Integrated Monte Carlo Microstructure and Analytical Temperature Simulations of Additive Manufacturing

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Additive Manufacturing Benchmark 2022

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Outline

Introduction / Background / Objective

Kinetic Monte Carlo Modeling of Microstructure Evolution

Analytical vs. Numerical Temperature Field Simulation

- Overview
- Impact of Time Step Choice

Simulation of Ti-6Al-4V PBF-LB Microstructure Evolution

- Comparisons with Experiment
- Effect of Processing Parameters

Conclusions and Summary

Introduction

- Laser beam powder bed fusion (PBF-LB) additive manufacturing (AM) forms complex, impactful microstructures
  - The microstructure impacts the final part performance and is not guaranteed to be removed through post-processing
- The domain space for PBF-LB is massive
  - Hatch spacing, layer thickness, power, velocity, beam diameter, scan rotation angle, scan strategy, pre-heat temperature, material system, etc…
- Surveying the microstructure design space experimentally is difficult, time-consuming, and costly
- Computational microstructure evolution techniques are a way to try to get a handle on the domain space challenge
- This work will focus on the Monte Carlo technique

Generations of SPPARKS-Based PBF-LB Monte Carlo Simulations

SPPARKS: Stochastic Parallel PARticle Kinetic Simulator

- Sandia National Laboratory developed Monte Carlo framework
- https://spparks.github.io/

Generation 1 (2017) [1]

Kinetic Monte Carlo (kMC) method

- Temperature field approximated by ellipsoid and exponential decay
- Solidification approximated by Monte Carlo grain coarsening
- Nucleation of new grains based on melt pool randomization
- Difficult to link laboratory and simulation reference frames

Generation 2 (2021) [2]

Physically-Based Monte Carlo (PBMC) method*

- Temperature field implemented analytically or numerically
- Solidification modeled by dendritic growth approximation
- Nucleation based on undercooling
- Links laboratory and simulation reference frames

[1] Rodgers, T.M., et al. "Simulation of metal additive manufacturing microstructures using kinetic Monte Carlo." *Computational Materials Science* 135 (2017): 78-89. https://doi.org/10.1016/j.commatsci.2017.03.053

[2] Rodgers, T.M., et al. "Simulation of powder bed metal additive manufacturing microstructures with coupled finite difference-Monte Carlo method." *Additive Manufacturing* 41 (2021): 101953. https://doi.org/10.1016/j.addma.2021.101953

While originally called Finite Difference Monte Carlo [2], this work extends the model to use an analytical temperature field so a more general name is used

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Focus of this work

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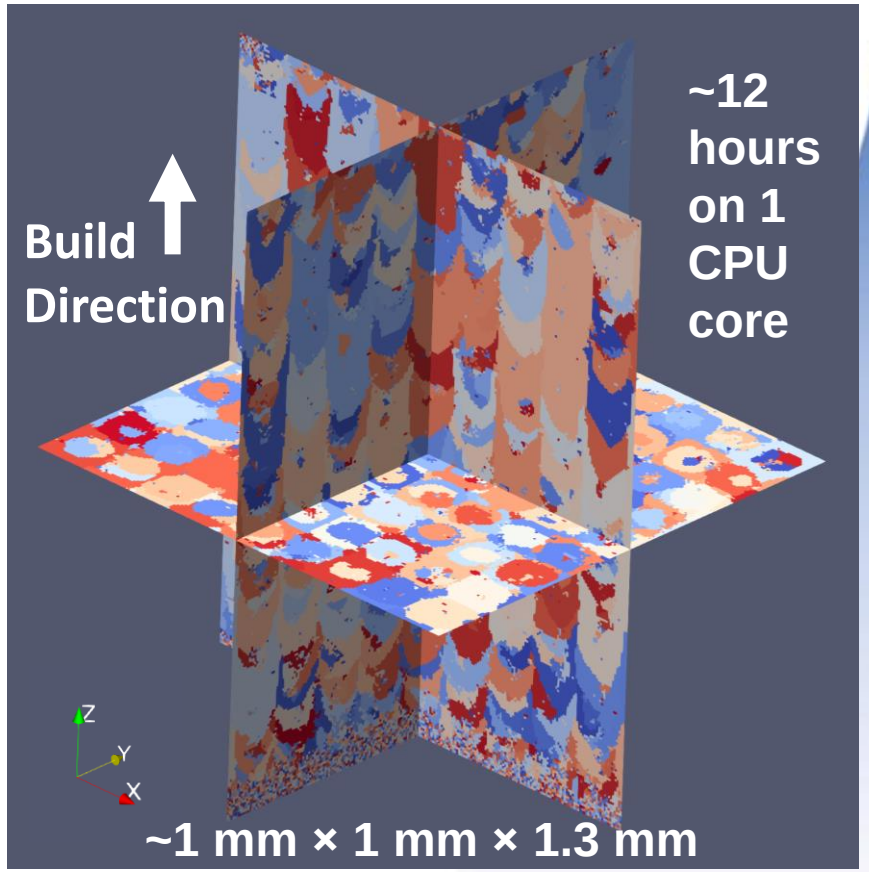
Objectives of This Work

- Demonstrate the applicability of the PBMC method for process-to-microstructure modeling of PBF-LB
- Present details on the integration of the model with analytical temperature fields
- Highlight the differences between the analytical and numerical temperature field implementations
- Compare analytical-temperature field PBMC Ti-6Al-4V PBF-LB simulations to experiments
- Present the impact of processing parameters on resulting grain statistics

AMBench Region #2 of Inconel 718 Build



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PBMC Modeling of Microstructure Evolution

Solidification Texture Nucleation Grain Coarsening

Critical Components of the PBMC Method

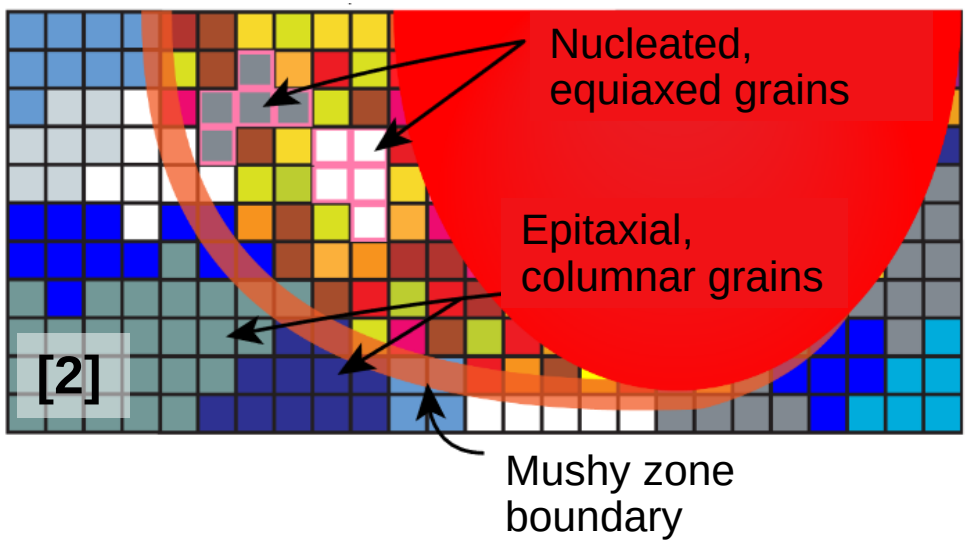
*Texture modeling represents a new addition to the PBMC method based on previous work incorporating texture [3]

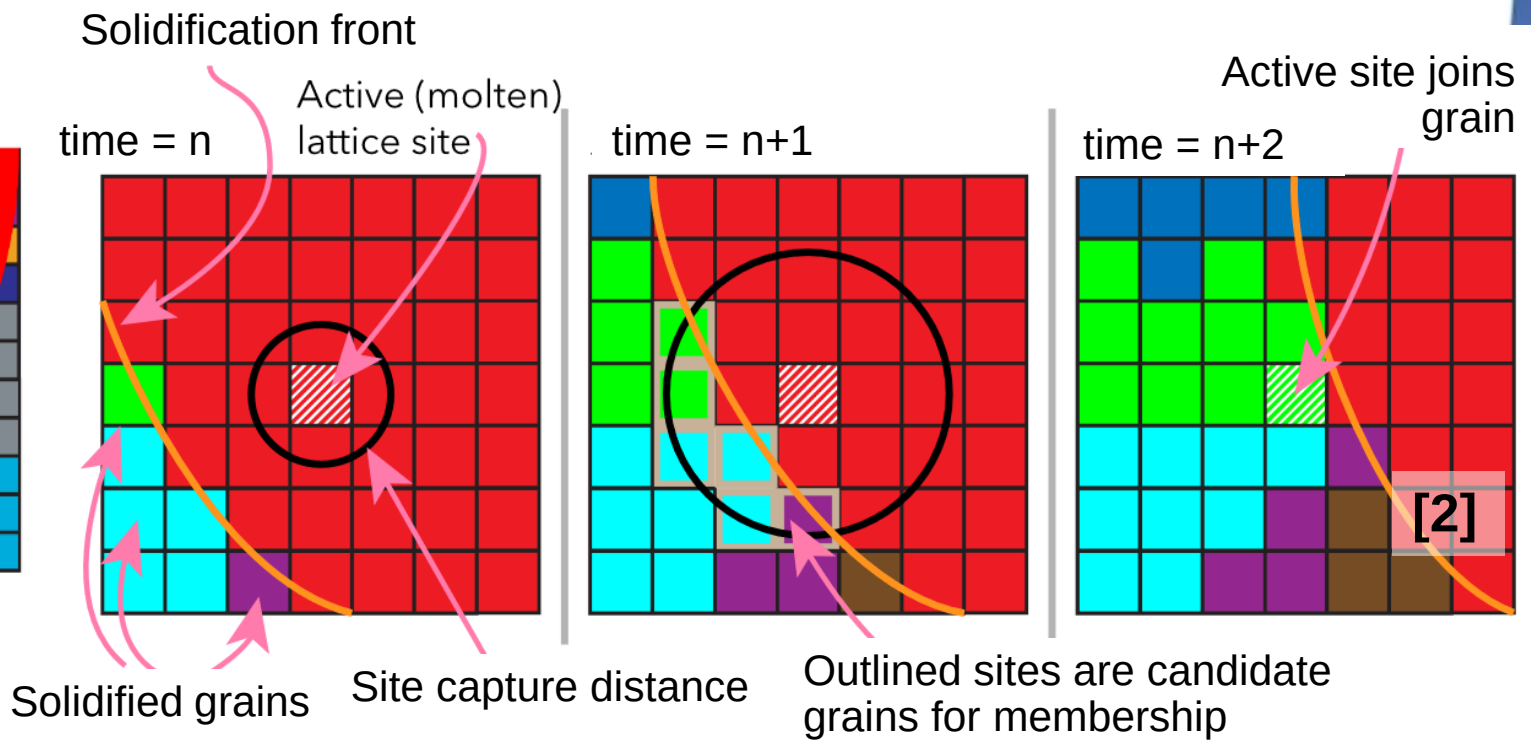
[3] Pauza, J.G. et al., "Computer simulation of microstructure development in powder-bed additive manufacturing with crystallographic texture." *Modelling and Simulation in Materials Science and Engineering* 29.5 (2021): 055019. https://doi.org/10.1088/1361-651X/ac03a6

PBMC Modeling of Microstructure Evolution

Solidification Texture Nucleation Grain Coarsening

Melt pool & solidification overview





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PBMC Modeling of Microstructure Evolution

