Computational Characterization and Model Verification for 3D Microstructure Reconstruction of Additively Manufactured Materials

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OUTLINE

1. INTRODUCTION

- Motivation

2. THEORETICAL BACKGROUND & METHOD

- Microstructure reconstruction
- Mathematical quantification of microstructure
- Clustering method and image moments

3. RESULTS & DISCUSSION

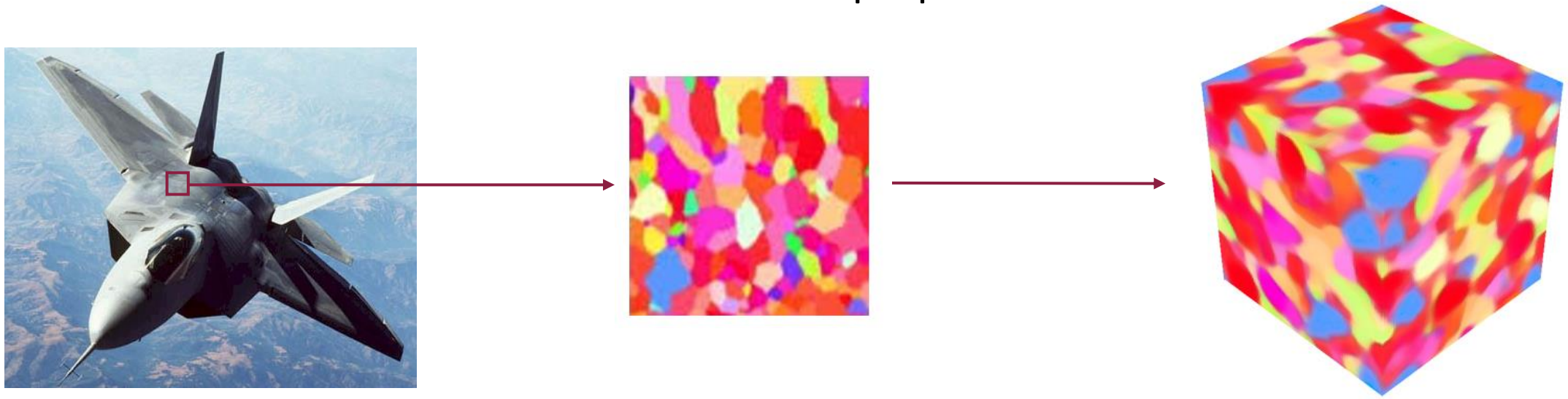
- Comparison of two-dimensional (2D) and three-dimensional (3D) grains
- Statistical measures for anisotropic features

4. CONCLUSION & FUTURE WORK

GOAL: Quantify uncertainty propagated in material properties

MOTIVATION

- Spatial reconstruction of larger microstructural domains from small experimental images to save cost and time and also determine material properties



- Computational techniques generate statistically equivalent reconstructed microstructures

- Markov random field (MRF) algorithm to reconstruct images

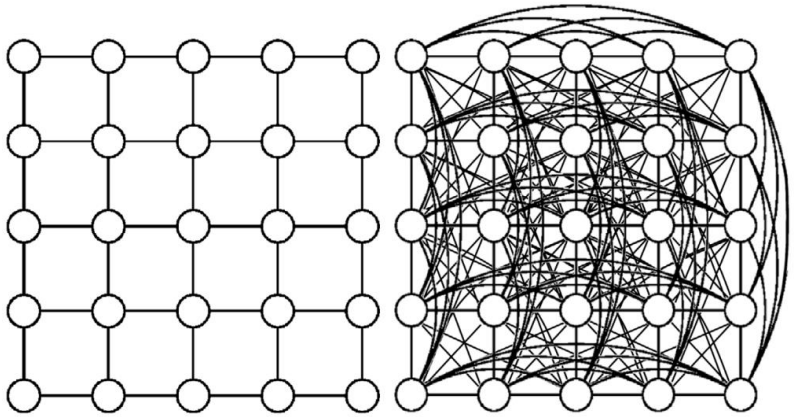
[Ref]: 1) Arulmurugan Senthilnathan, Iman Javaheri, Hengduo Zhao, Veera Sundararaghavan, Marc De Graef, Pınar Acar, "Uncertainty Quantification of Metallic Microstructures using Principal Image Moments", Computational Material Science

RECONSTRUCTION WITH MRF

- Undirected graphical model, unlike Bayesian, depends on current state
- Constructed using Ising model and Markov property
- ***Markov property:*** Probability of a value X is conditionally independent of all other values given its neighbors
- ***Reconstruction:*** Algorithm finds a window ($\boldsymbol{E}_v$) in the input image which resembles the neighborhood of unknown pixel ($\boldsymbol{S}_v$) the most
- Exhaustive search by comparing all possible windows in the input image

