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# Validation and application of crystal plasticity simulations to study effect of process-specific defects in additively manufactured polycrystalline materials


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# Presenter biography

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## Saikumar “Sai” Yeratapally

**Work Experience:**

Research engineer at National Institute of Aerospace (NIA) (10/2017- current)

Post-doctoral Research Associate at NIA (3/2016 – 10/2017)

**Education**:

Ph.D. in Aeronautics and Astronautics Engineering from Purdue University (12/2015)

M.S. in Mechanical Engineering from Carnegie Mellon University (12/2010)

B.E. (Honors) in Mechanical Engineering from Birla Institute of Technology and Science (Goa, India) (8/2009)

**Research Interests**:

Microstructure-performance linkage using crystal plasticity models

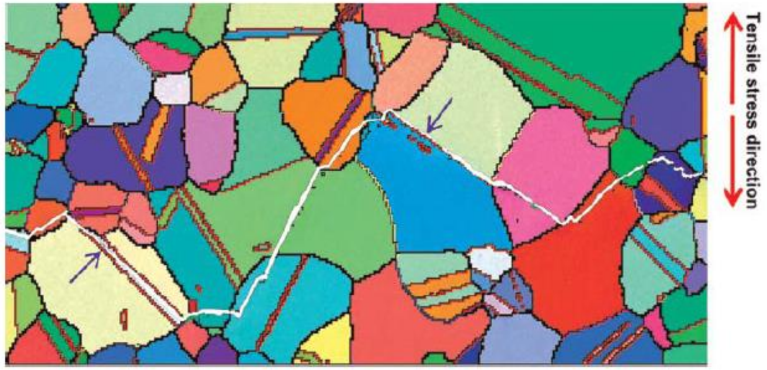
Effect-of-defects in additively manufactured polycrystalline materials

# Motivation

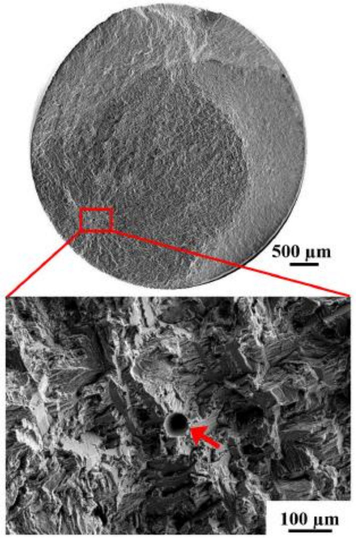
- Fatigue crack initiation (FCI) in polycrystalline materials is primarily dependent on microstructure, inclusion and defect attributes, in addition to other factors

*FCI at twin boundaries*



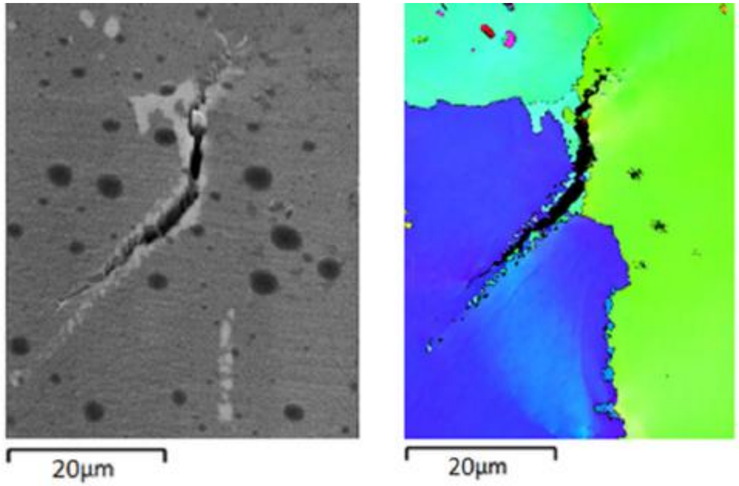

*Jiang et al. (2015)*

*FCI at pore*




*Shamir et al. (2020)*

*FCI at inclusion*




*Yeratapally et al. (2017)*

- Linking defect/microstructure attributes to failure mechanisms and hence performance is essential for rapid qualification
- Crystal plasticity (CP) simulations provide a platform to quantitatively link defect/microstructure attributes to performance
- Validation of CP models is important to be able to quantitatively understand the underpinning mechanisms of crack initiation

# Presentation outline

- Additive manufacturing (AM) modeling challenge
  - Comparing crystal plasticity finite element (CPFE) predictions with high-energy X-ray measurements
- CP-based investigation of process-specific defects Ti-6Al-4V alloy

# **AM modeling challenge**: Build configuration

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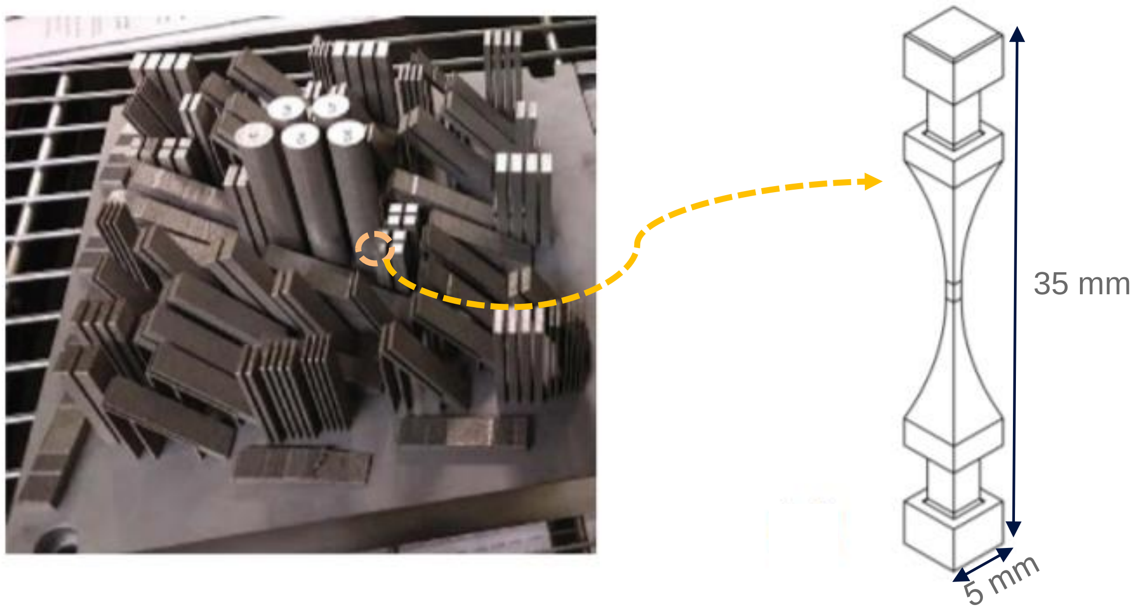
*Final build* | *Fully machined tensile coupon*




**<u>Material / AM Process</u>**: Inconel 625 (IN625) produced through Laser powder-bed fusion (L-PBF)
**<u>Machine</u>**: EOS M280
**<u>Powder</u>**: Commercially available IN625 gas atomized powder
**<u>Processing parameters</u>**: Nominal processing parameters
**<u>Machining</u>**: The sample was fully machined by wire electrical discharge machining (EDM)
**<u>Post processing</u>**: Stress relieved (SR)+ heat treated (HT)+ hot isostatic pressing (HIP), no surface treatment

***<u>Source</u>: ARFL's AM Challenge Series***

***https://materials-data-facility.github.io/MID3AS-AM-Challenge/***

# **AM modeling challenge**: High energy X-ray diffraction

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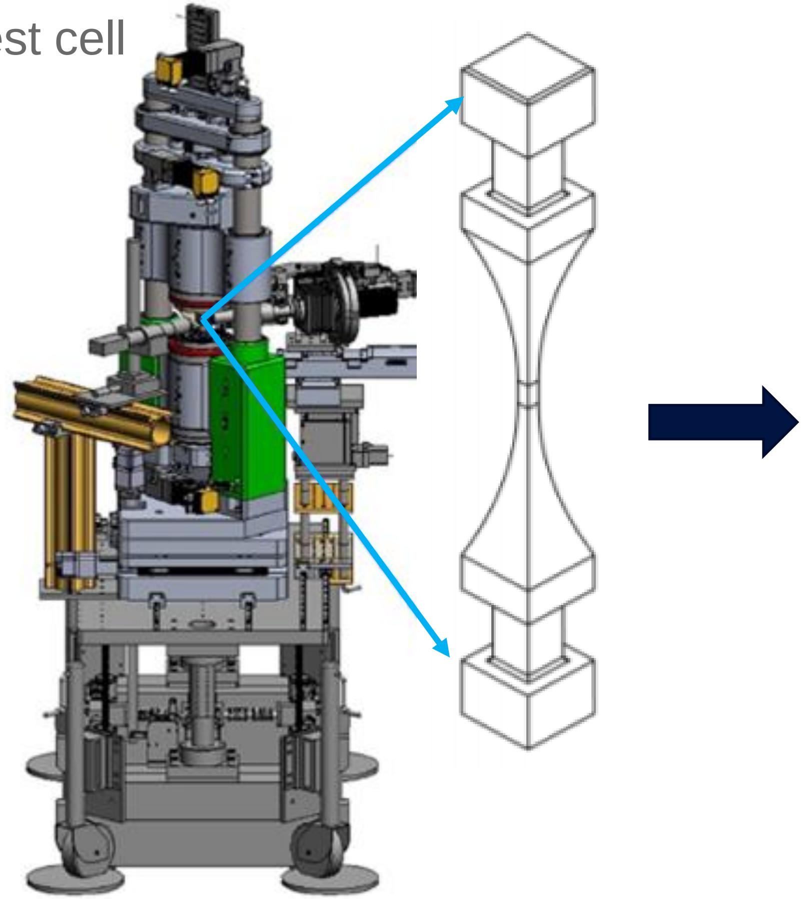