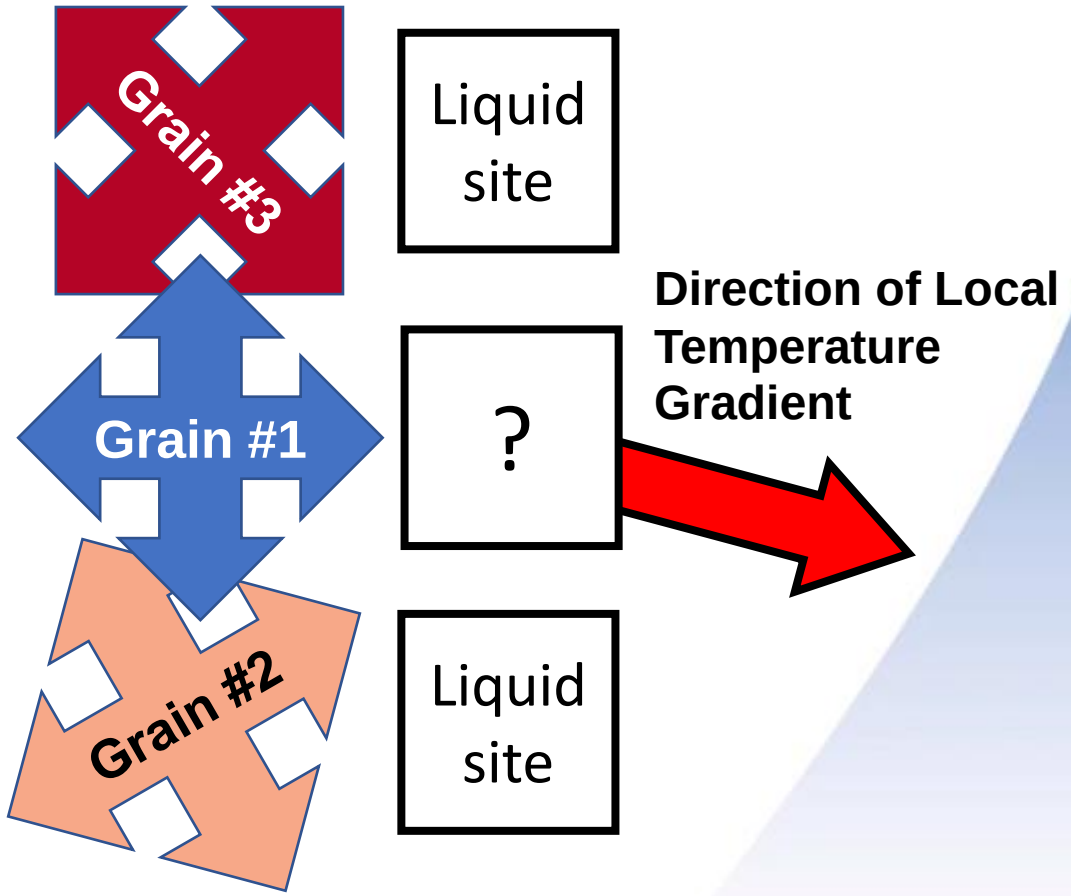
Solidification | **Texture** | Nucleation | Grain Coarsening

New addition in current work based on modification of previous implementation [3]

Each site is assigned Euler angles defining its crystallographic texture

The misorientation between a grain crystallographic orientation and the local temperature gradient impacts the capture distance

Favors <100> crystal growth



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PBMC Modeling of Microstructure Evolution

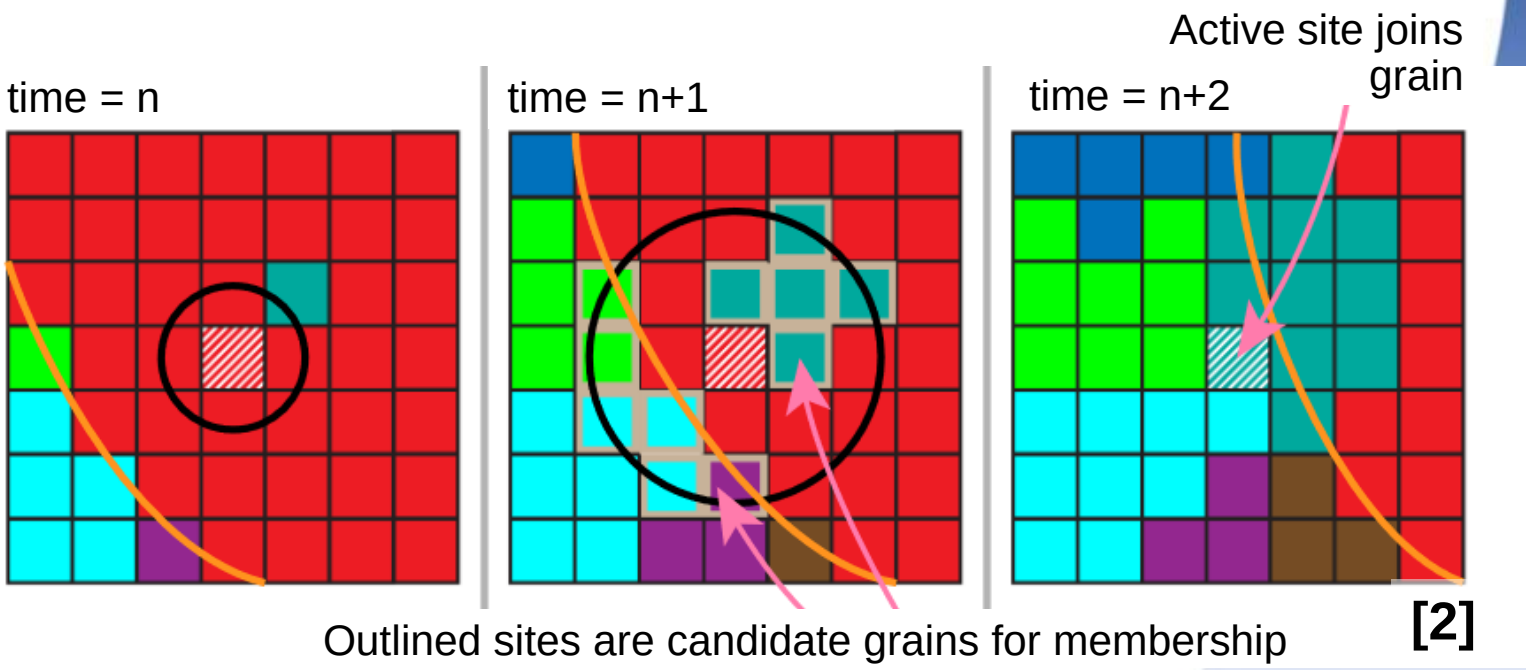
Solidification | Texture | **Nucleation** | Grain Coarsening

User defines:

1. Number of nucleation points per unit volume
2. Undercooling at which nucleation takes place

Before the simulation, nucleation sites are probabilistically assigned

If a possible nucleation site reaches the specified undercooling while molten, it solidifies



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PBMC Modeling of Microstructure Evolution

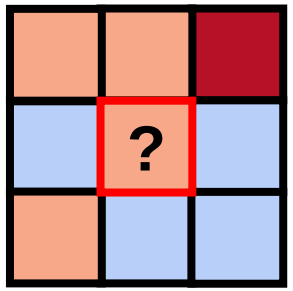
Solidification

Kinetic Potts Monte Carlo method

- Grain #1
- Grain #2
- Grain #3

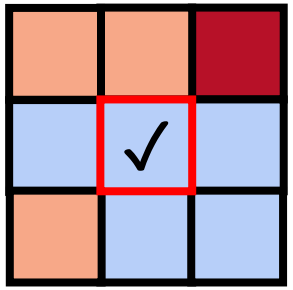
Texture

Initial Grains



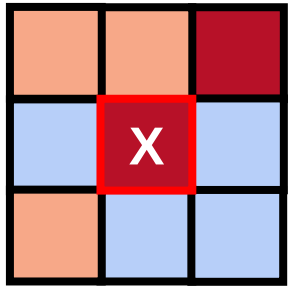
Nucleation

Flips to Grain #3
Accepted (lowers system energy)



Grain Coarsening

Flips to Grain #2
Rejected (Increases system energy)



δ_{ij} = Kronecker delta between spin i and nearest neighbor spin j
n_k = nearest neighbor k
N = All nodes in the system
E = Energy of system

$$E = \frac{1}{2}\sum_{i}^{N}\sum_{j}^{n_k}\left(1-\delta_{ij}\right)$$

$$\Delta E = E_{new} - E_{old}$$

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Analytical vs. Numerical Thermal Field Calculation

Analytical (Rosenthal)

$$T = T_0 + \frac{AP}{2\pi r k}\exp\left(-\frac{v(\xi + r)}{2\alpha}\right)$$

$$r = \sqrt{\xi^2 + y^2 + \left(\eta_{z,scale} z\right)^2}$$

$$\xi = x - vt$$

T = time & location specific temperature
T_0 = base temperature
A = absorptivity
P = laser power
v = scanning velocity
α = thermal diffusivity
c_p= specific heat capacity

Numerical (Finite Difference)

$$\rho c_p \frac{\partial T}{\partial t} = \nabla(-k\nabla T) + H_v = 0$$

Time Integration: Explicit Euler

Spatial Derivatives: Second Order Central Finite Difference

ρ = mass density
k = thermal conductivity
H_v = volumetric heat flux of laser
T_m = melt temperature
T_r = room temperature
$\eta_{z,scale}$ = scaling factor for melt pool shape
x, y, z = local coordinates with x in the direction of the laser movement
ξ = shifted coordinate frame with respect to time

Analytical vs. Numerical Thermal Field Calculation

Analytical (Rosenthal)

$$T = T_0 + \frac{AP}{2\pi r k}\exp\left(-\frac{v(\xi + r)}{2\alpha}\right)$$

- Analytical solution
  - **Stability Limit: N/A**
  - **Numerical Accuracy: N/A**
- **No boundary conditions**
- **Point source**
- **No radiation, convection, or powder conductivity**

Numerical (Finite Difference)

$$\rho c_p \frac{\partial T}{\partial t} = \nabla(-k\nabla T) + H_v = 0$$

- Explicit Euler implementation
  - **Stability Limit: $dt \leq dx^2/4\alpha$**
  - **Numerical Accuracy: $err \propto dt^2$**
- **Boundary conditions**
- **Volumetric beam**
- **Can include radiation, convection, and powder conductivity**

Both - Time Step Limitation: $dt \leq dx/v$

Positive
Neutral
Negative

Analytical vs. Numerical Thermal Field Calculation

Analytical (Rosenthal)

$$T = T_0 + \frac{AP}{2\pi r k}\exp\left(-\frac{v(\xi + r)}{2\alpha}\right)$$

- Anal[illegible]
  - S[illegible]
  - N[illegible] N/A
- No b[illegible]ons
- Poin[illegible]
- No radiation, convection, or powder conductivity

Numerical Speed

Numerical (Finite Difference)

$$\rho c_p \frac{\partial T}{\partial t} = \nabla(-k\nabla T) + H_v = 0$$

- Expl[illegible]ntation
  - S[illegible] $dx^2/4\alpha$
  - E[illegible] $err \propto dt^2$
- Bou[illegible]s
- Volu[illegible]
- Can include radiation, convection, and powder conductivity