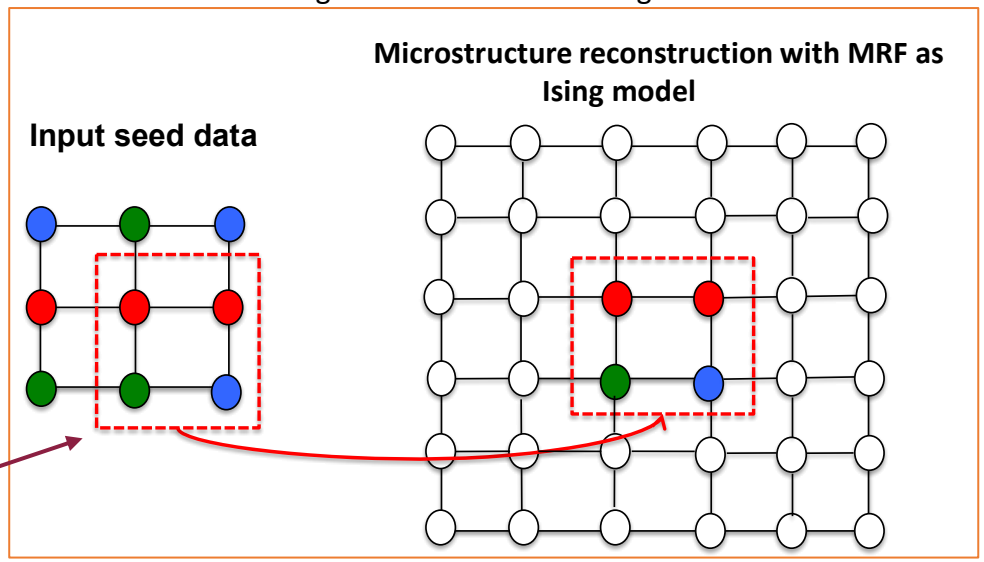
$$\boldsymbol{E}_v = \arg \min_{\boldsymbol{E}^w} \sum_u \omega_{v,u} (\boldsymbol{S}_{v,u} - \boldsymbol{E}_u^w)^2$$

- This search depends on 'window size'



Ising model with Nearest neighbor

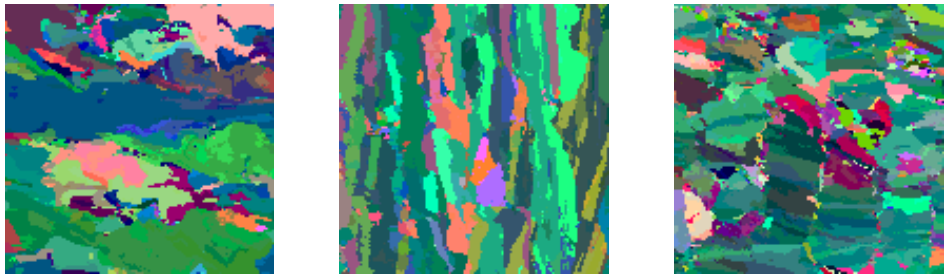
Higher order interactions in Ising model



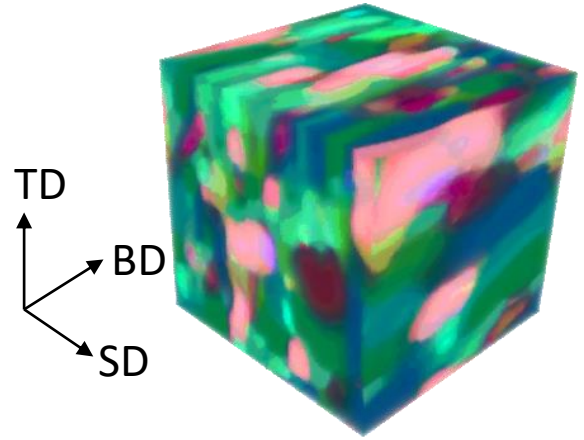
[Ref]: 2) P. Acar and V. Sundararaghavan, *Modelling and Sim. in Mat. Sci. Eng.*, **24** (7): 075005, 2016

RESULTS

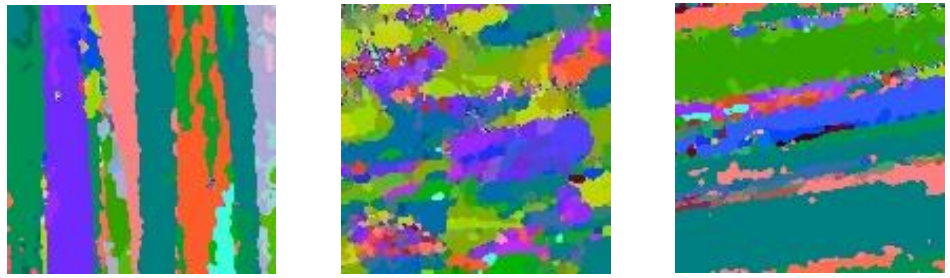
(a) Additively-manufactured (316L stainless steel)



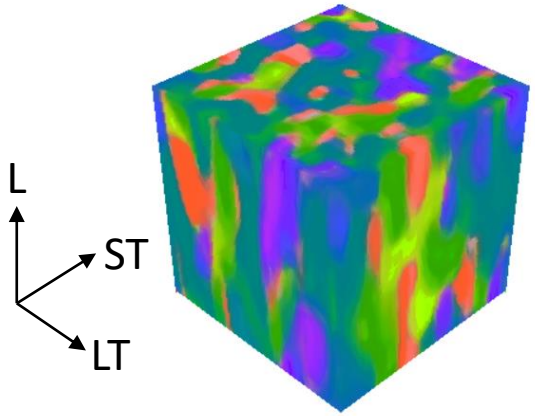
SD TD BD



(b) Rolled (Al-Li)

