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3D Characterization of the Columnar-to-Equiaxed Transition in Additively Manufactured Inconel 718

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Outline

- Background
- Three-dimensional Characterization
- Calibrating a Microstructure-Processing Map
- Summary

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Additive manufacturing (AM) provides enormous flexibility in design

Aerospace

Images courtesy Fraunhofer IWU, Lawrence Livermore National Lab, EOS, Added Scientific, and Imperial Machine & Tool Co.

Additive manufacturing (AM) provides enormous flexibility in design

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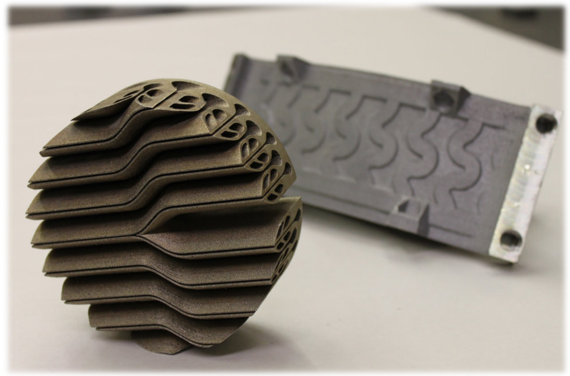
Biomedical

Images courtesy Fraunhofer IWU, Lawrence Livermore National Lab, EOS, Added Scientific, and Imperial Machine & Tool Co.