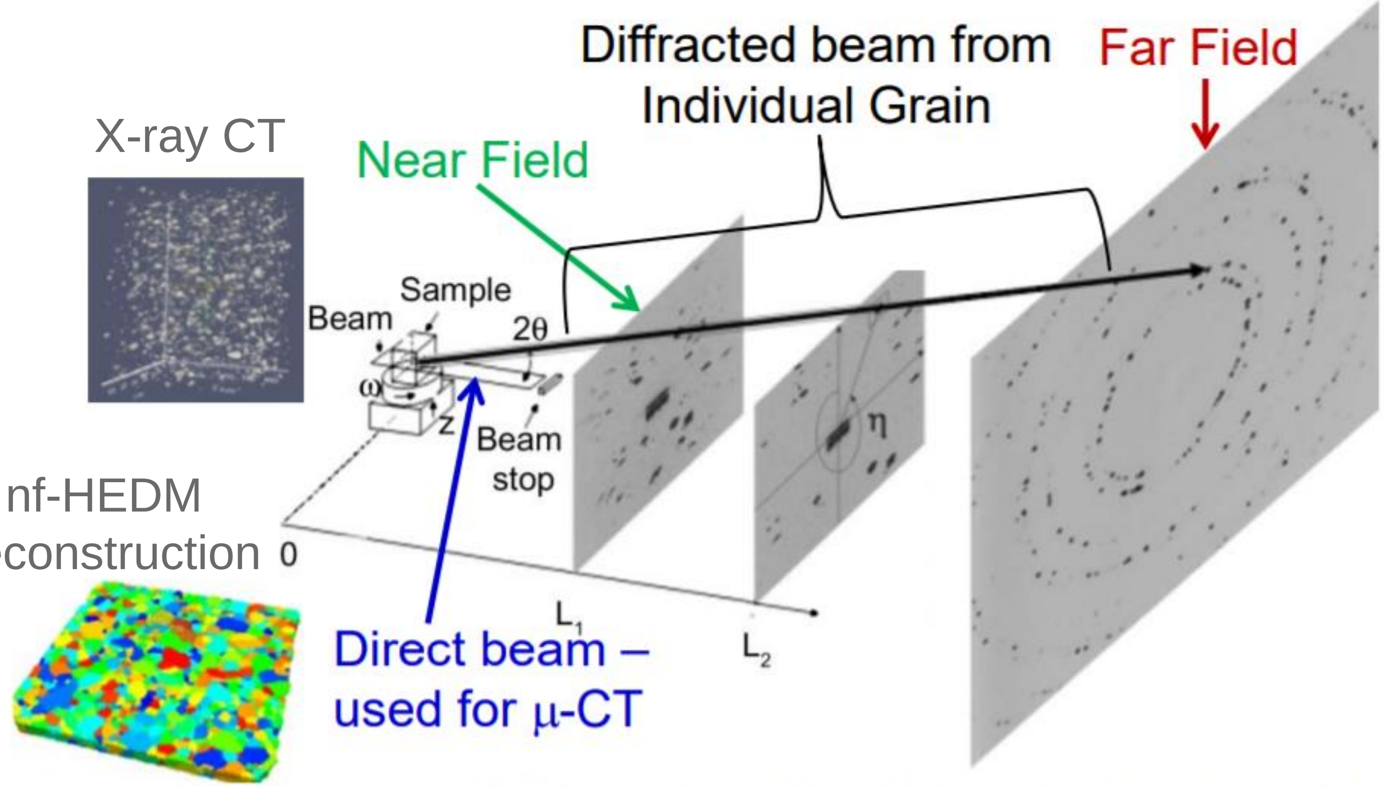


Adapted from: Poulsen HF. 2012. *J. Appl. Crystallogr.* 45:1084-1097

Variants of high-energy X-ray diffraction (HEDM) technique:

1) **near-field HEDM (nf-HEDM)**: provides data to reconstruct individual grain morphologies
2) **far-field HEDM (ff-HEDM)**: provides grain average orientations, elastic strains and centroids

  

# AM modeling challenge: Problem statement

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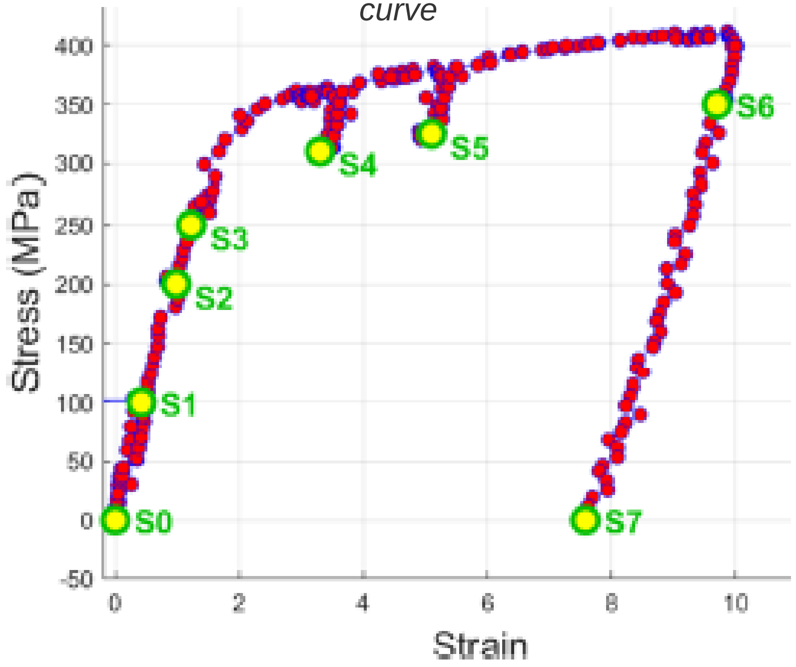
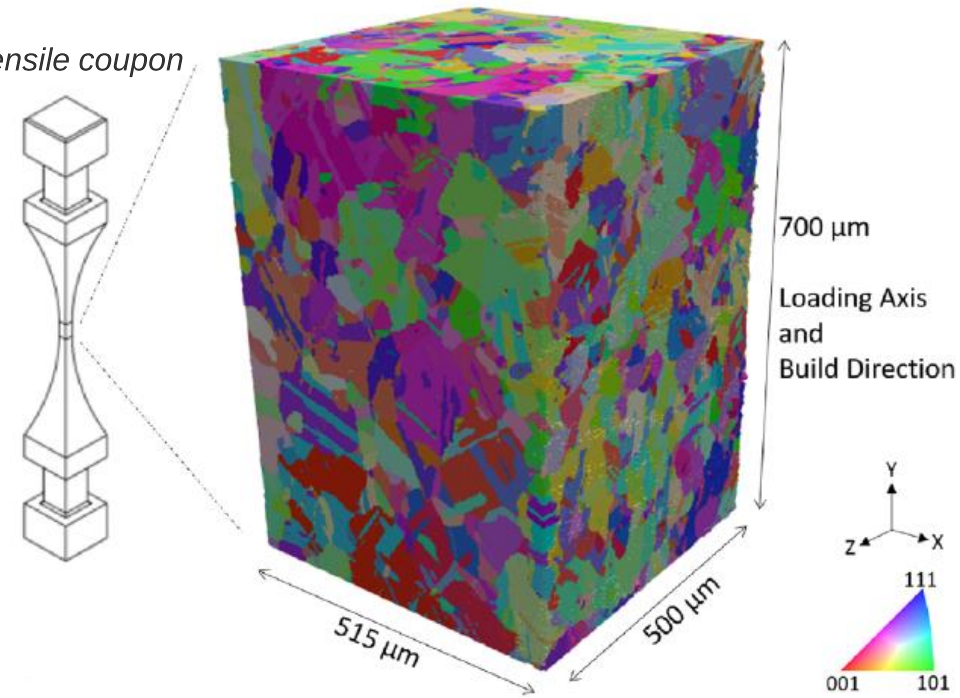
*Stress-strain curve*

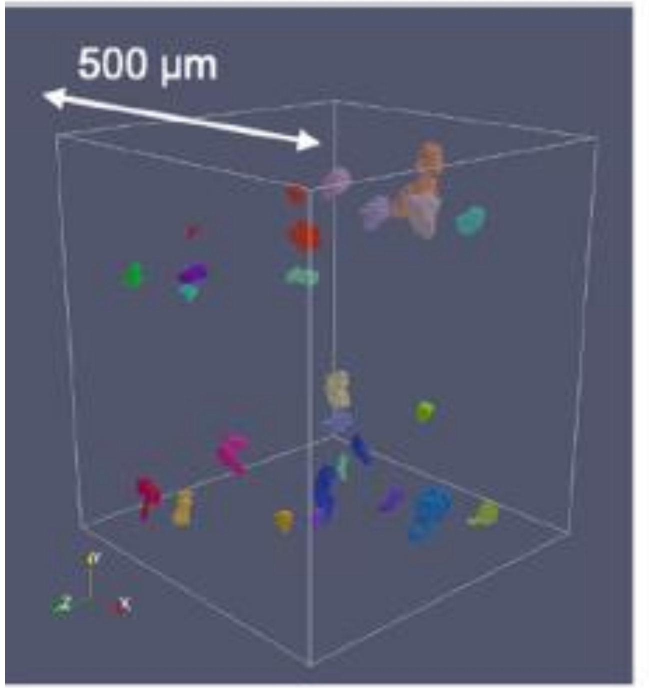



*Serial sectioned microstructure at gage section*

*Tensile coupon*




*28 "challenge" grains*




**Challenge problem**: Given the stress strain curve, serial-sectioned and reconstructed 3D microstructure, predict grain-average elastic strain tensor for 28 "challenge" grains at six different macroscopic load states, S1 through S6

