



Computational Microstructure Modeling for Powder Bed Fusion Additive Manufacturing

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Overview Presentation
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Introduction



Powder Bed Fusion (PBF) Additive Manufacturing (AM)

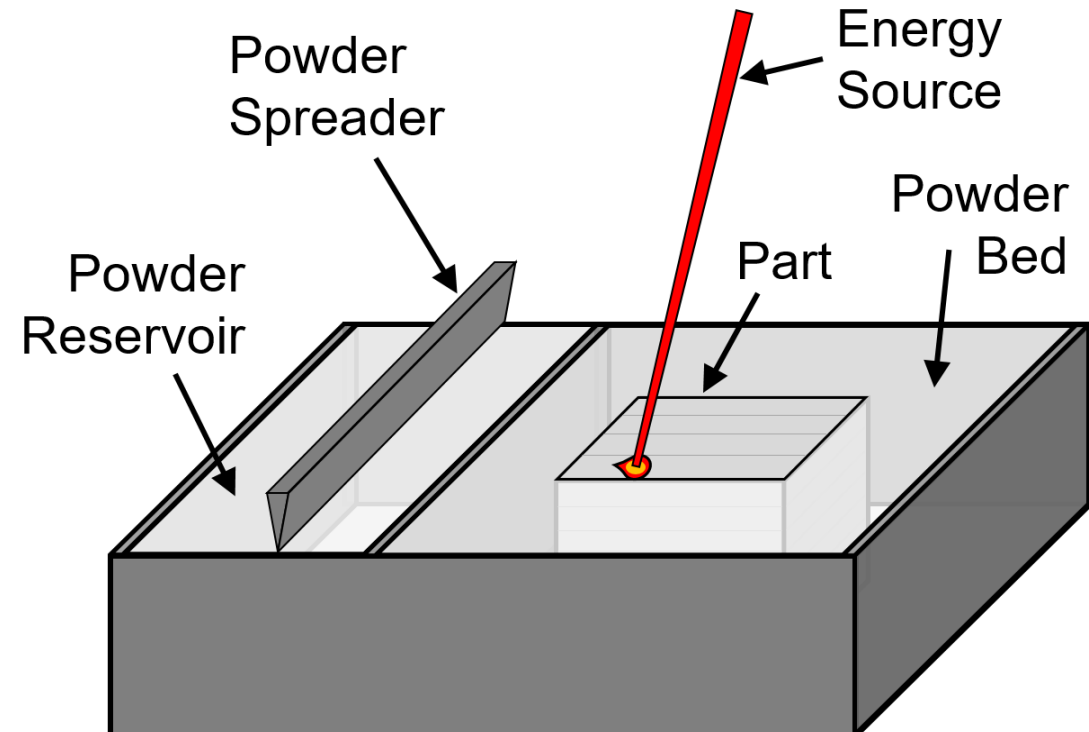
Advantages:

- Design complexity
- Feature resolution
- Near-net-shape creation
- Reduction in tooling
- Low concept-to-production time

Disadvantages:

- Build speed (low-to-medium runs)
- Part size
- Fatigue performance
- Performance uncertainty

Powder Bed Fusion AM Overview

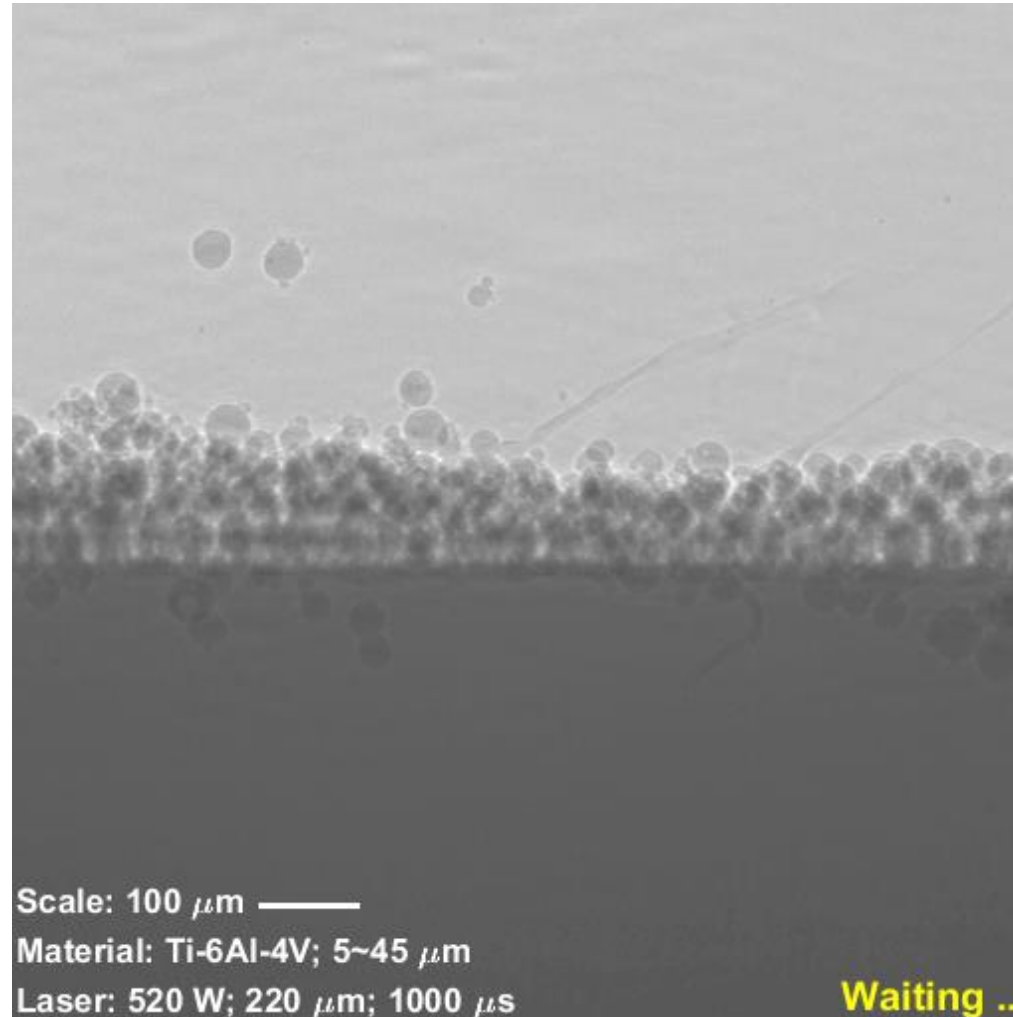


Complex Interaction of Multiple Phenomena in PBF



Simultaneous interactions between...

