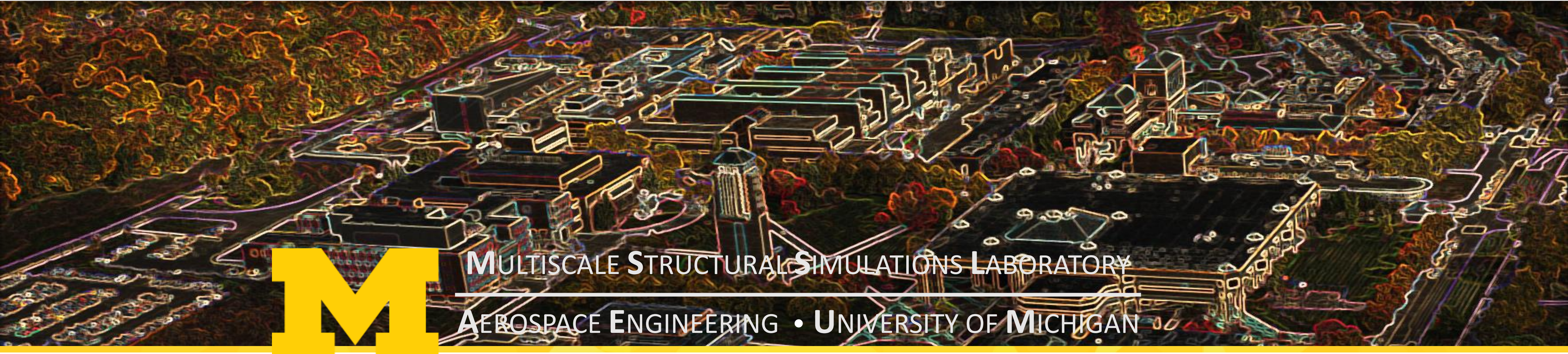

Generation of Large-Scale 3D Microstructures from Surface Images: Application to Additive Manufacturing

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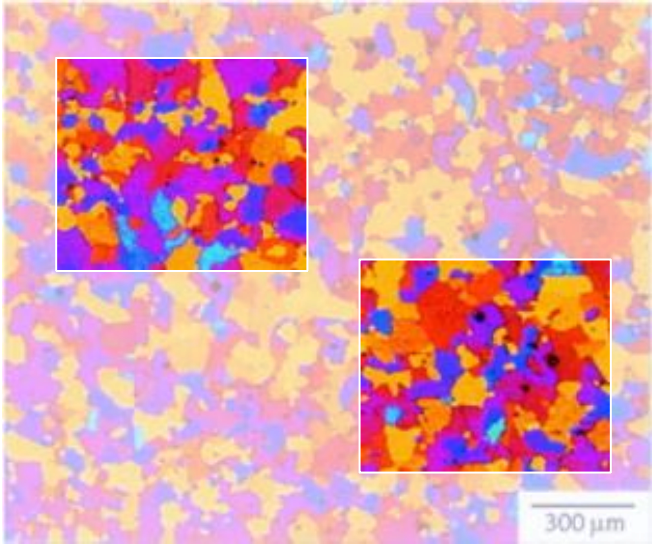
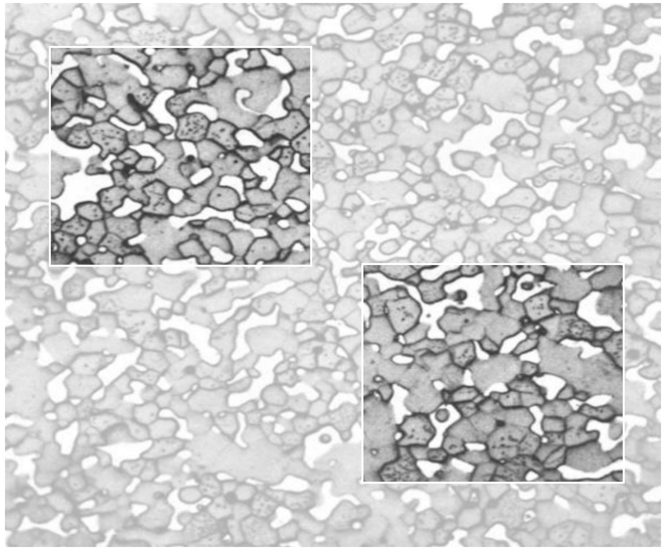
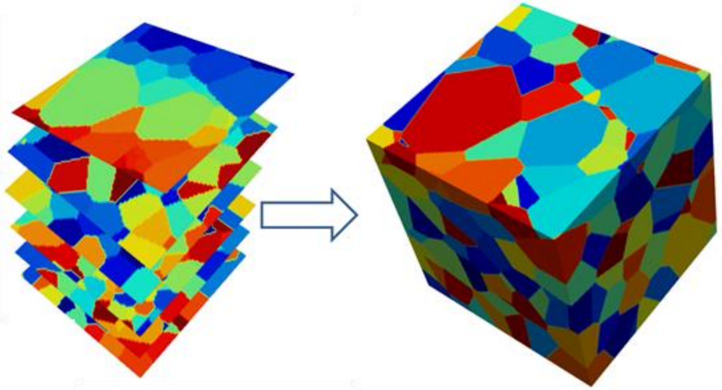
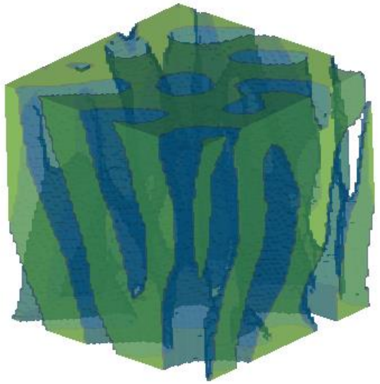
Background

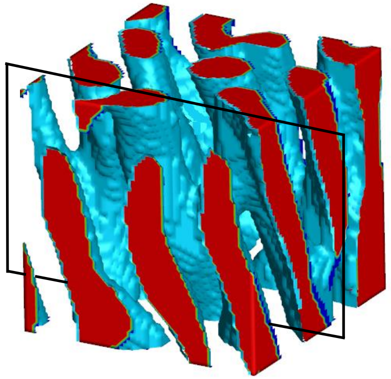
- Explore the notion of **stationary probability distribution** i.e., *Markov Random Fields (MRF)*:
  - Different windows on a 2D microstructure '*look-alike*'
  - Different sections on a 3D microstructure '*look-alike*'
- Reconstruction of 3D synthetic microstructural unit cells from orthogonal 2D images taken along x-, y-, and z- directions
- *Applications*:
  - Generation of larger synthetic images from small experimental exemplars
  - Reconstruction of large-scale *Computer Aided Design* (CAD) models with microstructural information using knowledge of grain formation
  - Analysis of process-property-microstructure relationships