***Source*: ARFL's AM Challenge Series**

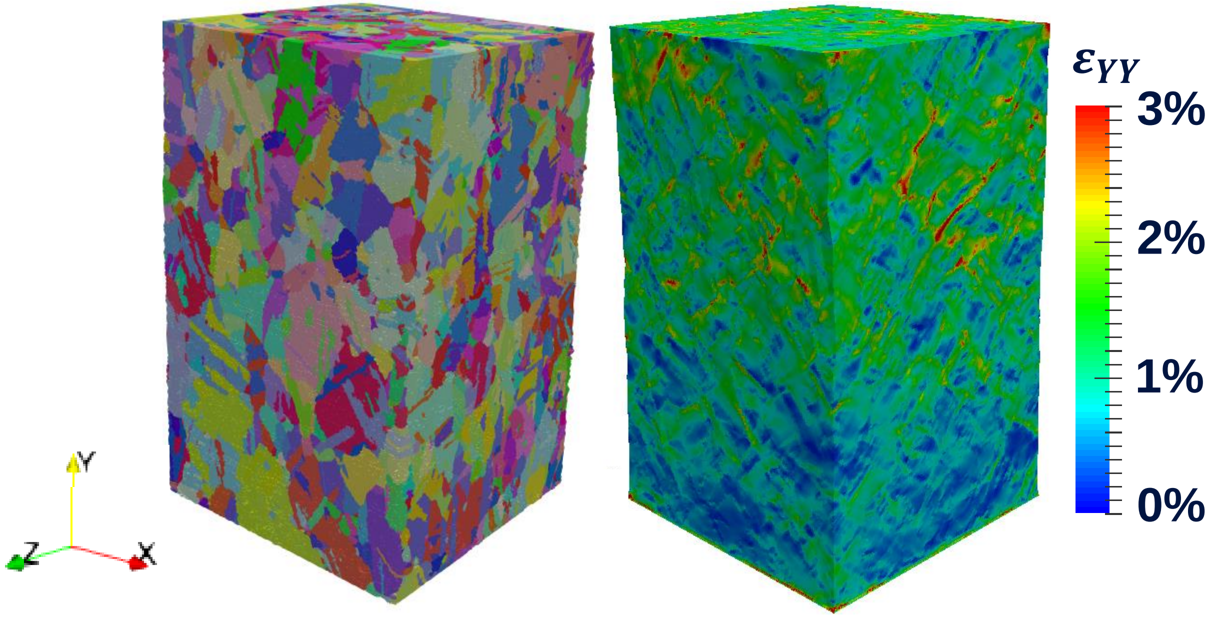
***https://materials-data-facility.github.io/MID3AS-AM-Challenge/***

# Presentation outline

- Additive manufacturing (AM) modeling challenge
  - ➢ Comparing crystal plasticity finite element (CPFE) predictions with high-energy X-ray measurements
- CP-based investigation of process-specific defects Ti-6Al-4V alloy

# Crystal plasticity (CP) for structure-property linkage

## ScIFEN: Scalable Implementation of Finite Elements by NASA




- ScIFEN[1] is built on PETSc[2]
- Leverages a suite of data structures and routines to achieve scalability.
- Utilizes open-source libraries like MOAB[3] and HDF5[4] for parallel I/O operations.
- Scales well over thousands of processers, compared to commercial packages
- Includes phenomenological CP models
- Interfaces with DREAM.3D[5], Gmsh[6] and SPPARKS[7]

- 3D microstructure* of IN625 obtained from serial-sectioning has 29,662 grains
- Finite element mesh has ~85 million degrees of freedom
- Global strain applied in YY direction: 1%
- CP model: Strain-gradient based[8]
- Simulation time: ~44 hours on 640 Intel Xeon E5-2670 processors

Boundary conditions:

- Fully fixed bottom (-Y) face
- Free X and Z faces
- Applied Y-displacement on top (+Y) face

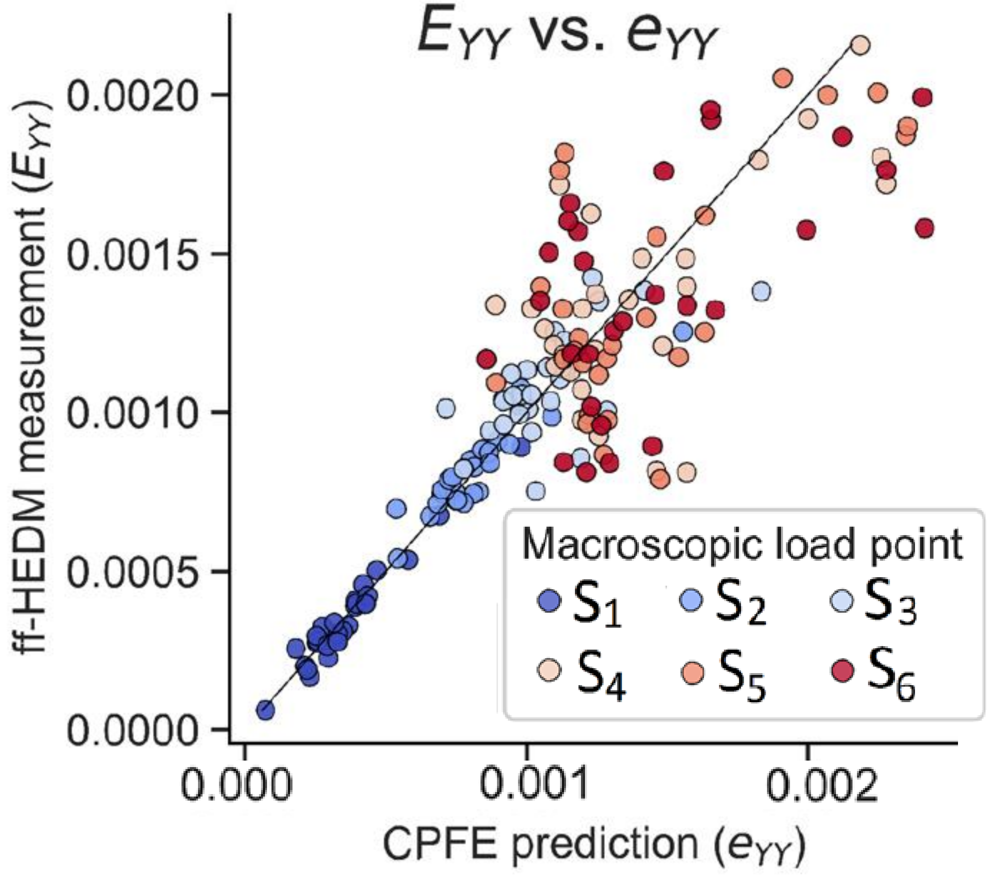
1. https://software.nasa.gov/software/LAR-18720-1
2. Scalable solutions for PDEs, www.mcs.anl.gov/petsc/
3. Mesh-Oriented dataBAse, http://sigma.mcs.anl.gov/moab-library/
4. Parallel file I/O, www.hdfgroup.com
5. DREAM.3D http://dream3d.bluequartz.net/
6. Gmsh, https://gmsh.info/
7. SPPARKS, https://spparks.github.io/
8. Acharya et al. (2000), J. Mech. Phys. Solids, 48(10), pp:2213-2230

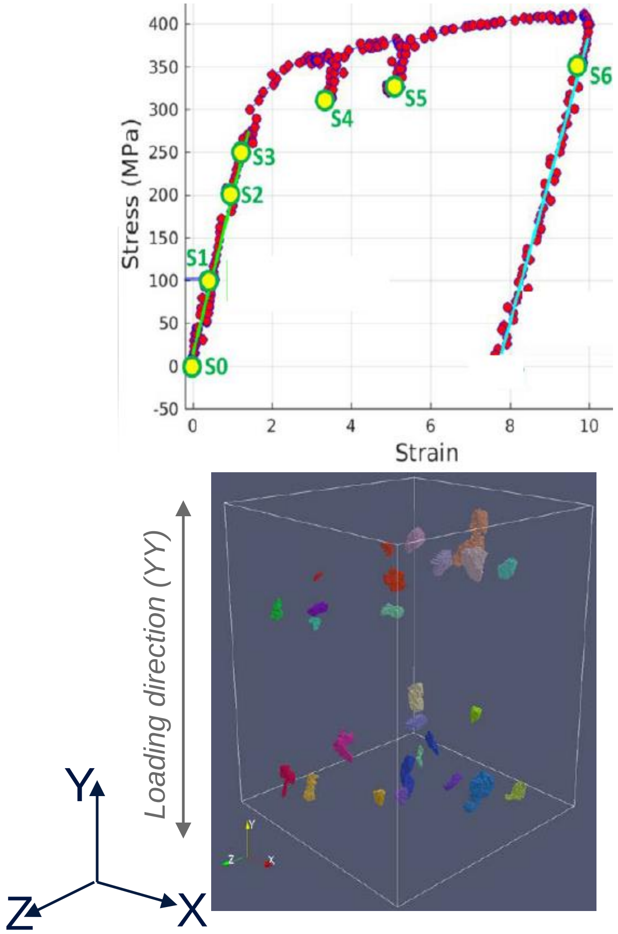
*Source of 3D microstructure: AFRL AM challenge series https://materials-data-facility.github.io/MID3AS-AM-Challenge/