- Gas dynamics
- Plasma formation
- Fluid dynamics
- Granular/powder effects
- Phase transformations
- Heat transfer
- And more...



- ❖ Occurring constantly for hours or days
- ❖ Thousands or millions of melt events

Powder Layer

Bulk Material

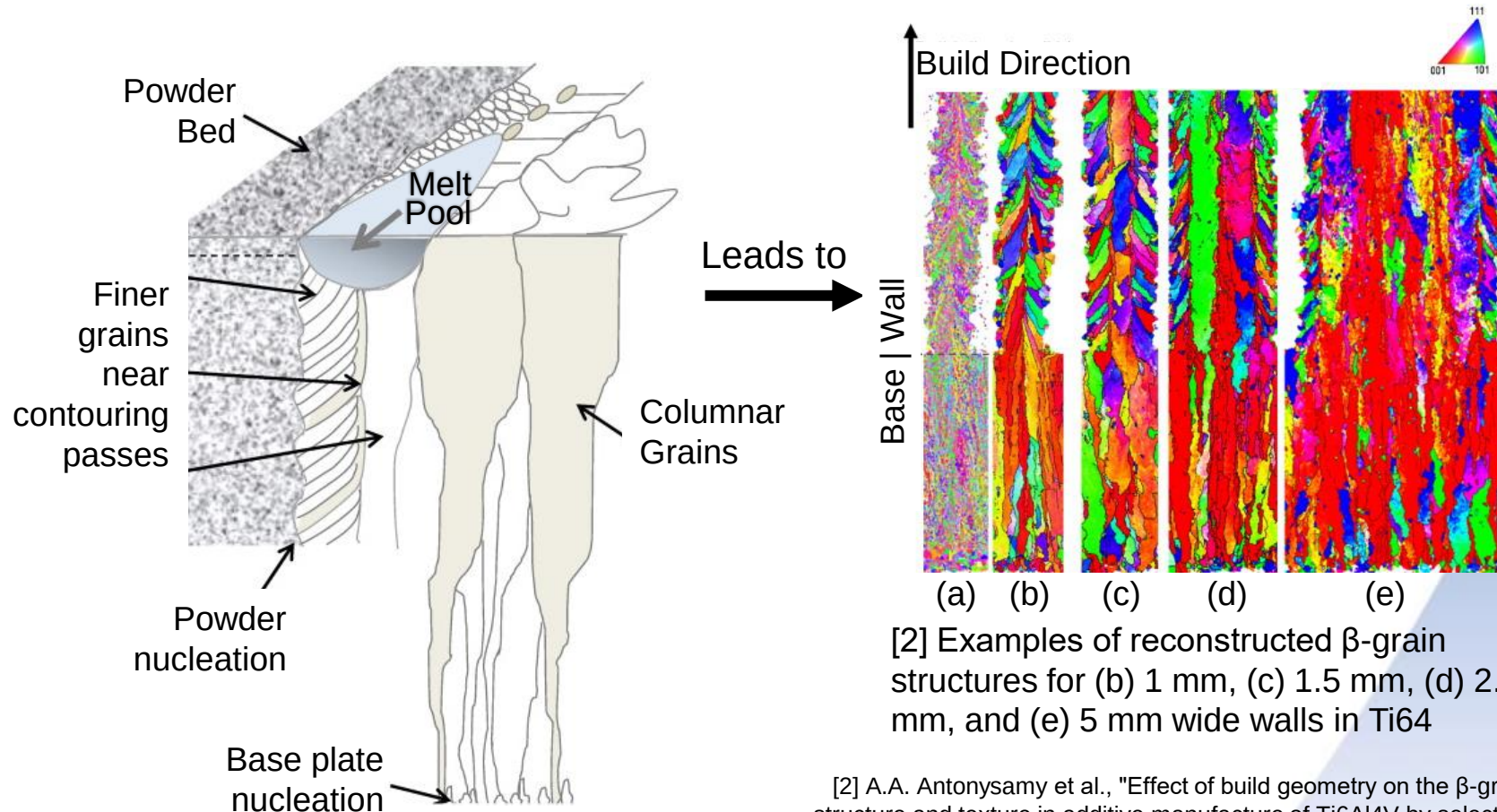
[1] C. Zhao, *et al.*, "Real-time monitoring of laser powder bed fusion process using high-speed X-ray imaging and diffraction." *Sci Rep* 7, 3602 (2017).
<https://doi.org/10.1038/s41598-017-03761-2>
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Bulk-Scale Effects of PBF on Microstructure



Process involves reiterative melting and solidification events

Causes the formation of large, columnar grains orientated in the build direction



[2] Microstructure Development Mechanism

[2] Examples of reconstructed β -grain structures for (b) 1 mm, (c) 1.5 mm, (d) 2.0 mm, and (e) 5 mm wide walls in Ti64

[2] A.A. Antonyasamy et al., "Effect of build geometry on the β -grain structure and texture in additive manufacture of Ti6Al4V by selective electron beam melting." *Materials characterization* 84 (2013): 153-168. <https://doi.org/10.1016/j.matchar.2013.07.012>, Figures 3 and 7 used under CC BY 3.0 license <https://creativecommons.org/licenses/by/3.0/> Figures cropped and relabeled vs. original