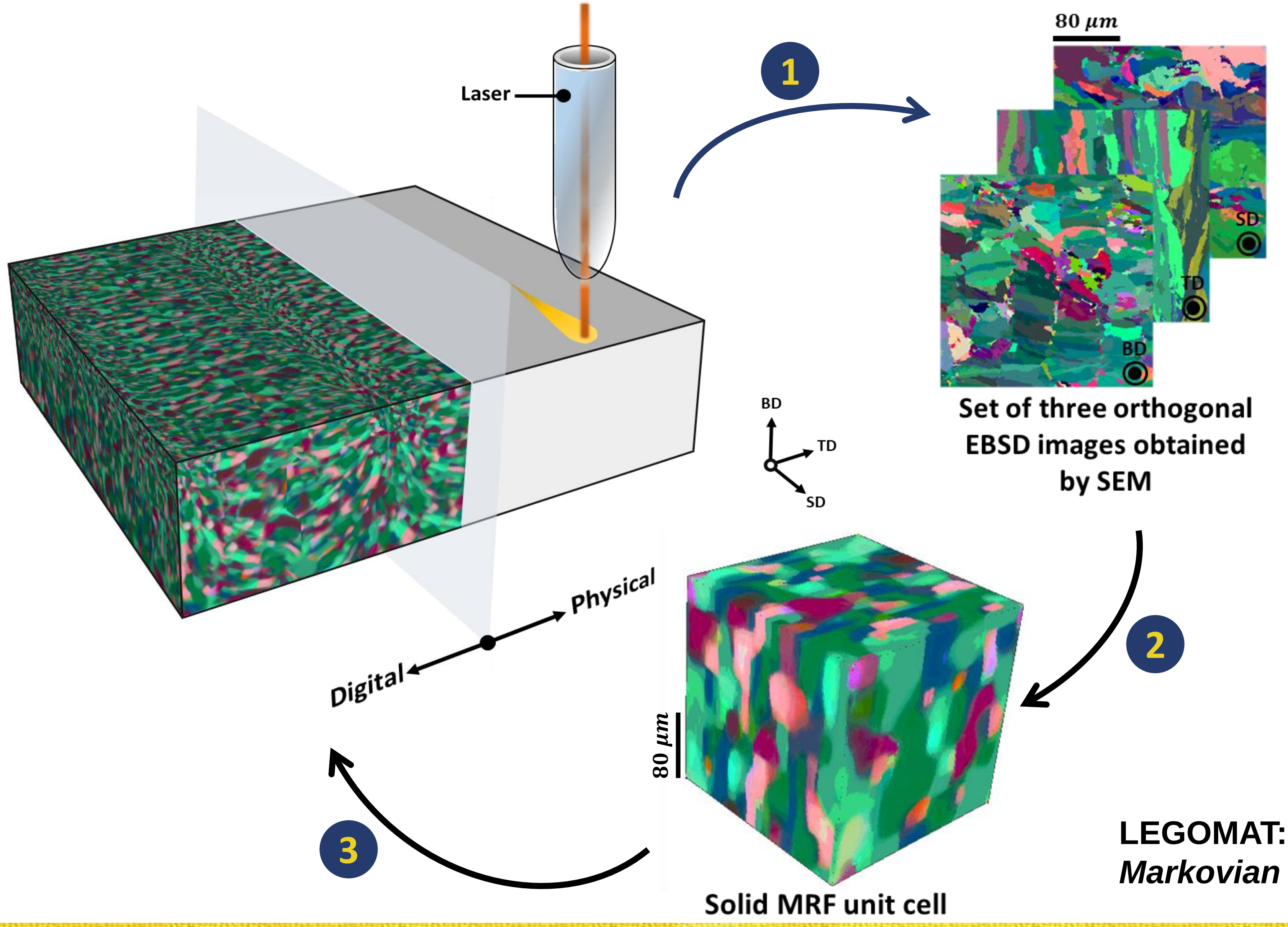








Overview



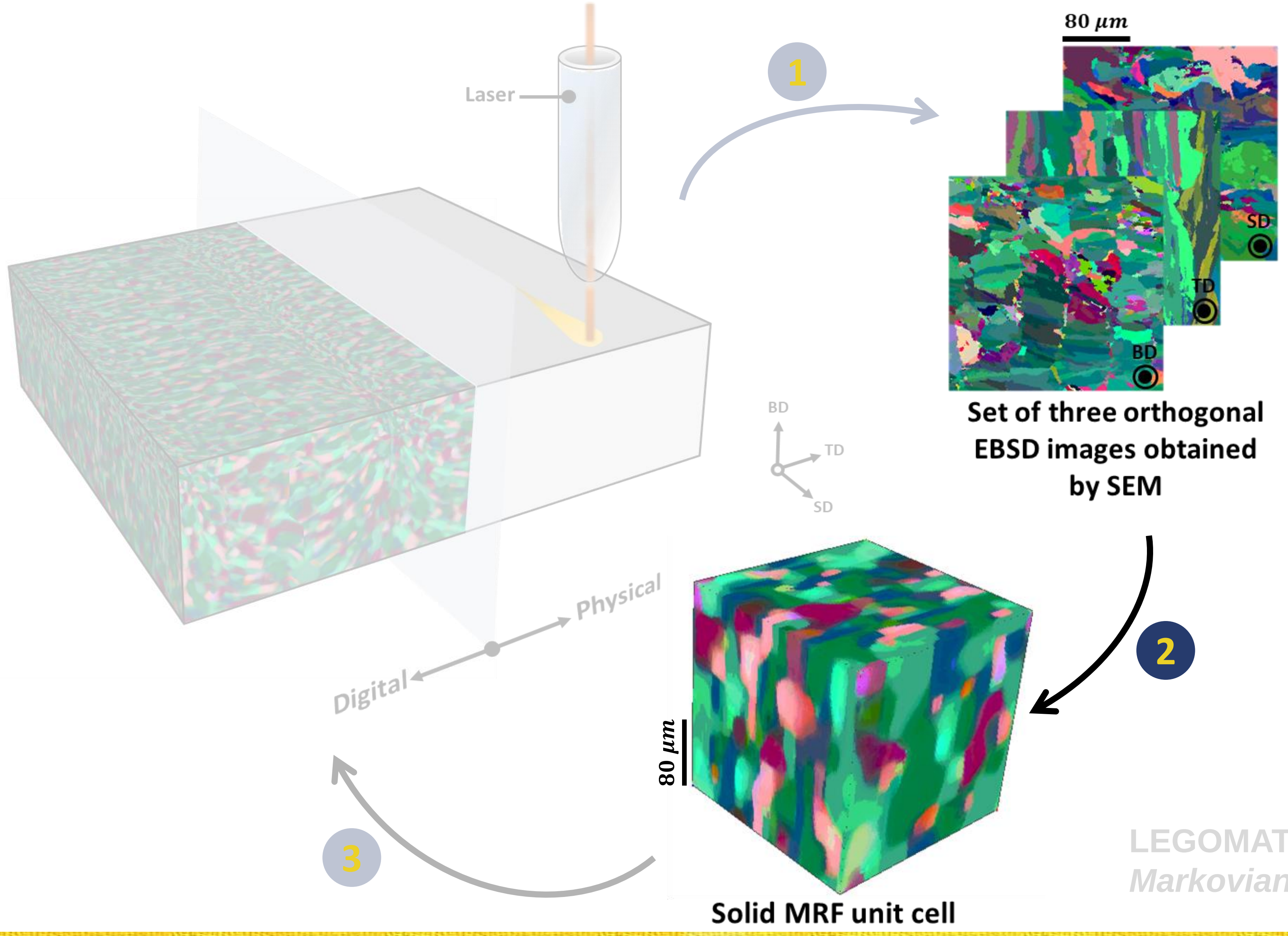
1. *Experimental EBSD imaging*

2. *Unit cell reconstruction algorithm*: 3D reconstruction from orthogonal surface images

3. *LEGOMAT algorithm*: embedding unit cell microstructure in part-scale geometries

LEGOMAT: ***Locally-Extracted Globally-Organized Markovian Material Models***

Unit Cell Reconstruction



1. *Experimental EBSD imaging*
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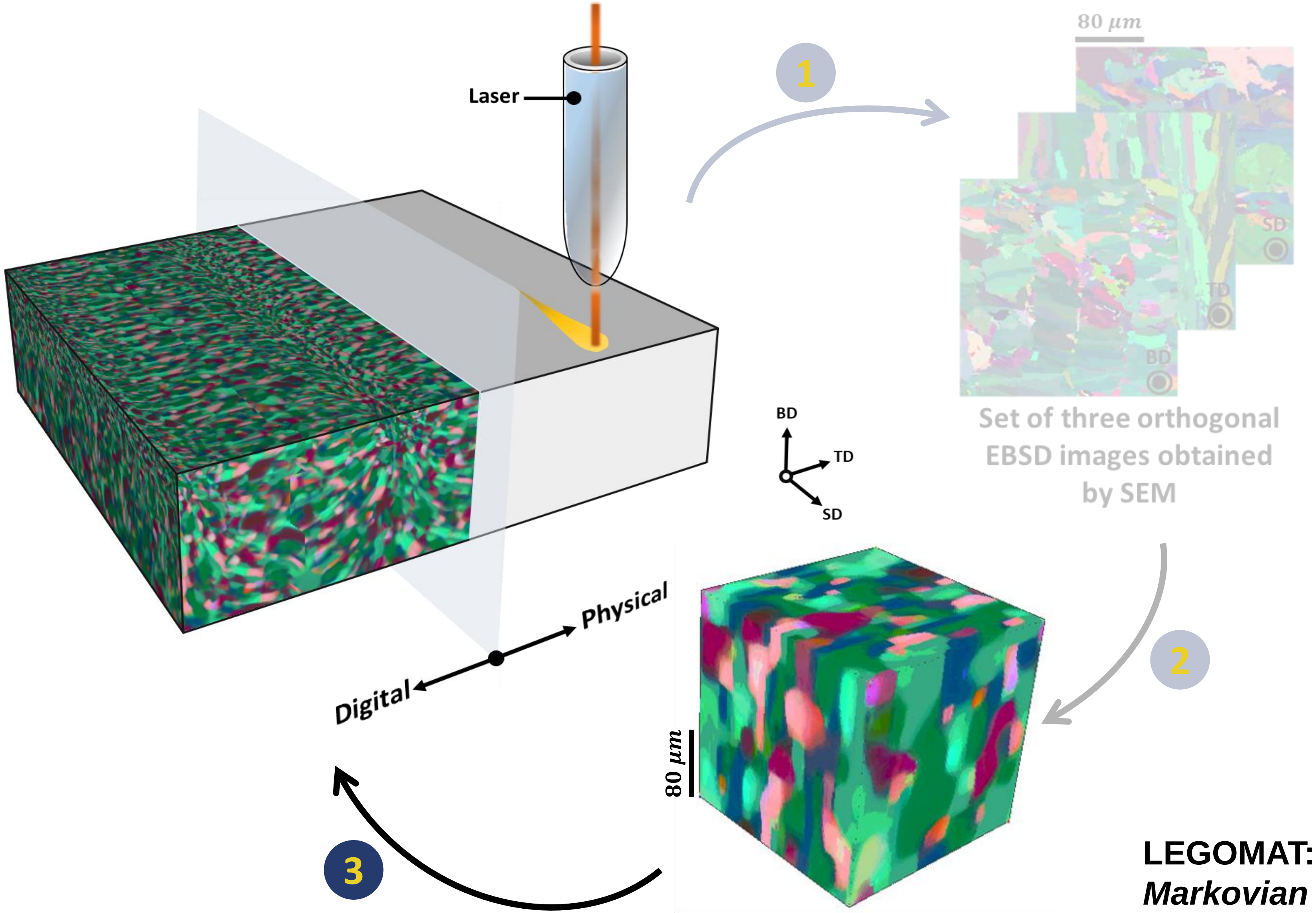
LEGOMAT: *Locally-Extracted Globally-Organized Markovian Material Models*

Large-Scale Generation



1. *Experimental EBSD imaging*
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LEGOMAT: *Locally-Extracted Globally-Organized Markovian Material Models*

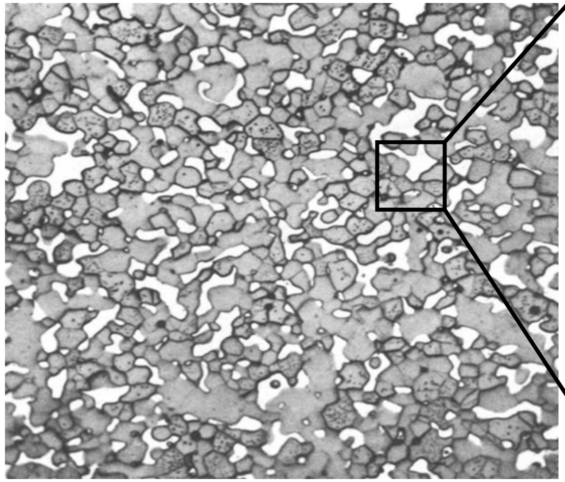
2D Markov Random Field

- Microstructures represented as *MRF* models (i.e., undirected graphs):
  - A set of n neighbors '*adequately*' determines the probability of the *unknown/center* pixel

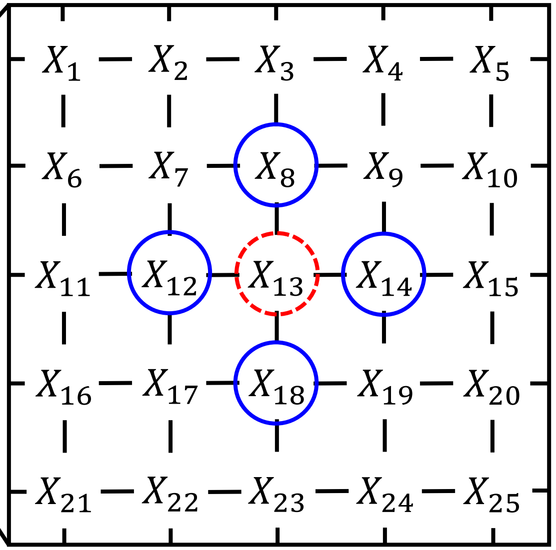
$$\mathbb{P}(X_{13}|X_8, X_{12}, X_{14}, X_{18}) \approx \mathbb{P}\left(X_{13}\middle|X_1, X_2, \dots, X_{N^2}\right)$$

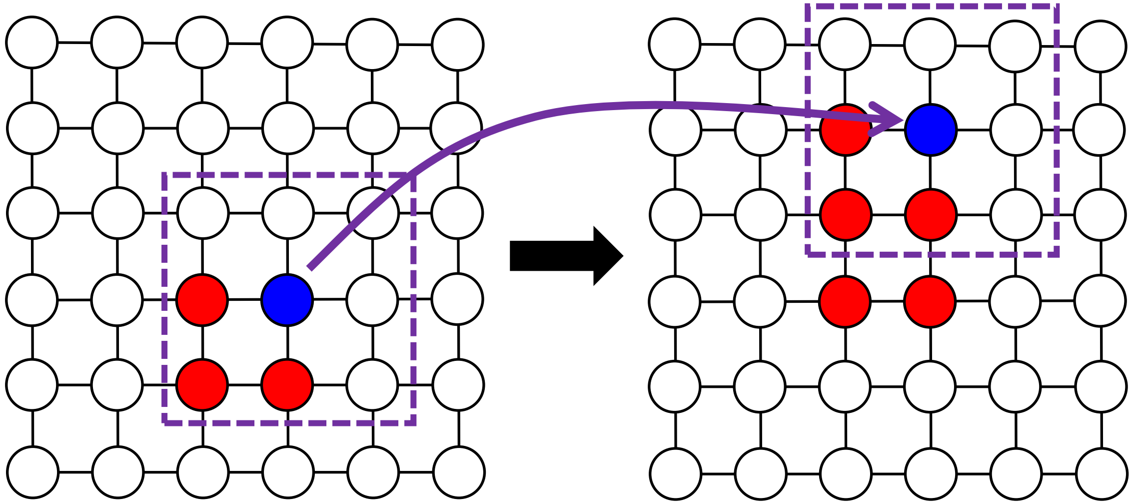
  - Building explicit probability tables from experimental exemplars is intractable, especially for higher-order interactions

W-Ag Composite from S. Umekawa (1965)



Ising Model (1st Order Interaction)





