Validation of Crystal Plasticity Simulations using High-Energy X-ray Diffraction Microscopy Measurements

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23rd May, 2023

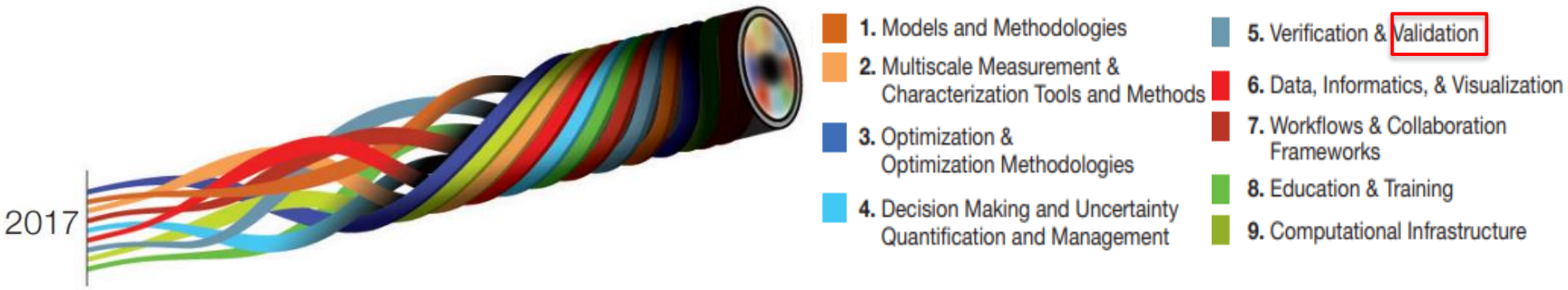
7th World Congress on Integrated Computational Materials Engineering (ICME 2023)
Orlando, Florida

Presentation Outline

- Introduction
- Air Force Research Lab (AFRL) Additive Manufacturing (AM) 2020 challenge series
  - Challenge problem
  - Data provided
  - Modeling approach
  - Model performance
- National Institute of Standards and Technology (NIST) AM-Bench 2022 challenge series
  - Challenge problem
  - Data provided
  - Modeling approach
  - Model performance
- Conclusions
- Acknowledgements

Introduction

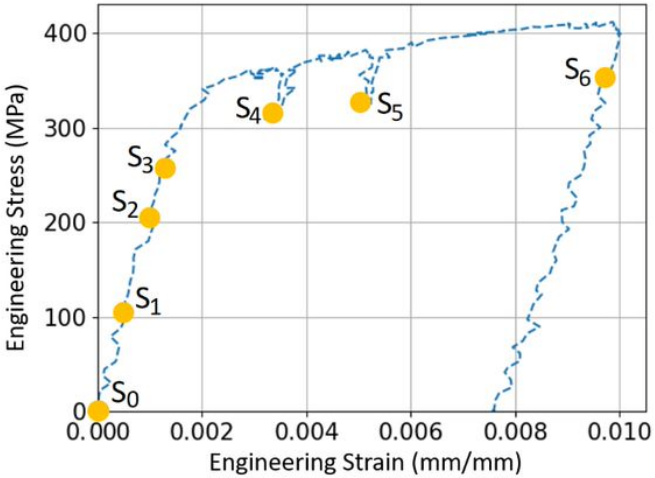
NASA Vision 2040: *"Accelerate model-based concurrent design, development, and deployment of materials and systems throughout the product lifecycle for affordable, producible aerospace applications."* -Liu, Furrer et al. (2018) NASA/CR—2018-219771



- Part of ongoing work at NASA LaRC is focused on verification and validation of micro-mechanical models by leveraging both internal and external resources
- High-fidelity data from materials community challenges organized by other government agencies (OGAs) are used for model validation
- A few examples include:
  - AFRL AM challenge series (2020)
  - NIST AM-Bench challenge (2022)

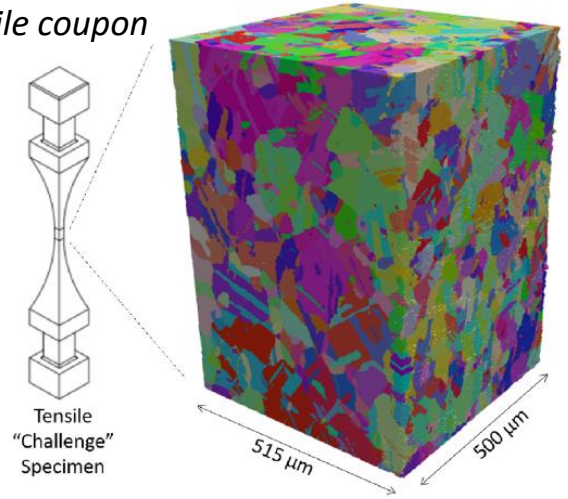
AFRL Additive Manufacturing (AM) Modeling Challenge

Stress-strain curve

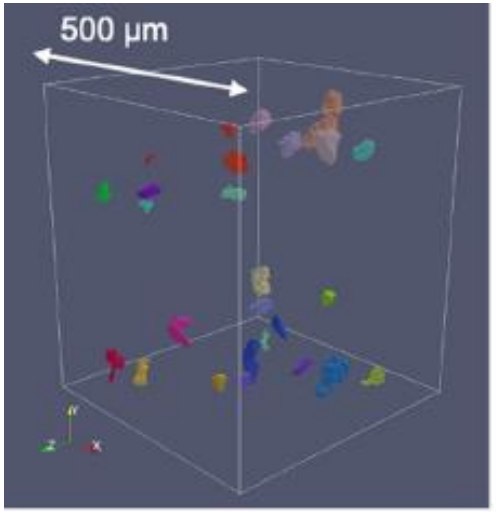


Tensile coupon

Serial sectioned microstructure at gage section



28 "challenge" grains



Challenge problem: Given the stress-strain curve, serial-sectioned and reconstructed three-dimensional (3D) microstructure, predict grain-average elastic strain tensor for 28 "challenge" grains at six different macroscopic load states, S_1 through S_6

Data provided:

- Stress-strain curve
- Serial-section electron backscatter diffraction (EBSD) data from gage section
- Grain IDs of the 28 "challenge" grains
- Type-II residual strains at macroscopic load state, S_0

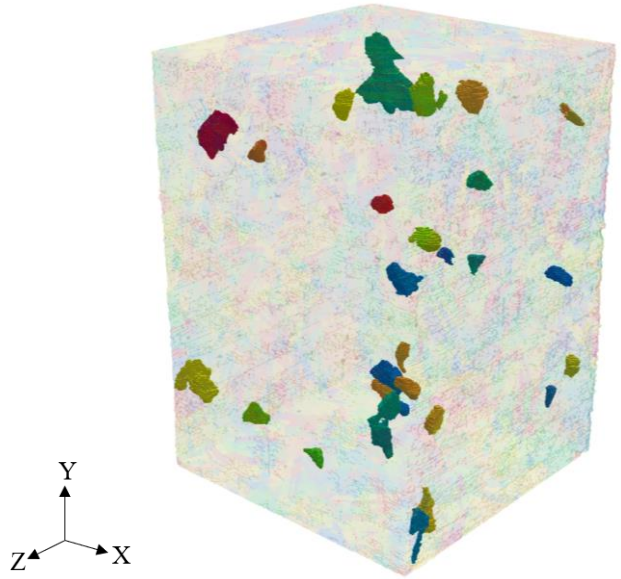
Answer Key (provided after challenge ended and individual team grading was completed):