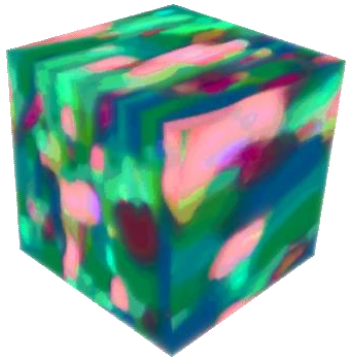


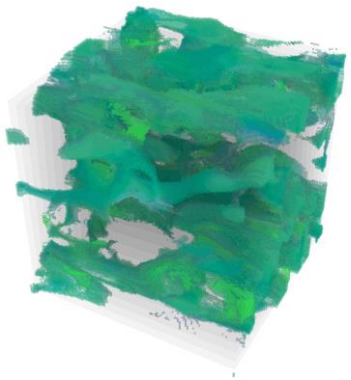
ST L LT



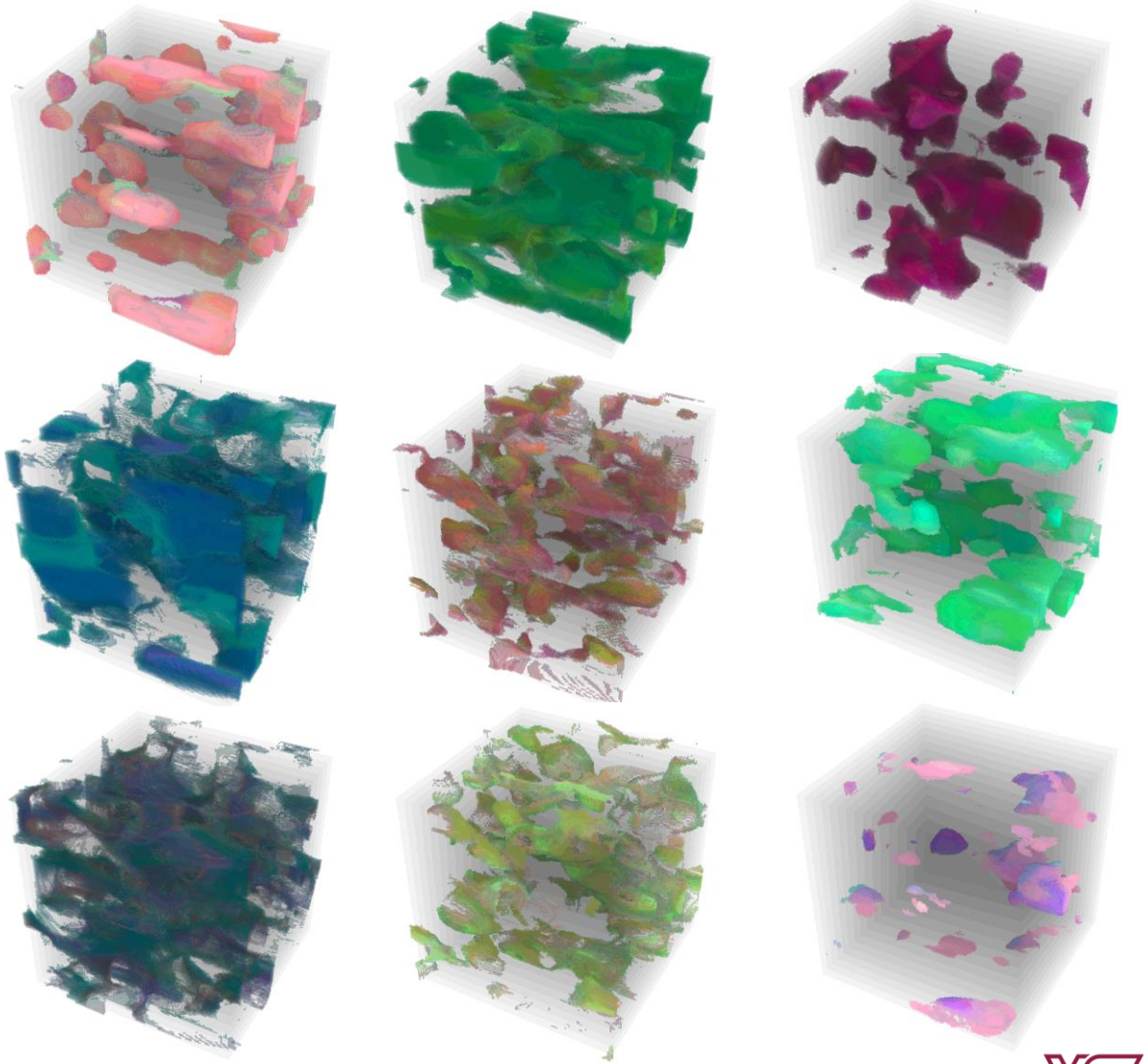
CLUSTERS

Reconstructed
3D microstructure





Clusters



MATHEMATICAL QUANTIFICATION OF MICROSTRUCTURE

- An image of N x N resolution is mathematically a matrix of N x N order
- Each element contains the pixel RGB intensity value
- For greyscale image, pixel intensity ranges from 0 – 255 with 1 channel
- For color image, pixel intensity ranges between 0 – 255 with 3 channels
- Moments are calculated for each pixel and total sum is taken as final moment value for the image. For color images, the average of total sum of three channels are taken to be the final moment value