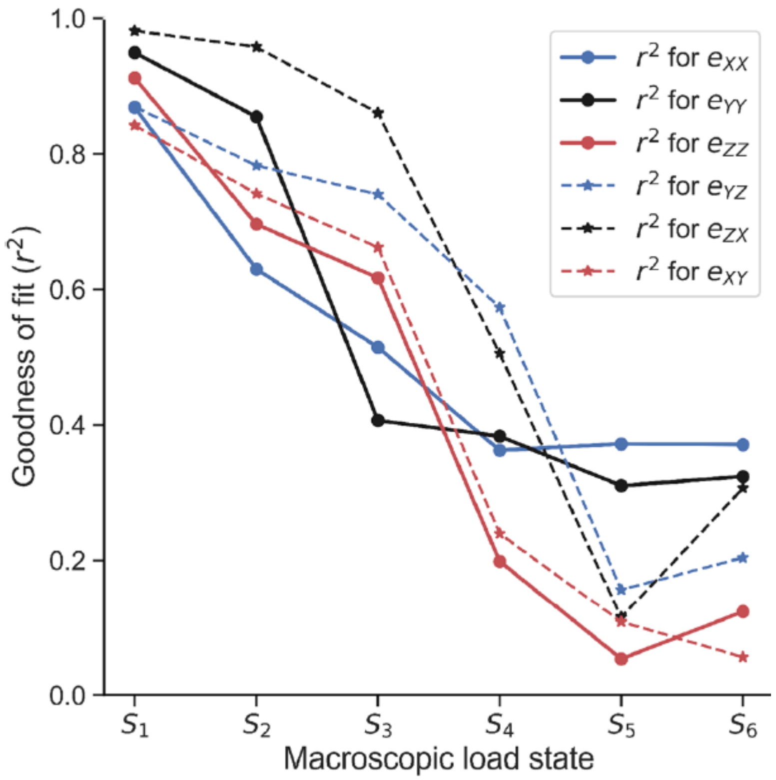
# CP predictions vs. ff-HEDM measurements

## CP predictions vs. ff-HEDM measurements




## Goodness-of-fit




**Observations:**

- There is a good agreement between CP predictions and ff-HEDM measurements in the elastic regime (S1-S3)
- Deviations start to develop in plastic regime (S4-S6)



*Yeratapally et al. (2021) IMMI, vol: 10(2):196-217*

# Discrepancy 1: Boundary conditions

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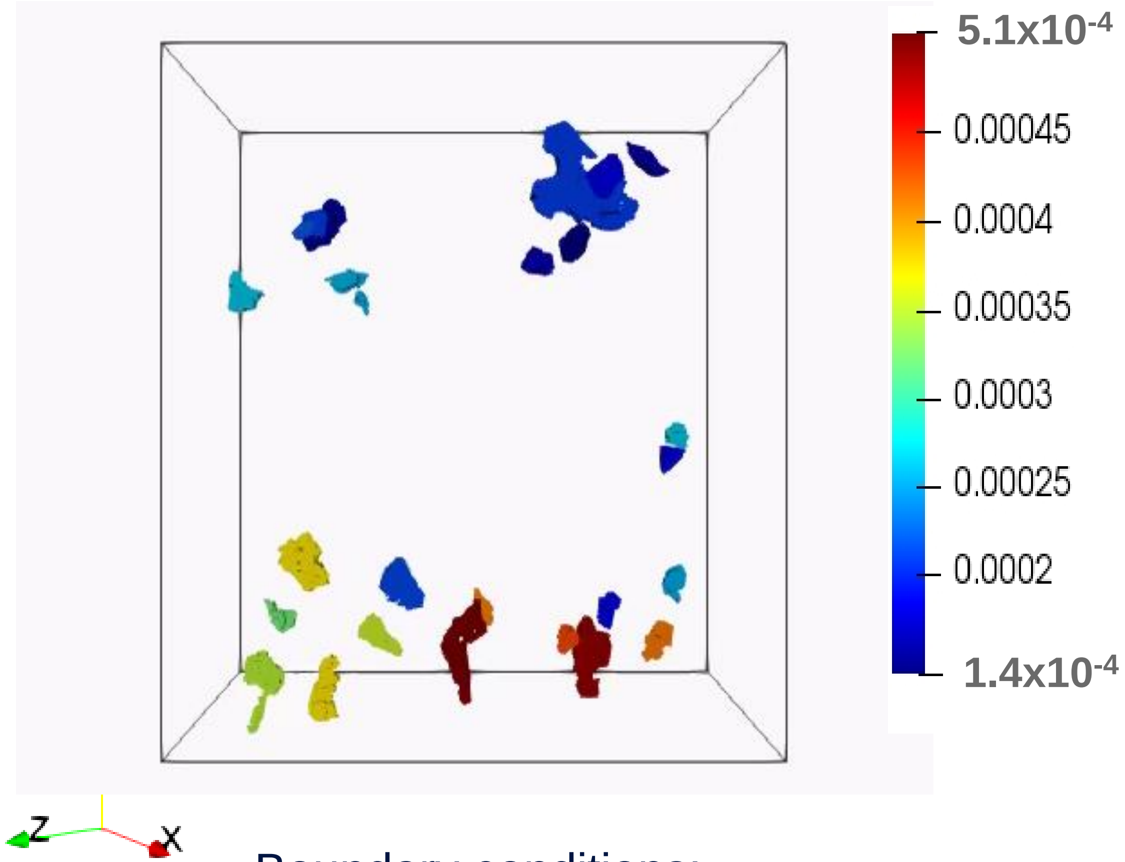
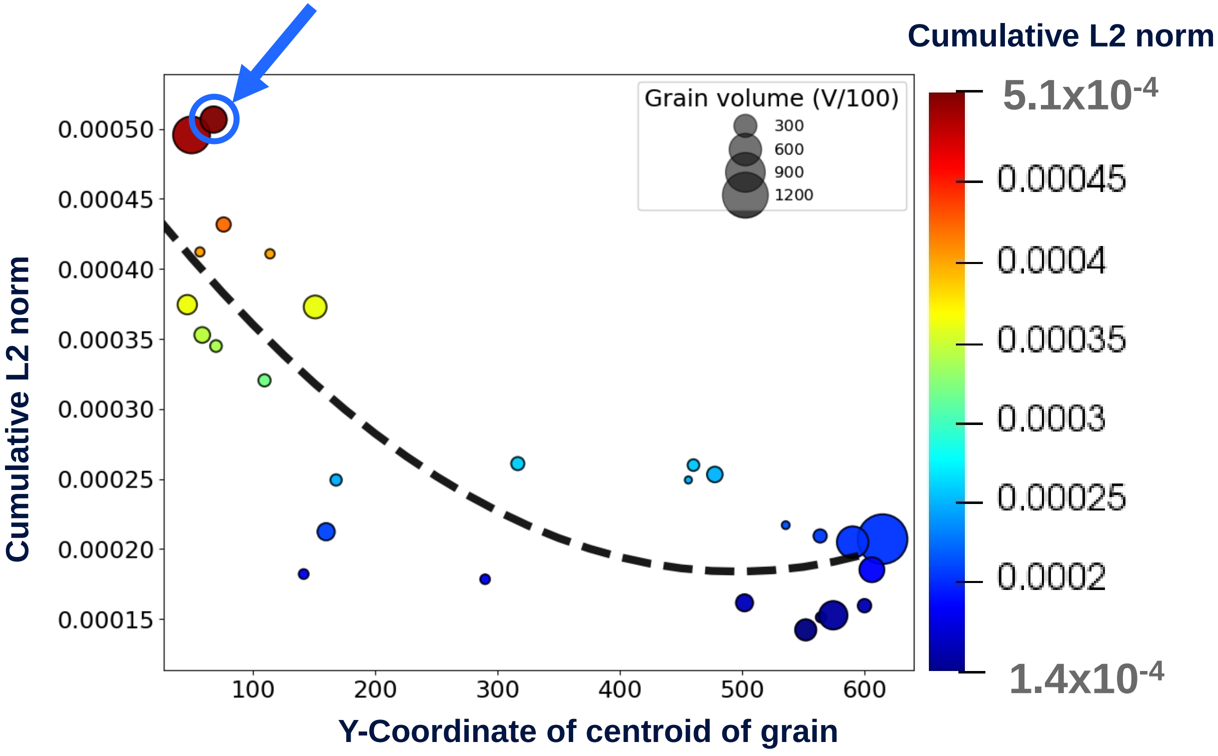


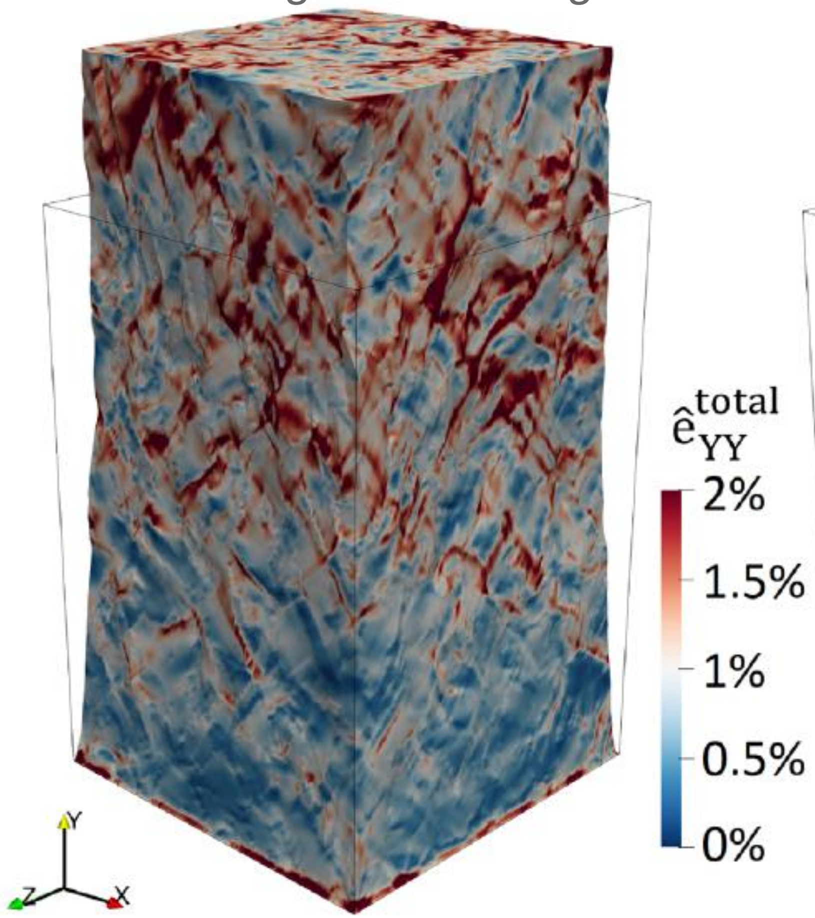




Boundary conditions:

- Fully fixed bottom (-Y) face
- Free X and Z faces
- Applied Y-displacement on top (+Y) face

# Discrepancy 1: Boundary conditions

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

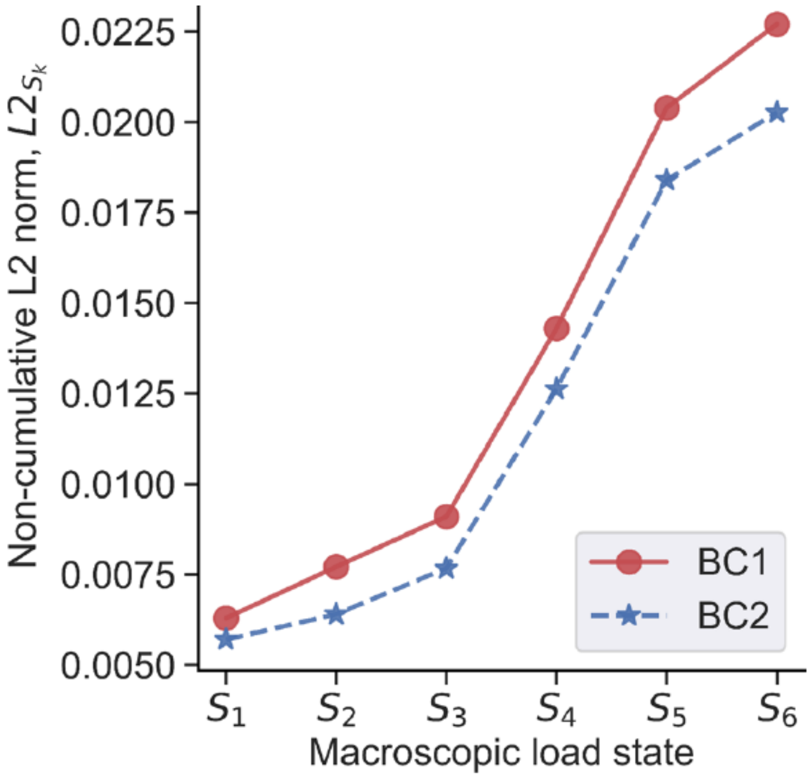



**BC1**: Fully constrained bottom face

**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, $S_k$*




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

$(E_i)_{S_k}^{g_n}$ ***is ff-HEDM measurement;*** $(e_i)_{S_k}^{g_n}$ ***is CP prediction;*** $N$ ***is # grains***

$S_k$ ***is macroscopic stress state;*** $g_n$ ***is grain ID***

# Discrepancy 2: Stress relaxation in grains

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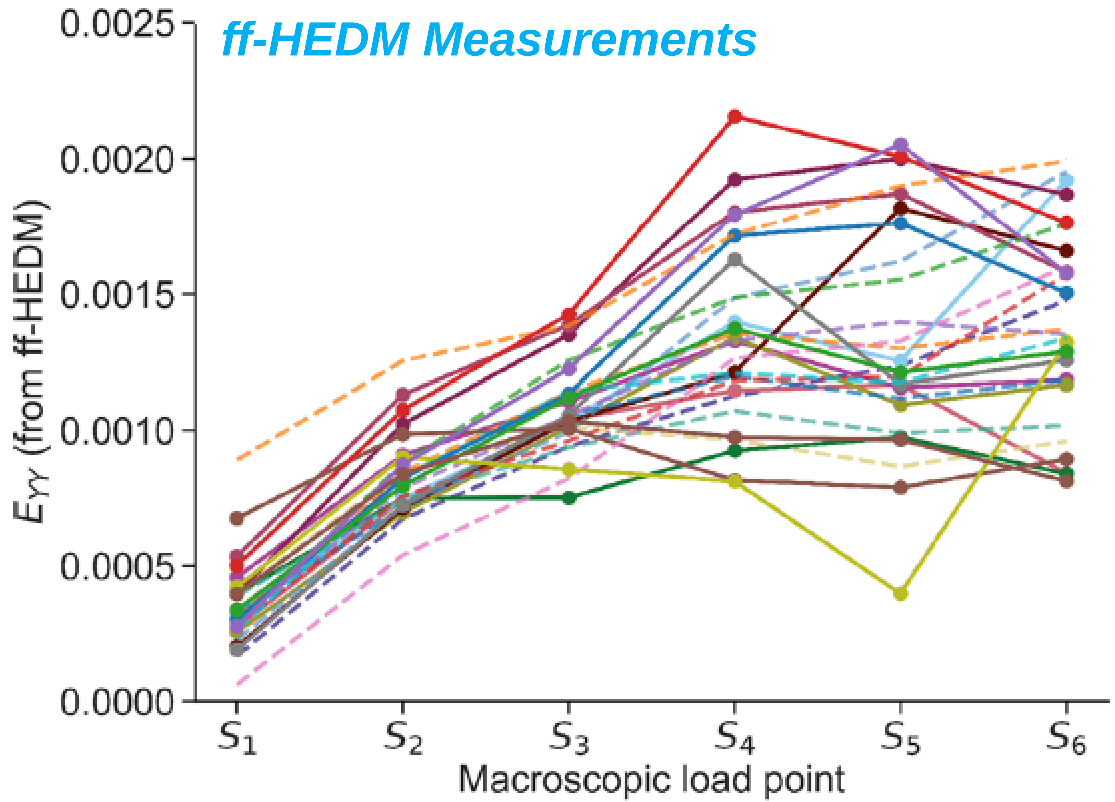
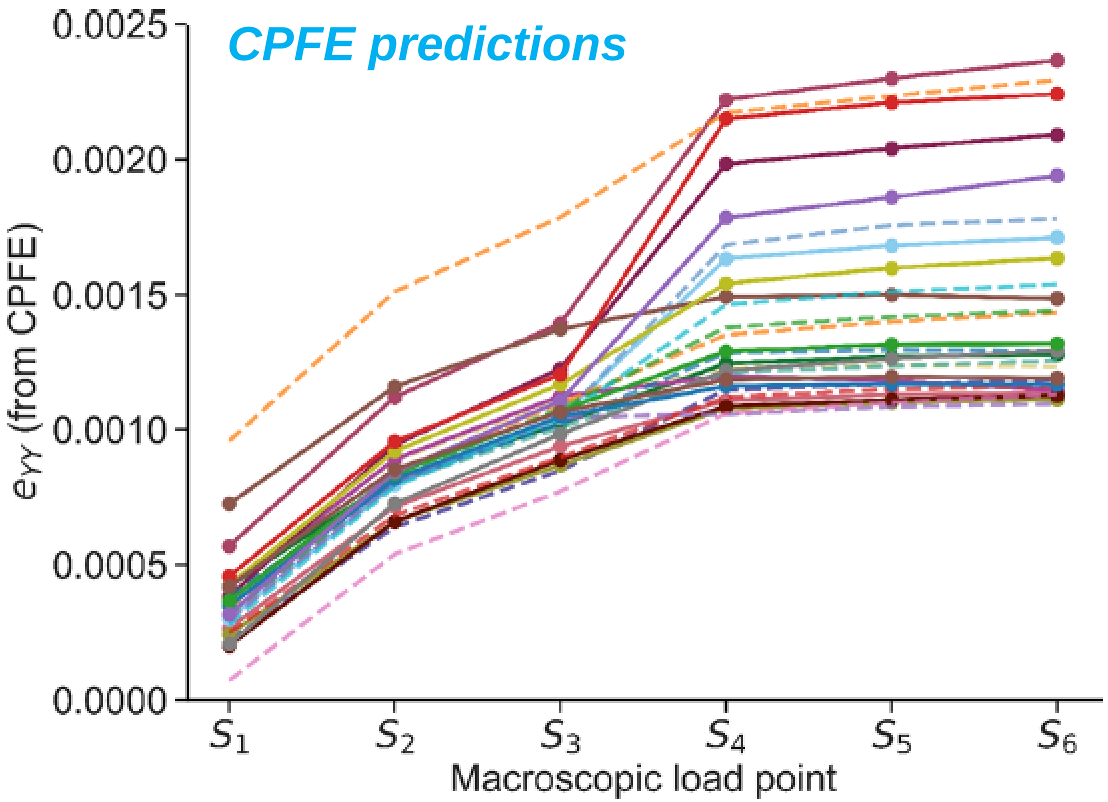
*ff-HEDM measurement of evolution of YY component of grain-average elastic strain in each of the 28 grains*

*CPFE prediction of evolution of YY component of grain-average elastic strain in each of the 28 grains*



