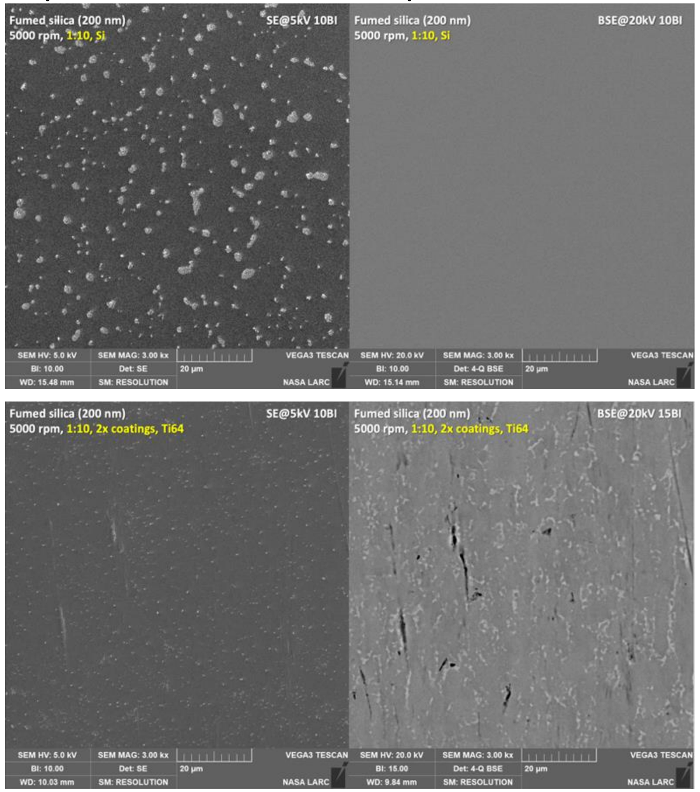
High-Temperature Micro Speckle Patterning

High-Temperature Speckle Pattern – Silica Nanoparticles

- High-temperature micro speckle patterns need **thermal stability and amorphous structure** for simultaneous acquisition of DIC and EBSD
- Fumed silica nanoparticles: amorphous, 200 nm, stable up to 1000°C



Fumed silica nanoparticles: amorphous, 200 nm in average size, thermally stable up to 1000°C



High-temperature speckle patterns of fumed silica nanoparticles on (top) silicon wafer and (bottom) Ti64 (left: SEM image; right: BSE image)

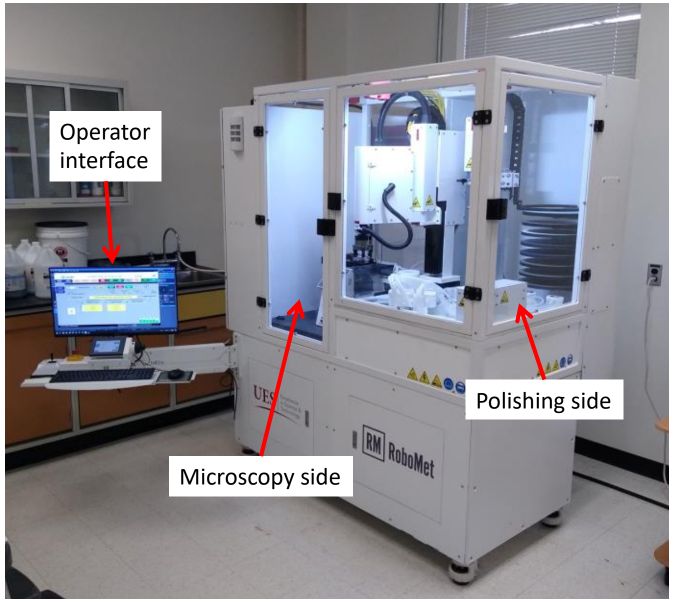
POCs: Sang-Hyon Chu / Andy Newman

Microstructure Characterization and Residual Stress Analysis

Microstructure Characterization Tools

Microstructure Analysis and Fabrication

- Microstructure/composition analysis:
  - SEM: Secondary and Backscattered Electron Imaging
  - Electron Back Scatter Diffraction (EBSD)
  - Energy Dispersive Spectroscopy (EDS)
- Nanofabrication:
  - Plasma Focused Ion Beam (PFIB)
- 3D microstructure investigation
  - RoboMet to identify pores and cracks



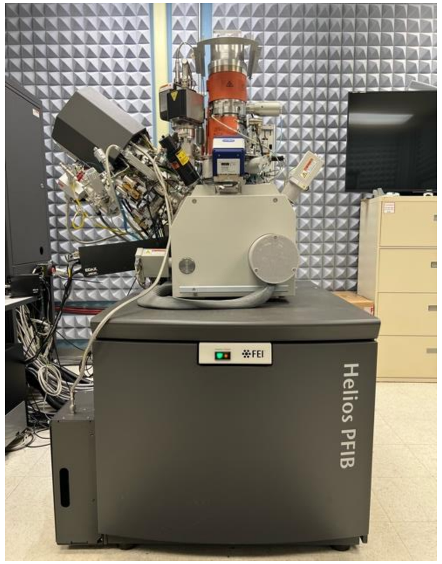
RoboMet

- Automated Polishing and Microscopy Image Capturing
- Rapid sample preparations
- 3D microstructure imaging
- Serial sectioning for grain size and pore distribution in AM materials
- EBSD sample preps
- Interrogation volumes: FIB 0.001 mm^3 vs. RoboMet 1000 mm^3