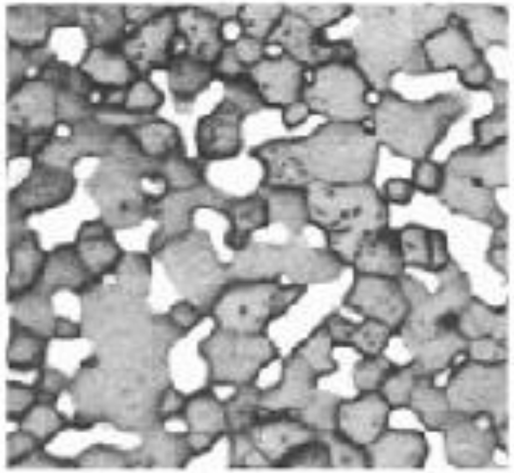
Experiment Exemplar **Synthetic Image**

- <u>Harder problem</u>: given the experimental exemplar, generate a new synthetic image of the same size:
  - Start from a small '*seed image*' and '*fill in*' the unknown pixel based on its known neighbors:

$$\mathbb{P}(X_i|\text{known neighbors}) = ?$$

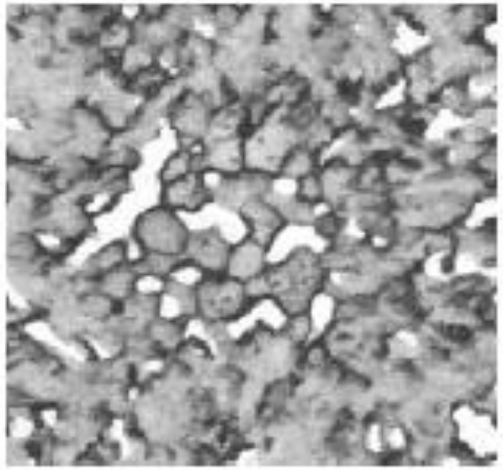
  - Iterate until convergence i.e., colors remain unchanged

Sampling Window Size

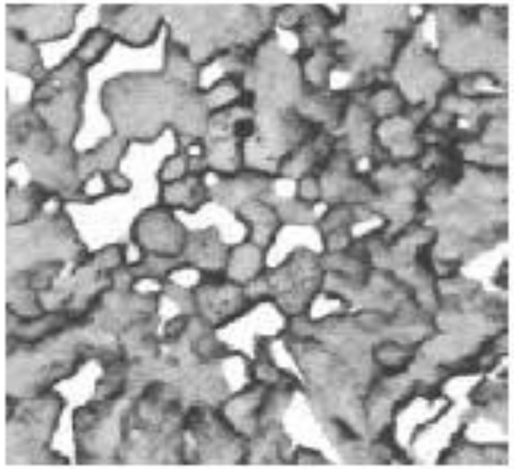


Exemplar

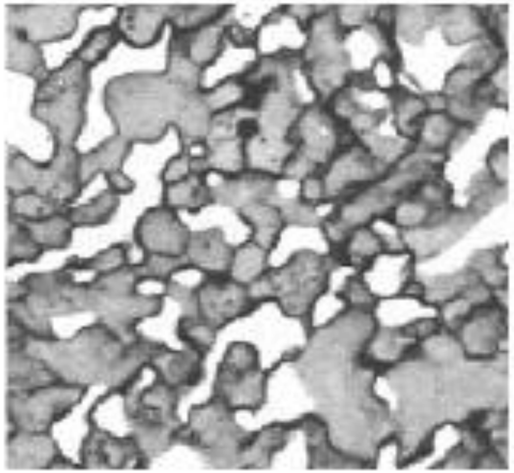
Window Size 3x3



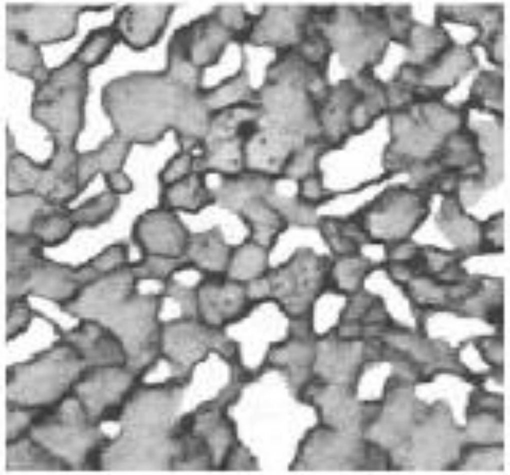
Window Size 5x5



Window Size 7x7



Window Size 9x9



Window Size 11x11

3D Reconstruction Formulation

- The 3D microstructure is to be synthesized by solving the following ℓ_2 optimization problem:
  - Where $\omega^i_{v,u}$, $\boldsymbol{V}^i_{v,u}$, and $\boldsymbol{S}^i_{v,u}$ denote the weight, color of voxel u in neighborhood of $\boldsymbol{V}^i_{\boldsymbol{v}}$, and color of pixel u in neighborhood of $\boldsymbol{S}^i_{v}$, respectively

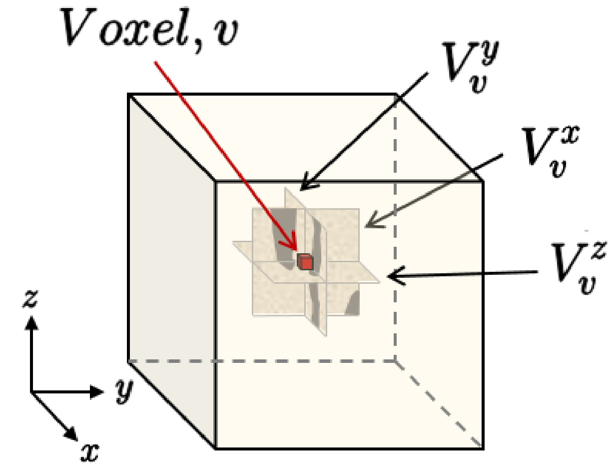
$$E(\boldsymbol{V}) = \sum_{i\in\{x,y,z\}} \sum_{v} \sum_{u} \omega^i_{v,u} \left\| \boldsymbol{V}^i_{v,u} - \boldsymbol{S}^i_{v,u} \right\|^2$$

- Each iteration for the optimization problem is carried out in two steps:
  - *Searching Step:* Minimize the *cost function* w.r.t. the set of input neighborhoods, $\boldsymbol{S}^i_v$. Here, the ***best-matching neighborhood*** of voxel v, along each orthogonal direction is identified by solving the following:

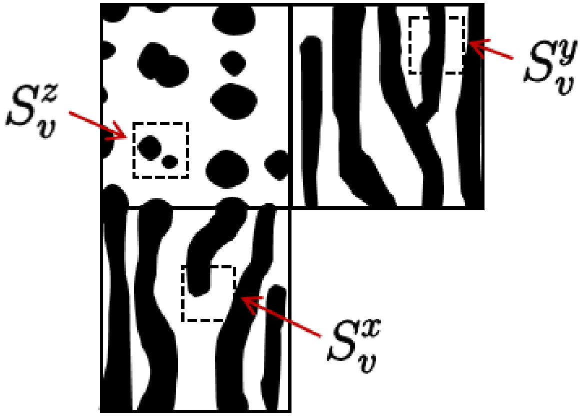
$$\boldsymbol{S}^i_v = \arg\min_{\boldsymbol{S}^{i,w}} \sum_{u} \omega^i_{v,u} \left\| \boldsymbol{V}^i_{v,u} - \boldsymbol{S}^{i,w}_u \right\|^2$$

  - *Expectation Step*: Minimize the *cost function* w.r.t. $\boldsymbol{V}_{\boldsymbol{v}}$. In this step a ***unique value*** for the voxel v is found:

$$V_v = \Big(\sum_{i\in\{x,y,z\}} \sum_{u} \omega^i_{u,v} \boldsymbol{S}^i_{u,v} \Big) \Big/ \Big(\sum_{i\in\{x,y,z\}} \sum_{u} \omega^i_{u,v} \Big)$$



Synthetic Unit Cell (Output)

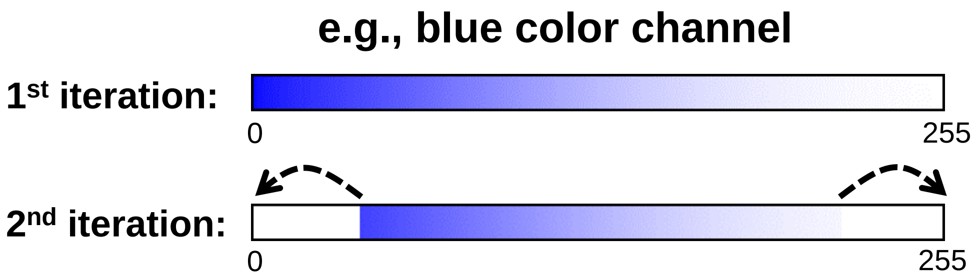


Orthogonal Exemplars (Input)

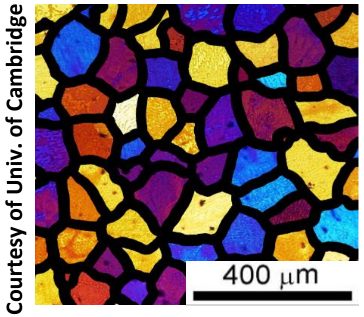
Javaheri et al., CAD, 120 (2020)

Histogram Matching

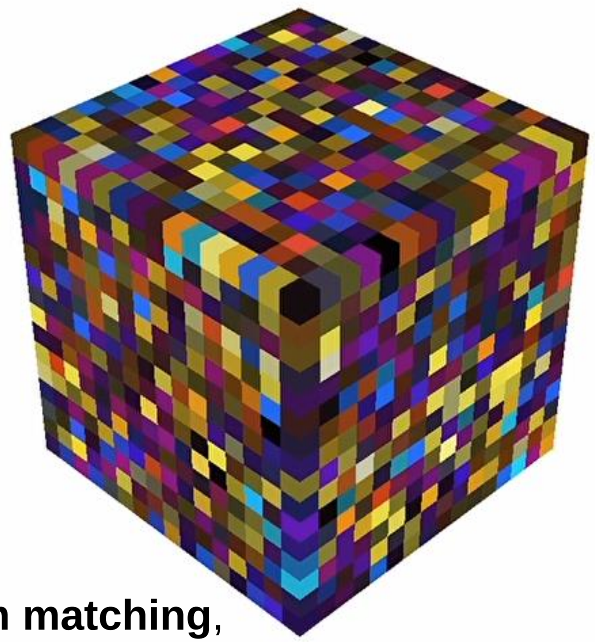
- The *Expectation Step* tends to shrink the *Red-Green-Blue* (RGB) color levels. ***Histogram matching*** is performed after every iteration such that color levels are stretched back properly



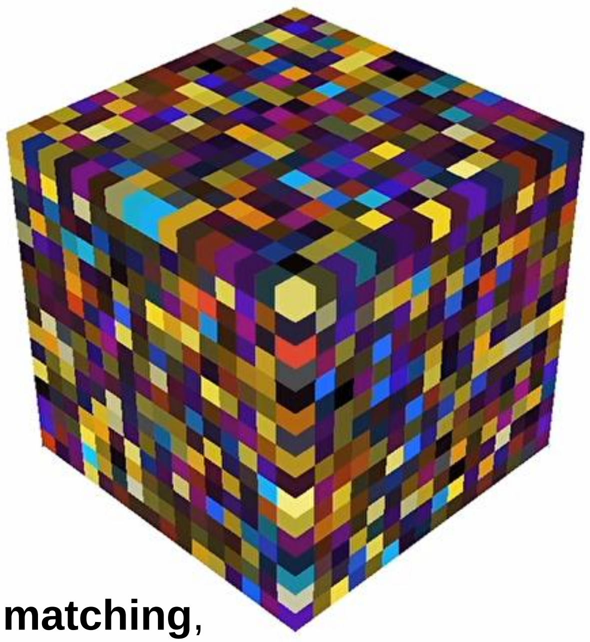
- Histogram matching modifies the MRF algorithm's color density such that the ***cumulative distribution function* (CDF)** of each color channel matches with the input exemplars after every iteration