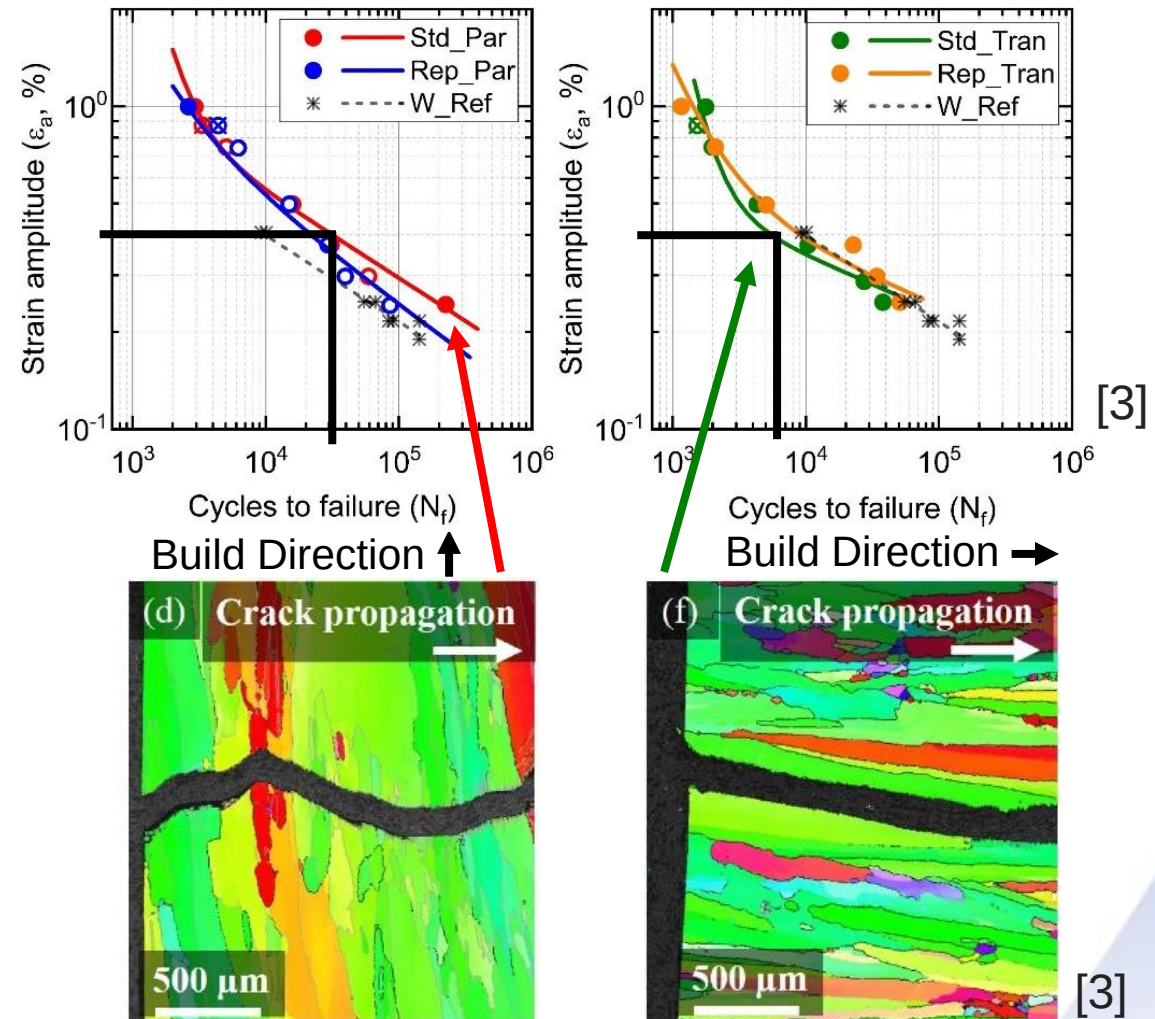
Importance of AM Microstructure



Columnar grains cause performance anisotropy and uncertainty based on part orientation

Renders qualification and certification (Q&C) of aerospace parts difficult

Want to relate final performance back to grain structure and processing

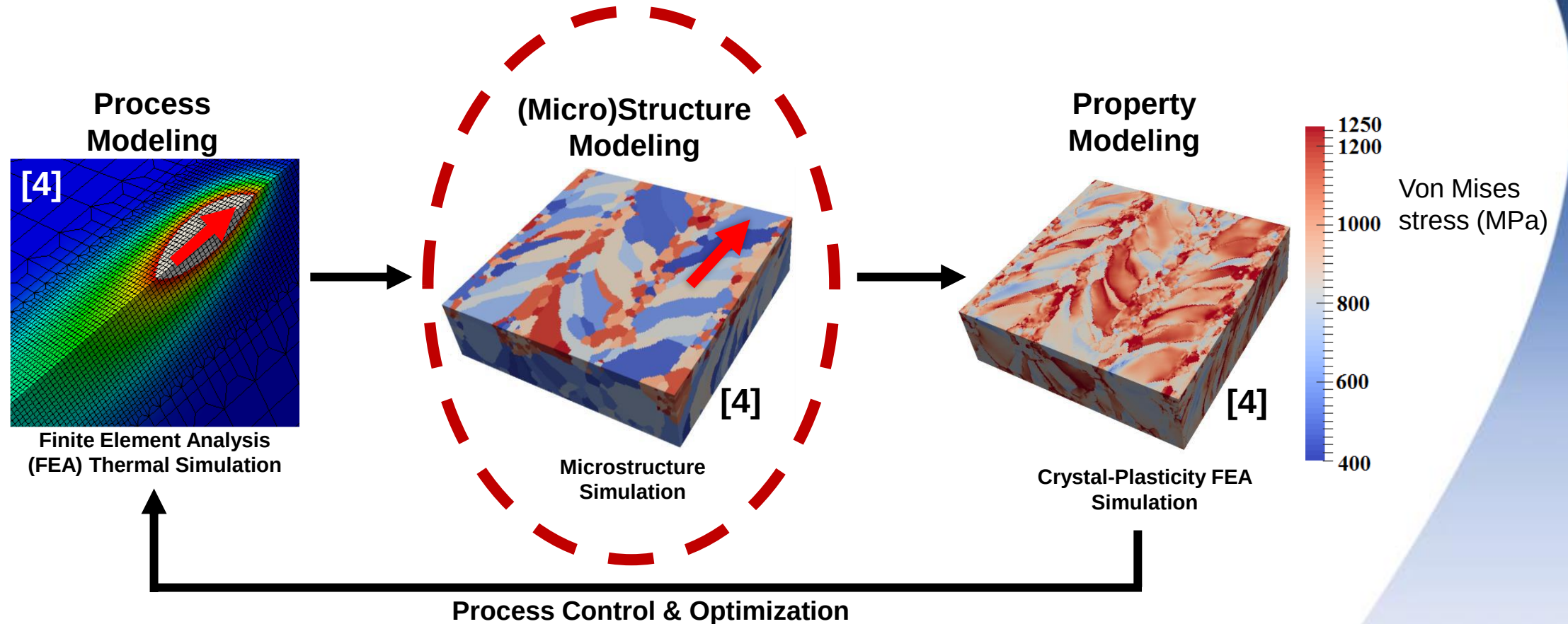


[3] A.R. Balachandramurthi, "Anisotropic fatigue properties of Alloy 718 manufactured by Electron Beam Powder Bed Fusion," Int. J. Fatigue 141 (2020)