- Grain-average elastic strain tensors in all 28 challenge grains at macroscopic load states S_1-S_6

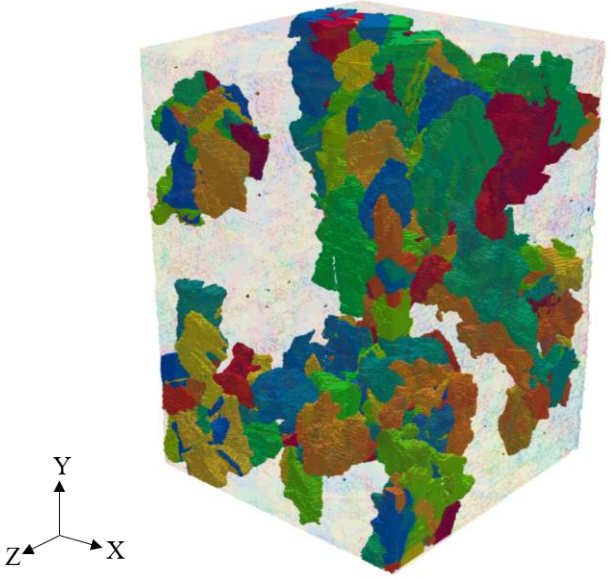
Pre-processing: Microstructure Reconstruction

- DREAM.3D*,# was used to reconstruct the microstructure
- The reconstructed 3D microstructure consisted of 29,665 grains
- A “minimum size” filter was applied to reduce the number of grains to ease meshing
- 28 “challenge” grains were not modified in any way
- 854 first neighbor grains were also untouched
- The final reconstruction of the microstructure had 9,369 grains (including “challenge” grains and their first neighbors)