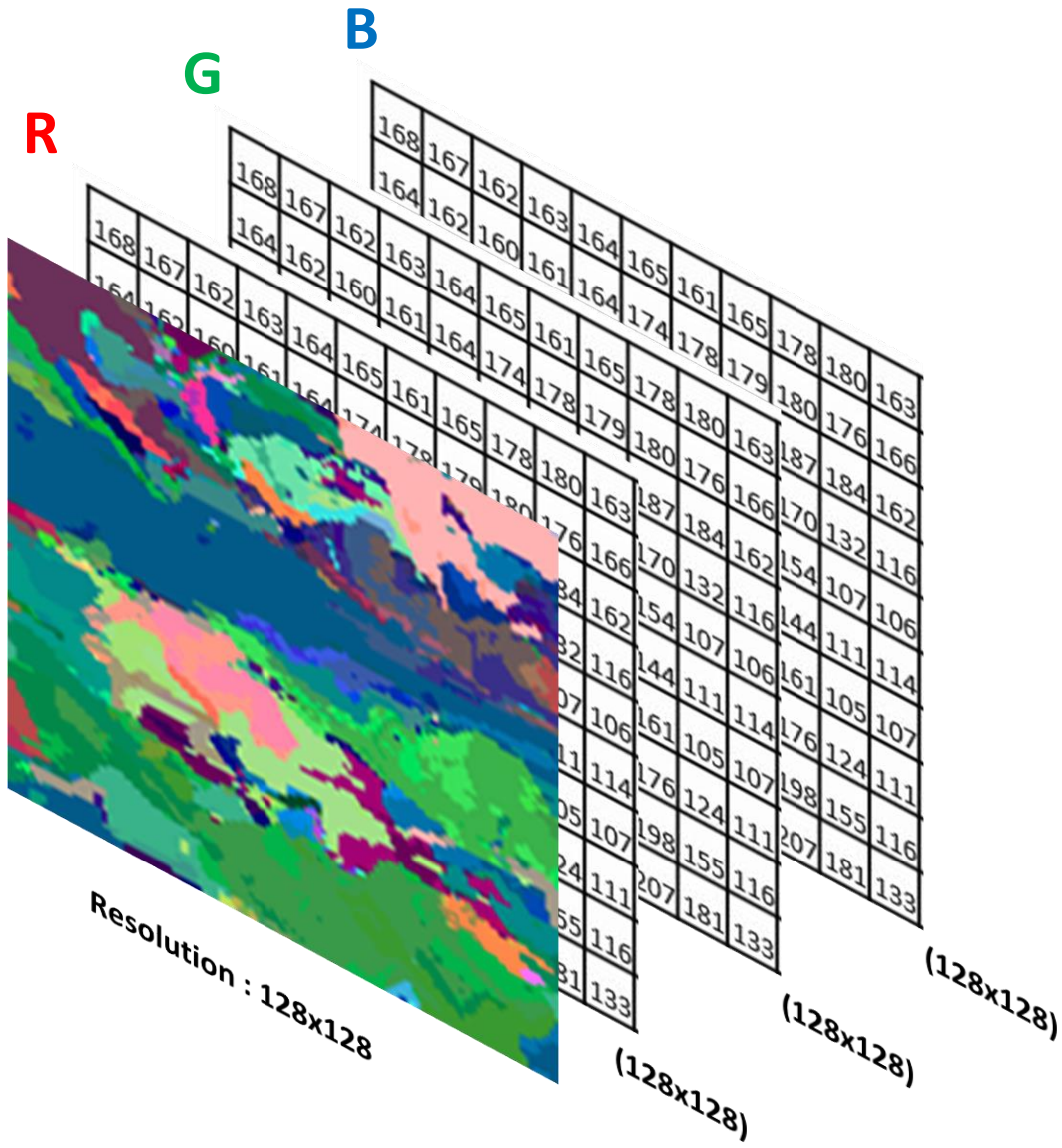


IMAGE MOMENTS

- A measure of an average weightage number based on each pixel intensity and location
- ***Types of moments:***

Raw moments

$$m_{ij} = \sum\sum x^i y^j I(x,y)$$

Centroid

$$\bar{x} = \frac{m_{10}}{m_{00}} \quad \bar{y} = \frac{m_{01}}{m_{00}}$$

Image area

$$m_{00} = \sum\sum I(x,y)$$

Expected value

$$m_{ij} = E[X]$$

(1^{st} order)

Central moments

$$\mu_{ij} = \sum\sum (x - \bar{x})^i (y - \bar{y})^j I(x,y)$$

Variance

$$\mu_{ij} = E[(X - E[X])^2]$$

(2^{nd} order)

Normalized central moments

$$\eta_{ij} = \frac{\mu_{ij}}{A^{\gamma}}, \quad \gamma = \frac{i+j+2}{2}$$

Where i, j = 0,1,2… representing order of the moment

Skewness

(3^{rd} order)

COMPARING 2D AND 3D GRAINS

- 2D and 3D grains are compared through the same measure called: Normalized central moments (η)

2D	3D
$\eta_{ij} = \frac{\sum\sum (x-\bar{x})^i (y-\bar{y})^j I(x,y)}{A^\gamma}$	$\eta_{ijk} = \frac{\sum\sum\sum (x-\bar{x})^i (y-\bar{y})^j (z-\bar{z})^k I(x,y,z)}{V^\gamma}$