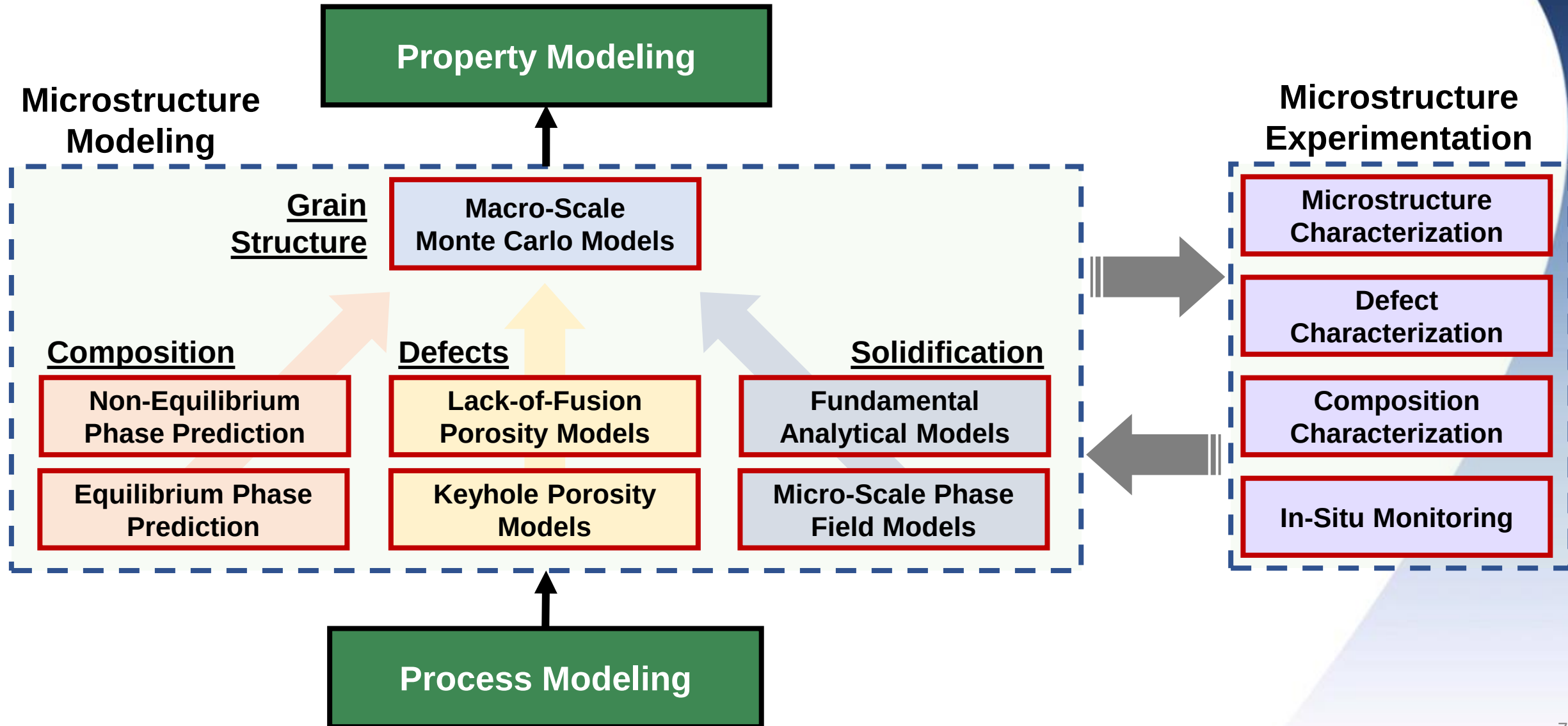
Figures 10 & 13 used under CC BY 4.0 license <https://creativecommons.org/licenses/by/4.0/>

<https://doi.org/10.1016/j.ijfatigue.2020.105898> Figures cropped, re-arranged, and lines added vs. original

Process-Structure-Property (PSP) Frameworks



Components of Microstructure Modeling



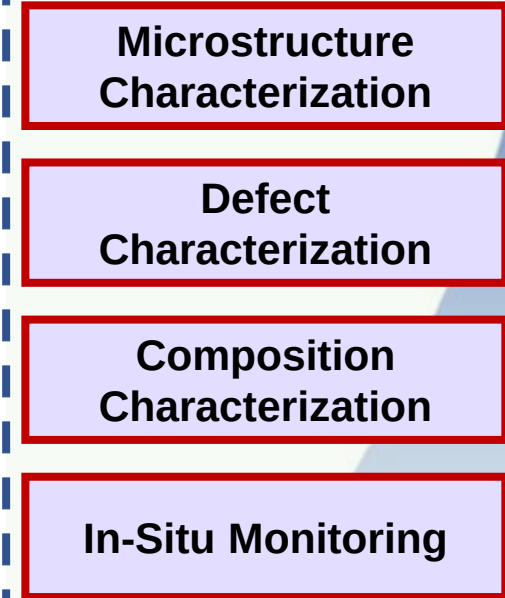
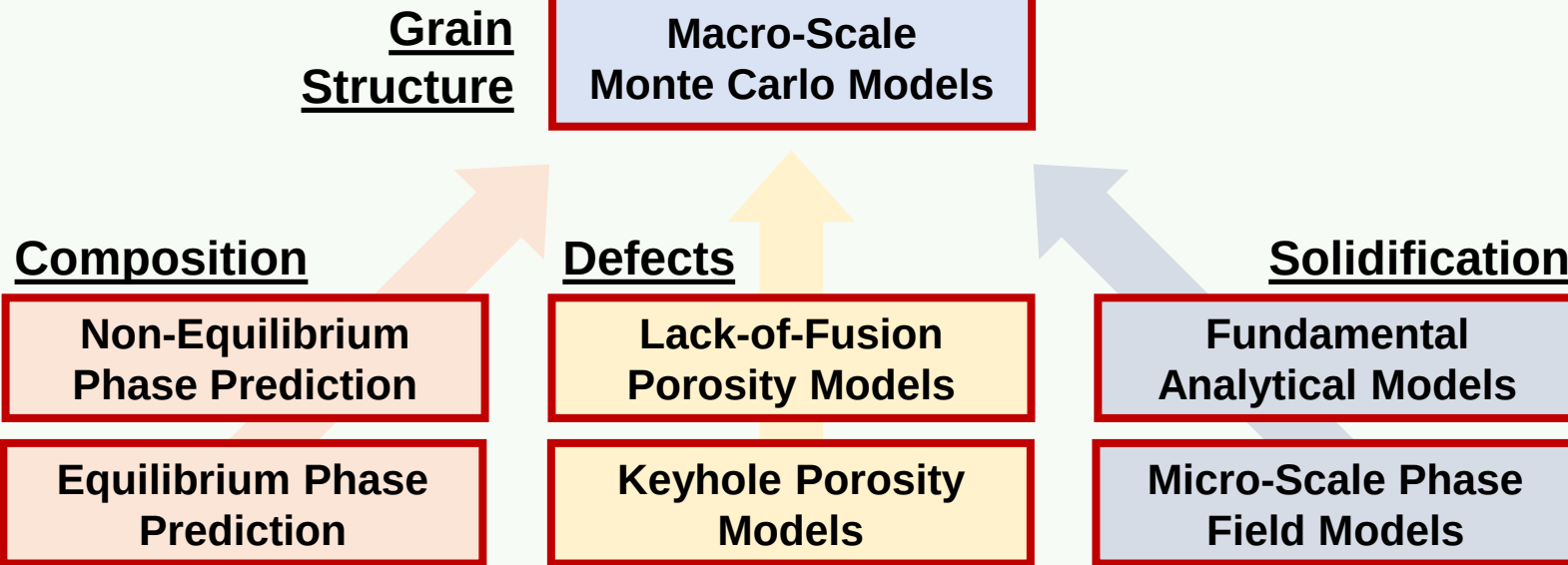
Components of Microstructure Modeling