28 “challenge” grains



Challenge grains and their first neighbors

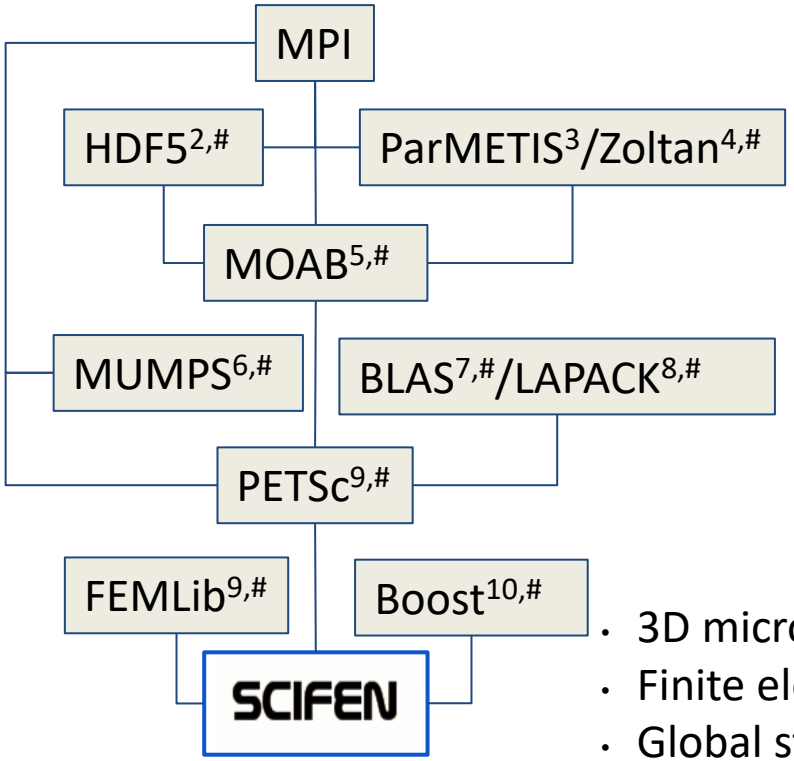


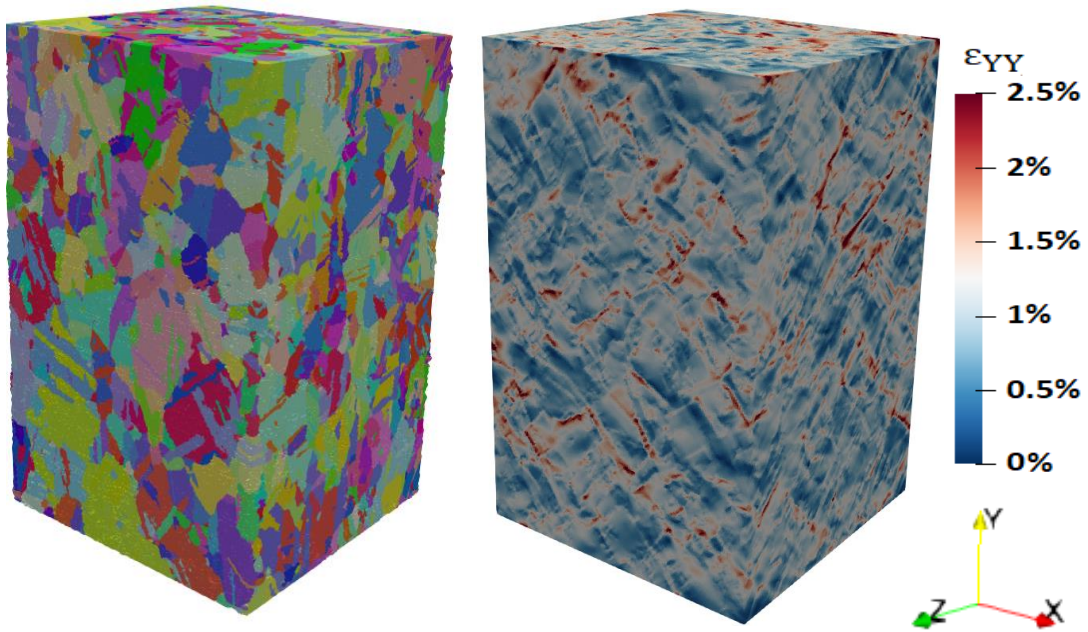
*http://dream3d.bluequartz.net

#This is not an endorsement by NASA

CP Simulations using ScIFEN

ScIFEN[1]: Scalable Implementation of Finite Elements by NASA





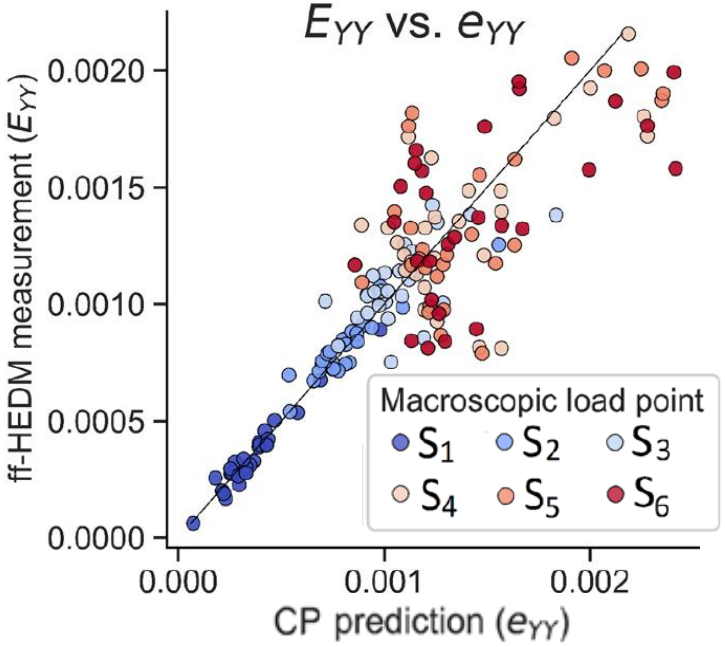
- 3D microstructure of additively produced Inconel alloy
- Finite element mesh has ~85 million degrees of freedom
- Global strain applied in YY direction: 1%
- CP formulation: Strain-gradient based[11]
- Simulation time: ~44 hours on 640 processors

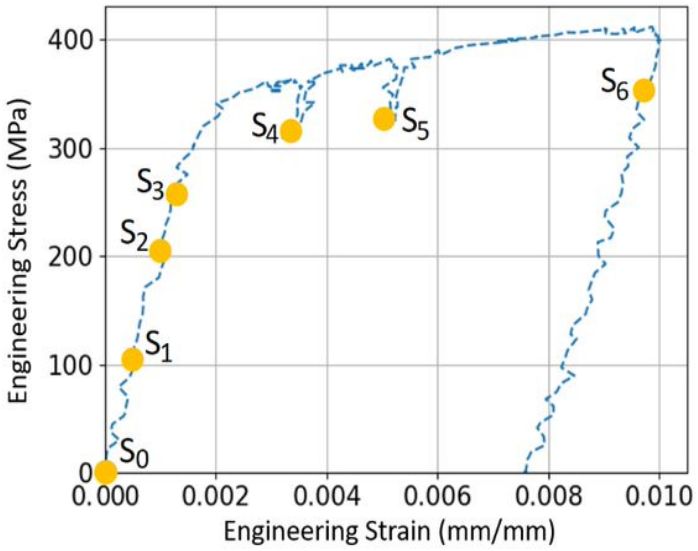
1. https://software.nasa.gov/software/LAR-18720-1
2. www.hdfgroup.com
3. http://glaros.dtc.umn.edu/gkhome/metis/parmetis/overview
4. http://www.cs.sandia.gov/zoltan/
5. http://sigma.mcs.anl.gov/moab-library/
6. http://mumps.enseeiht.fr/
7. www.netlib.org/blas/
8. www.netlib.org/lapack
9. www.mcs.anl.gov/petsc/
10. www.boost.org/
11. Acharya et al. (2000), JMPS 48

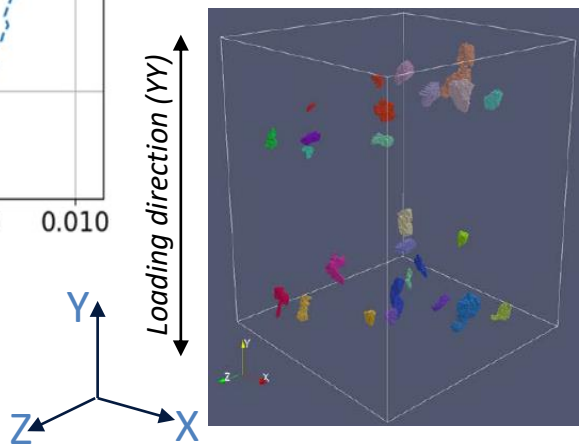
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ScIFEN's Predictions vs. ff-HEDM Measurements

CP predictions vs. ff-HEDM measurements





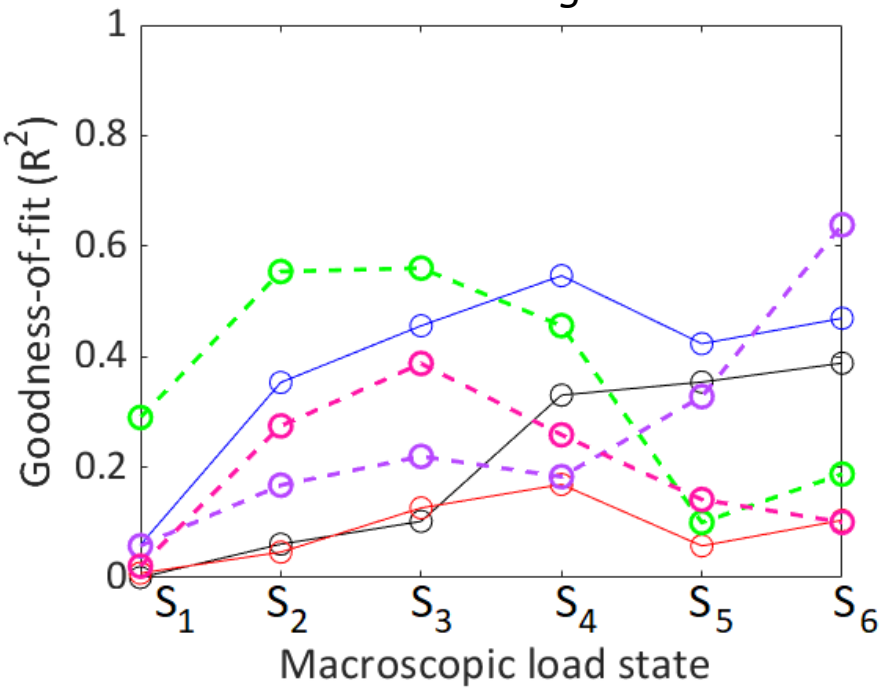


Observations:

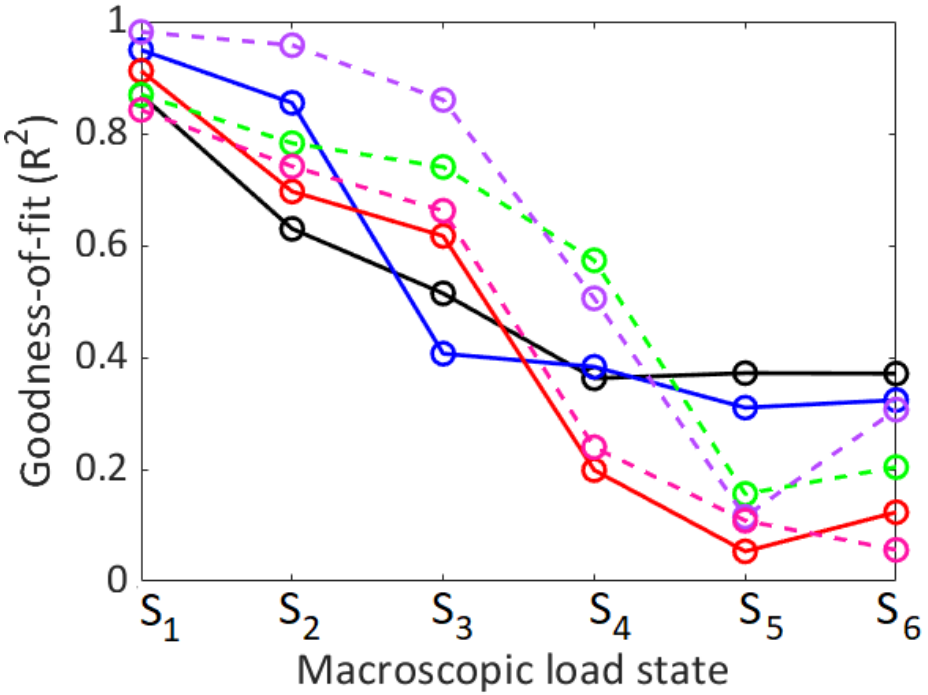
- There is a good agreement between CP predictions and far-field high-energy X-Ray diffraction microscopy (ff-HEDM) measurements in the elastic regime (S_1-S_3)
- Deviations start to develop in plastic regime (S_4-S_6)

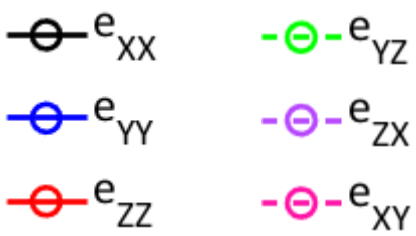
Discrepancy 1: Residual Strains

Grain-average (type-II) residual strains ignored



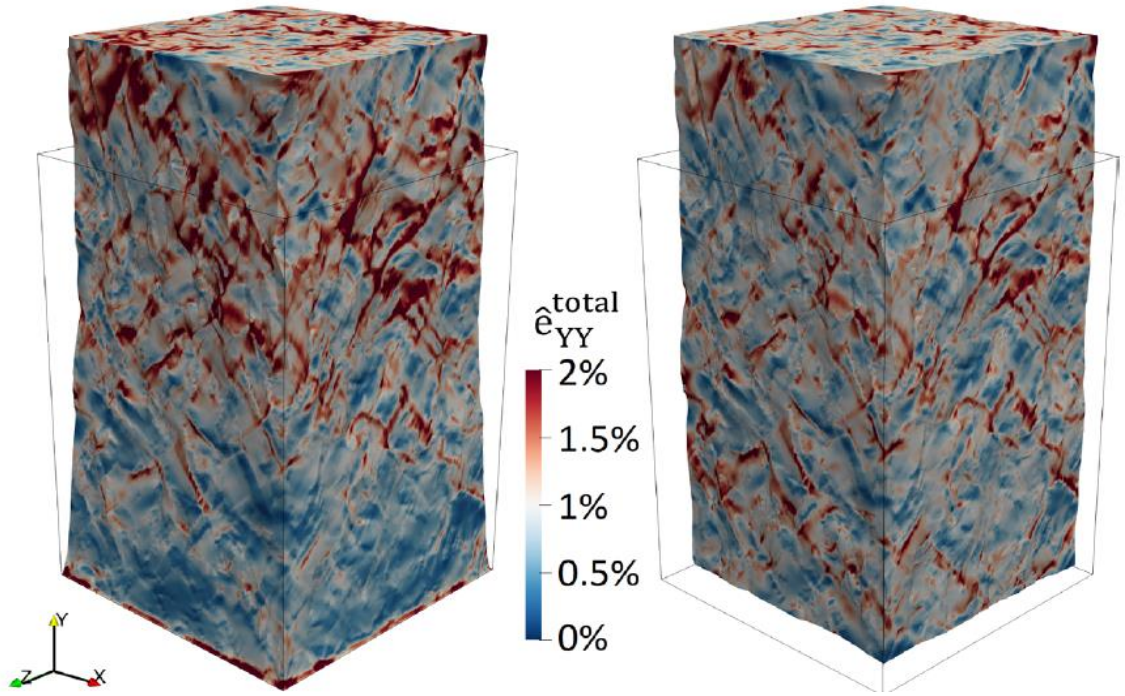
Grain-average (type-II) residual strains added to CP predictions





Discrepancy 2: Boundary Conditions

Strain maps of total strain in YY direction, generated at global strain of 1%

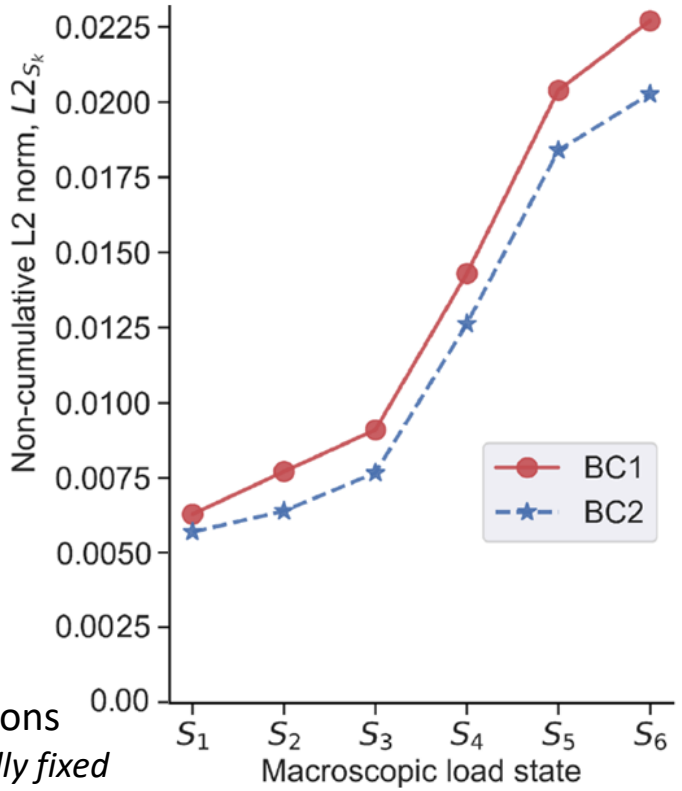


BC1: Fully constrained bottom face

BC2: Relaxed boundary conditions

(Only one corner node on –Y face fully fixed and one edge fixed in X and Y directions)

Non-cumulative L2 norm calculated at each macroscopic load state, S_k



$$L2_{S_k} = \sum_{n=1}^{N} \sqrt{\sum_{i=1}^{6} \left(\left(E_i\right)_{S_k}^{g_n} - \left(e_i\right)_{S_k}^{g_n} \right)^2}$$