Input Exemplar
Al-Mg-Fe-Si alloy (cross-polarized light microscopy)



Without histogram matching, the color space shrinks, phase information is lost

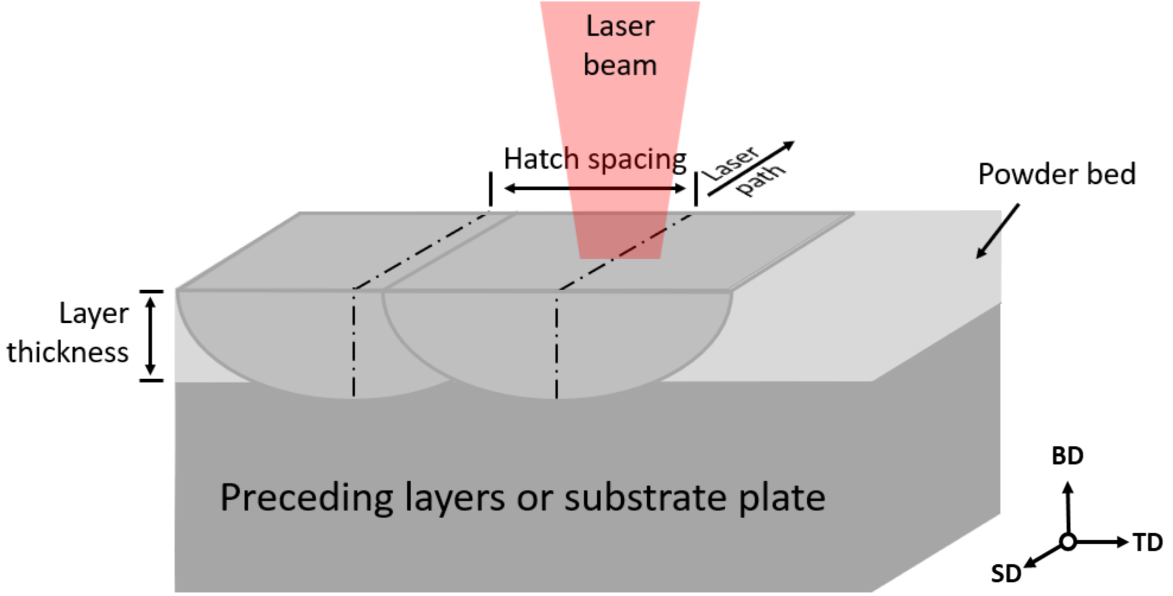


With histogram matching, the color space remains consistent with input exemplar

Additive Manufacturing (AM)

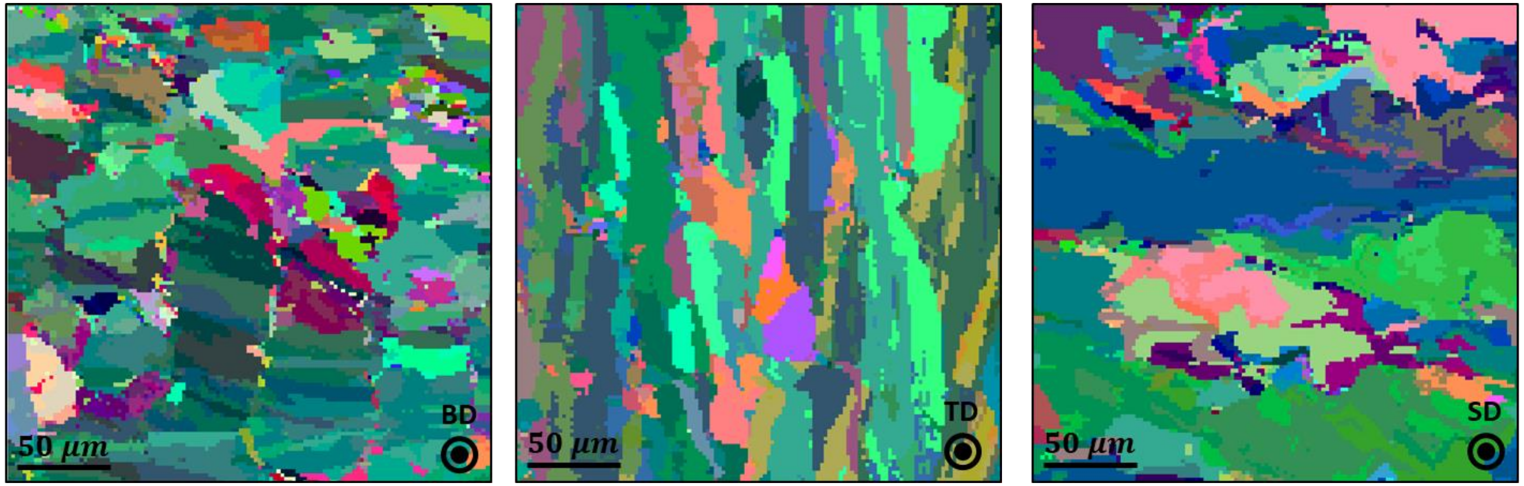
- *Process*: *Selective Laser Melting* (SLM)
- *Material*: 316L stainless steel

- *Process Parameters*:
  - Effective laser power: $200\ W$
  - Layer thickness: $30\ \mu m$
  - Scan velocity: $800\ \frac{mm}{s}$
  - Hatch spacing: $120\ \mu m$
  - Zig-zag rastering pattern



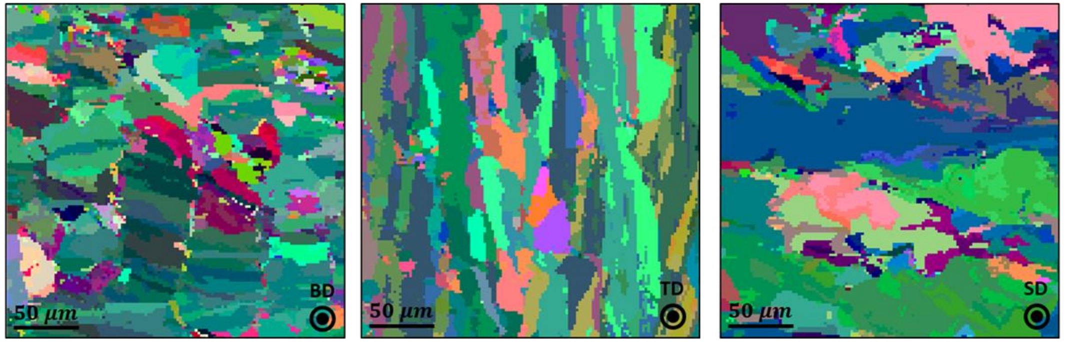
Laser Powder-Bed Fusion (LPBF) manufacturing process

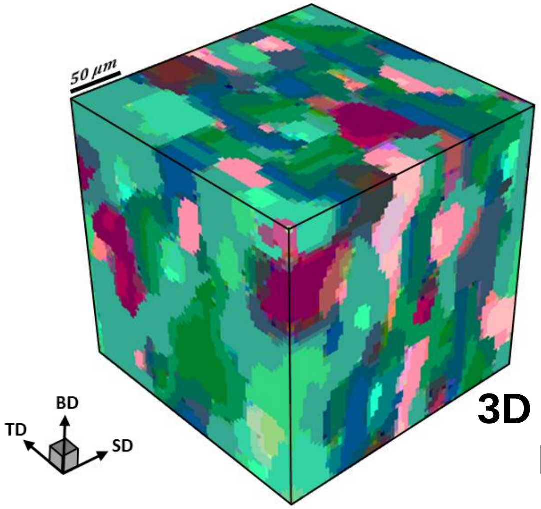
Orthogonal EBSD exemplars obtained by SEM:



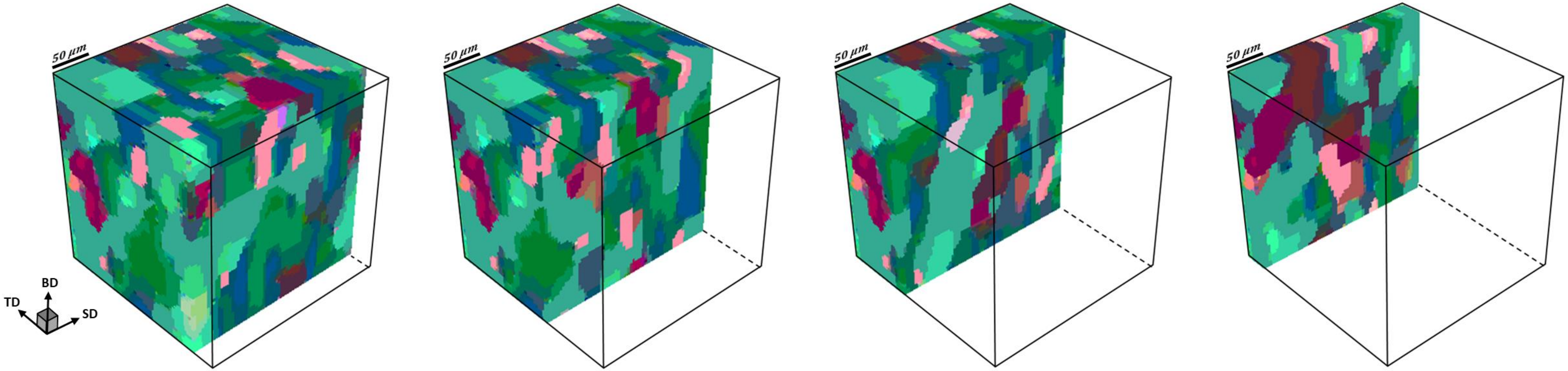
3D Reconstruction of AM

Orthogonal EBSD exemplars





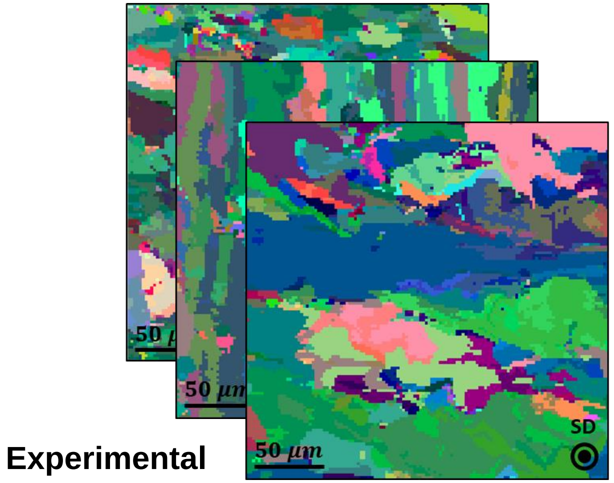
3D reconstructed MRF model

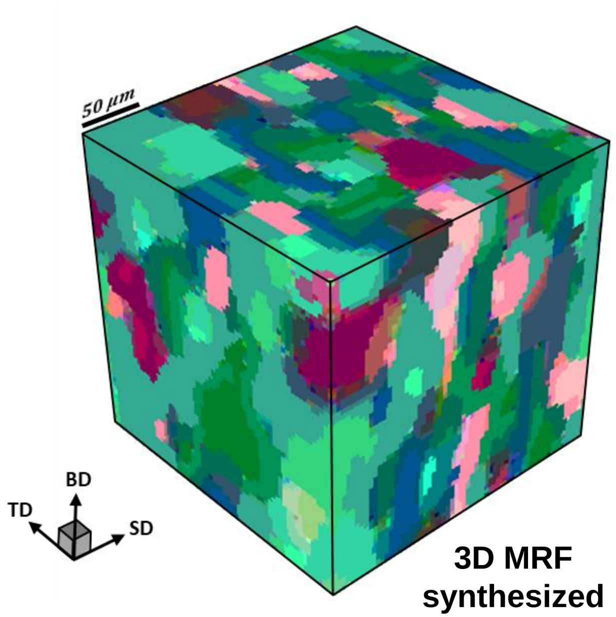


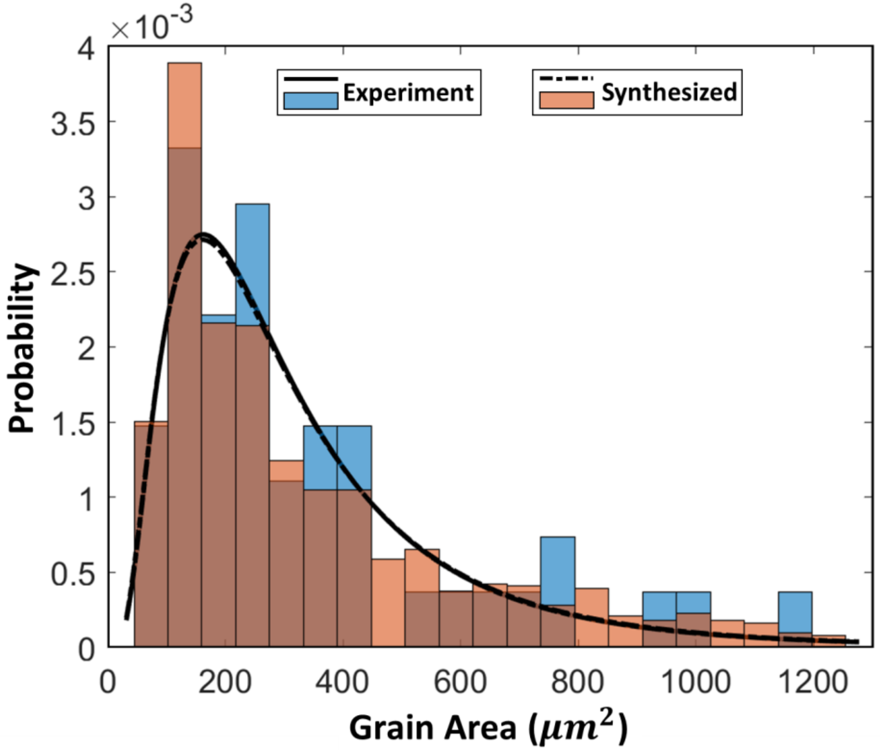
Cross-sections of MRF model

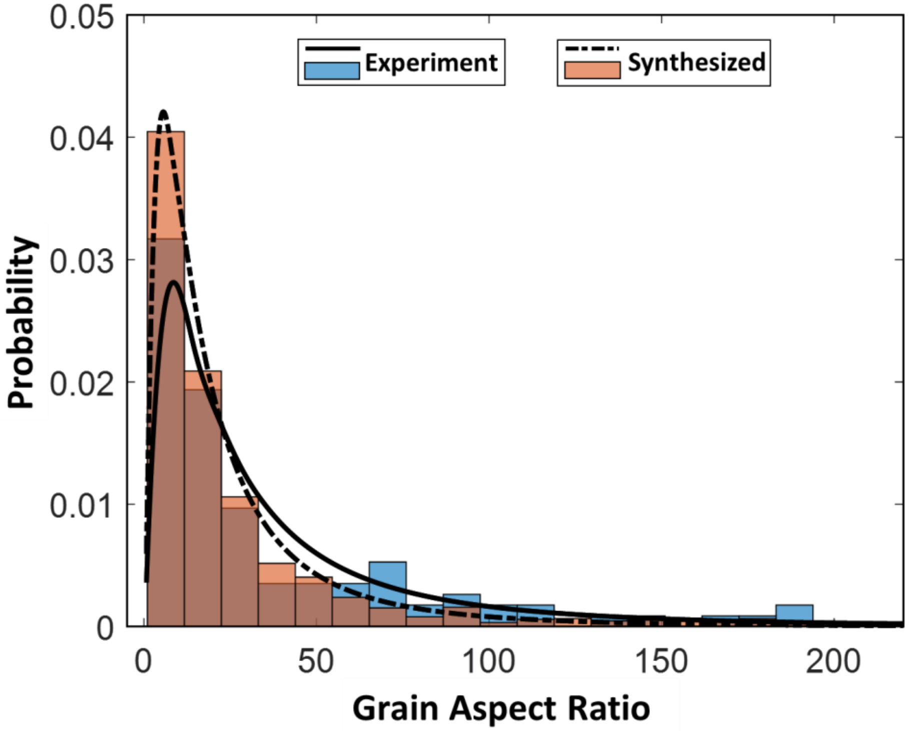
Grain Size Distribution

- Remove incomplete grains along the external borders of the image
- Aspect ratio computed by measuring the ratio of major over minor diameters
- Ratios near 1 represent near-circular (i.e., equiaxed), while values close to ∞ mimic needle-like cross-sections



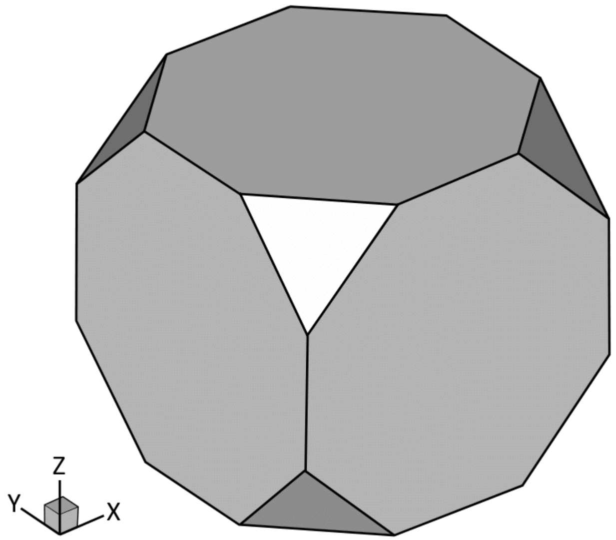




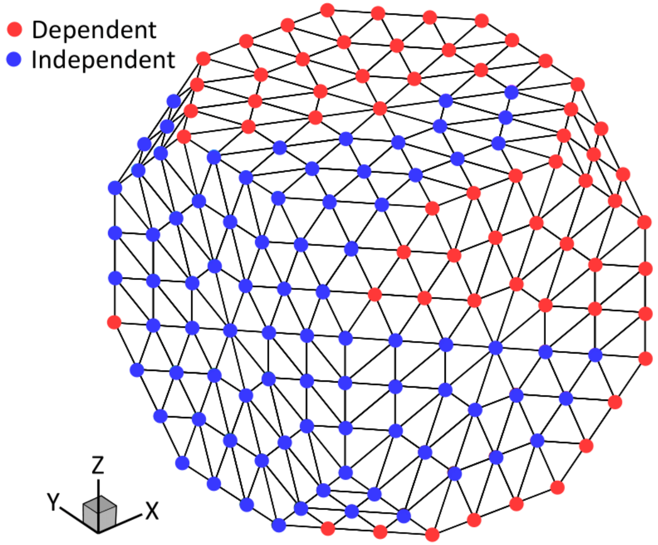


Modeling Crystal Orientation

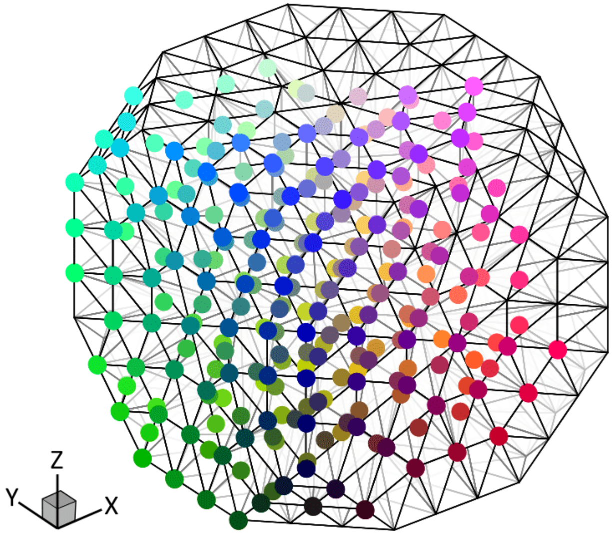
- Textures colored according to the **nearest nodes** in the orientation space (i.e., Rodrigues space)
- Nearest node may not be independent, so a symmetry map is used
- Number of colors in an *Electron Backscatter Diffraction* (EBSD) image controlled by the discretization of the fundamental region