$\gamma = \frac{i+j+k+2}{2}$, k=0 for η_{ij}

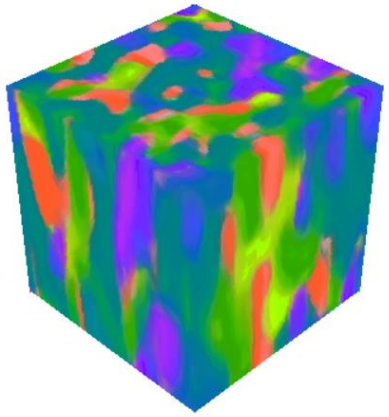
- Why?
  - Invariant to shape transformations such as scale and translation
  - Statistically equivalent to variance normalized to the image area
  - Ability to use the same parameter for both two and three dimensions

$\eta_{20} \approx \eta_{200} \approx \eta_x$ → Normalized variance in x direction

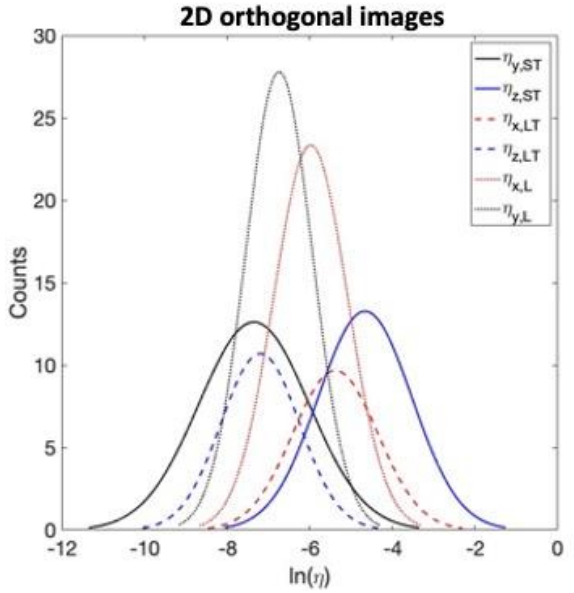
$\eta_{02} \approx \eta_{020} \approx \eta_y$ → Normalized variance in y direction