$(E_i)_{S_k}^{g_n}$ ***is ff-HEDM measurement***

$(e_i)_{S_k}^{g_n}$ ***is CP prediction***

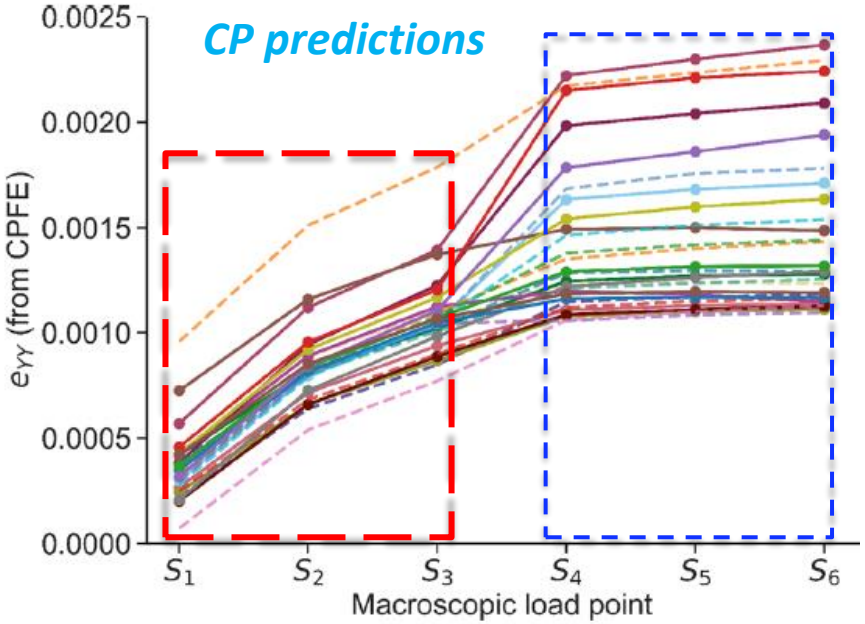
S_k ***is macroscopic stress state***

g_n ***is grain ID***

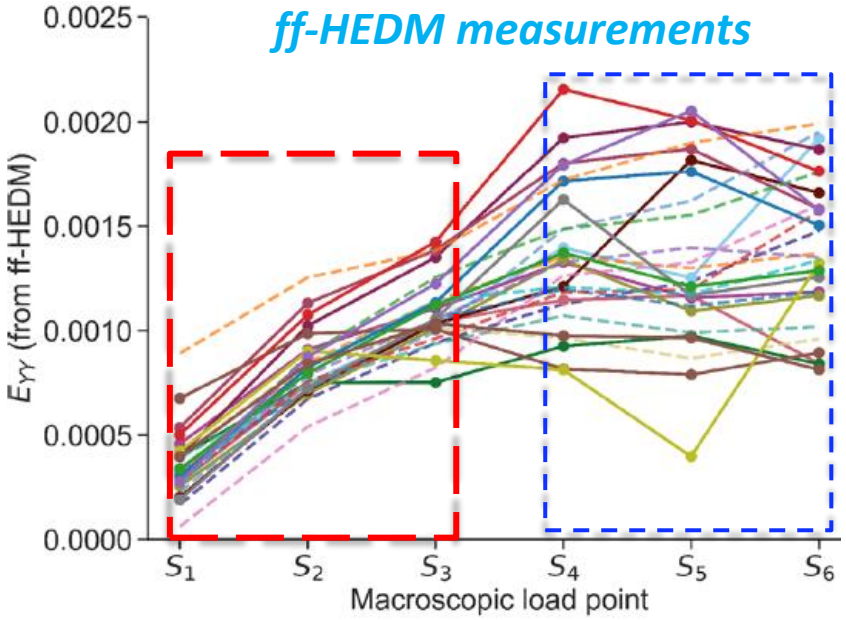
N is # grains

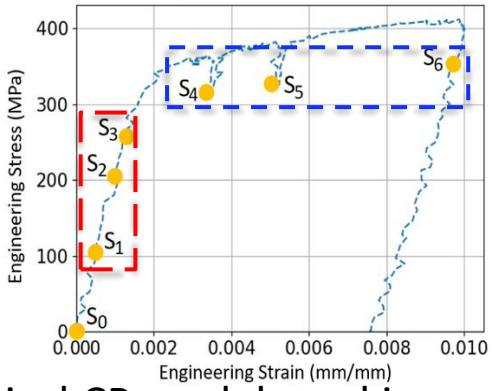
Discrepancy 3: Missing Physics (Stress Relaxation)

CP prediction of evolution of YY component of grain-average elastic strain in each of the 28 "challenge" grains



ff-HEDM measurement of evolution of YY component grain-average elastic strain for the 28 "challenge" grains

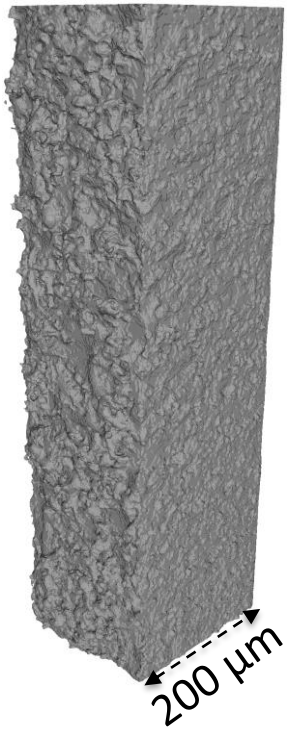




Observation: Phenomenological CP model used is unable to predict stress relaxation

NIST AM-Bench 2022 Challenge

XCT scan of gage section



Challenge:

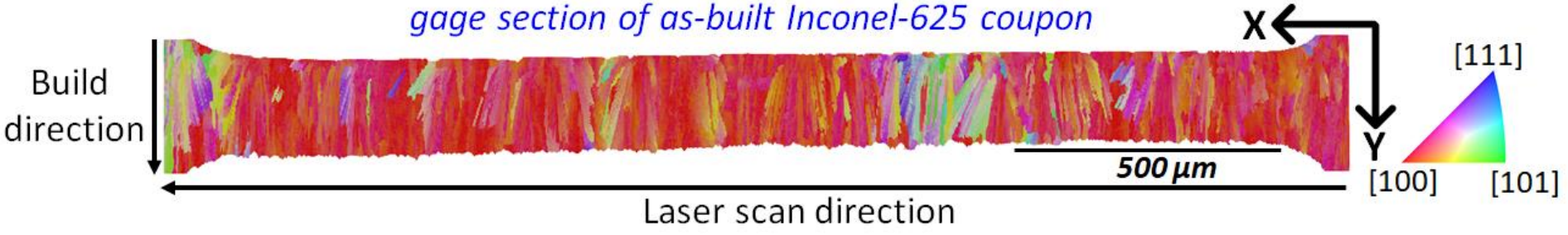
Predict subcontinuum stress-strain behavior, fracture location, and post failure width reduction of an as-built Inconel-625 meso-scale specimen

Data provided:

- EBSD scan of entire gage section of meso-scale coupon
- X-Ray computed tomography (XCT) data of the meso-scale coupon
- Tensile stress-strain curve of as-built macroscale Inconel-625 coupons

Reference direction for IPF map is [100]