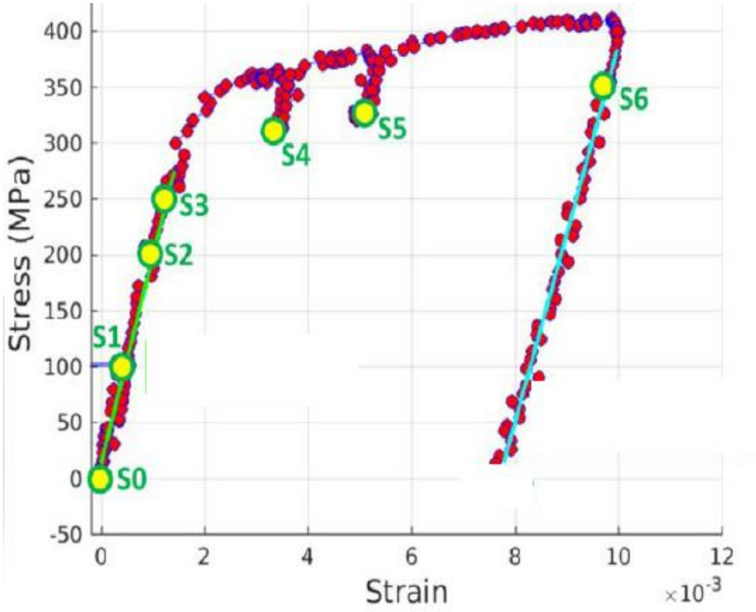

**Observation**: Phenomenological CP model used is unable to predict stress relaxation

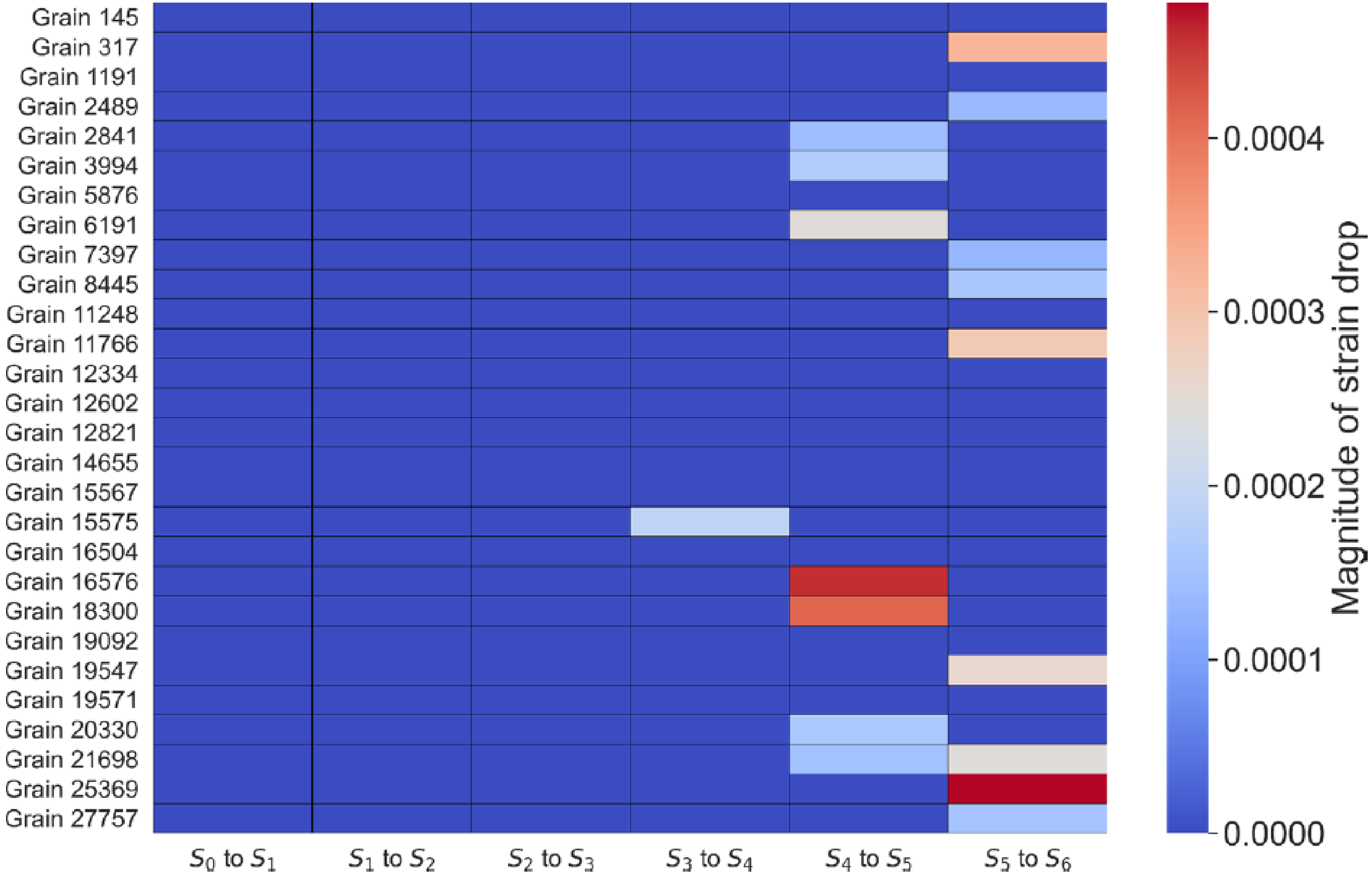
  

*Yeratapally et al. (2021) IMMI, vol: 10(2):196-217*

# Discrepancy 2: Stress relaxation in grains

- Heatmap showing strain drop in grains
- Heatmap created using ff-HEDM data.




**Observation**: Stress relaxation is predominant in the plastic regime and is non-existent in the elastic regime

*Yeratapally et al. (2021) IMMI, vol: 10(2):196-217*

# Illustration: Grain-level stress relaxation in Ti-7Al

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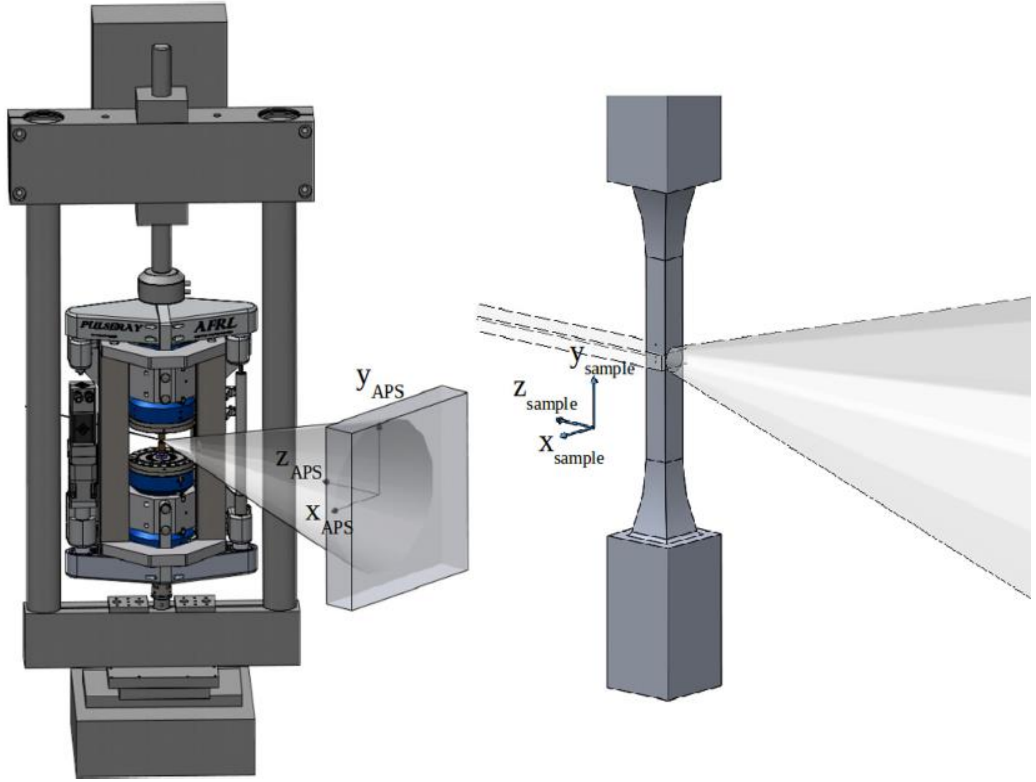
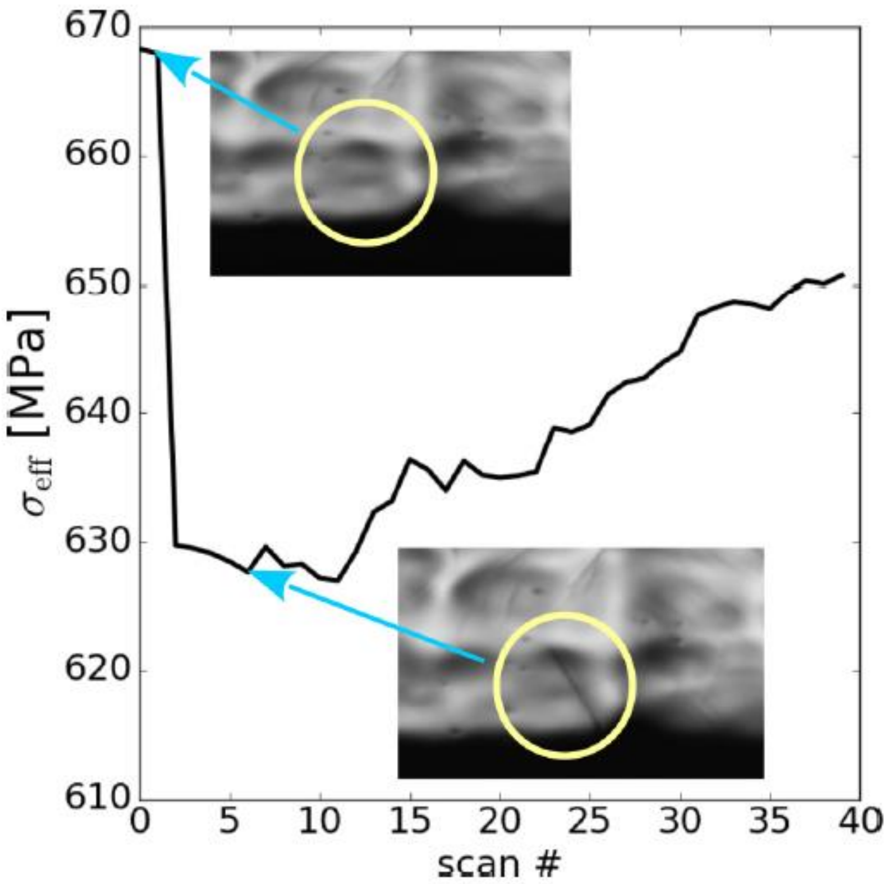