Additive manufacturing (AM) provides enormous flexibility in design

Aerospace

Industrial

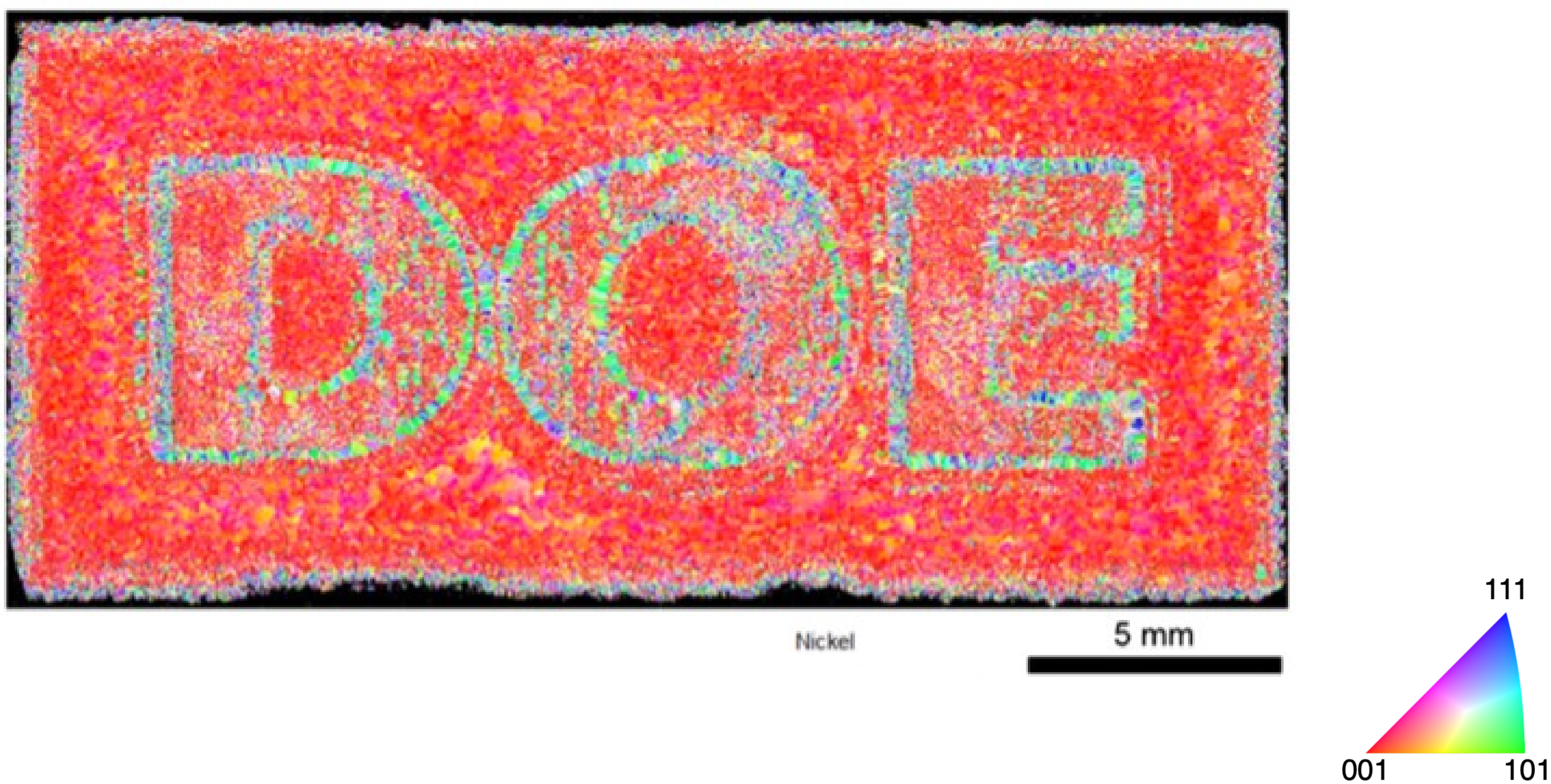


Biomedical

Images courtesy Fraunhofer IWU, Lawrence Livermore National Lab, EOS, Added Scientific, and Imperial Machine & Tool Co.

Scan strategy can be manipulated for site-specific microstructure

- Founded in parametric studies that are not easily generalizable to complex geometries



RR Dehoff, MM Kirka, WJ Sames, H Bilheux, AS Tremsin, LE Lowe, and SS Babu, *Materials Science and Technology*, 2015

Scan strategy can be manipulated for site-specific microstructure

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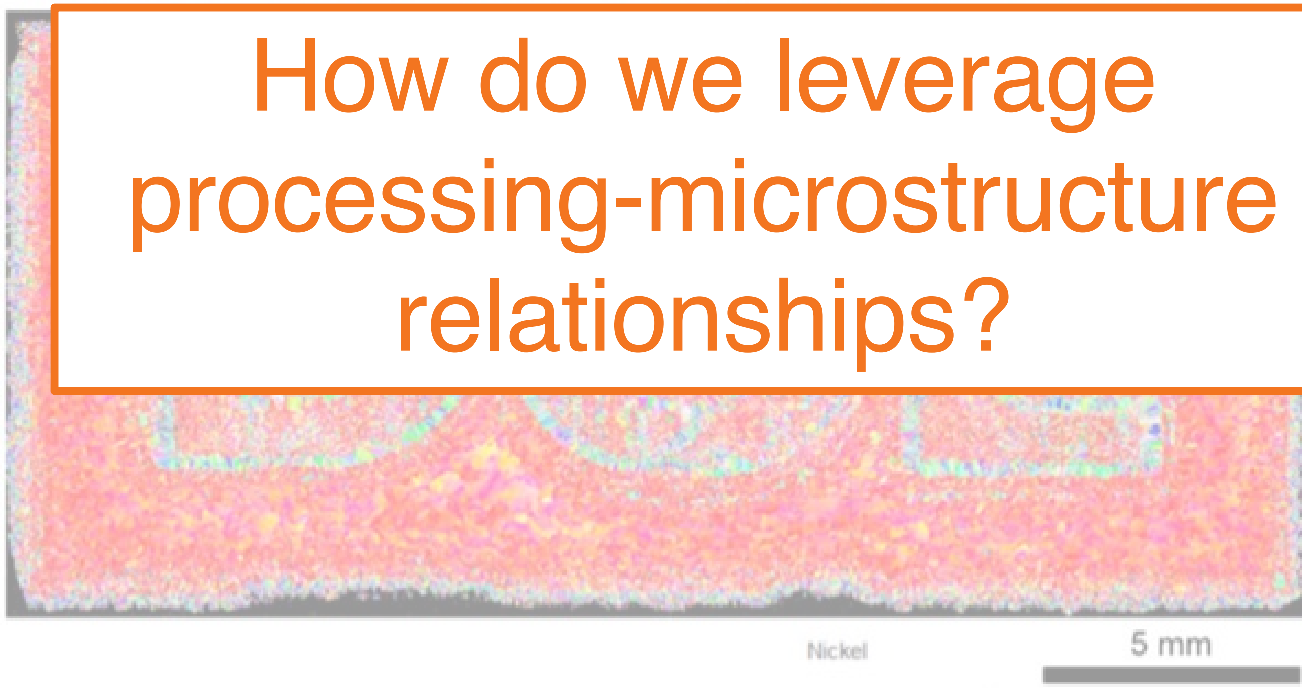
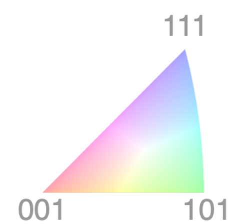
How do we leverage processing-microstructure relationships?