Fundamental Rodrigues space for cubic lattice structure

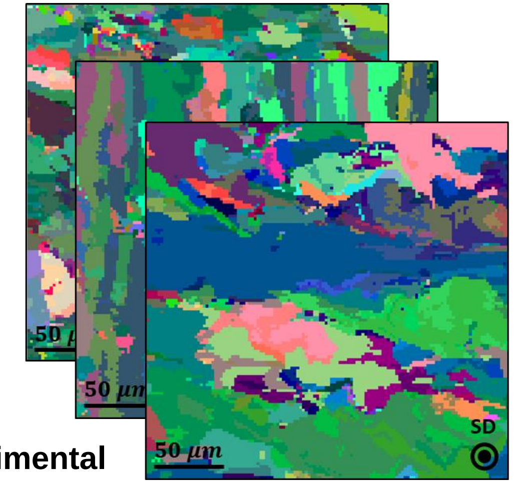


399 nodes, 254 independent nodes

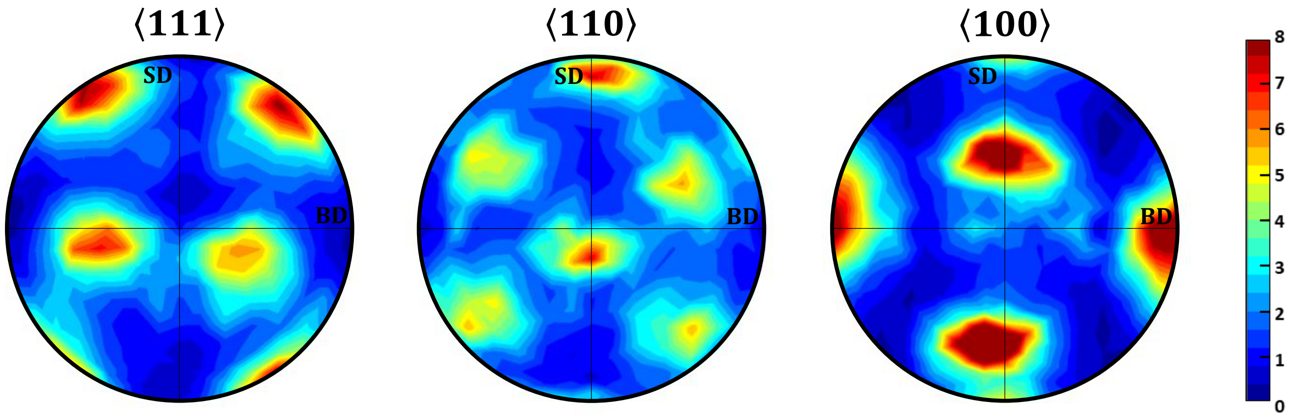


Texture coloring based on distances in fundamental region

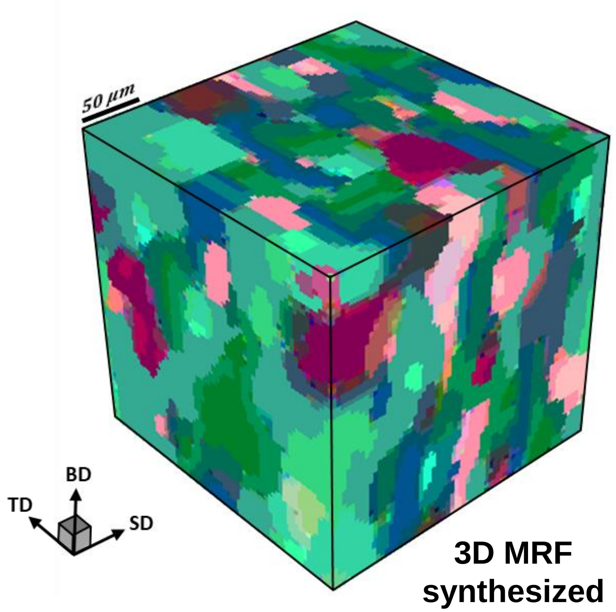
Orientation Distribution



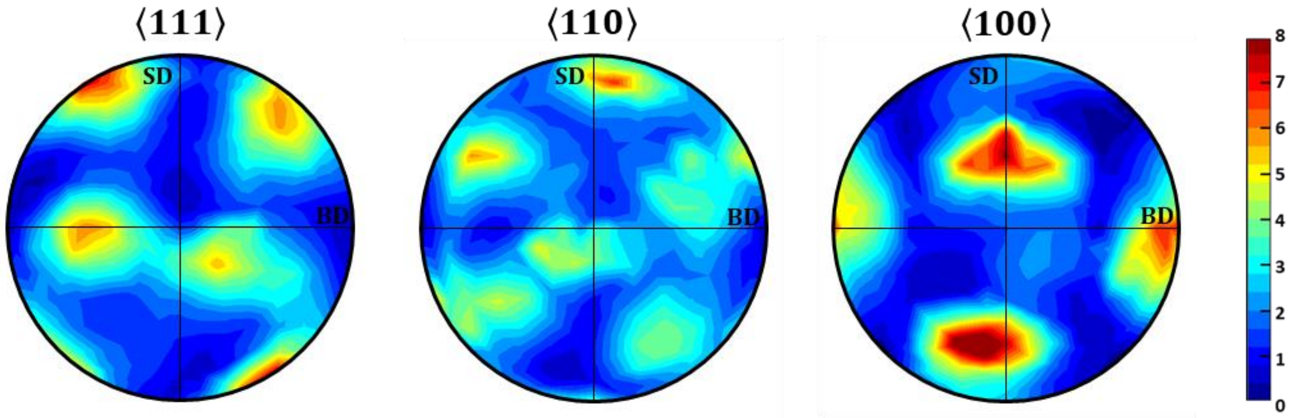
Experimental



Texture (experiment)



3D MRF synthesized



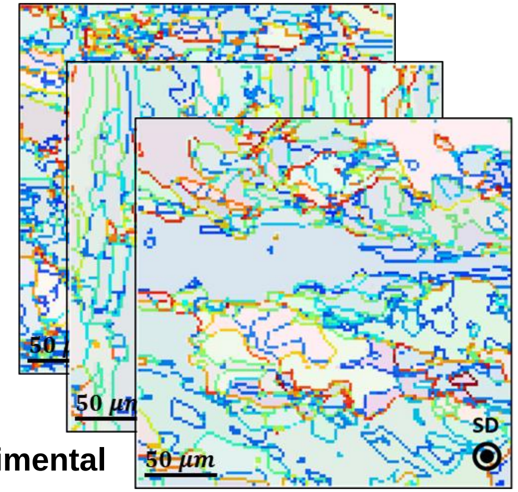
Texture (MRF reconstruction)

Misorientation Distribution

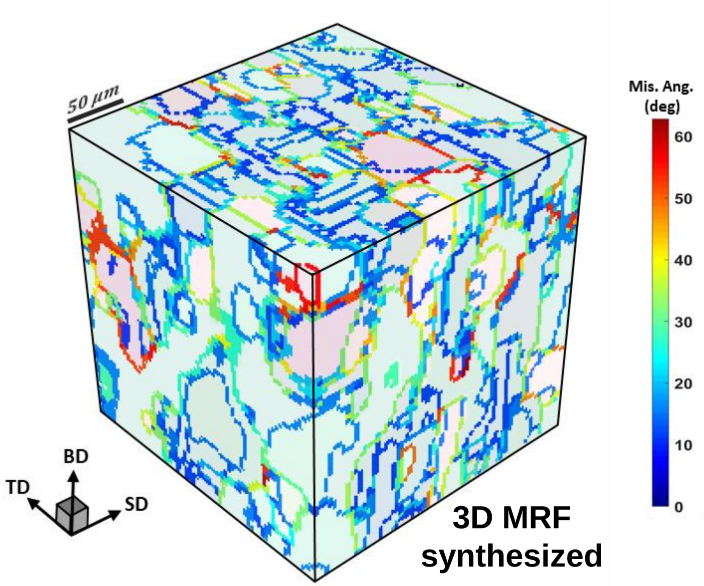
- Misorientation angle is defined as the required angle ϕ to bring the two neighboring grains into coincidence about an axis common to both lattices

$$2\cos\phi + 1 = \mathrm{tr}(\boldsymbol{M})$$

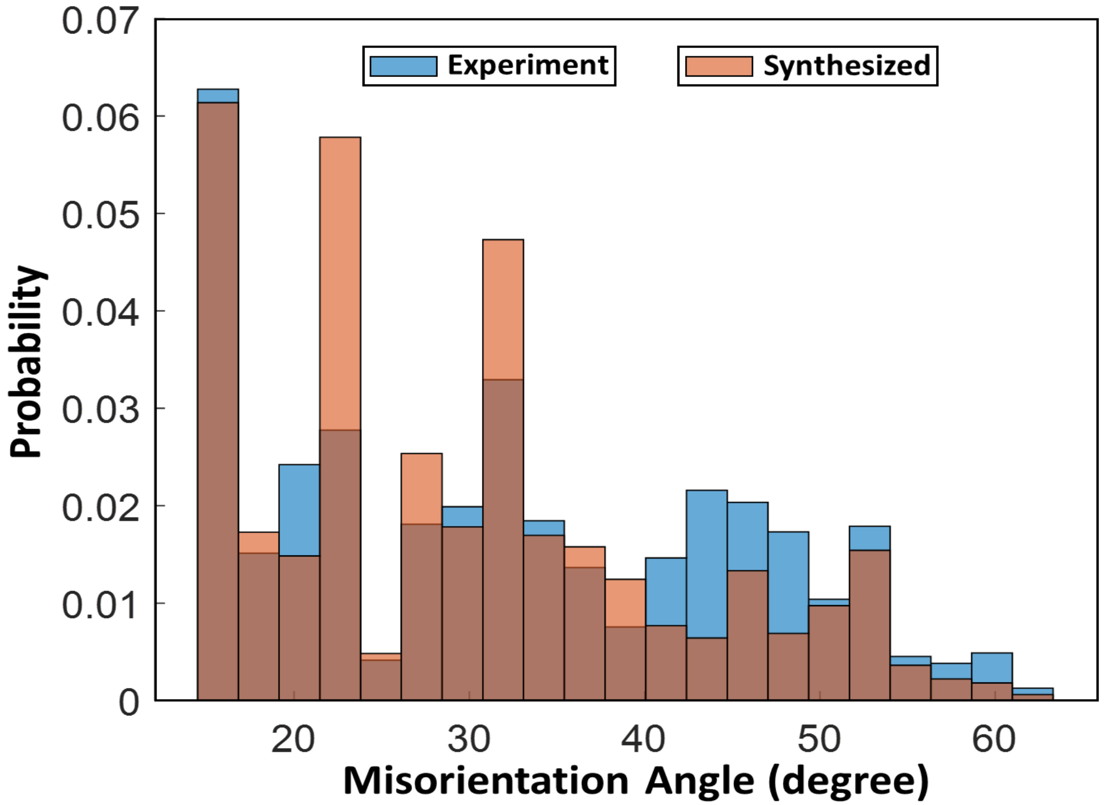
- High-Angle Grain Boundary (HAGB) angle values are $\phi \geq 15^o$