Physical Fidelity

Positive

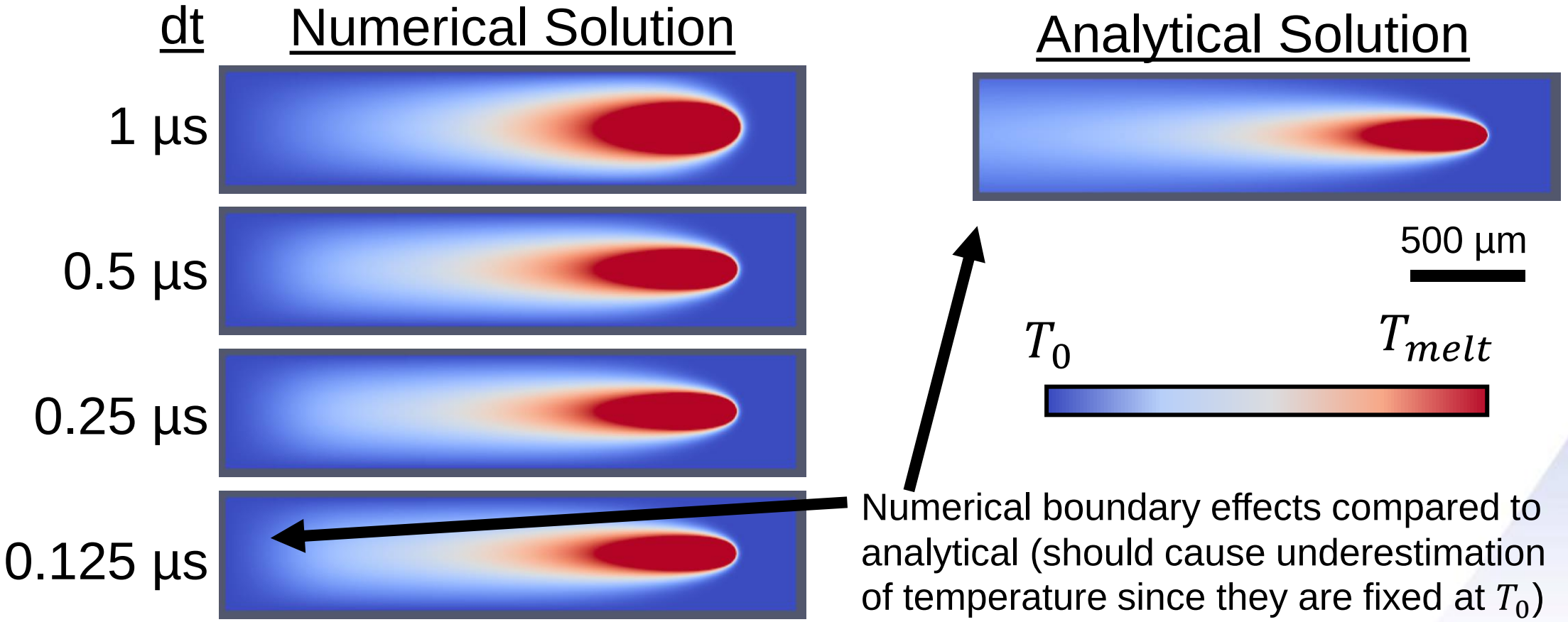
Neutral

Negative

Both - Time Step Limitation: $dt \leq dx/v$

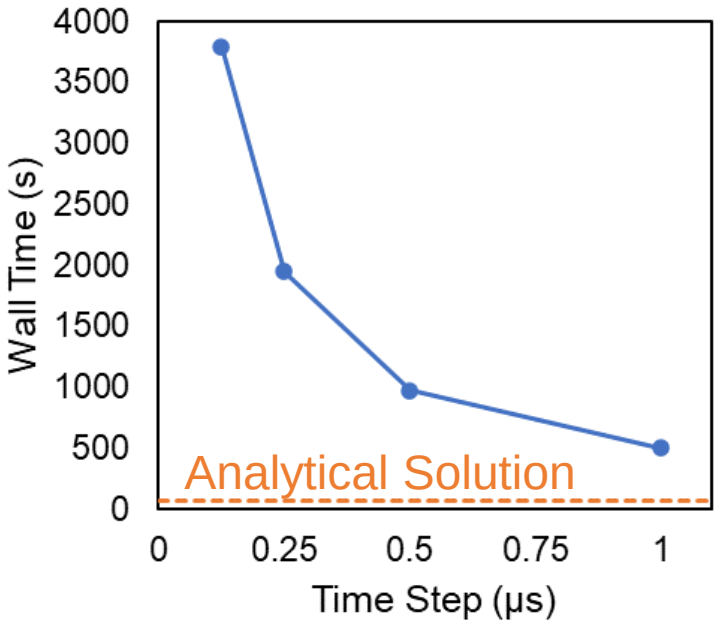
Influence of Time Step on Temperature

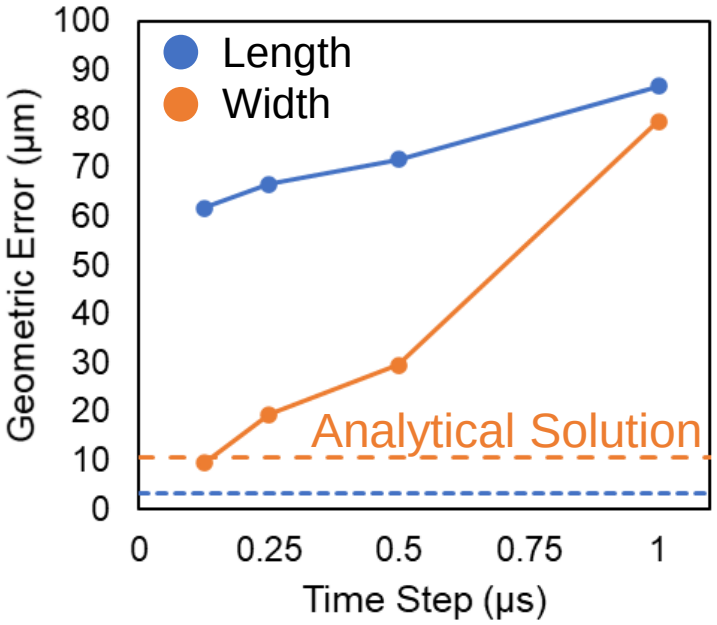
The numerical solution was compared to the analytical solution to estimate accuracy and characterize speed trade-off

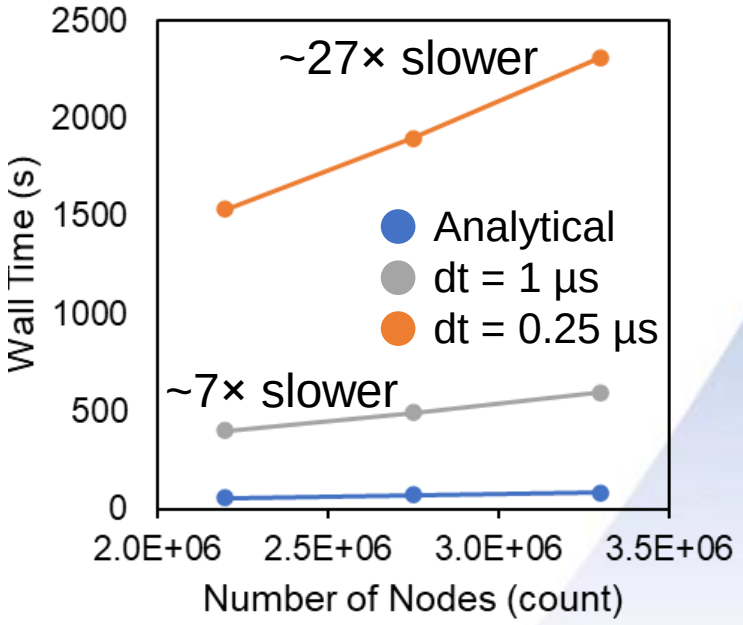


Influence of Time Step on Melt Pool Geometry

- Same voxel size, same thermophysical parameters
  - Analytical solution has geometric error due to voxel size (5 μm)
- Numerical solution approaches analytical solution as time step approaches zero
  - 0.125 μs time step requires ~50× more wall time





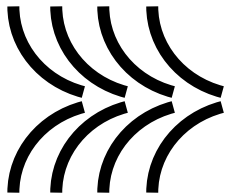


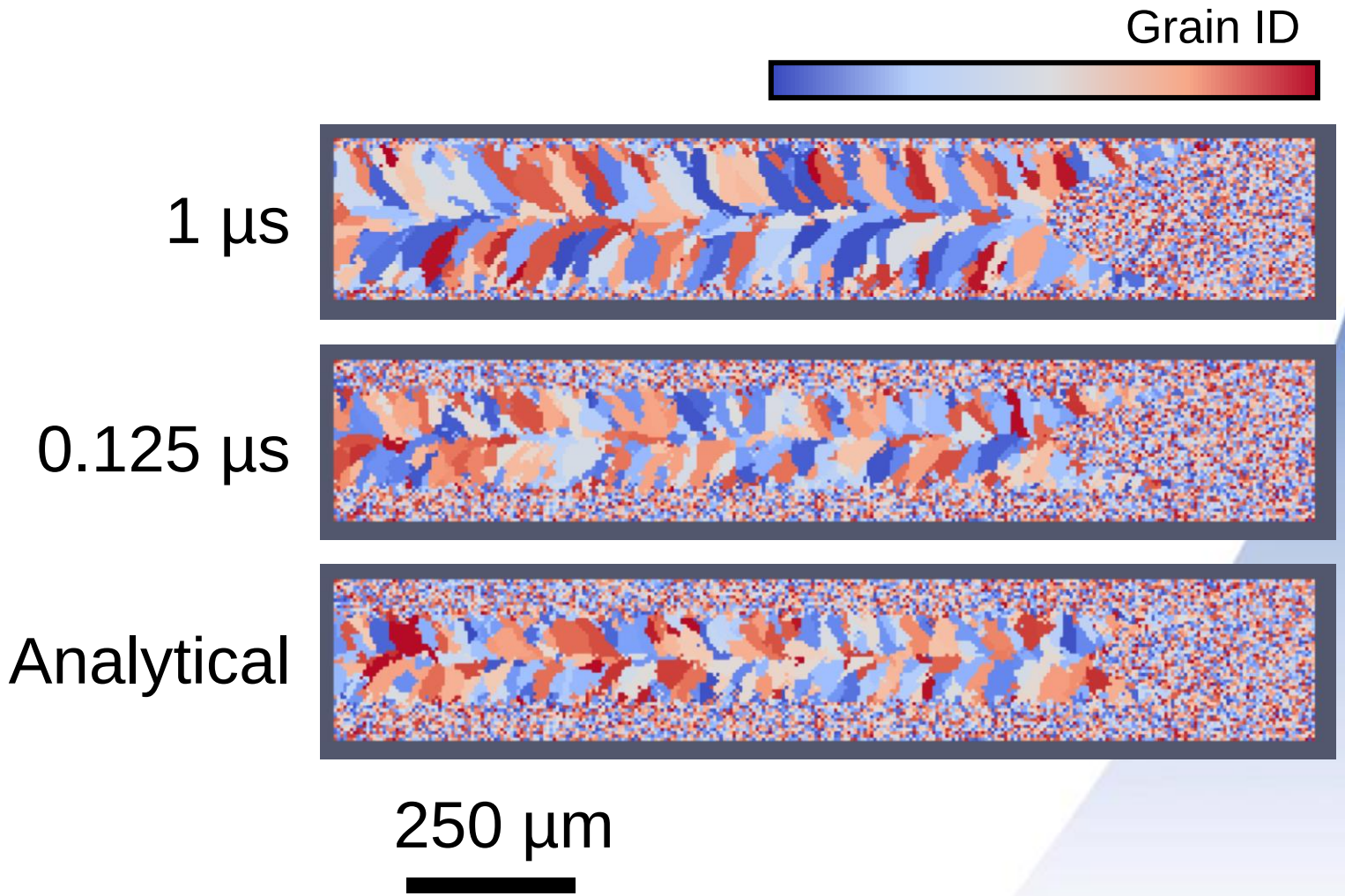
Influence of Time Step on Grain Structure