RESULTS

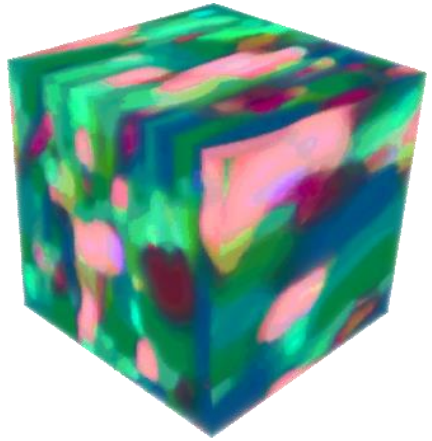
Rolled



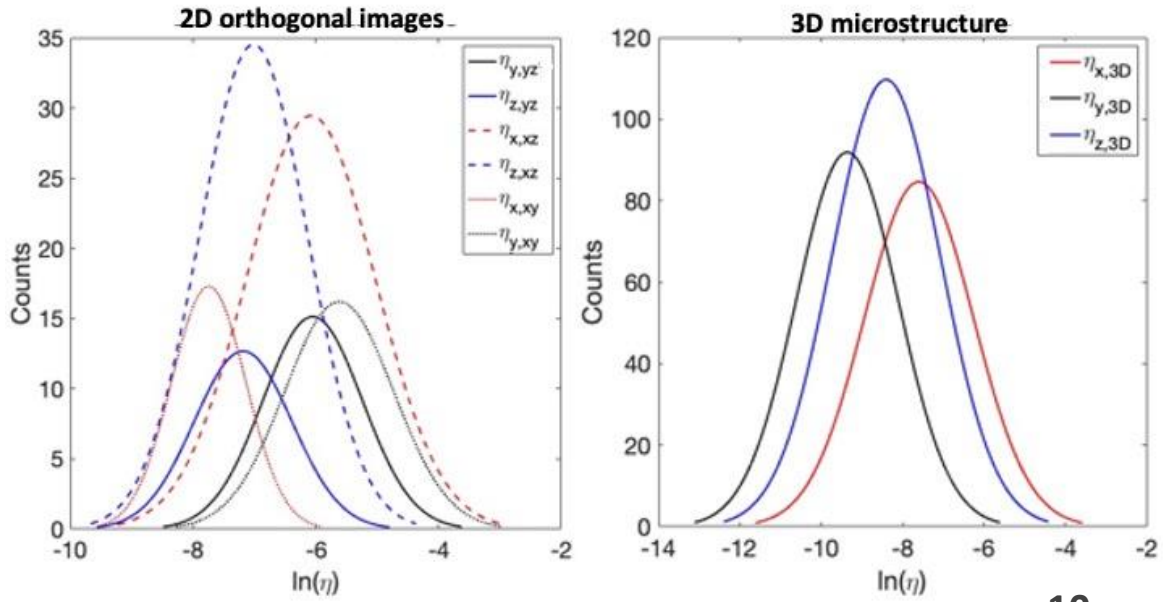




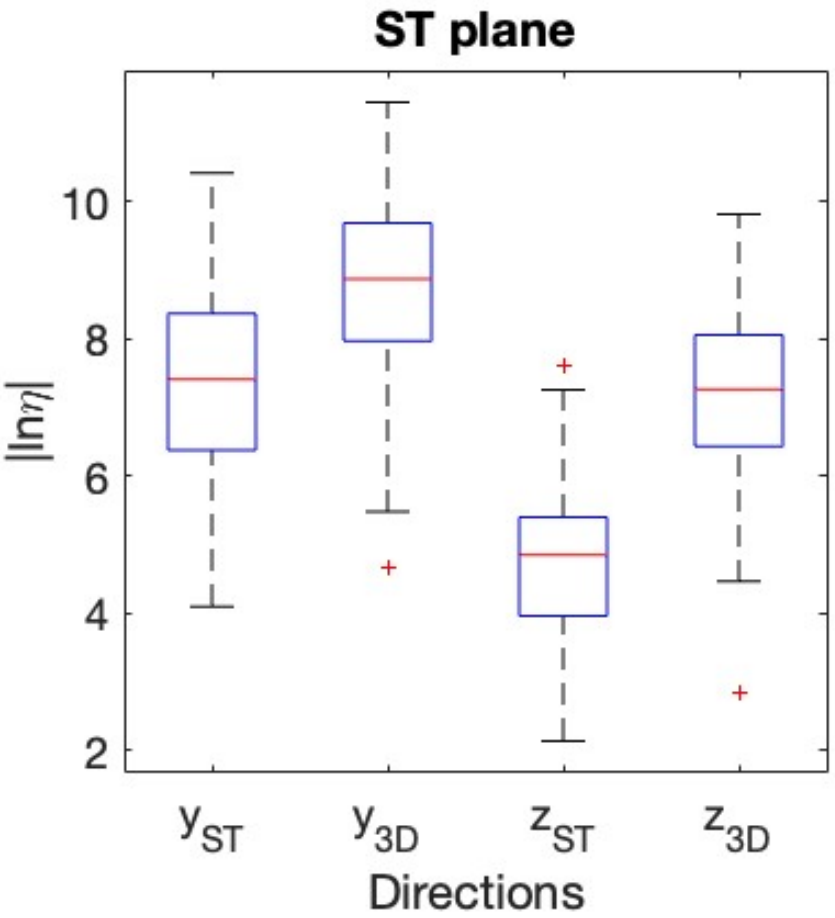
Additively manufactured

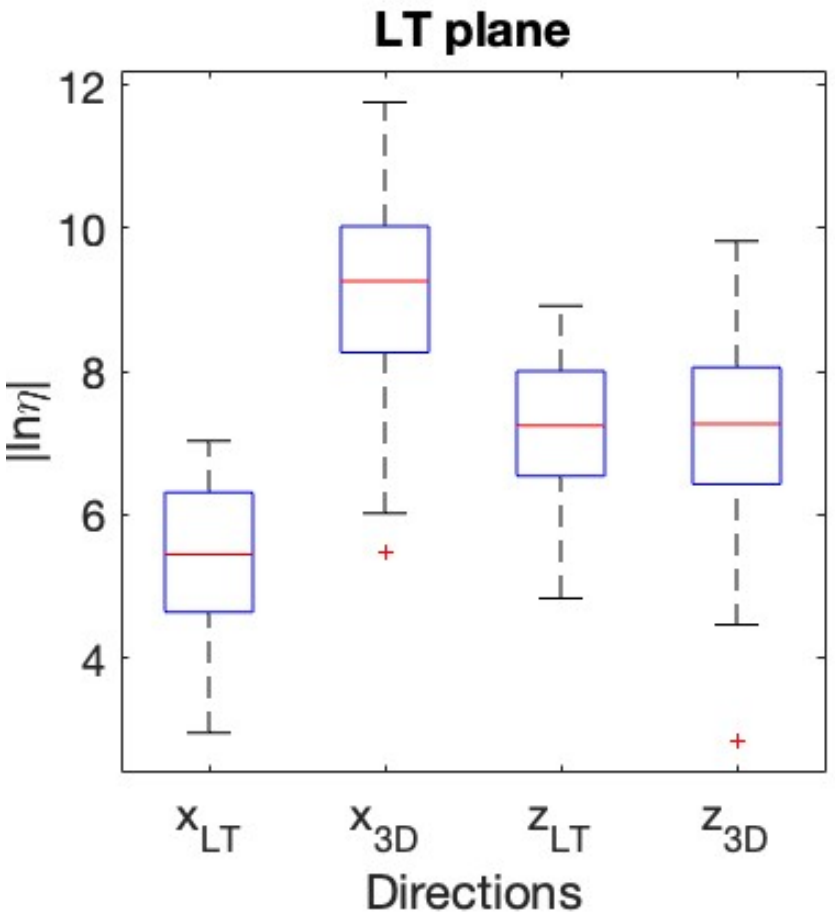


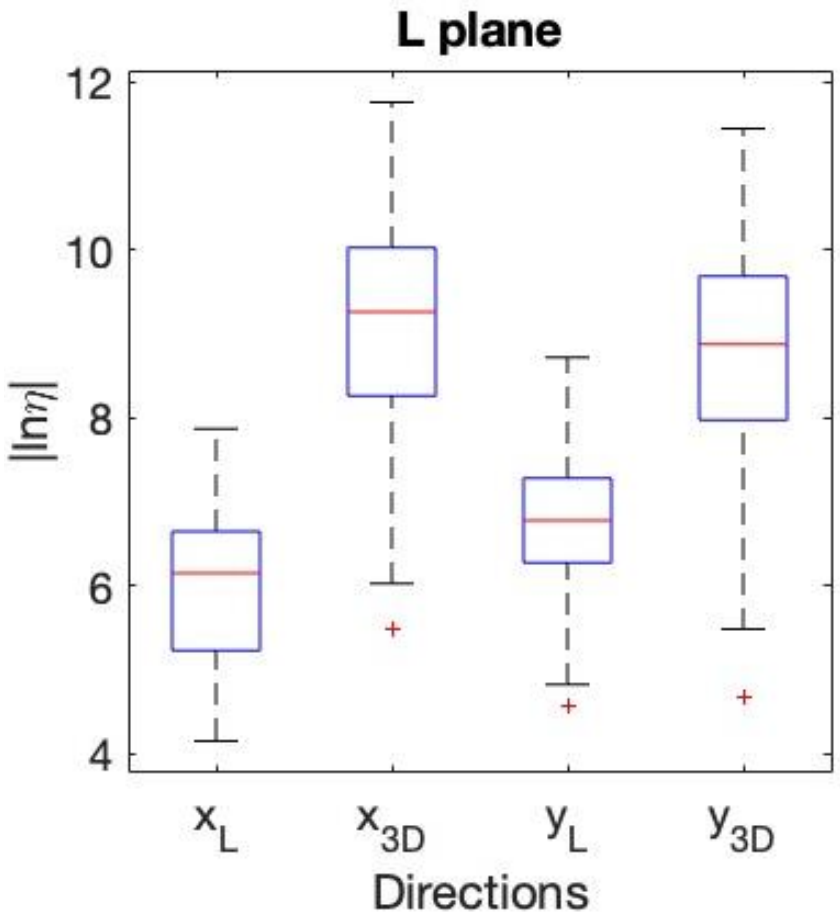




RESULTS – ROLLED

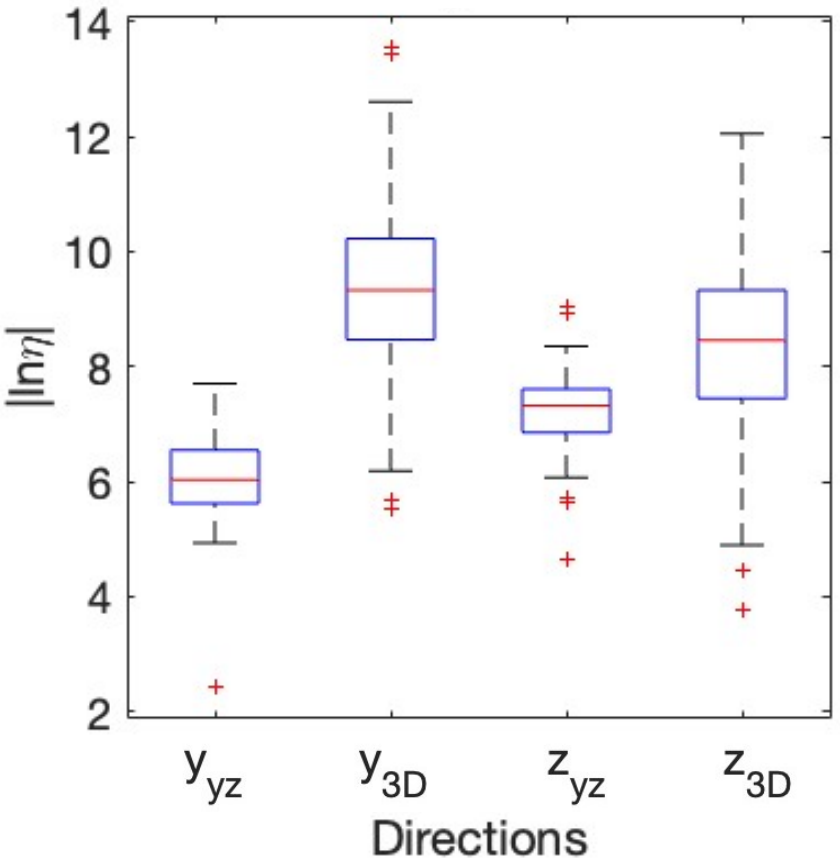




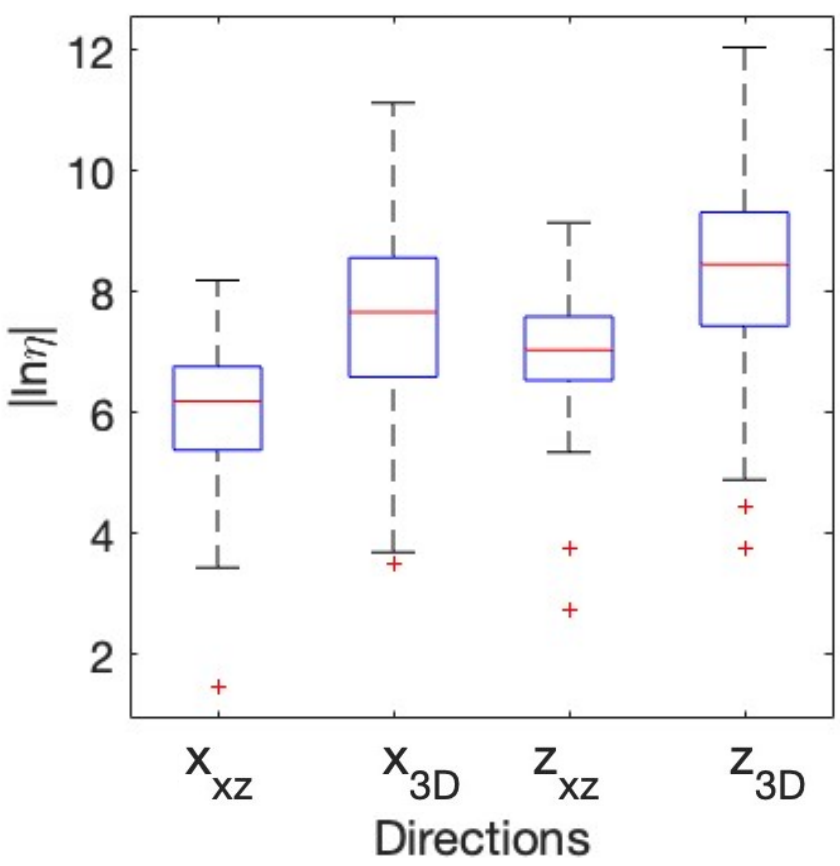


RESULTS – ADDITIVELY MANUFACTURED

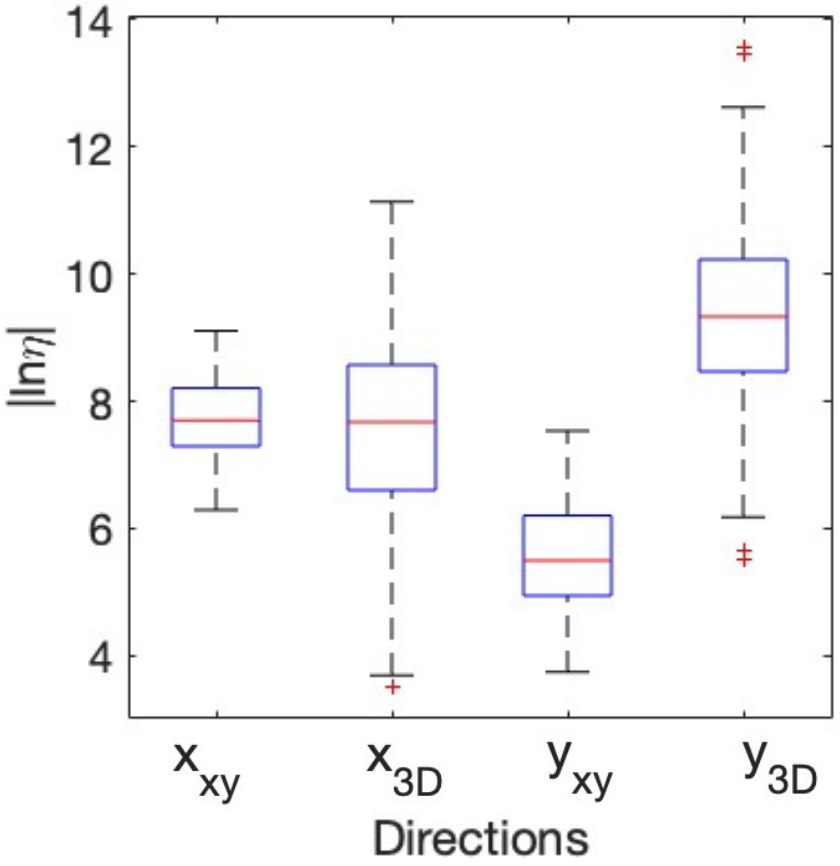
YZ plane (SD)



XZ plane (BD)



XY plane (TD)



RESULTS

		X			Y			Z		
		3D	X,xz	X,xy	3D	Y,yz	X,xy	3D	Z,yz	X,xz
Rolled	Mean	9.13848	5.380784	5.976988	8.779185	7.350776	6.743291	7.231071	4.660436	7.197765
	Std dev	1.242754	1.028651	0.89541	1.228236	1.334567	0.808697	1.164793	1.13509	0.951241
	Variance	1.544438	1.058122	0.80176	1.508564	1.78107	0.65399	1.356743	1.288429	0.90486
Additively manufactured	Mean	7.595243	6.080227	7.747056	9.357121	6.049683	7.747056	8.402375	6.049683	6.080227
	Std dev	1.339053	1.051975	0.608671	1.251892	0.811646	0.608671	1.330783	0.811646	1.051975
	Variance	1.793062	1.106652	0.370481	1.567235	0.65877	0.370481	1.770984	0.65877	1.106652

SUMMARY

- 3D microstructures are reconstructed from a set of three orthogonal 2D images using the Markov random field (MRF) algorithm
- The microstructure data is characterized by normalized central moments that are invariant to the scale and translation of shapes
- Graphical methods based on a common metric are developed to compare 2D and 3D grains of the anisotropic microstructure
- ***Future work*** will involve generating additional synthetic anisotropic microstructures in order to understand the uncertainty propagated into the microstructure

ACKOWLEDGEMENTS

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Thank you

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