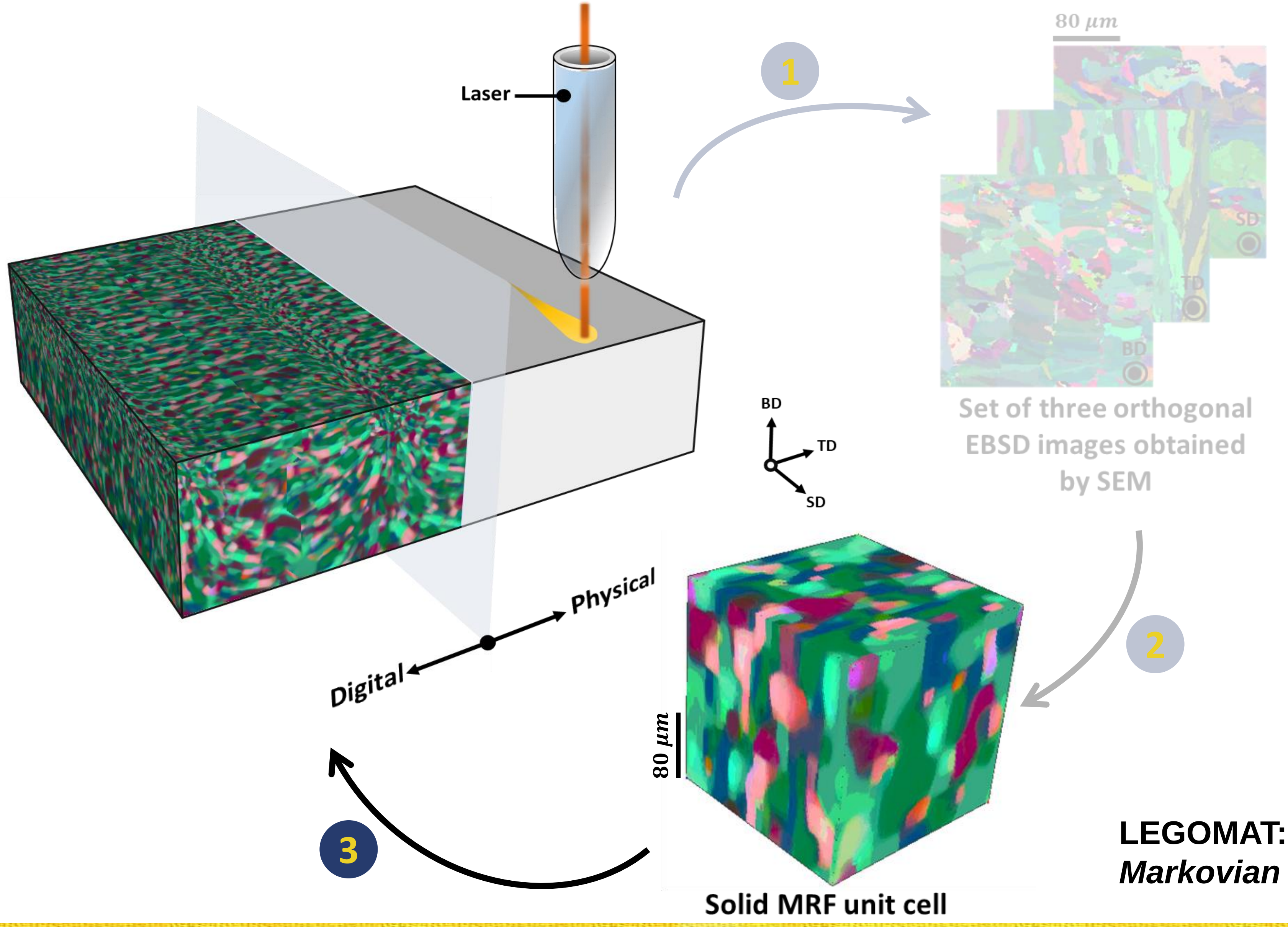
Experimental



3D MRF synthesized



Large-Scale Generation



1. *Experimental EBSD imaging*
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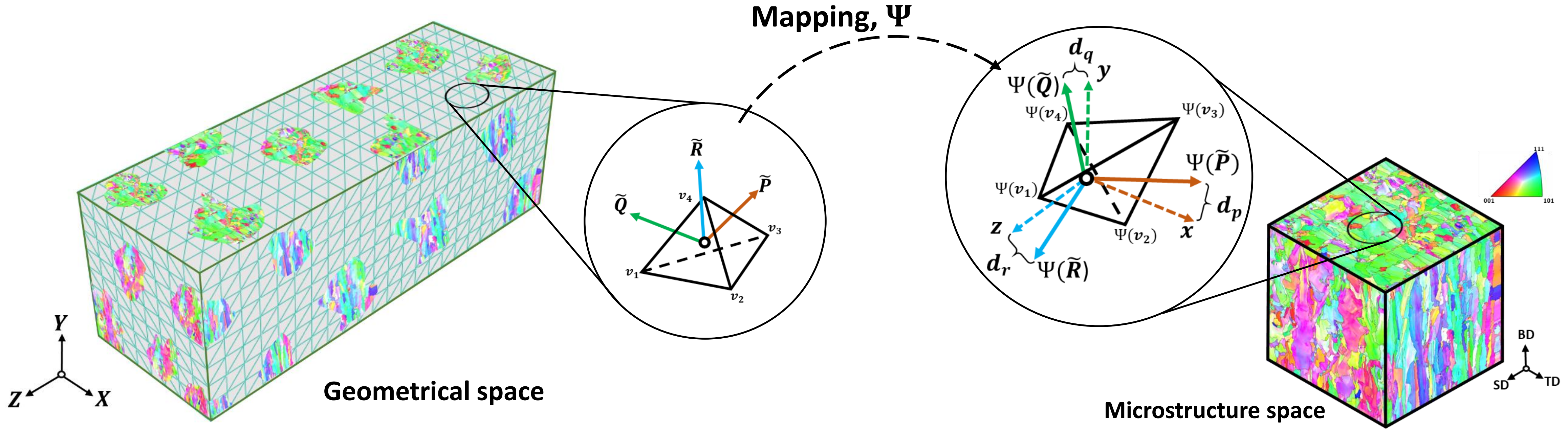
LEGOMAT: *Locally-Extracted Globally-Organized Markovian Material Models*

LEGOMAT Technique

- **Patch-based** MRF algorithm:
  - Discretization of geometrical space via *Delaunay tetrahedralization*
  - Growing each patch while minimizing difference vectors for all T_i elements

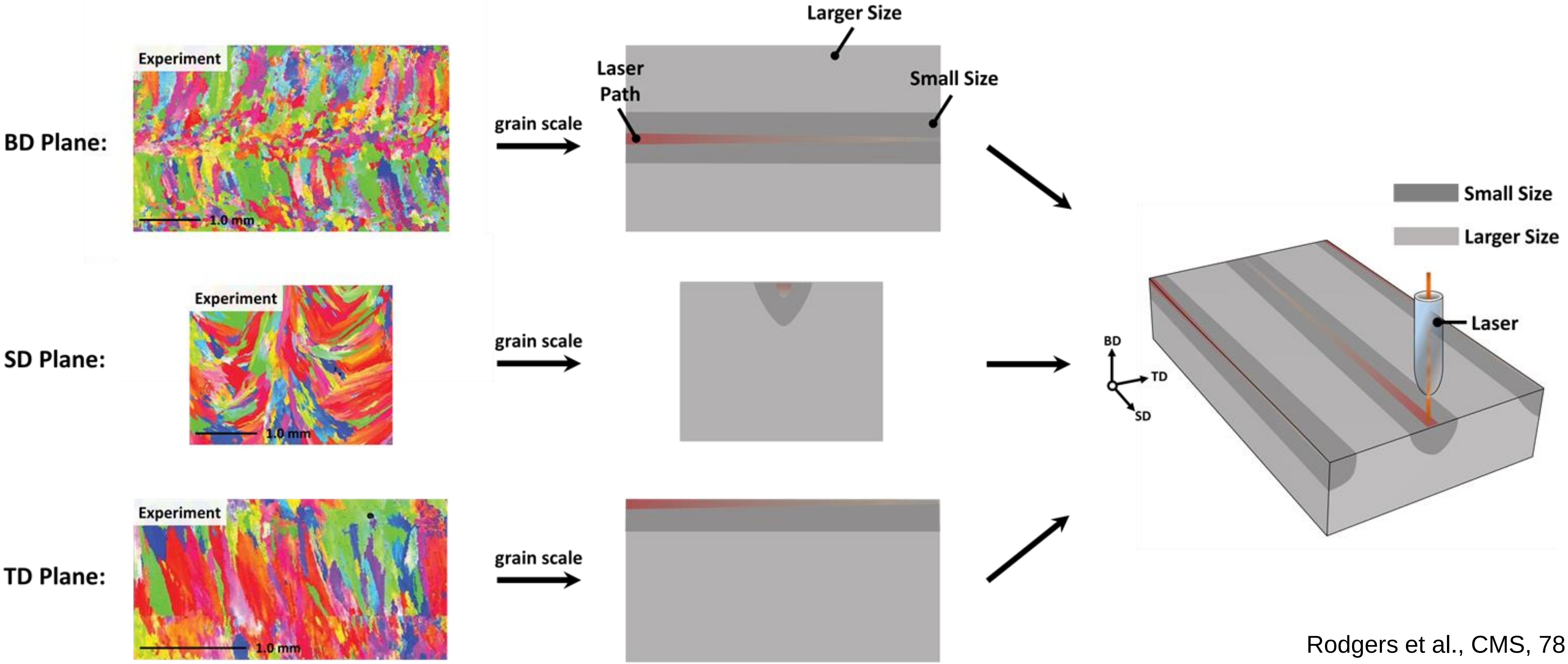
$$\mathcal{F} = \sum_{i=0}^{N-1} \|\boldsymbol{d}_p^i\| + \|\boldsymbol{d}_q^i\| + \|\boldsymbol{d}_R^i\|$$

- *Approach:*
  - Utilize grain size **scaling** and **growth direction** to simulate microstructural formation in AM



Grain Size Scaling

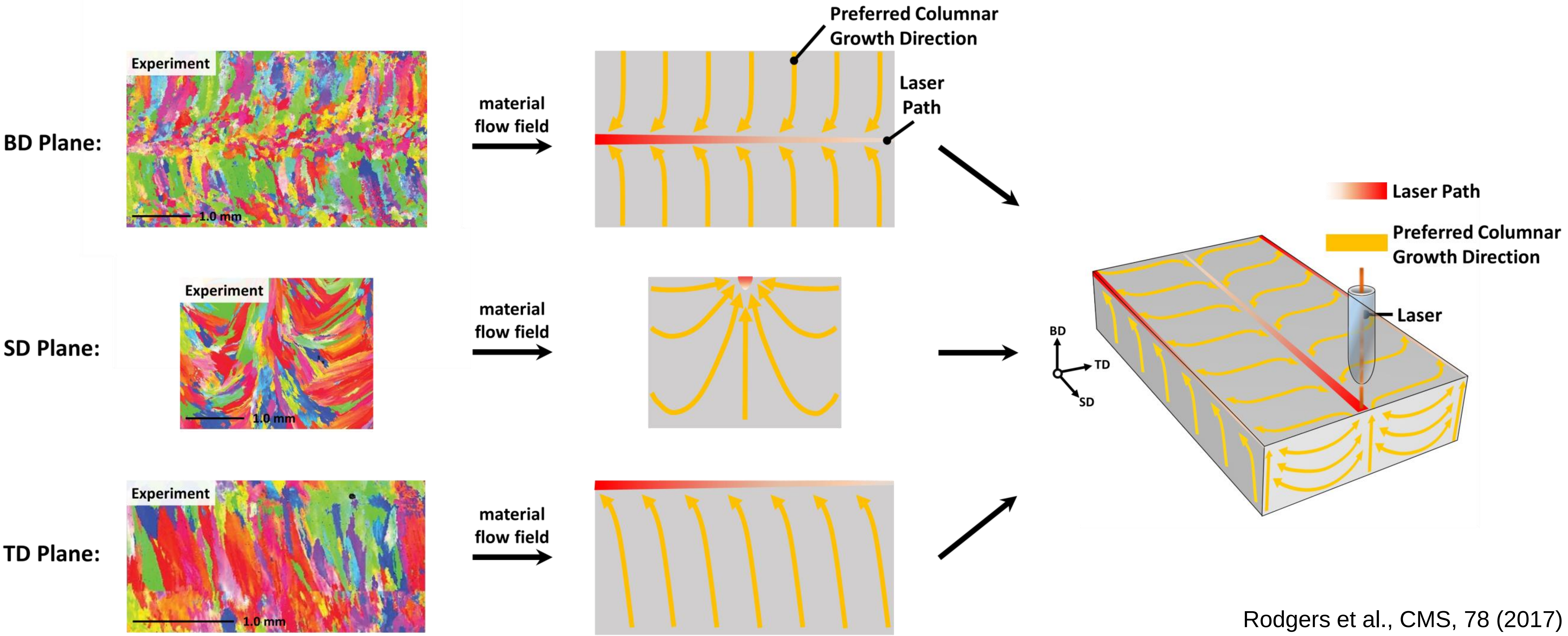
- Small grains along laser path tend to nucleate during solidification while transitioning to larger grains in between each laser path



Rodgers et al., CMS, 78 (2017)