The time step has a big influence on the resulting simulated grain structure

Larger time steps cause longer and wider melt pools

These melt pools cause a smoother grain structure with a characteristic shape





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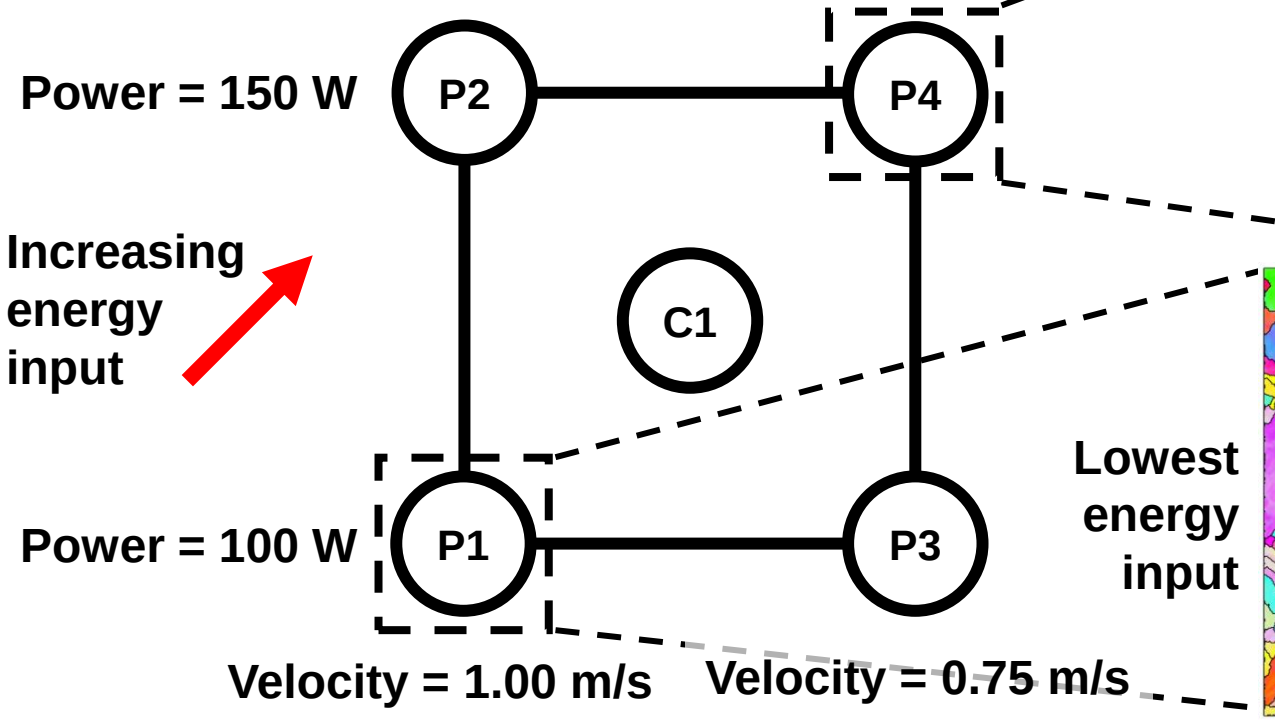
Experimental Samples and Numerical Study

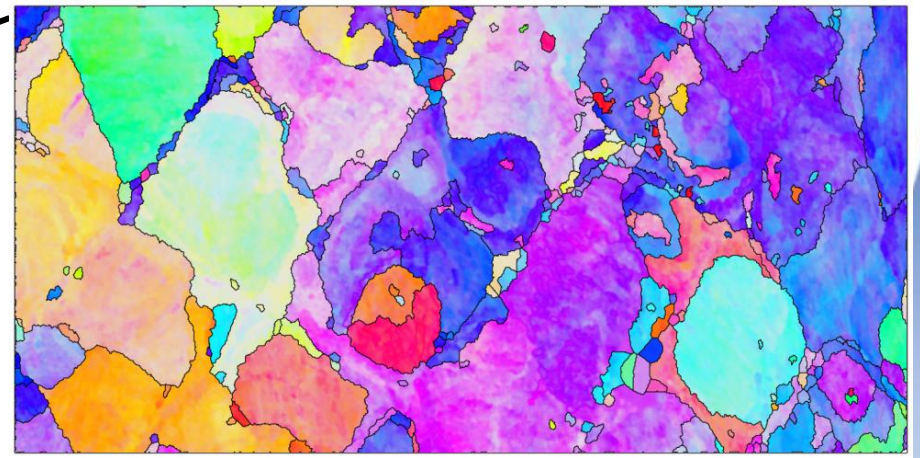
2^2 Factorial Design with Center Point (values half-way between end points)

- 600 µm x 600 µm x 695 µm numerical domain (20 layers)
- Experimentally characterized P1 & P4
- Hatch Spacing = 100 µm
- Layer Thickness = 30 µm
- Rotation between layers = 67°

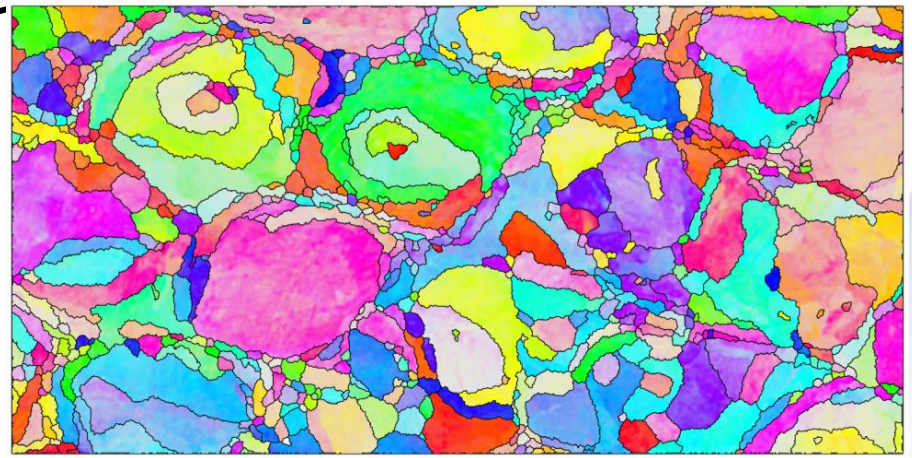


256 µm × 512 µm X-Y Plane

Highest energy input



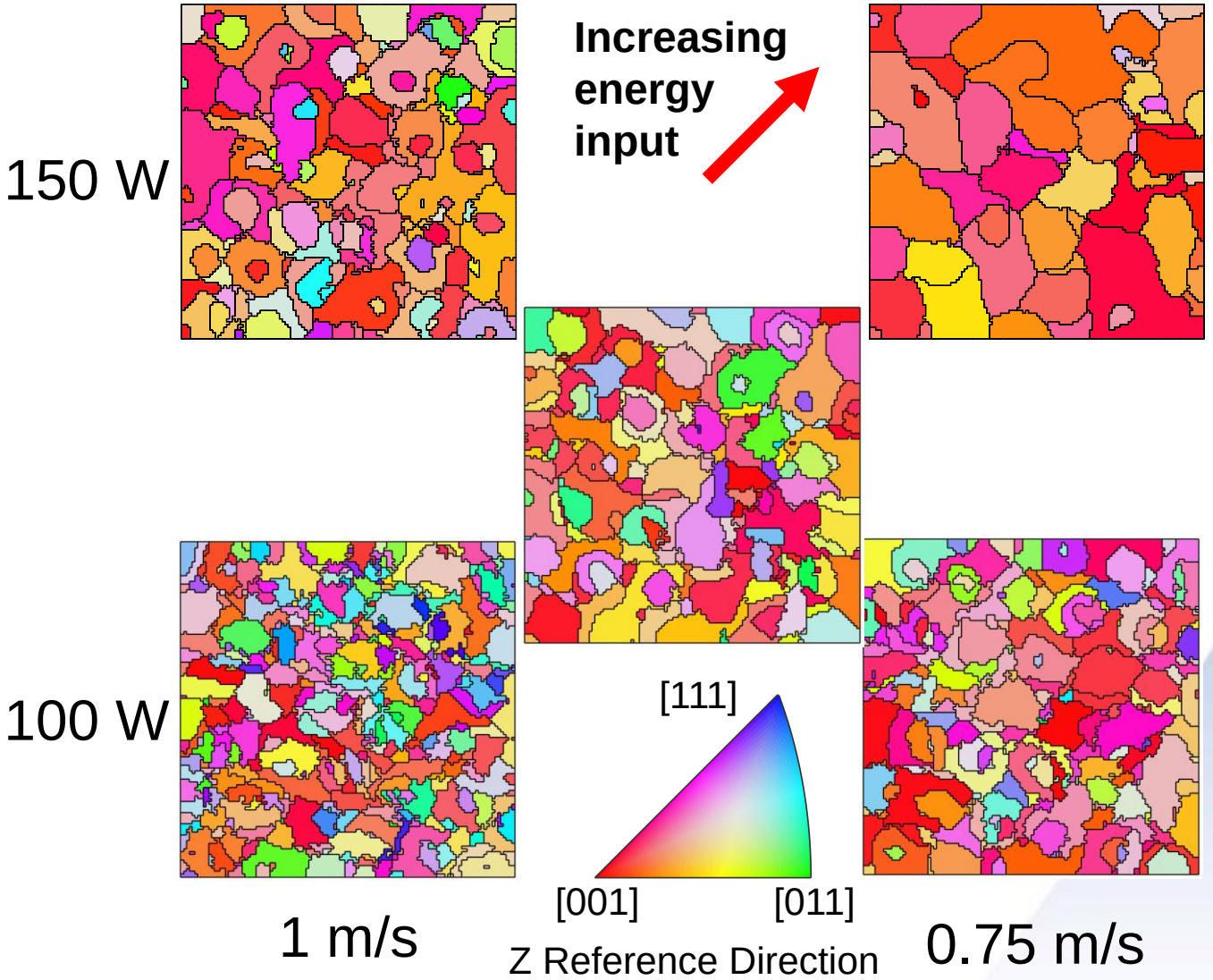
Lowest energy input



Simulated Regions – X-Y Plane

As the input energy gets higher (low velocity and high power):

- The average grain size gets larger
- The <001> texture becomes dominant
- Inner circular regions appear then disappear

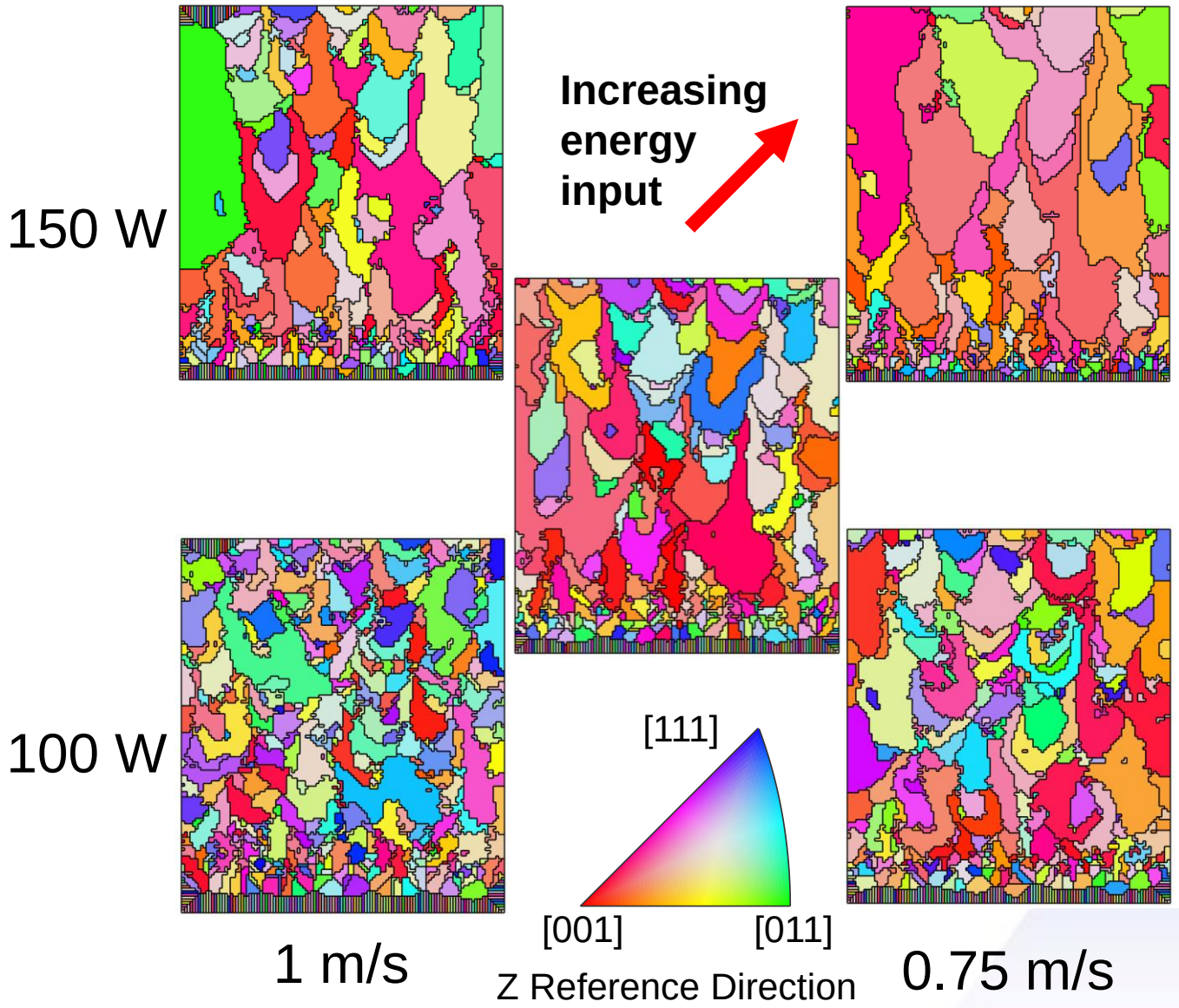


Simulated Regions – X-Z Plane

As the input energy gets higher (low velocity and high power):