Database Linkages Applied to Microstructure Modeling

Microstructure Modeling

Microstructure Experimentation



Integrated with
entire framework

Process
Models

Property
Models

Uncertainty
Quantification

Experiments /
Monitoring

Equilibrium and Non-Equilibrium Phase Prediction

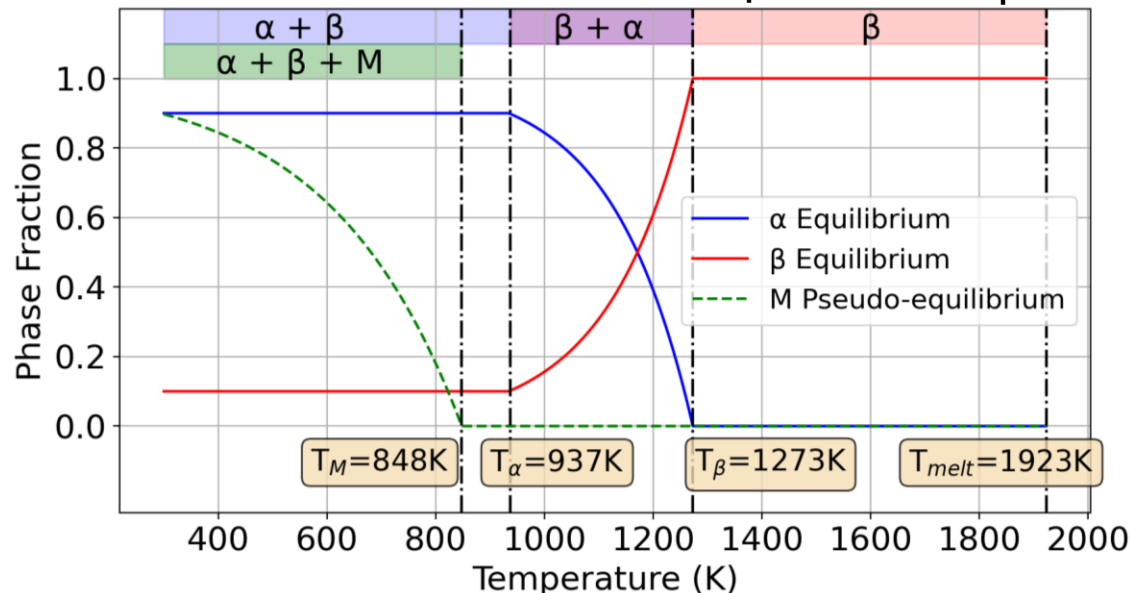
❖ Phase Prediction

Simulates phase composition through free energy and kinetics

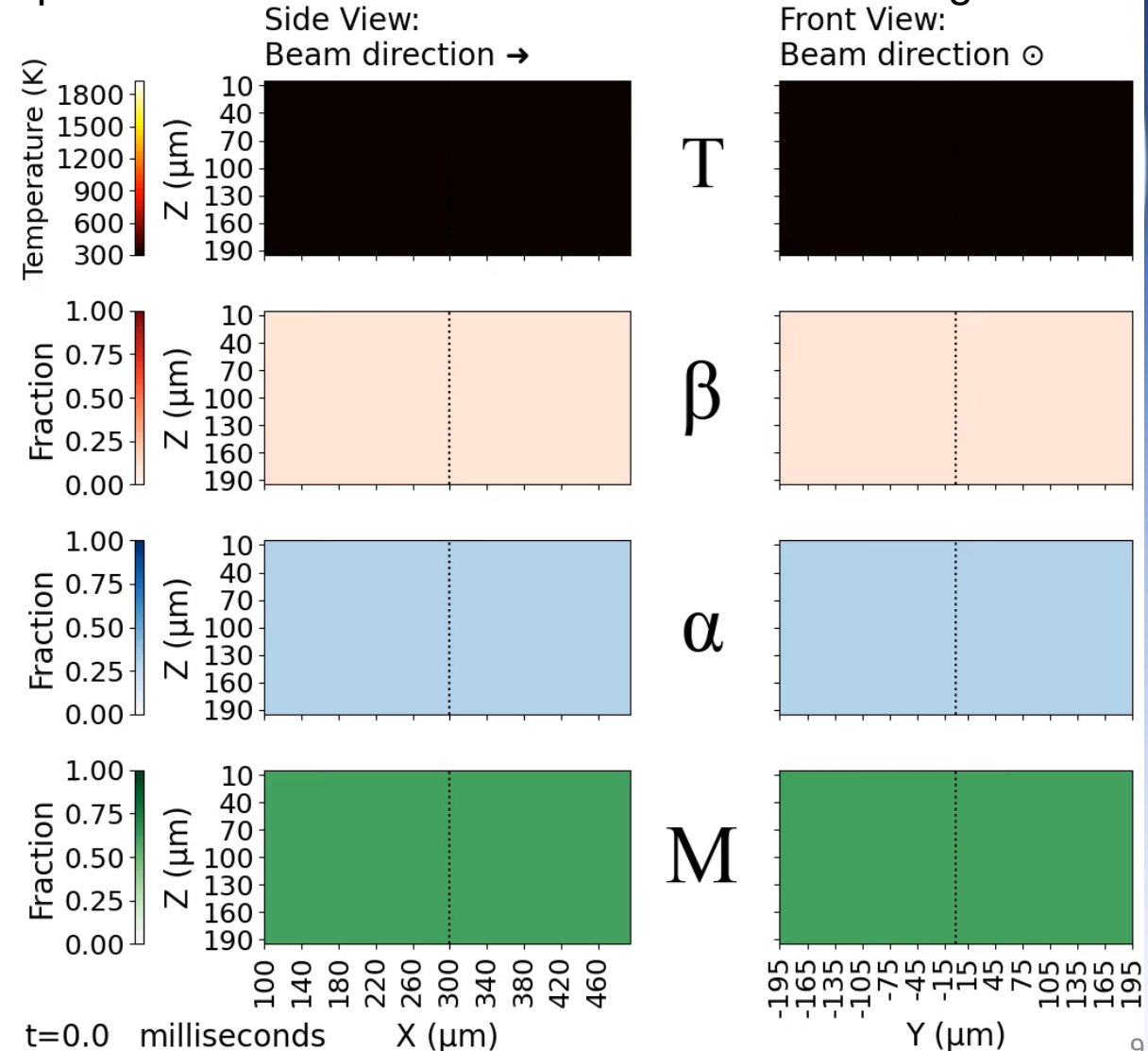
- Occurrence of deleterious phases
- Provides phases for property models