Residual Stress Analysis

Residual Stress Analysis of AM builds

- Hole drilling method
  - Hole drilling with PFIB and measuring the resulting strains
  - Local residual stress can be measured
  - Destructive method
- XRD method
  - Nondestructive determination of surface/subsurface residual stress of AM build samples
  - Only shallow (<0.001 inch) surface layer is measured, requiring electrolytic polishing to remove top layers of subsurface



Helios PFIB for nanofabrication

XRD for residual stress analysis

The TRUST-AM Platform

Platform for prototyping Computational Materials-informed Qualification and Certification

State of the Discipline: Qualification and Certification (Q&C)

Industry needs learned from the CM4QC Steering Group

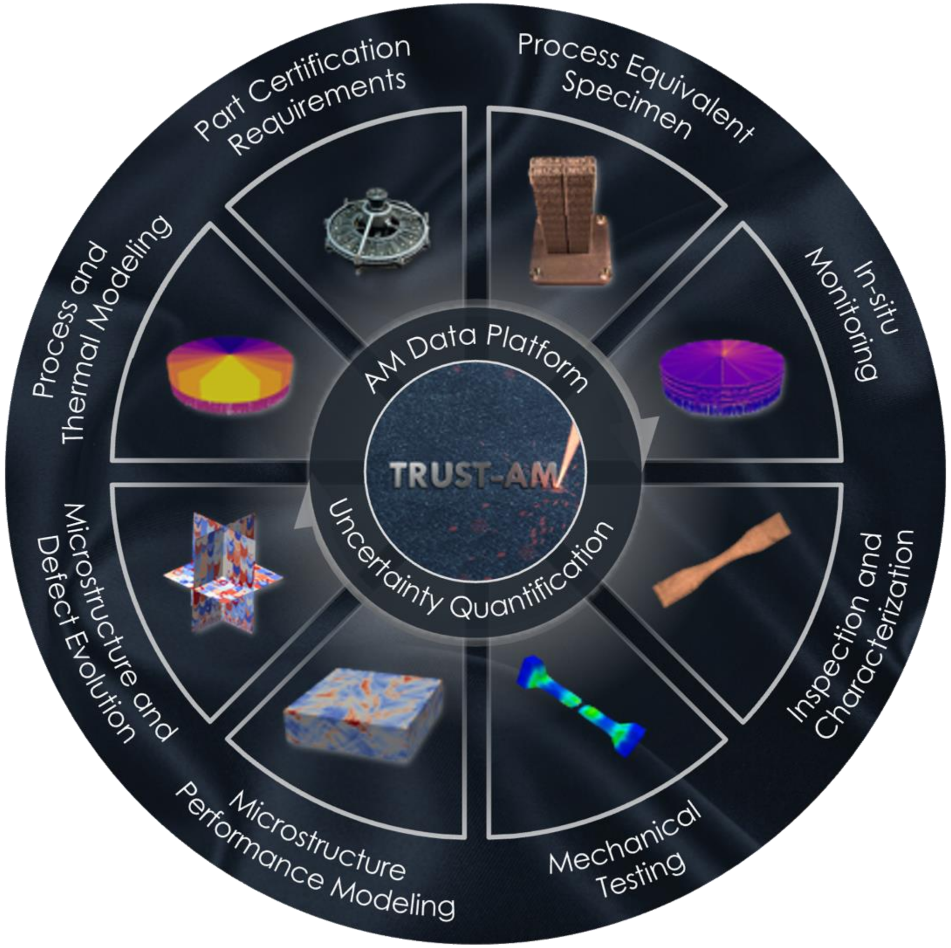
- Time and cost of Q&C limits adoption of additive manufacturing
- Manufacturing technology is outpacing regulatory environment

TRUST-AM

- An agile response from NASA’s Transformational Tools and Technologies (T^3) Project to address industry needs for digitally accelerated Q&C
- Augments physical testing requirements with modeling, simulation, uncertainty quantification, and data science
- A platform for prototyping Computational Materials-informed capabilities as part of a Q&C package

Impact

- Rapidly mature and transition Computational Materials research and development as the foundation for OEM-relevant engineering technologies
- Increase trust in modeling and simulation while reducing cost of Q&C



POCs: Andrew Kitahara/ George Weber

Summary

- CM4QC Steering Group and Roadmap
- Work of the Computational Materials-informed Qualification and Certification Research Group

Contact for more information
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