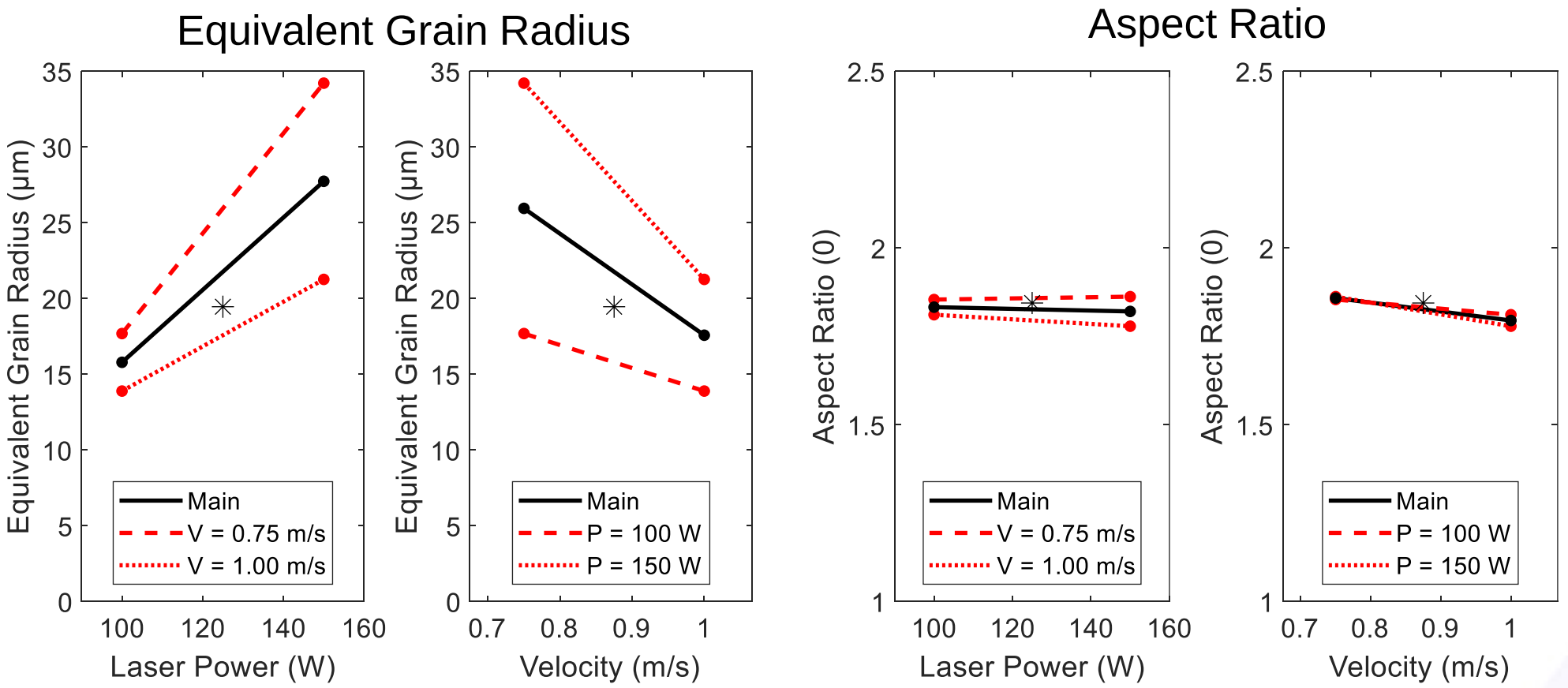
- A columnar grain structure appears
- The <001> texture becomes stronger

A pseudo-steady state in grain structure is reached in the middle of the simulation domain



Simulated Main and Interaction Effects

- Strong main effect of power and velocity on equivalent grain radius
- Medium interaction effect between power and velocity on equivalent grain radius
- Weak main effect velocity on aspect ratio

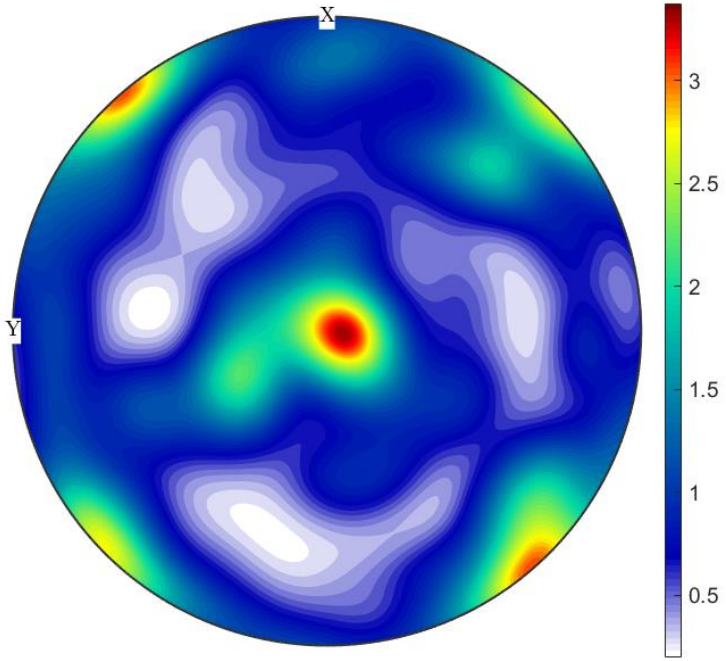


X-Y Plane, 14 layers up (420 μm up from build plate

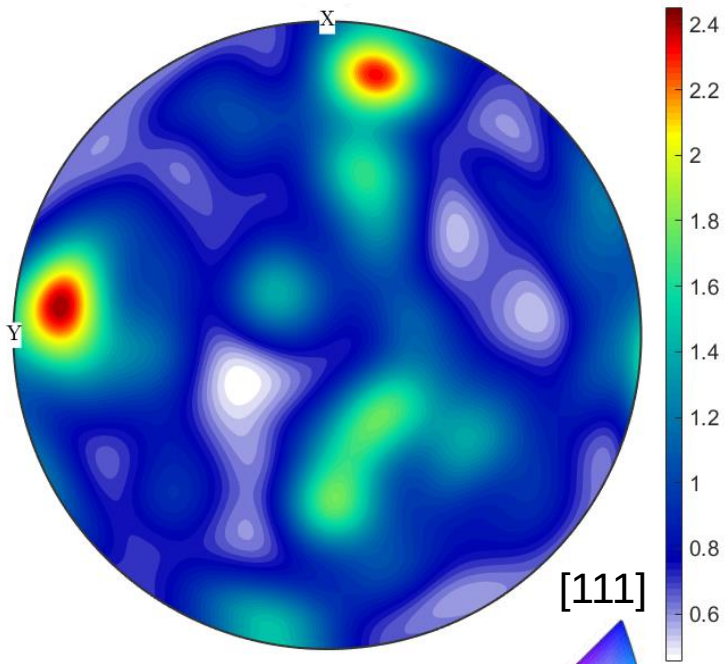
Comparison with Experiment – Low Energy

- Simulation overestimates <001> texture development (analyzed with MTEX [4])

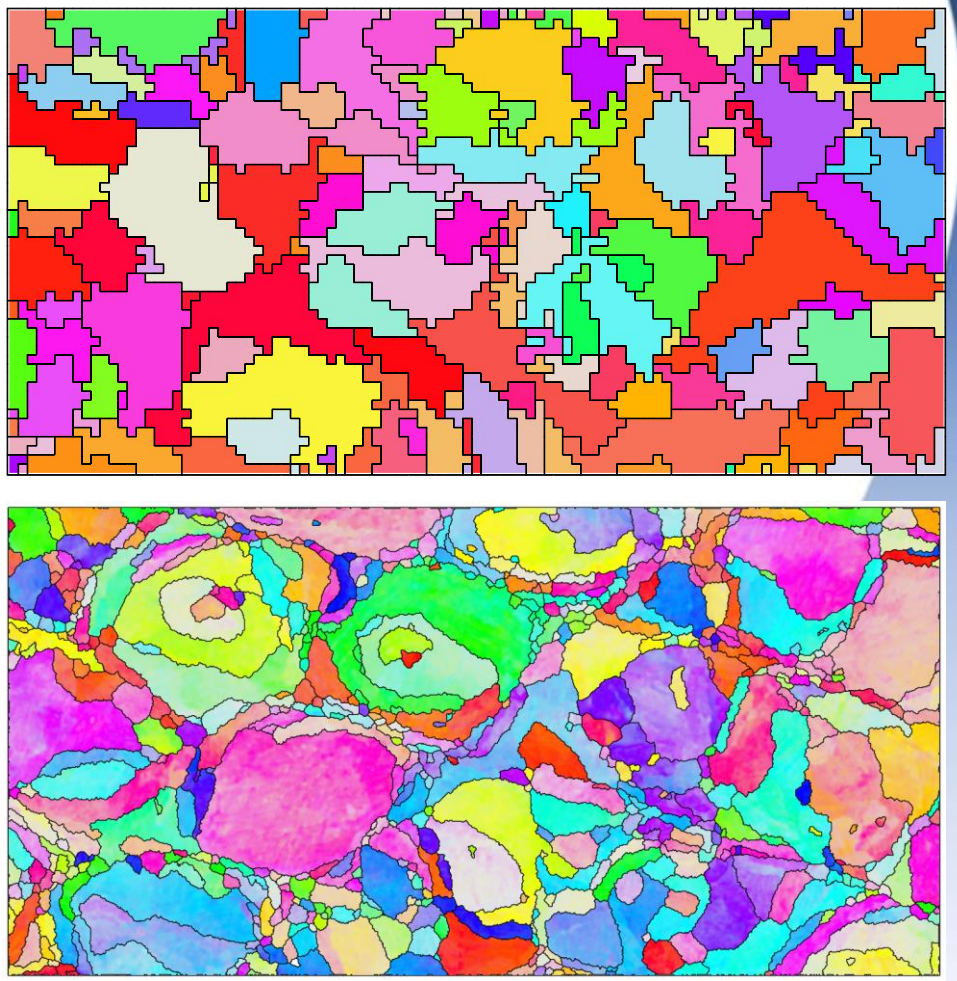
Simulation
(100)

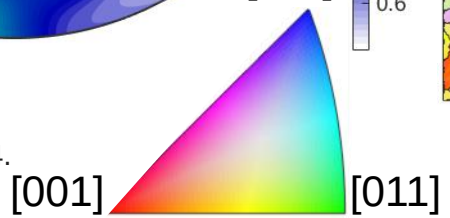


Experimental
(100)



Simulation (top) and Experiment (bottom)