*Setup of creep experiment at advanced photon source (APS)*




- ➢ *Stress relaxation during creep loading at 85% of the yield stress*
- ➢ *Corresponding slip band developed at the location of the grain*

Source: Beaudoin et al. Physical Review B. 96, 174116 (2017)

# For more detailed discussion

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**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

Journal: Integrating Materials and Manufacturing Innovation (IMMI)

Special Issue: Metal Additive Manufacturing Modeling Challenge Series 2020

# Presentation outline

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# Fatigue crack initiation at pores

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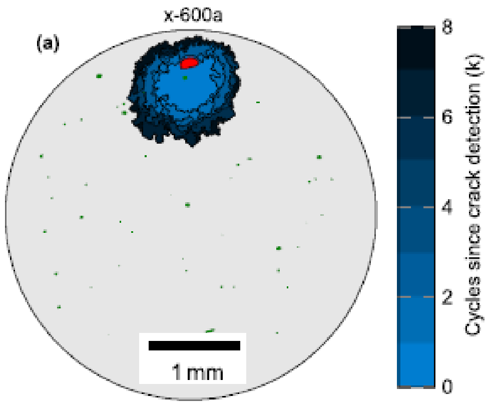
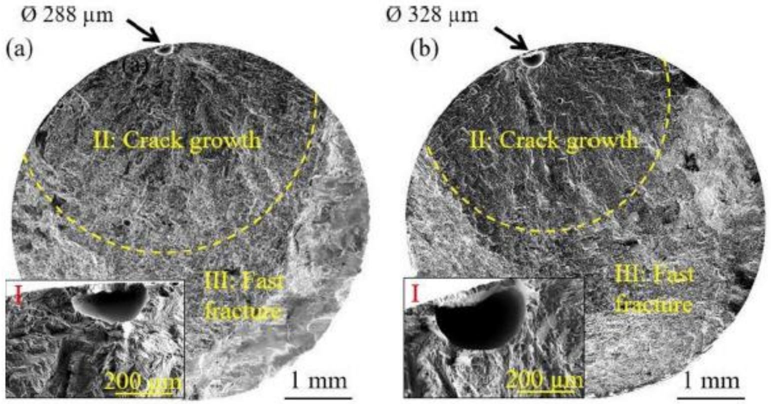
**Ti6Al4V, EBM**



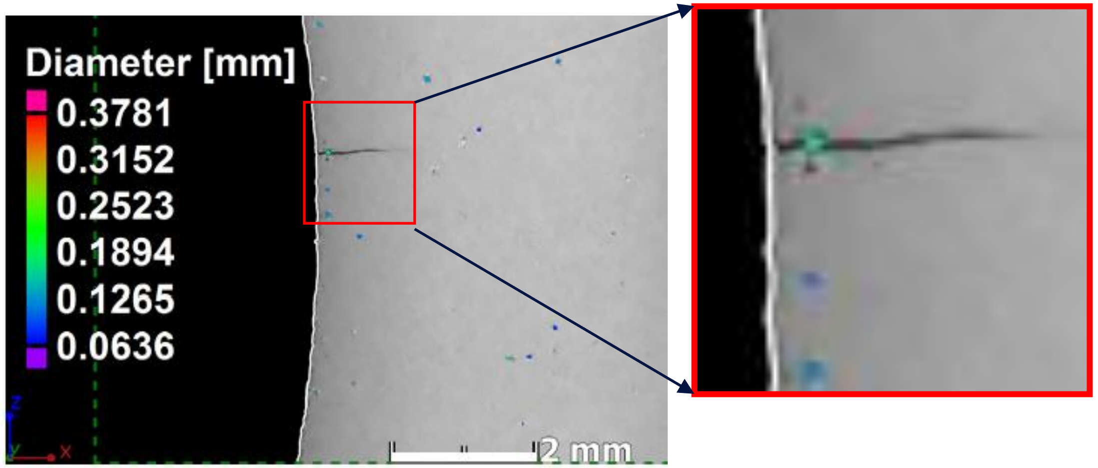

*Williams et al. (2017) Scientific Report| 7: 7308*

**Ti6Al4V, WAAM**



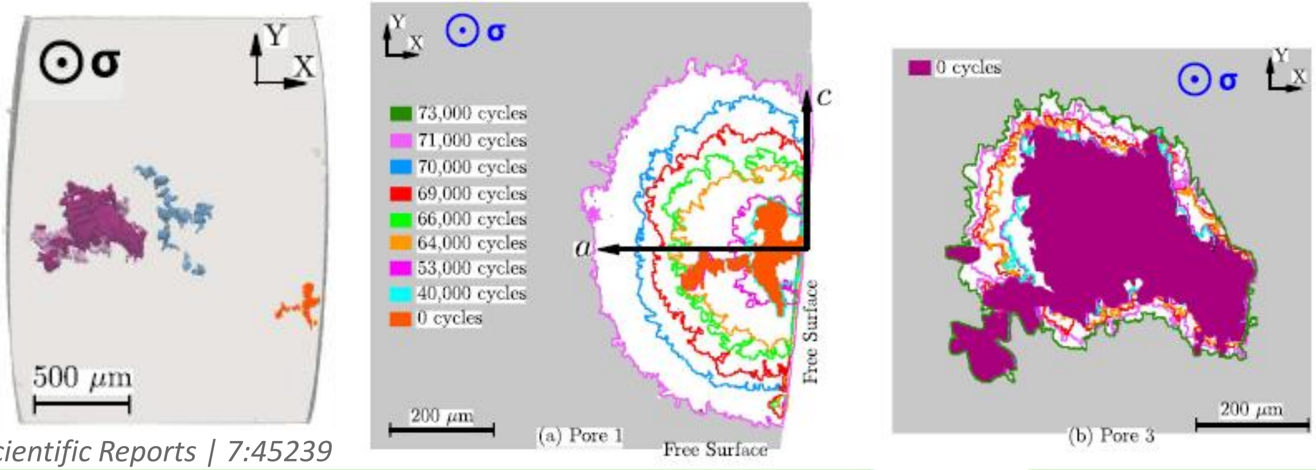

*Biswal et al. (2019)* Additive Manufacturing 28:517–52

**AlSi10Mg, L-PBF**




*Du Plessis et al. (2020) Materials and Design 187 (2020) 108385.*

**A357-T6, Cast**




*Munoz et al. (2016) Scientific Reports | 7:45239*

EBM: electron beam melting
WAAM: wire arc additive manufacturing
L-PBF: Laser powder-bed fusion