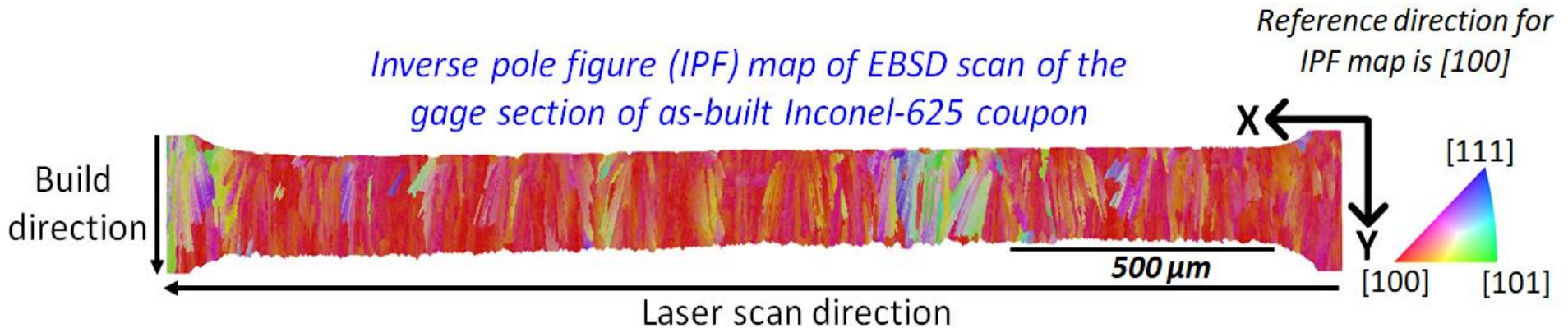
Inverse pole figure (IPF) map of EBSD scan of the gage section of as-built Inconel-625 coupon

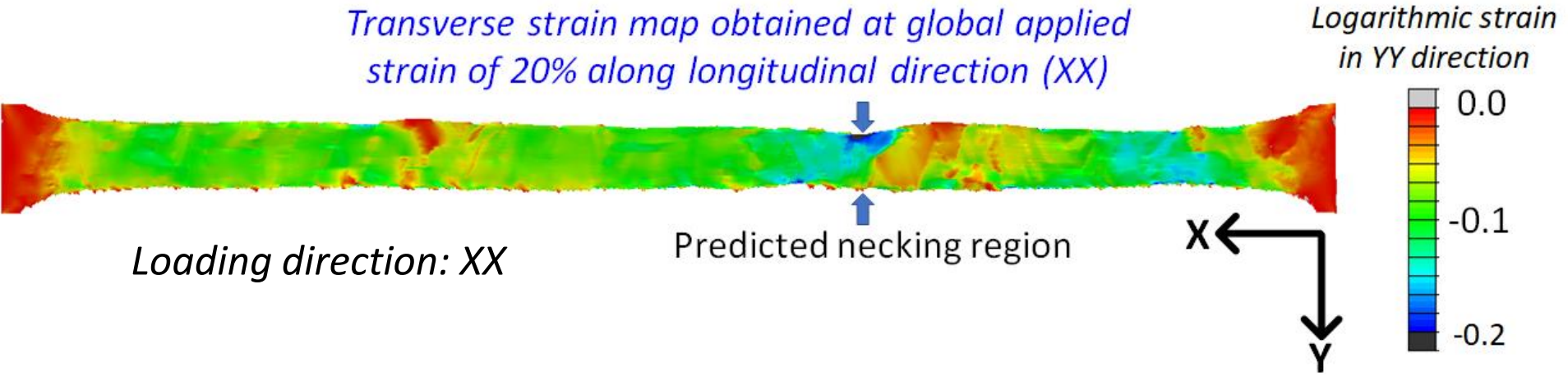


Modeling Assumptions

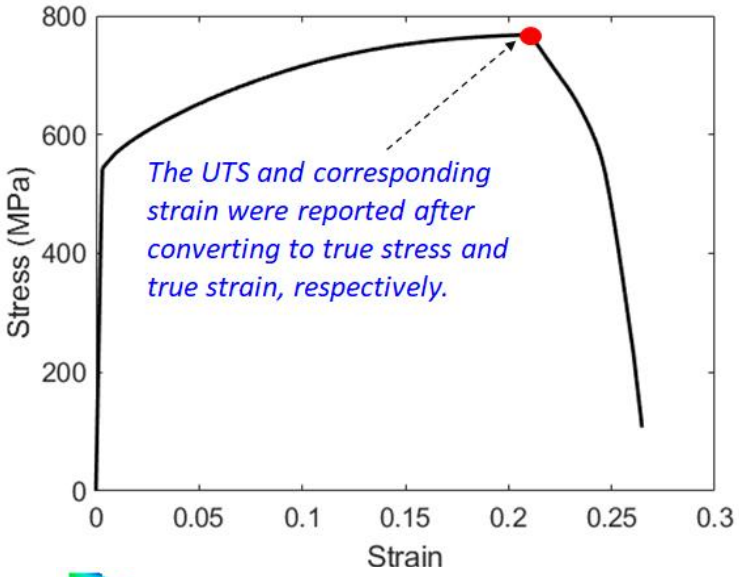
- Finite strain formulation
- No damage model considered within the CP simulations
- Residual strains not available
- Only 12 octahedral slip systems considered active
- Secondary phases were not modeled explicitly
- Sub-surface microstructure was not accounted for
- XCT data provided was not used