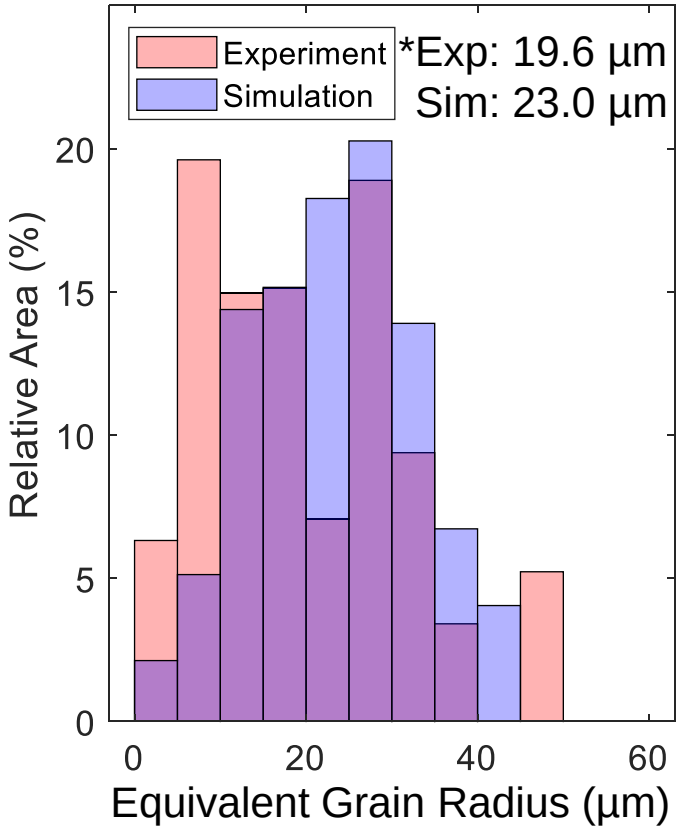


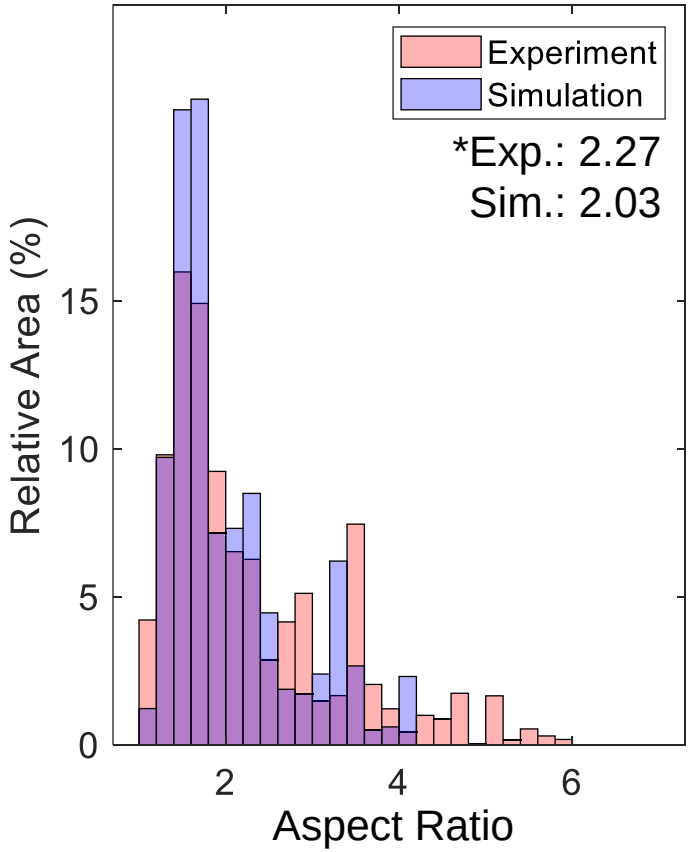
Z Reference Direction

[4] Niessen, F., et al. "Parent grain reconstruction from partially or fully transformed microstructures in MTEX." *Journal of Applied Crystallography* 55.1 (2022). 180-194. https://doi.org/10.1107/S1600576721011560

Comparison with Experiment – Low Energy

- Simulation overestimates equivalent radius approximately 17%
- Good agreement for aspect ratio (~12% difference)





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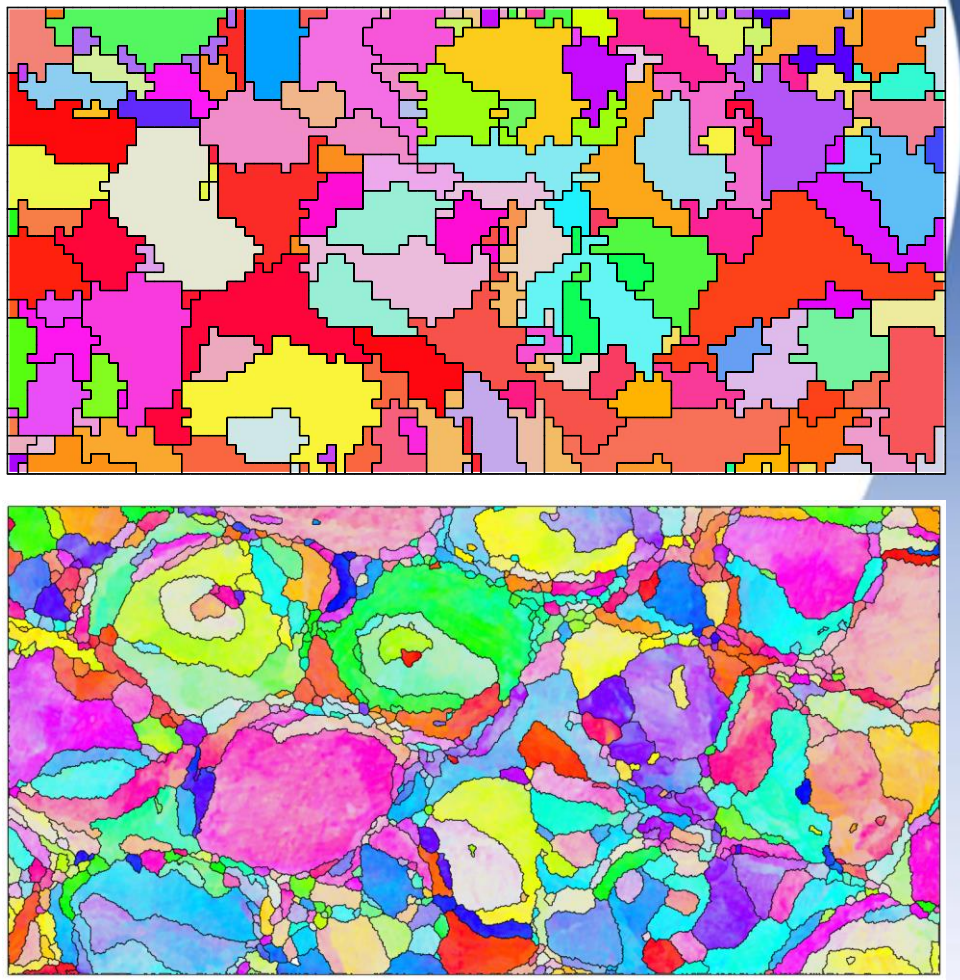
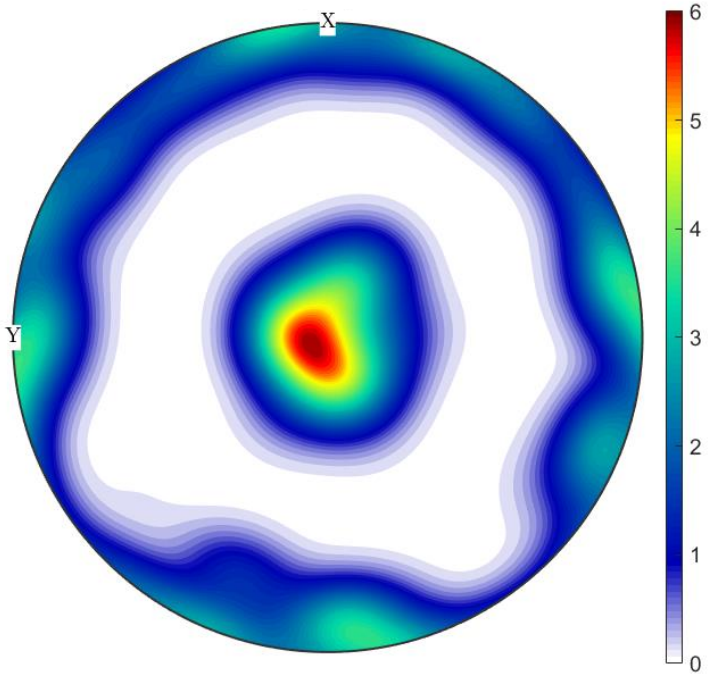


*Area Weighted Mean Values

Comparison with Experiment – High Energy

- Simulation overestimates <001> texture development (analyzed with MTEX [4])

Simulation
(100)



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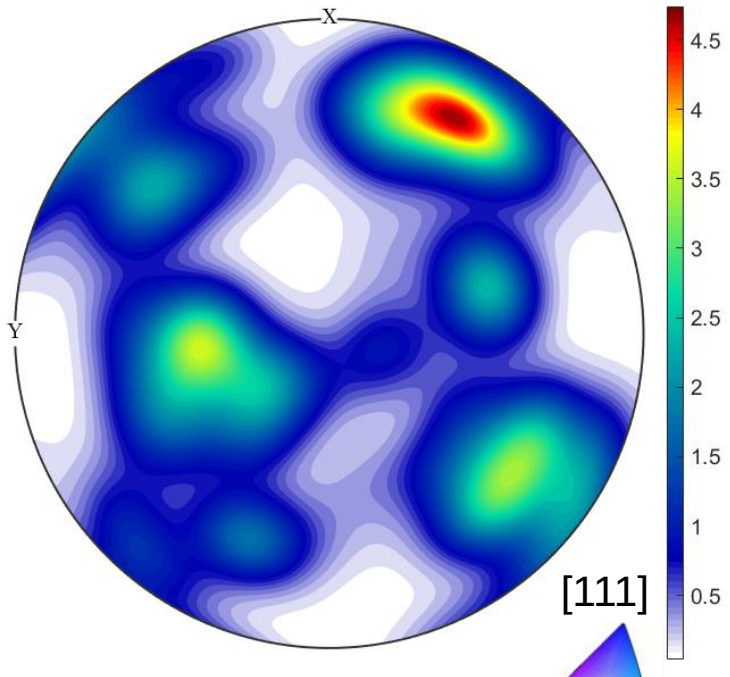

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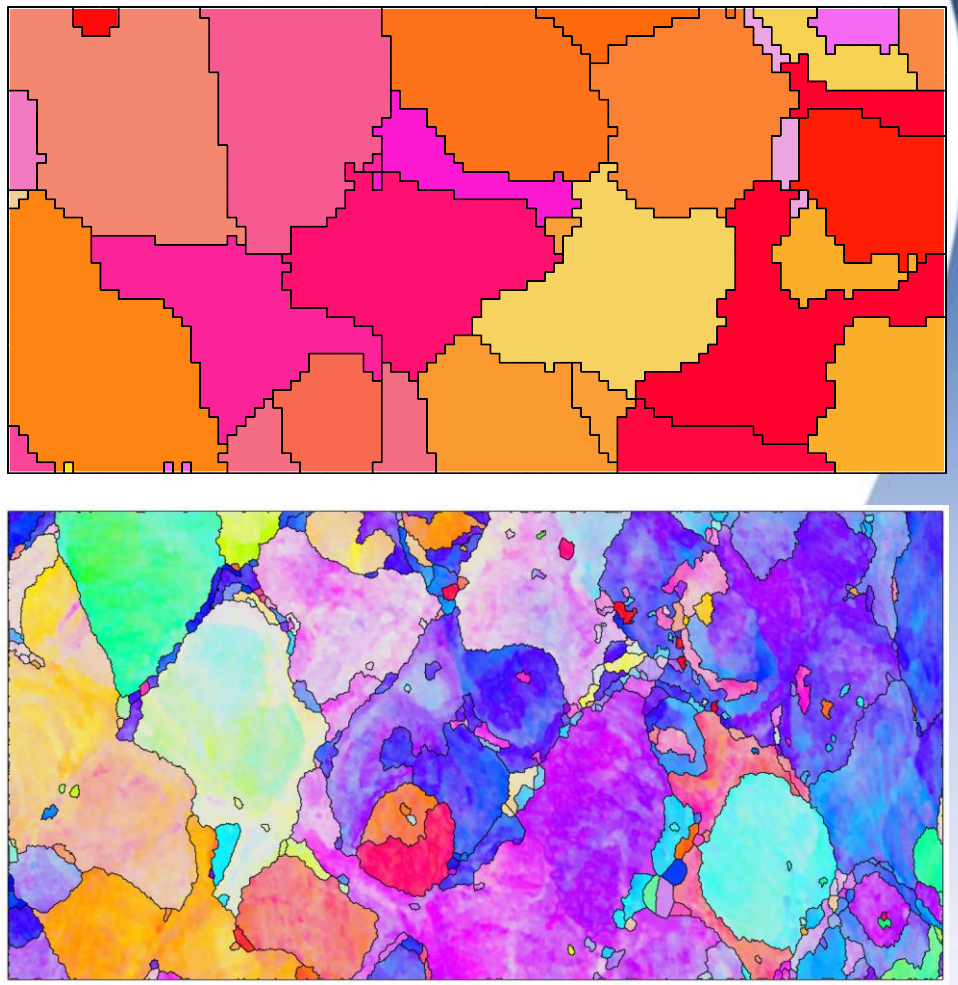
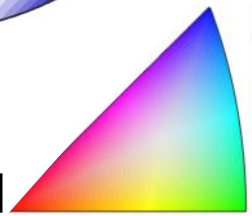