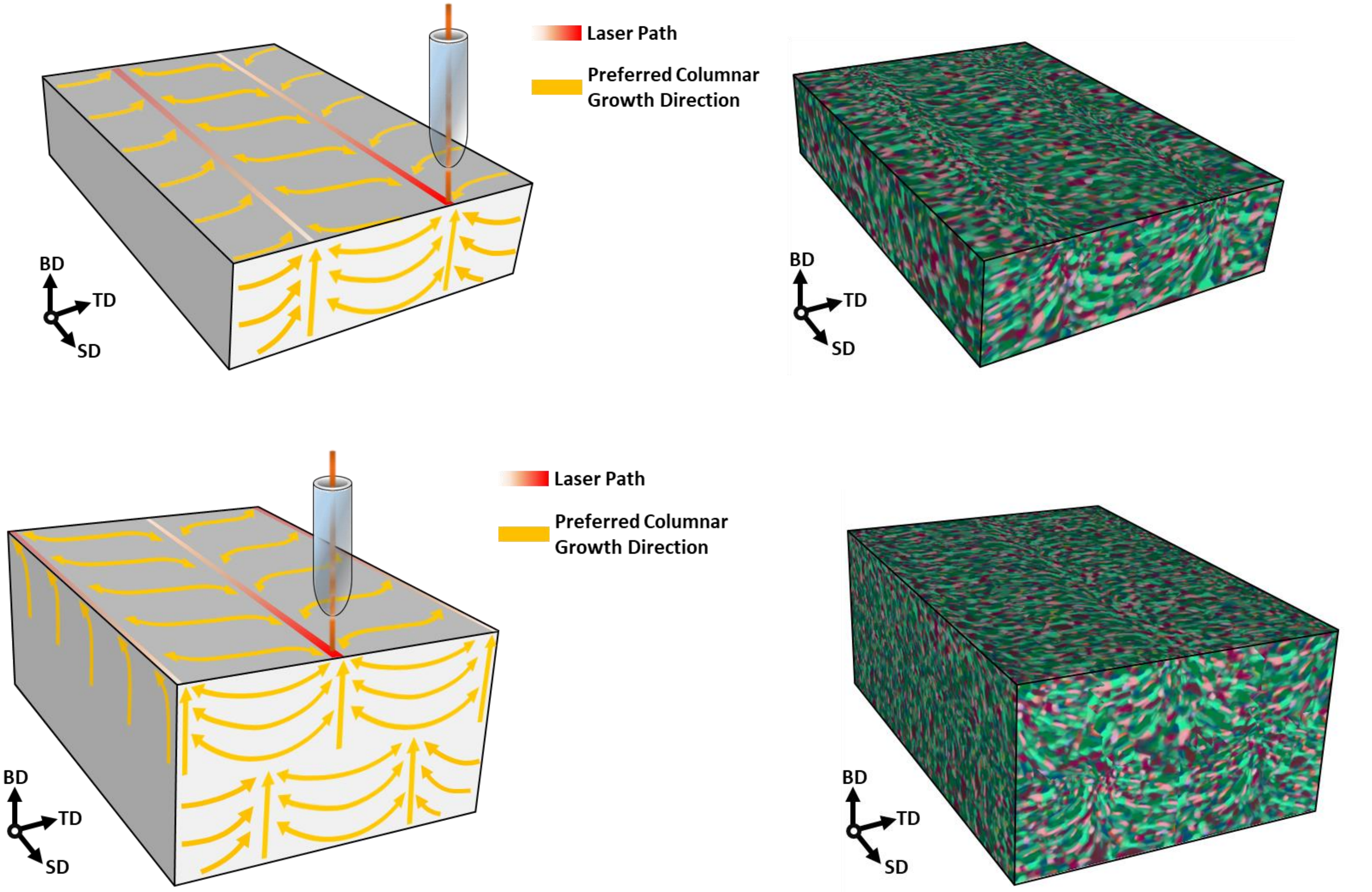
Columnar Growth Direction

- Preferred crystallographic growth direction tend to align columnar grains in the direction of increasing temperature



Rodgers et al., CMS, 78 (2017)

Large-Scale Reconstructions

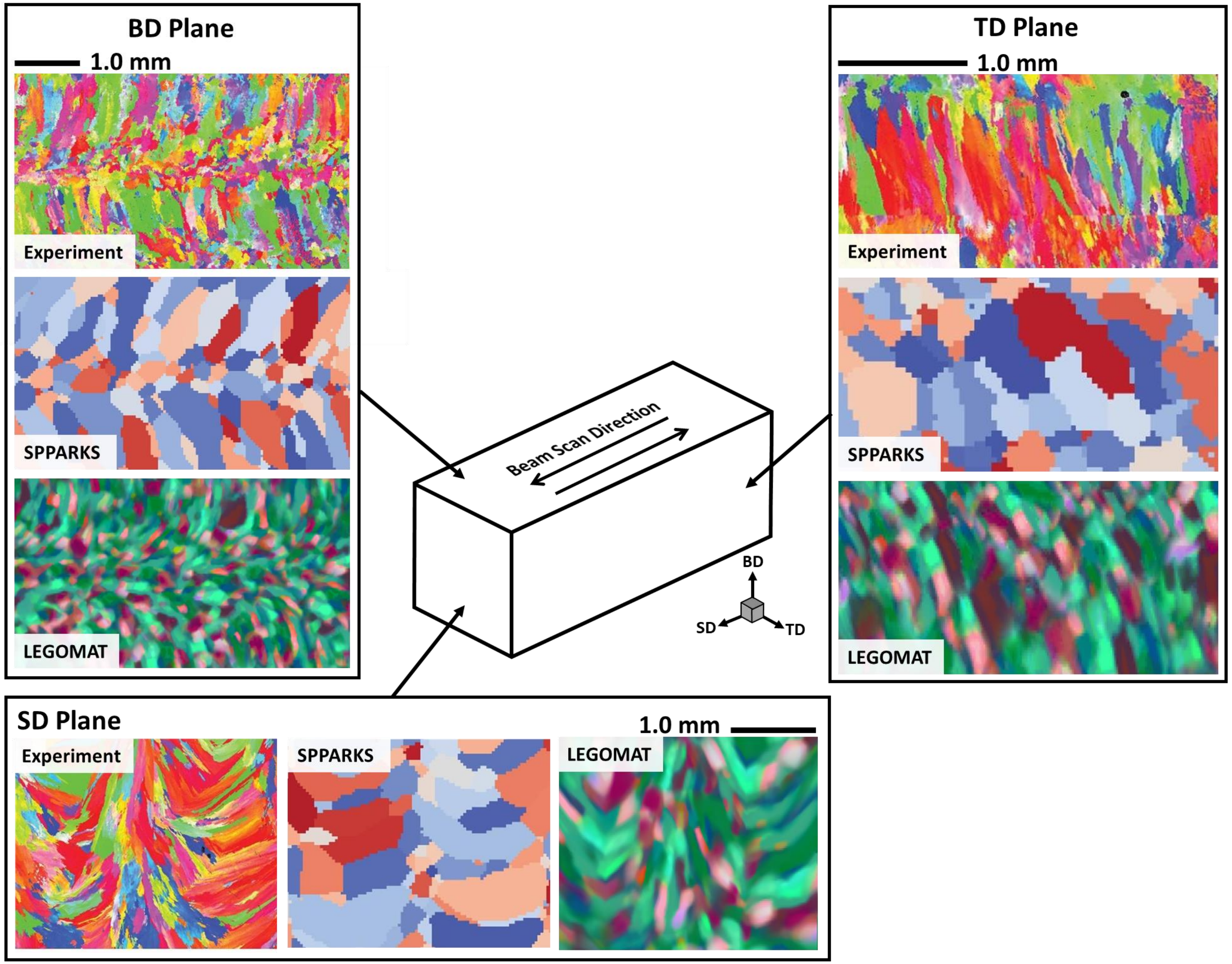


Javaheri et al., CMS, 206 (2022)

Microstructure Simulations

Method	Computational Cost	Benefits	Challenges
Phase-field	Extremely high	Physics-based	Small-scale prediction
Cellular Automata	High	Texture prediction	Accuracy depends on cell size
Kinetic Monte Carlo (e.g., SPPARKS)	Intermediate	Allows large-scale prediction	Texture prediction
LEGOMAT	Low	Allows large-scale prediction	Data-driven and requires knowledge of grain growth directions

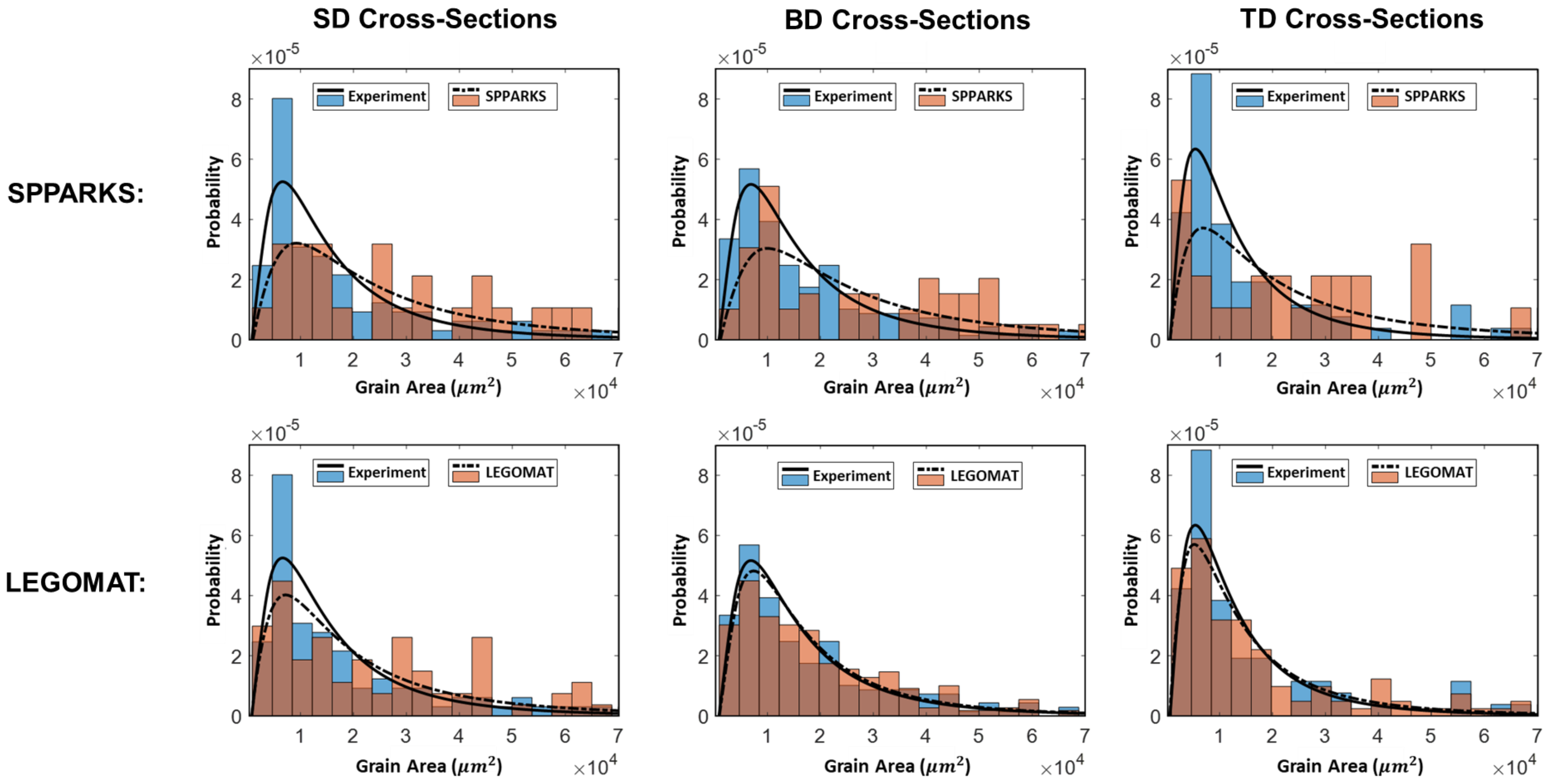
LEGOMAT vs. SPPARKS



Javaheri et al., CMS, 206 (2022)

Grain Size Statistics

- Comparison of grain size distributions for SPPARKS (top) and LEGOMAT (bottom) against experiments in three directions



Summary

- MRF approach reconstructs 3D microstructures from 2D EBSD images
- Grain size distribution, crystal orientations (e.g., ODFs and pole figures), and misorientation angles for 3D reconstructions are consistent with experiment
- LEGOMAT embedding process simulates real-time descriptions of additively-manufactured microstructures by combining flow fields and grain size scaling
- Future work:
  - Utilize thermal field predictions for flow field generation
  - Create microstructural libraries and use machine learning for adaptive microstructure selection based on laser parameters

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Thank You

Questions can be directed to imanajv@umich.edu