Ti-6Al-4V Equilibrium Phase Diagram

β : Beta M: Martensite
 α : Alpha T: Temperature



Non-Equilibrium Phase Prediction for Ti-6Al-4V during PBF



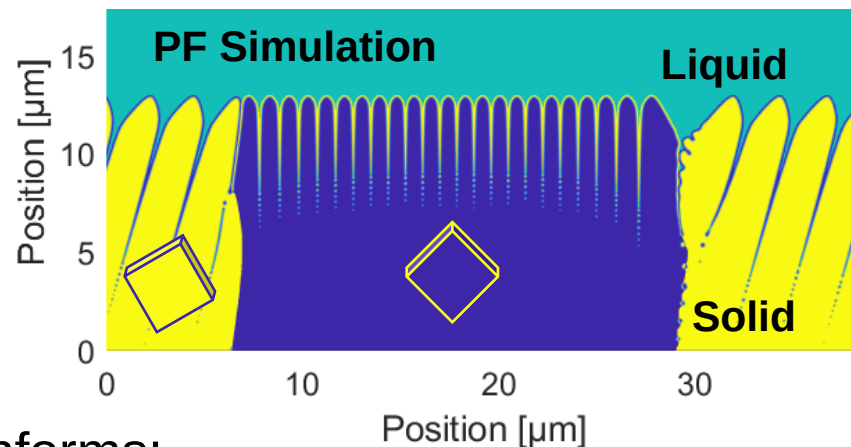
Micro-Scale Phase Field Models



❖ Phase-Field (PF)

Simulates solidification by solving governing partial differential equations

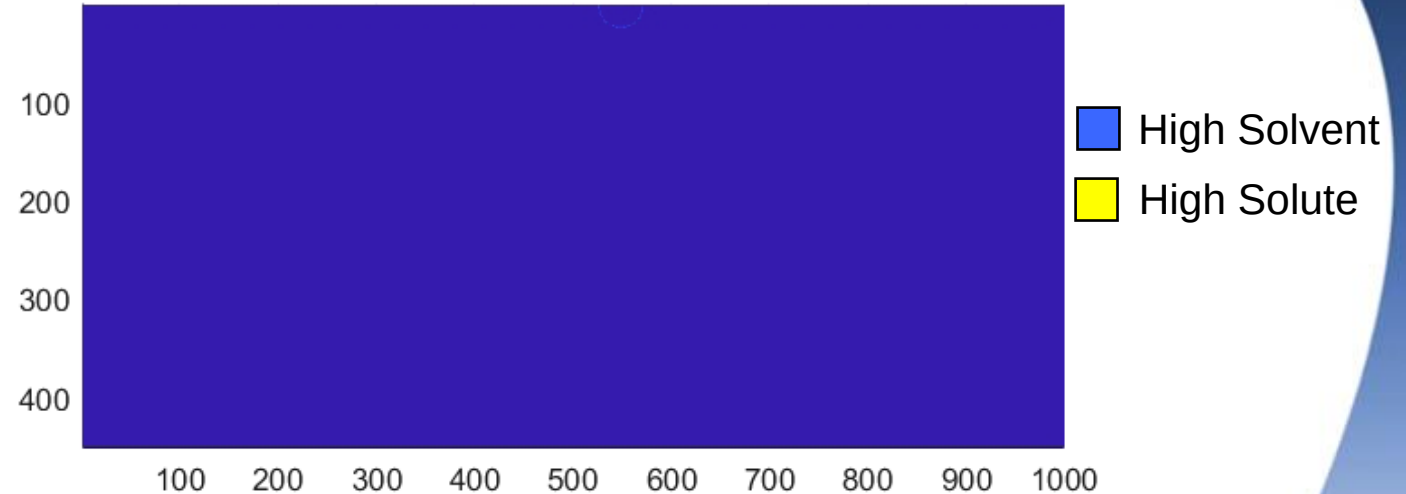
- High accuracy and resolution
- Computationally expensive
- Strong physical basis



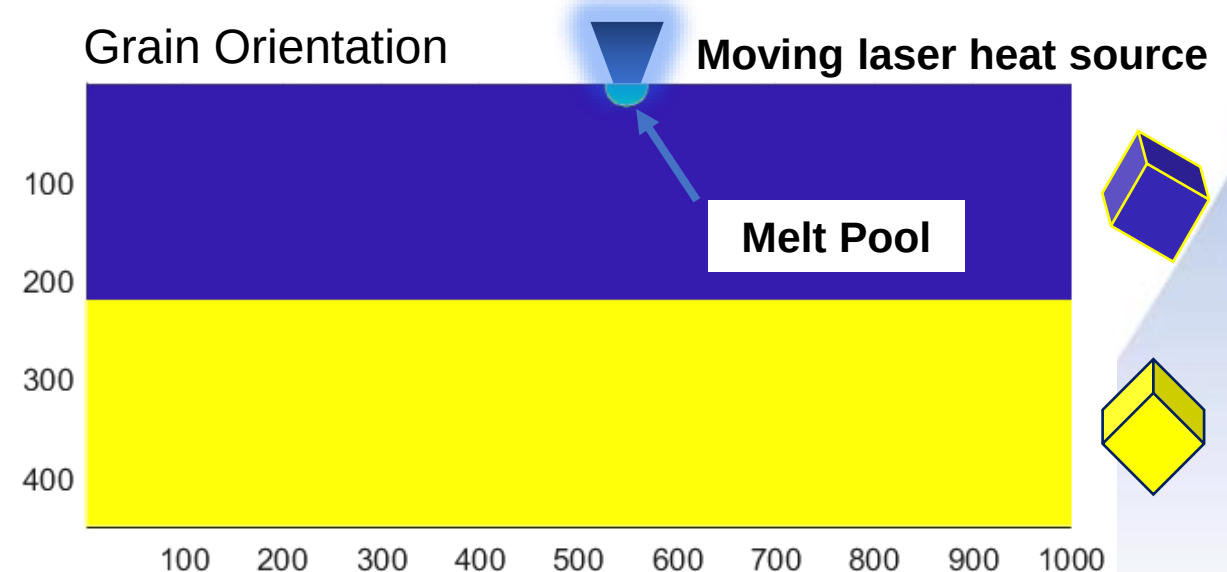
Informs:

- Dendritic velocity
- Texture evolution
- Solute buildup

Concentration Surface Map



Grain Orientation



Fundamental Analytical Models

❖ Analytical Models

Various analytical models are used in conjunction with computational models to:

- Provide inputs for more complex models
- Allows verification of more complex models

Columnar-to-Equiaxed Transition

$$G_{equiaxed} < 0.617 N_0^{1/3} \left(1 - \frac{\Delta T_N^3}{\Delta T_c^3} \right) \Delta T_c$$

Dendrite Velocity vs. Undercooling

$$v_s = c_1 \Delta T_c^{c_2}$$

N_0 : Nucleation particles per unit volume

ΔT_N : Nucleation temperature

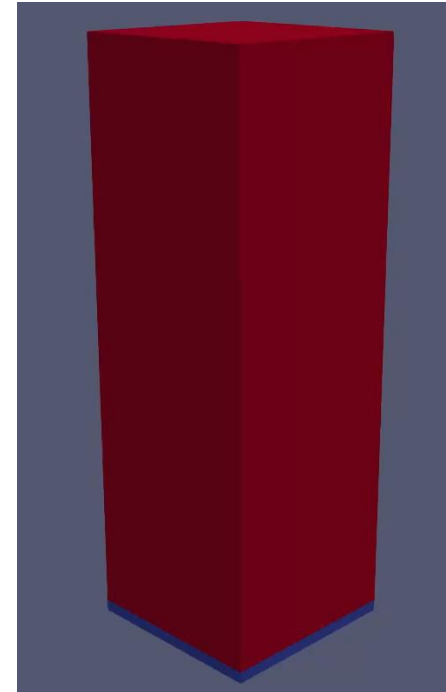
ΔT_c : Undercooling temperature

c_1, c_2 : Material growth constants

v_s : Dendritic growth velocity

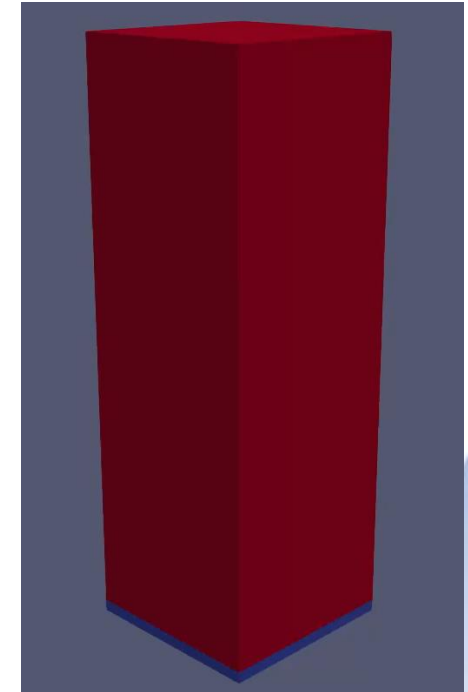
G : Thermal gradient

$G: 10^5 \text{ K/m}$
 $v_s: 0.1 \text{ m/s}$



Equiaxed
Region

$G: 10^7 \text{ K/m}$
 $v_s: 0.1 \text{ m/s}$



Columnar
Region

- Liquid
- Columnar grains
- Equiaxed grains

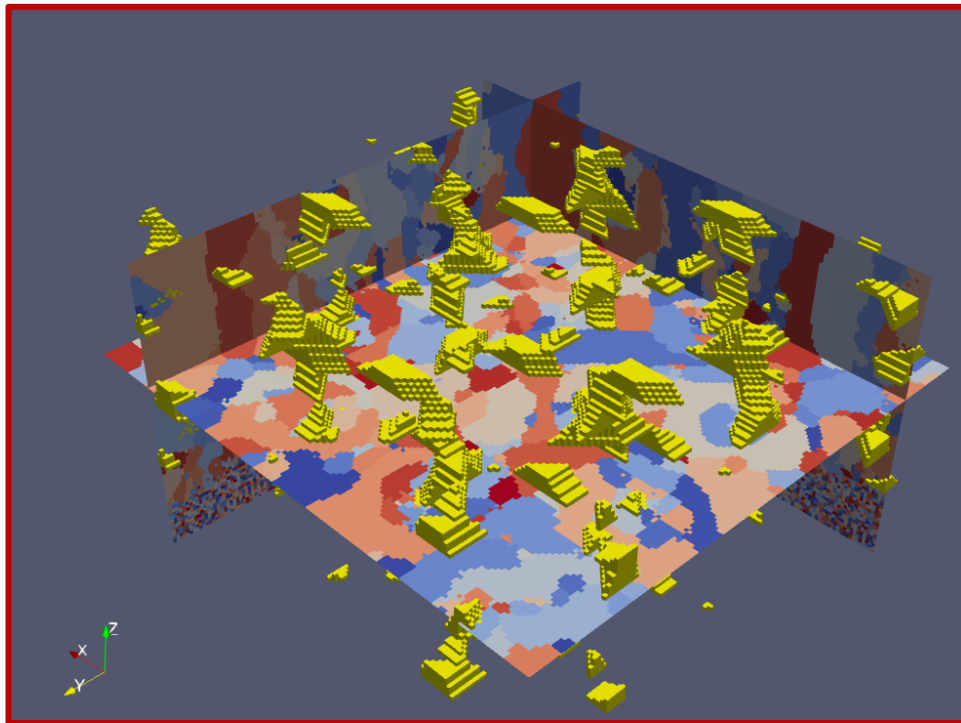
Keyhole and Lack-of-Fusion Defect Modeling