[111]

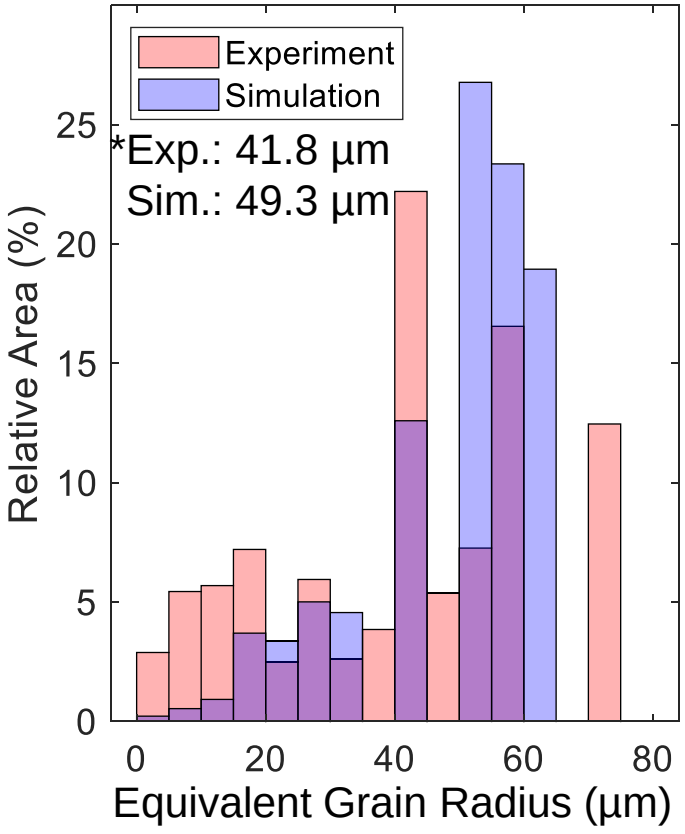


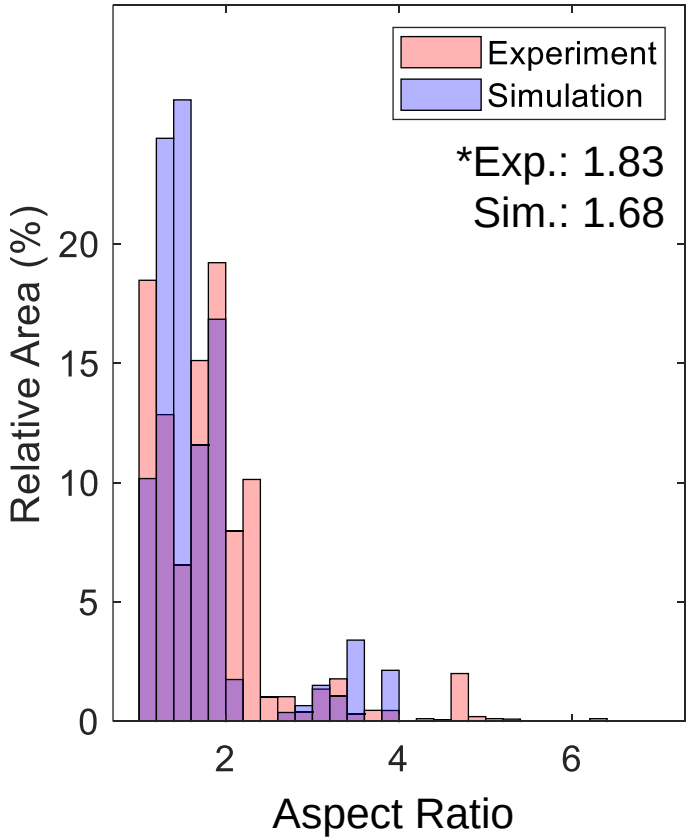
[001] [011] Z Reference Direction

[4] Niessen, F., et al. "Parent grain reconstruction from partially or fully transformed microstructures in MTEX." *Journal of Applied Crystallography* 55.1 (2022). 180-194. https://doi.org/10.1107/S1600576721011560

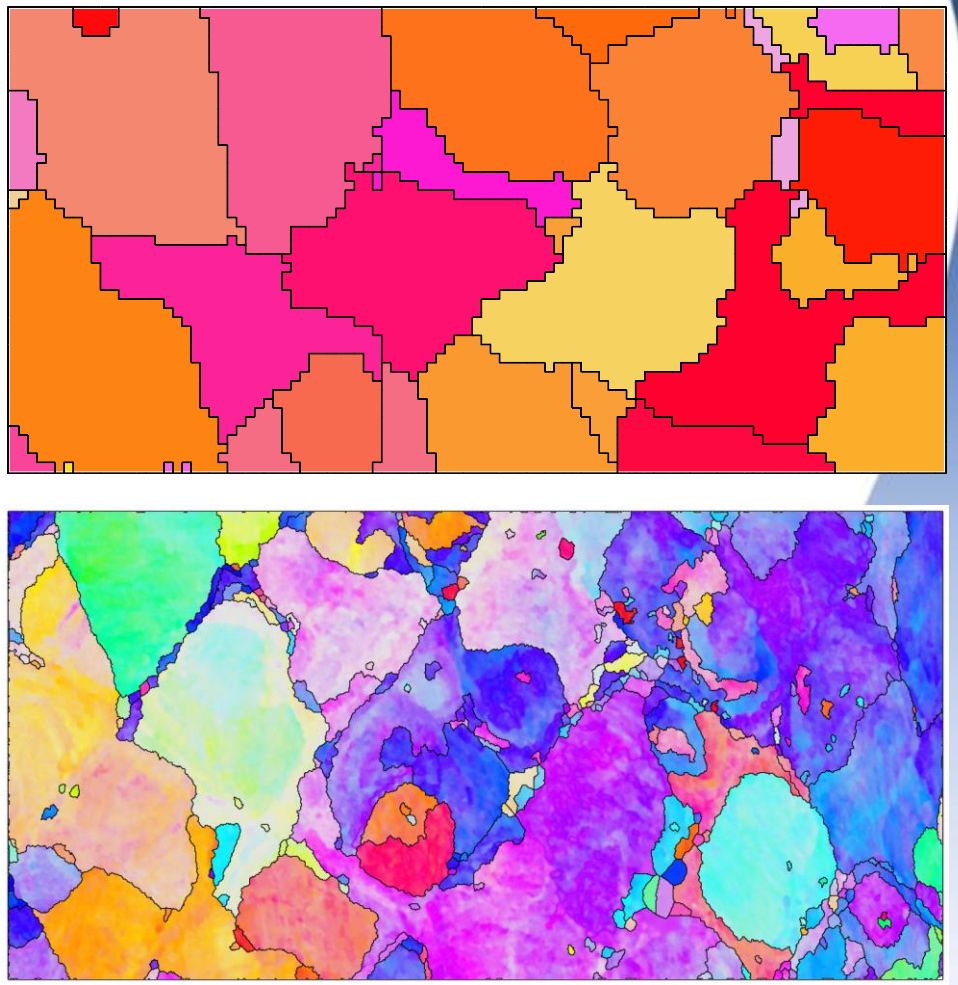
Comparison with Experiment – High Energy

- Simulation overestimates equivalent radius approximately 18%
- Good agreement for aspect ratio (~9% difference)





Simulation (top) and Experiment (bottom)



*Area Weighted Mean Values

Outline

Introduction / Background / Objective

Kinetic Monte Carlo Modeling of Microstructure Evolution

Analytical vs. Numerical Temperature Field Simulation

- Overview
- Impact of Time Step Choice

Simulation of Ti-6Al-4V PBF-LB Microstructure Evolution

- Comparisons with Experiment
- Effect of Processing Parameters

Conclusions and Summary

Summary of Findings

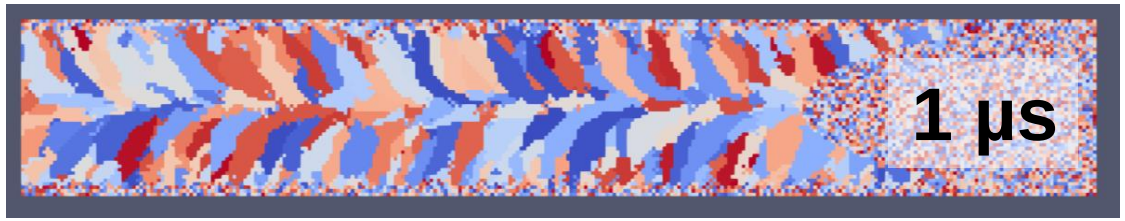
- Analytical temperature field tied Monte Carlo simulations were used to simulate Ti-6Al-4V PBF-LB
- Reasonable grain structure agreement between the simulation and experiment were observed
- A high laser power and low scanning velocity caused an increase in equivalent grain radius
- Aspect ratio was weakly impacted by the laser parameters
- The simulated crystallographic texture developed too quickly in the <001> direction compared to experimental measurements

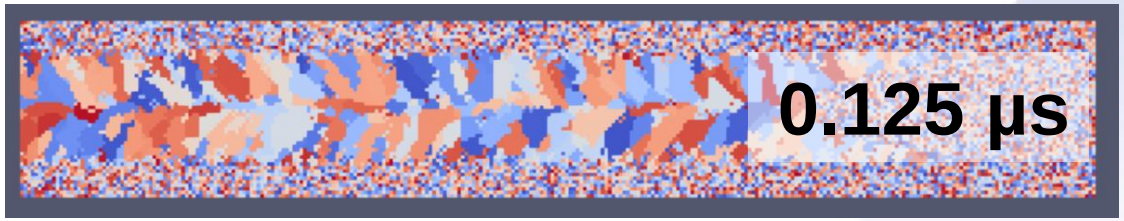
Key Takeaways

- The Monte Carlo method represents a suitable technique for simulating PBF-LB microstructure evolution

- There are advantages and disadvantages to using either an analytical or numerically-calculated temperature field
  - Analytical: higher computational efficiency, lower physical fidelity
  - Numerical: greater physical fidelity, numerical accuracy considerations

- If a numerical-temperature field is used, careful consideration of time step is required





End & Acknowledgements

Thank you!

Questions?

If you have further questions, I will be at AMBench on Wednesday and Thursday or email me at:

brodan.m.richter@nasa.gov

This work was supported by the NASA Aeronautics Research Mission Directorate (ARMD) Transformational Tools and Technologies (TTT) project

Interested in this work and engaging with us on it?
Reach out to us….