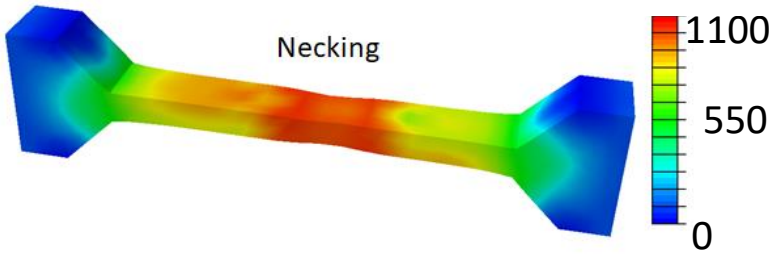
Stress-Strain Behavior and Necking

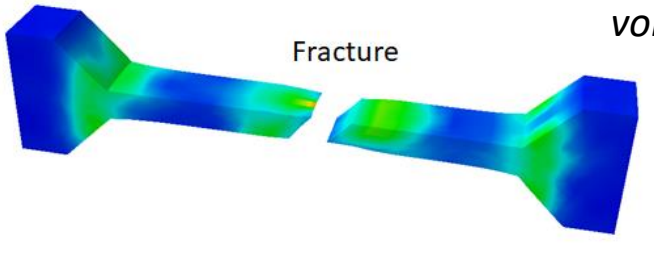


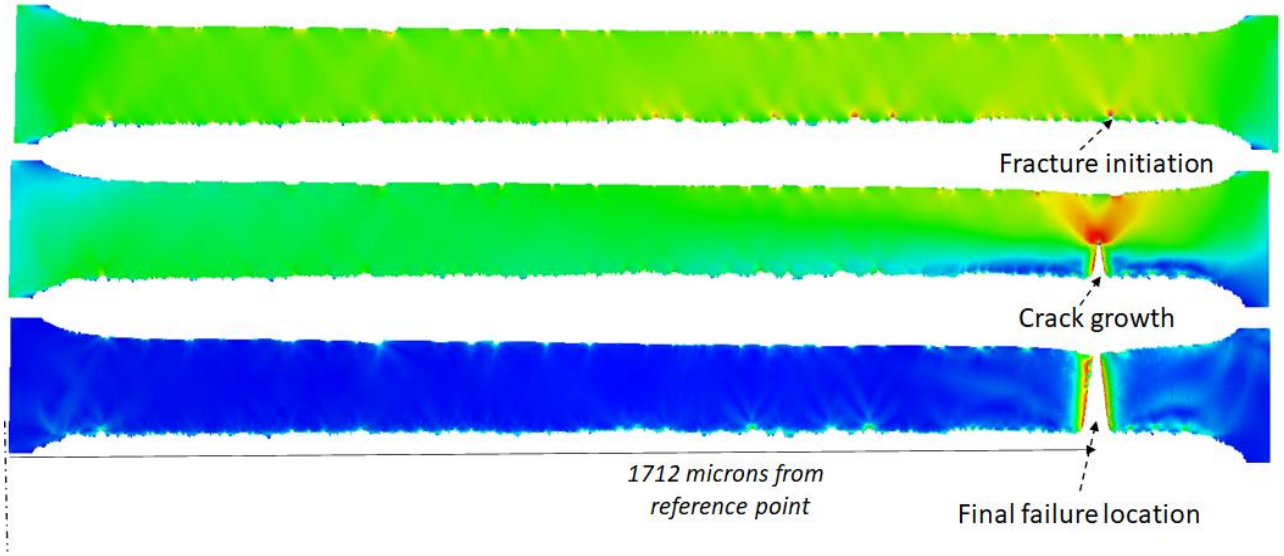


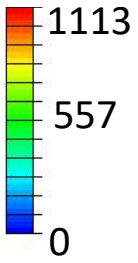
Fracture and Width Reduction Predictions



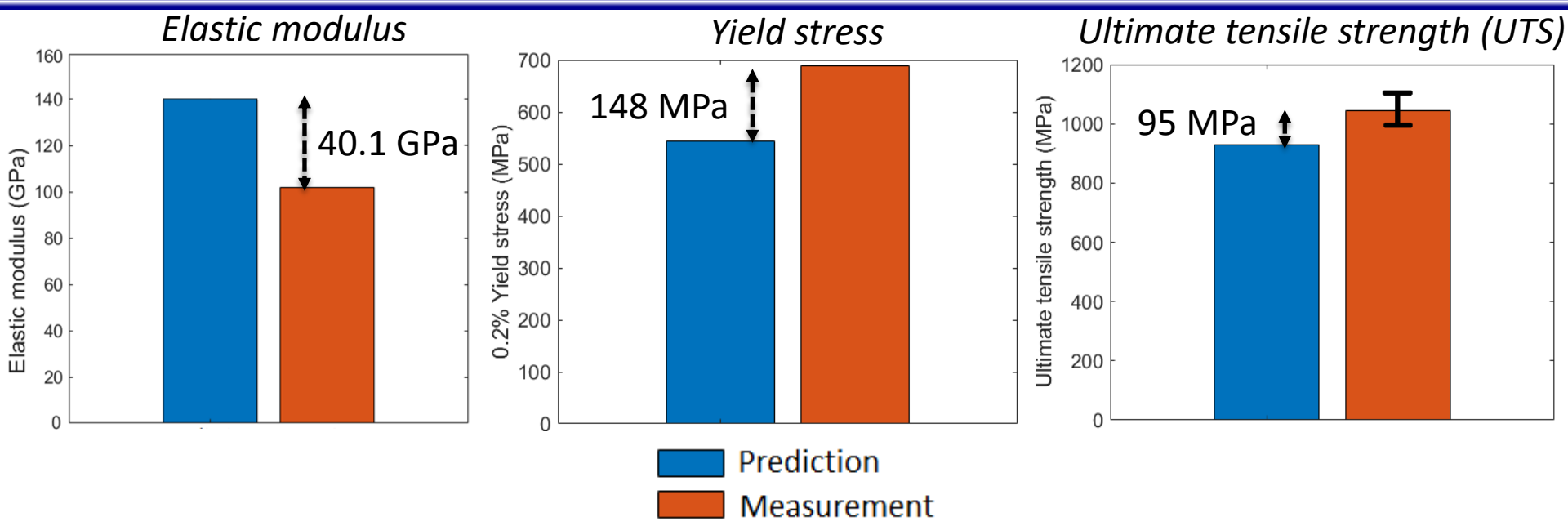


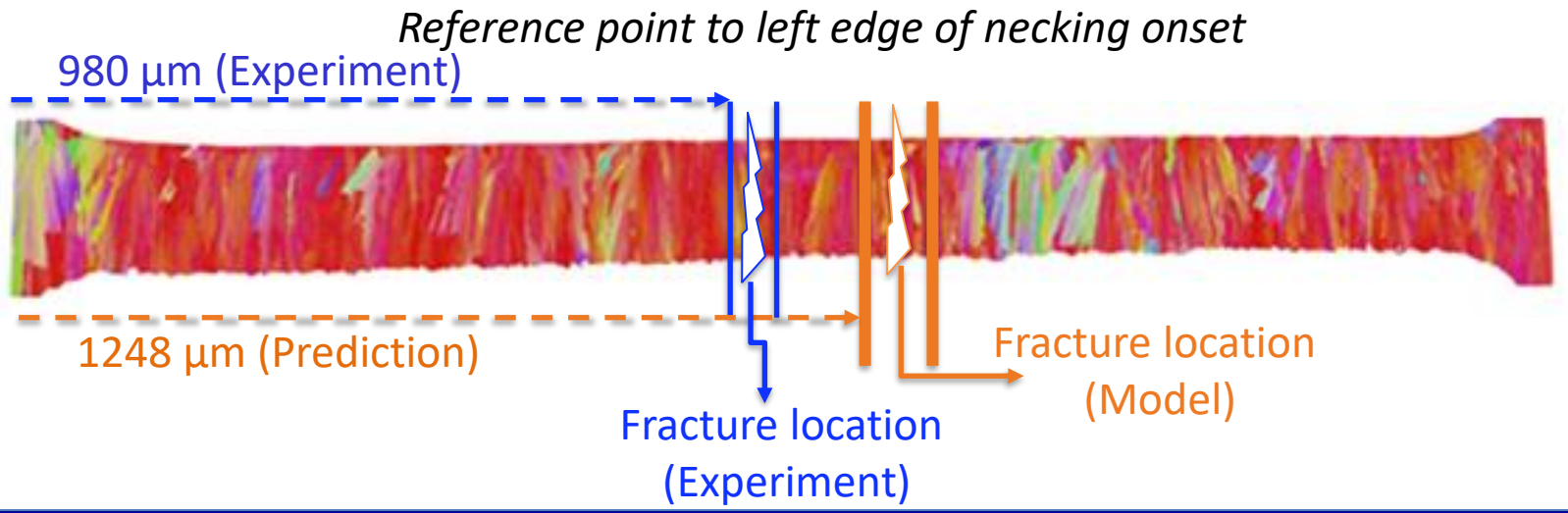






Prediction vs. Measured Properties





Conclusions

- High-fidelity deformation measurements and microstructure datasets from the AFRL and NIST AM related challenge series were leveraged to evaluate the following aspects using CP simulations:
  - predicting grain-average behavior
  - various types of model discrepancies to be aware of (residual strains, boundary conditions, stress relaxation etc.,)
  - sub-continuum stress-strain behavior and fracture
- Considering the residual strains and avoiding using over-constrained boundary conditions helped in improving the predictive capabilities of CP simulations (AFRL challenge)
- Not accounting for the sub-surface microstructure can lead to significant discrepancy in predicted elastic modulus (NIST AM-Bench challenge)
- Less than 2% error was observed in elastic modulus predicted by considering the 3D microstructure in AFRL challenge