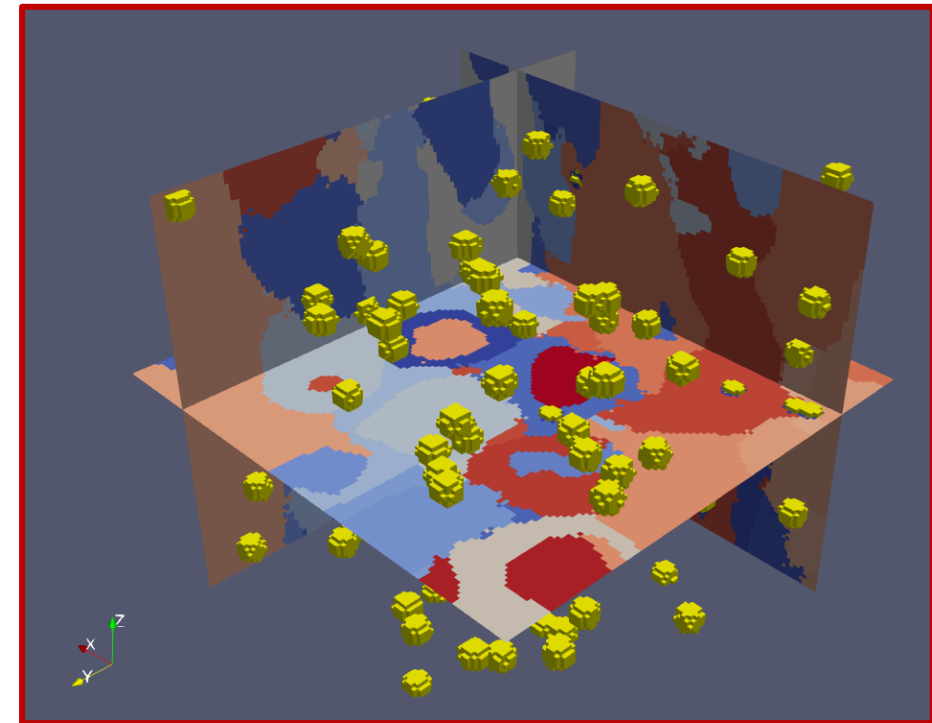
❖ Defect Modeling

- Simulates defect formation during processing based on processing parameters
- Allows for estimating part density and impact of defects on performance

Lack-of-Fusion Porosity (Deterministic)



Keyhole Porosity (Stochastic)

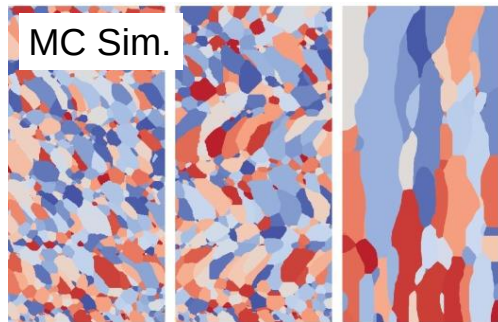
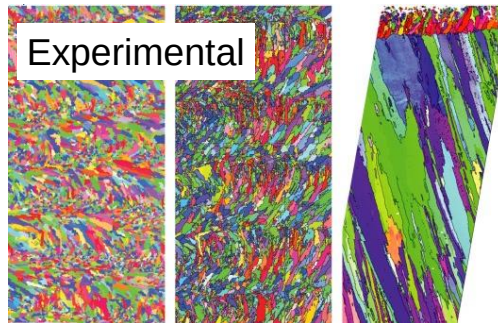


Porosity  Grain # 

Macro-Scale Monte Carlo Models



❖ Monte Carlo (MC) [6]



Build Direction ↑
[6]
Low-Power Unidirectional Low-Power Bidirectional High-Power Bidirectional

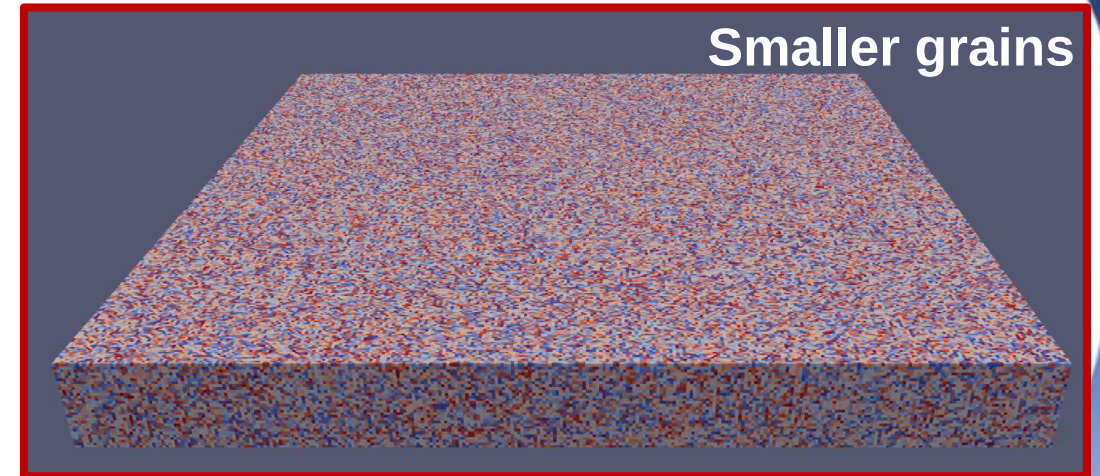
Simulates grain evolution through a series of probabilistic flips

- Micrometer resolution
- Highly flexible
- Cheap
- Weak physical basis

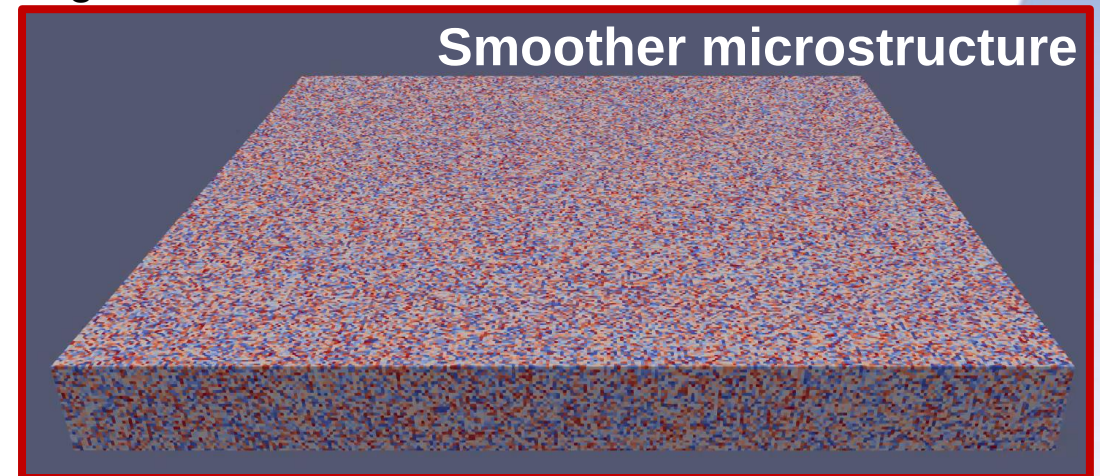
Informs:

- Grain growth

Low Laser Power



High Laser Power



Grain #

[6] T.M. Rodgers et al., Simulation of metal additive manufacturing microstructures using kinetic Monte Carlo, *Comp. Mater. Sci.* (2017) <https://doi.org/10.1016/j.commatsci.2017.03.053>
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Key Takeaways and Framework Linkages



- Process-Structure-Property modeling frameworks enable process understanding and the relating of part processing to performance
- Microstructure modeling involves many interconnected components
- Models and experiments can leverage database linkages to provide further advantages

Simulated Grain Structure Overview