# Influence of pore neighborhood

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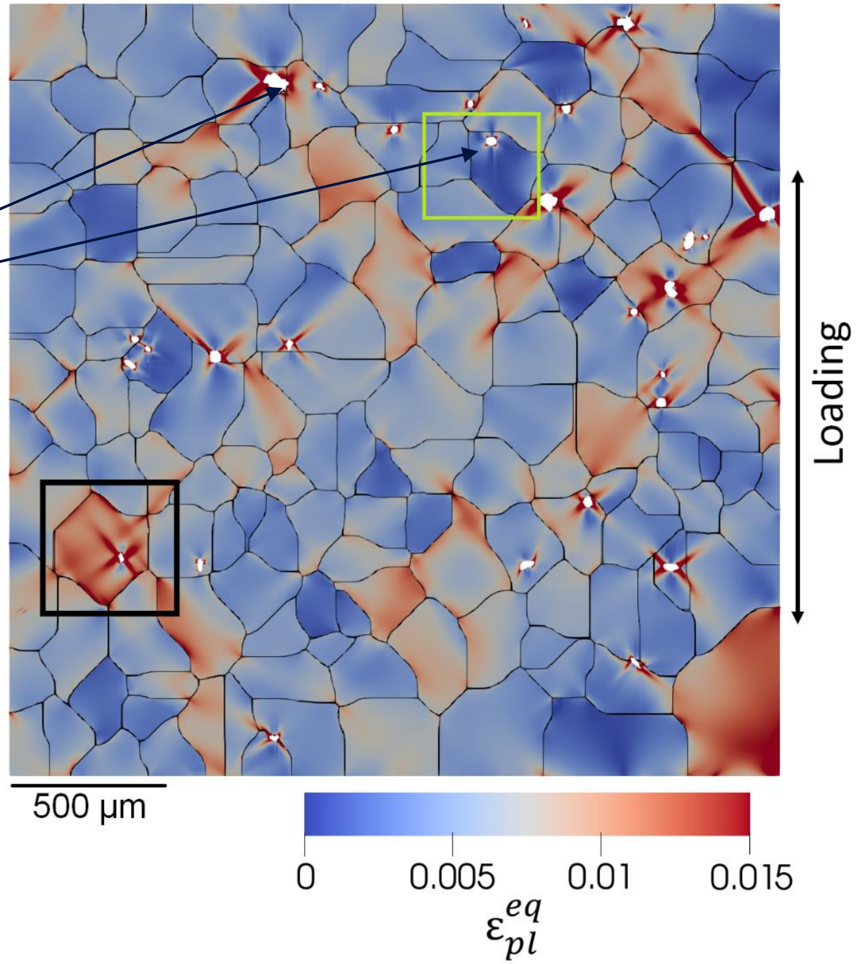
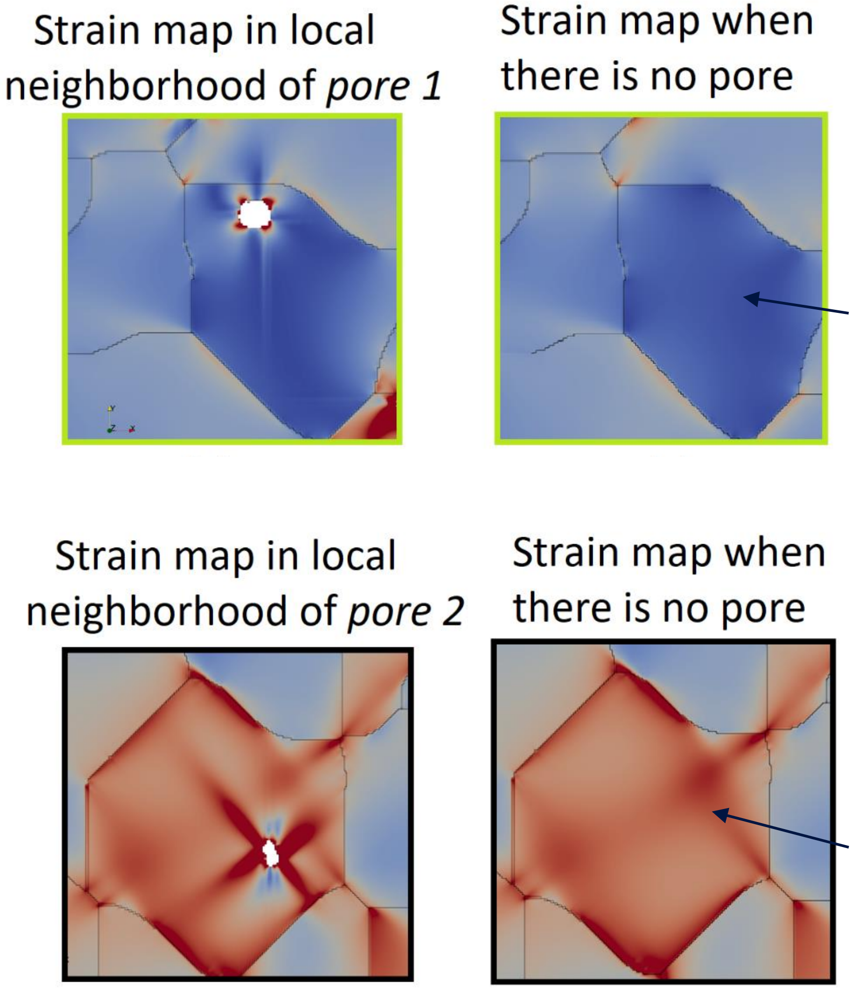
*Equivalent plastic strain map*
*(at 1% global strain)*




L-PBF process-specific pores in as-built Ti-6Al-4V alloy, obtained from backscatter electron images of metallographic sections



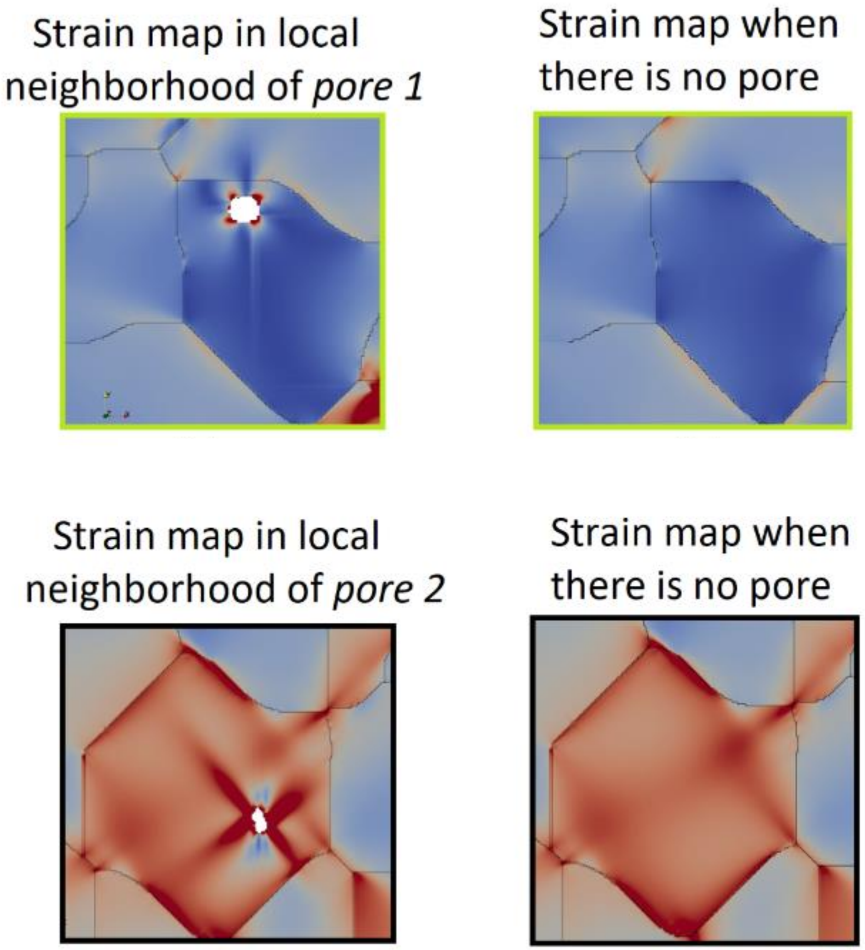

*Pore 1* is embedded in a "hard" grain

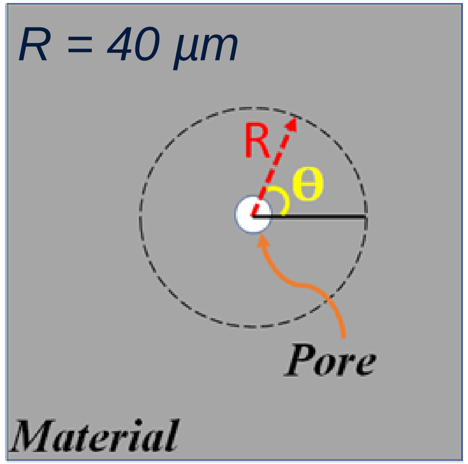
*Pore 2* is embedded in a "soft" grain

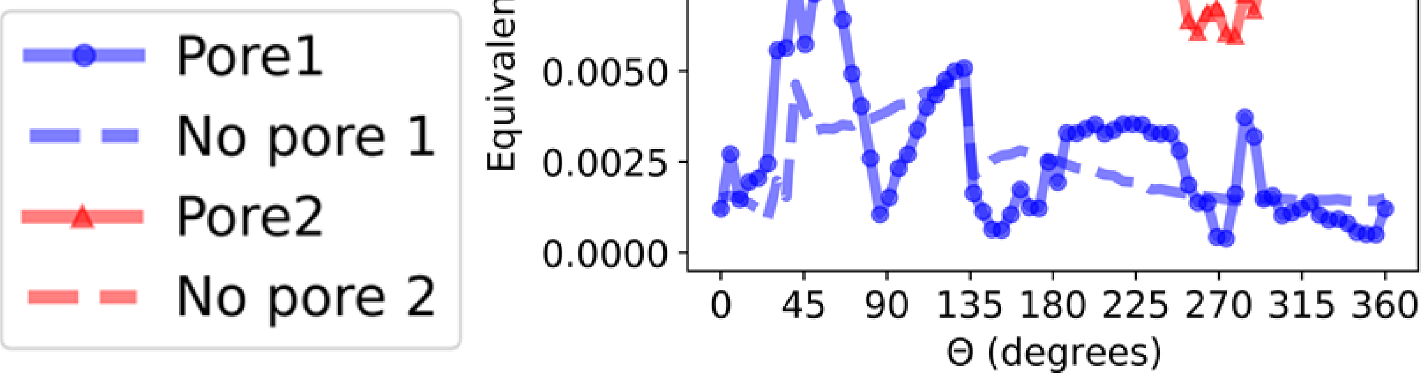
  

# Influence of pore neighborhood






**Observation**: Pore fully embedded in "soft" grain accumulates significant plastic strain in its vicinity compared to a similar sized pore located within a "hard" grain

# Summary



- Grain-average elastic strain measurements from crystal plasticity finite element (CPFE) are compared with far-field high energy X-ray diffraction (ff-HEDM) measurements.
  - ScIFEN's CPFE solver predictions (in the elastic regime) agree with ff-HEDM measurements
  - The results qualitatively agree in the elastic regime, but increased level of discrepancy is observed in the plastic regime
  - Sources of discrepancy between CPFE and ff-HEDM are discussed

- CP simulations are used to understand the influence of local microstructure on the accumulation of plastic strain.
  - Pore fully embedded in "soft" grain accumulates significant plastic strain compared to a similar sized pore located within a "hard" grain

- Ongoing work to validate and apply high-fidelity CP models will be used to develop certification by analysis

# Acknowledgements

The work presented is supported by NASA Aeronautics Research Mission Directorate's (ARMD) Transformative Tools and Technologies (TTT) project

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# Thank you.

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