Acknowledgements

- This work was supported by the NASA Aeronautics Research Mission Directorate (ARMD) through the Transformational Tools and Technologies (T^3) project

- We thank AFRL for organizing the 2020 Additive Manufacturing challenge series

- We thank NIST for organizing the AM-bench 2022 challenge series

Reference to AFRL challenge modeling work

Saikumar R. Yeratapally, Albert R. Cerrone, Edward H. Glaessgen, "*Discrepancy between crystal plasticity simulations and far-field high energy X-Ray diffraction microscopy measurements*" Integrating Materials and Manufacturing Innovation 2021; 10(2):196-217. DOI: 10.1007/s40192-021-00216-5



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Back-up Slides

Gurson-Tvergaard-Needlman (GTN) Model: Yield Potential

The yield potential (ϕ) of GTN model is expressed as:

$$\Phi = \frac{\sigma_e^2}{\sigma_M^2} + 2fq_1 \cosh\left(\frac{q_2\sigma_k^k}{2\sigma_M}\right) - \left(1 + q_3 f^2\right) = 0$$

- f is the void volume fraction
- σ_e and σ_M are the effective stress and yield stress, respectively
- σ_k^k is three times the hydrostatic stress
- q_1, q_2, and q_3 are yield surface parameters introduced by Tvergaard et al.* as a modification to the Gurson** model.
- Typically, for metals, the ranges of the parameters q_1, q_2, and q_3 are (1.0 to 1.5), (1.0), and (1.0 to 2.25), respectively***.

The void volume fraction (*f*) is the damage parameter, and it evolves according to the following rate equations:

$$\dot{f} = \dot{f}_{\text{gr}} + \dot{f}_{\text{nucl}}$$

$$\dot{f}_{\text{gr}} = (1 - f)\,\dot{\varepsilon}^{pl} : \mathbf{I}$$

$$\dot{f}_{\text{nucl}} = A\,\dot{\bar{\varepsilon}}_m^{pl}$$

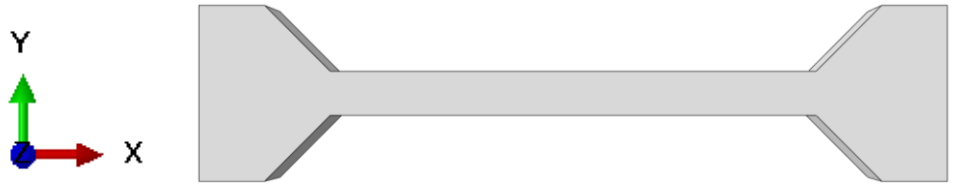
$$A = \frac{f_N}{s_N\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\bar{\varepsilon}_m^{pl} - \varepsilon_N}{s_N}\right)^2\right]$$

- $\dot{f}_{nucl}$ and $\dot{f}_{gr}$ are the rate of void nucleation and growth, respectively
- $\dot{\varepsilon}^{pl}$ is the plastic strain rate tensor
- I is the Identity tensor
- *A* represents a normal distribution of void nucleation
- $\dot{\varepsilon}_m^{pl}$ is the equivalent plastic strain
- ε_N and s_N represent the mean, standard deviation of nucleation strain, respectively
- f_N represents the nucleated void volume fraction

*Tvergaard et al. (1981)Int. J. Fracture 17,389–407. **Gurson (1977) Journal of Engineering Materials and Technology, 99: 2–15. ***ABAQUS User manual

GTN Model: Modeling Assumptions

- GTN model assumes isotropic material and hence ignores microstructure heterogeneities
- An idealized model of the subcontinuum coupon (shown below) was created. The model doesn't account for the surface roughness present in the as-built coupon.
- Isotropic parameters were assigned to the entire model.



- The Youngs modulus and stress-strain curve predicted from CP simulation is provided as input to the GTN model
- q_1 = 1.5, q_2 = 1.0, and q_3 = 2.25
- ε_N = 0.3, s_N=0.1 and f_N=0.004
- Void coalescence starts to occurs when f attains a value greater than or equal to 0.10
- A total failure at the material point was assumed to occur when f attains value of 0.25
- The porous plasticity model within ABAQUS[#] software has GTN plasticity model implemented
- ABAQUS Explicit solver was used to solve the idealized fracture problem

Crystal Plasticity Model

Flow rule: $$\dot{\gamma}^{\alpha} = \dot{\gamma}_{o}\left|\frac{\tau^{\alpha}}{g^{\alpha}}\right|^{m} \operatorname{sgn}(\tau^{\alpha})$$

- $\dot{\gamma}^{\alpha}$ is the slip rate along slip system α
- $\dot{\gamma}_{o}^{\alpha}$ is the reference slip rate on slip system α
- g^{α} is the slip resistance on slip system α
- m is the shear rate sensitivity parameter

Hardening law: $$\dot{g}^{\alpha} = H\sum_{\beta=1}^{N} q^{\alpha\beta}\left|\dot{\gamma}^{\beta}\right| - Rg^{\alpha}\sum_{\beta=1}^{N}\left|\dot{\gamma}^{\beta}\right|$$

- g^{α} is the resolved shear strengths of slip system α
- γ^{α} is the slip accumulated on slip system α
- H is the direct hardening coefficient
- R is dynamic recovery coefficient
- N represents the number of slip systems
- $q^{\alpha\beta}$ is the latent hardening coefficient

CP Model: Calibration (NIST AM-Bench)

- Understandably, no calibration stress-strain data was provided as a part of this challenge.
- There is very limited tensile stress-strain data available in the literature pertaining to as-built mesoscale Inconel-625 coupons
- Robbins et al. (2019)* reported stress-strain behavior of sub-size Inconel-625 coupons with gage section area of 1.1 mm^2
- Hence, the data from Robbins et al. (2019) was leveraged to calibrate the CPFE model in the current study
- It must be noted that only the yield stress and hardening values were fit using the data published in the aforementioned work

NOTE: Critical resolved shear stress, g_o^α, was assumed the same for any given slip system α

Calibrated CP parameters

Parameter	*Calibrated value (units)*
$\dot{\gamma}_o^\alpha$	0.001
g_o^α	172 MPa
m	15
H	215 MPa
R	10 MPa
$q_{\alpha\beta}$	1 (for self hardening)
	1.4 (for latent hardening)

*Robbins, Aron. "Mechanical Characterization of Additively Manufactured Inconel 625 and AlSi10Mg via High-Throughput Tensile Testing." (2019). https://digitalrepository.unm.edu/me_etds/177