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Additional Slides

Meso-scale Modeling of Microstructure Evolution

Solidification Texture Nucleation **Grain Coarsening**

Linking the numerical and laboratory domains are critical for conducting accurate simulations. It is very easy to overestimate the amount of coarsening present

Numerical spatial and temporal domain  Laboratory spatial and temporal domain

dx= Voxel side length
dt_{MC} = Numerical/Monte Carlo time step
dt_{lab} = Laboratory time step
K_{MC}= Simulation Constant
K_0= Experimental pre-exponential
Q =Experimental activation energy
$\bar{R}$= Ideal Gas Constant
T_{max} = Maximum simulation temperature

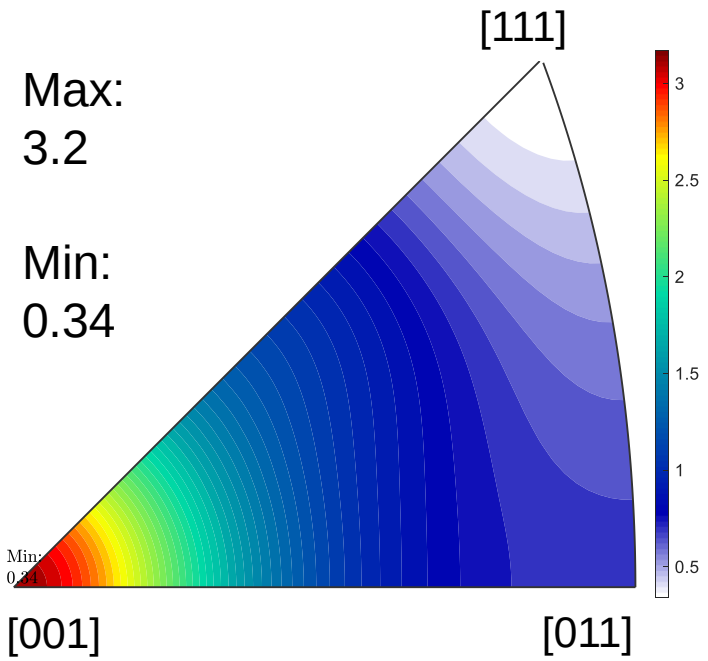
$$dt_{MC} = \frac{dx^2 K_{MC}}{K_0} \exp\left(\frac{Q}{\bar{R}T_{max}}\right) dt_{lab}$$

Domains are linked through heat treatment studies of grain size vs. time vs. temperature

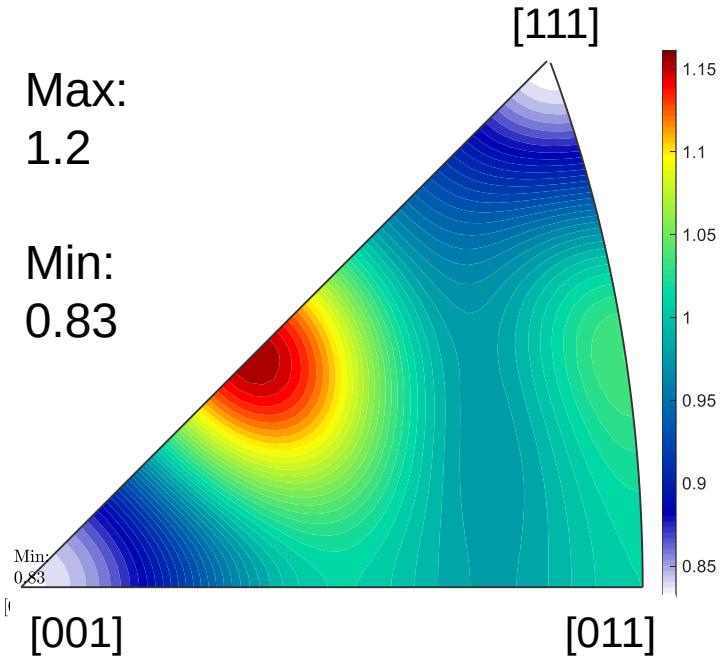
Comparison with Experiment – Low Energy

- Simulation overestimates <001> texture development and overall texture strength

Simulation
(100) Z-Direction IPF [4]



Experimental
(100) Z-Direction IPF [4]



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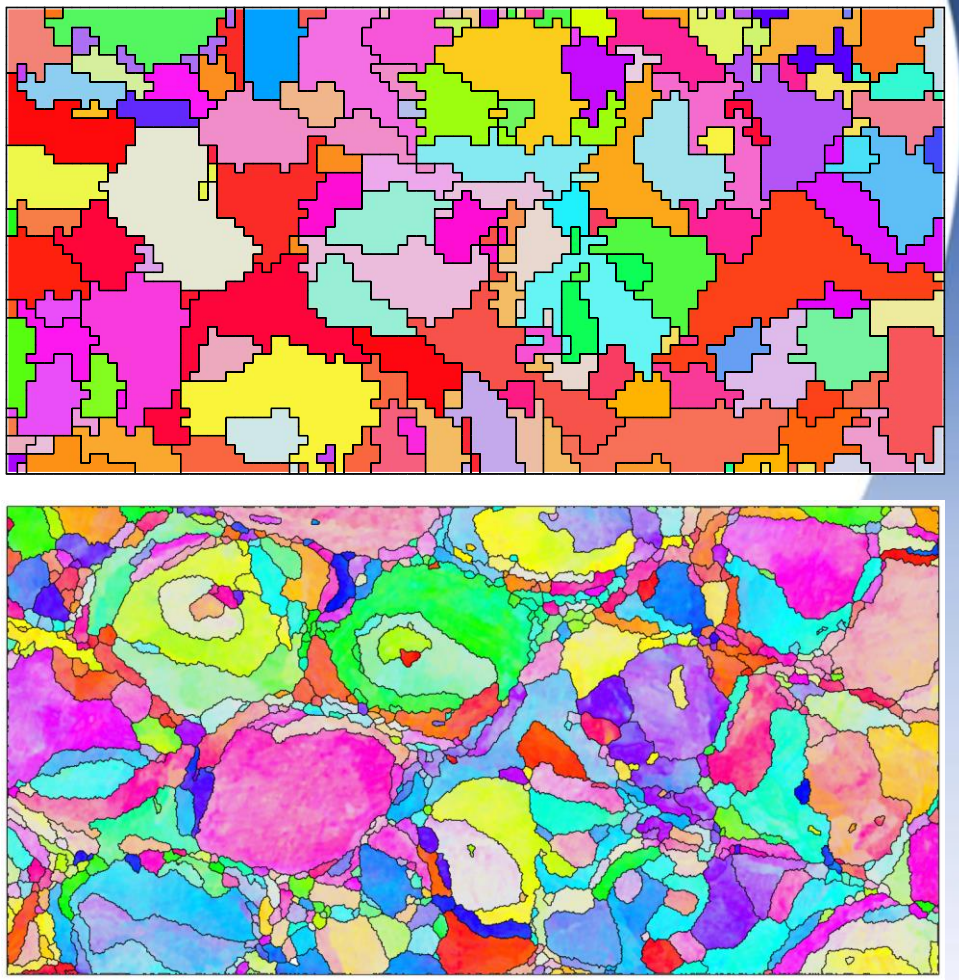

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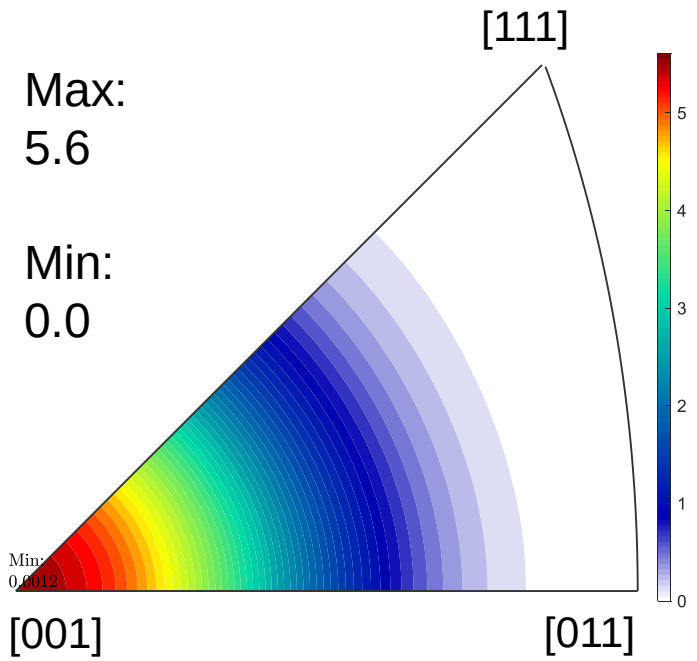

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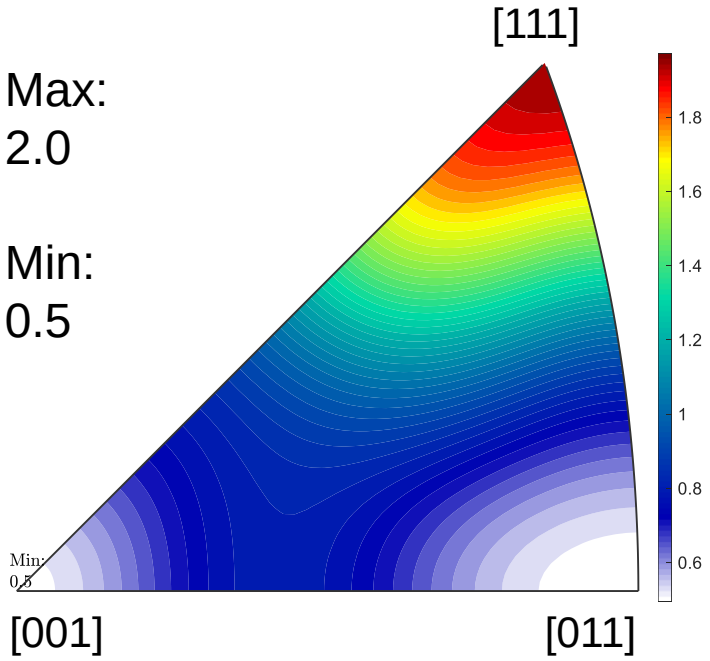
(100) Z-Direction IPF [4]



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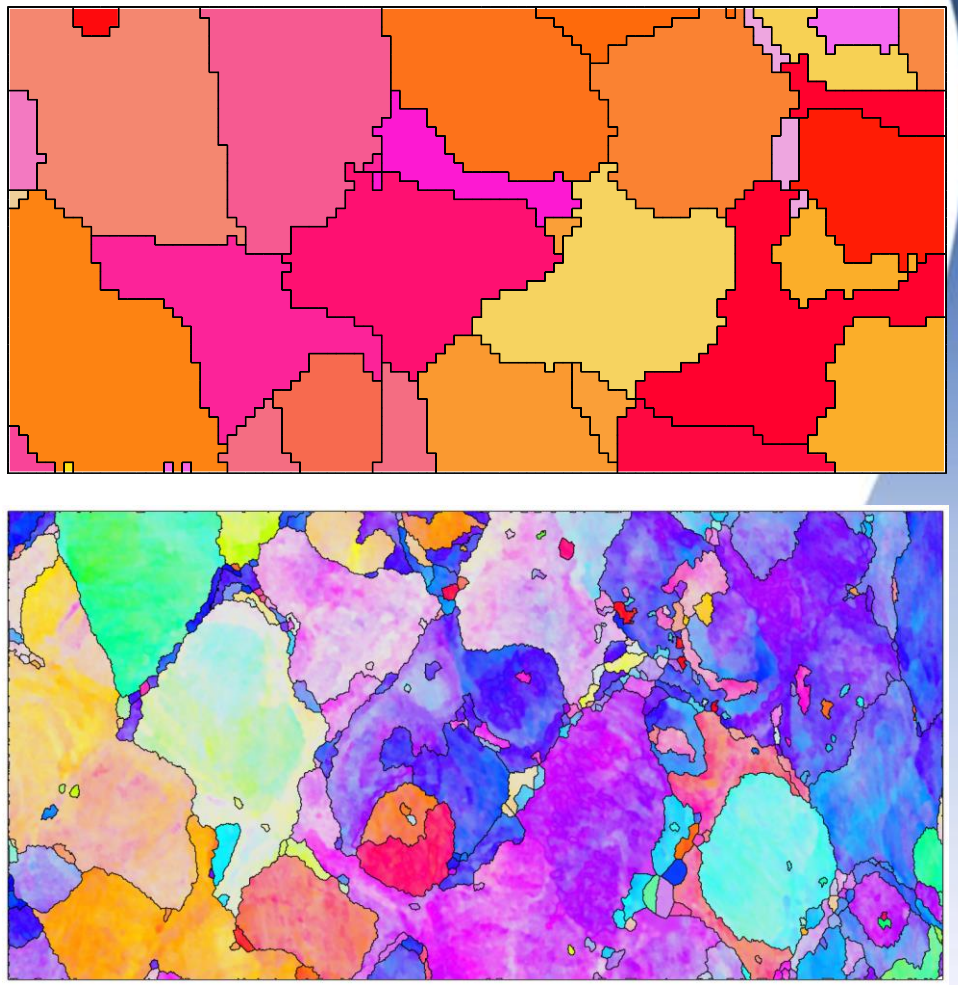

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