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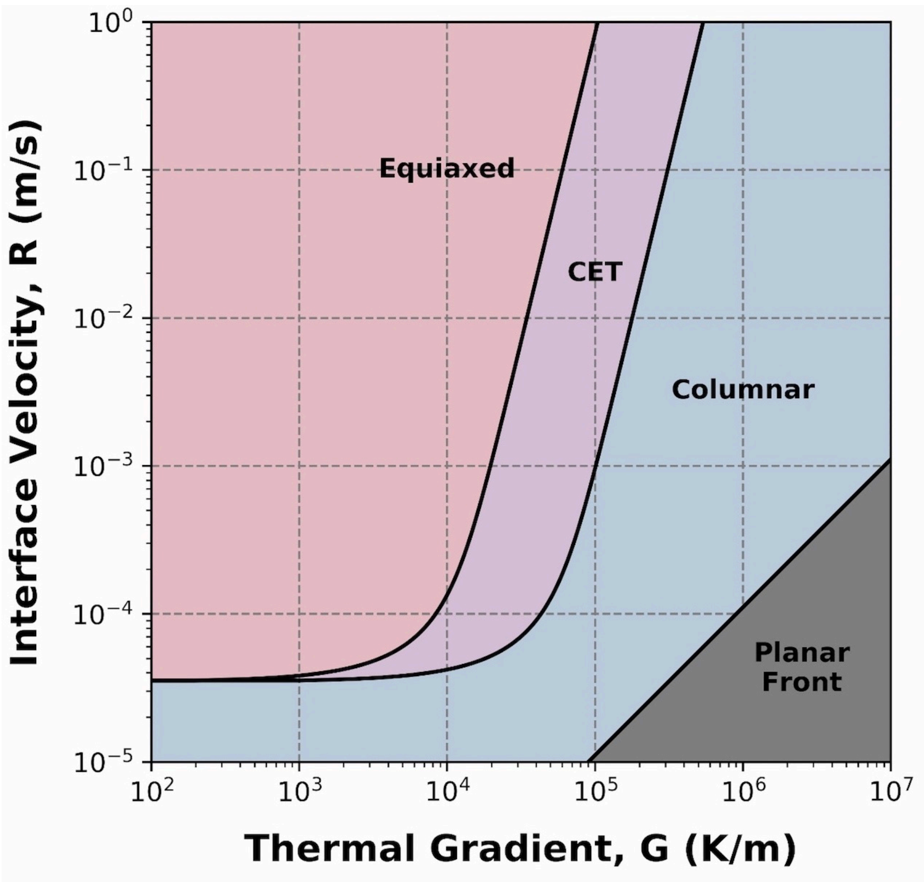
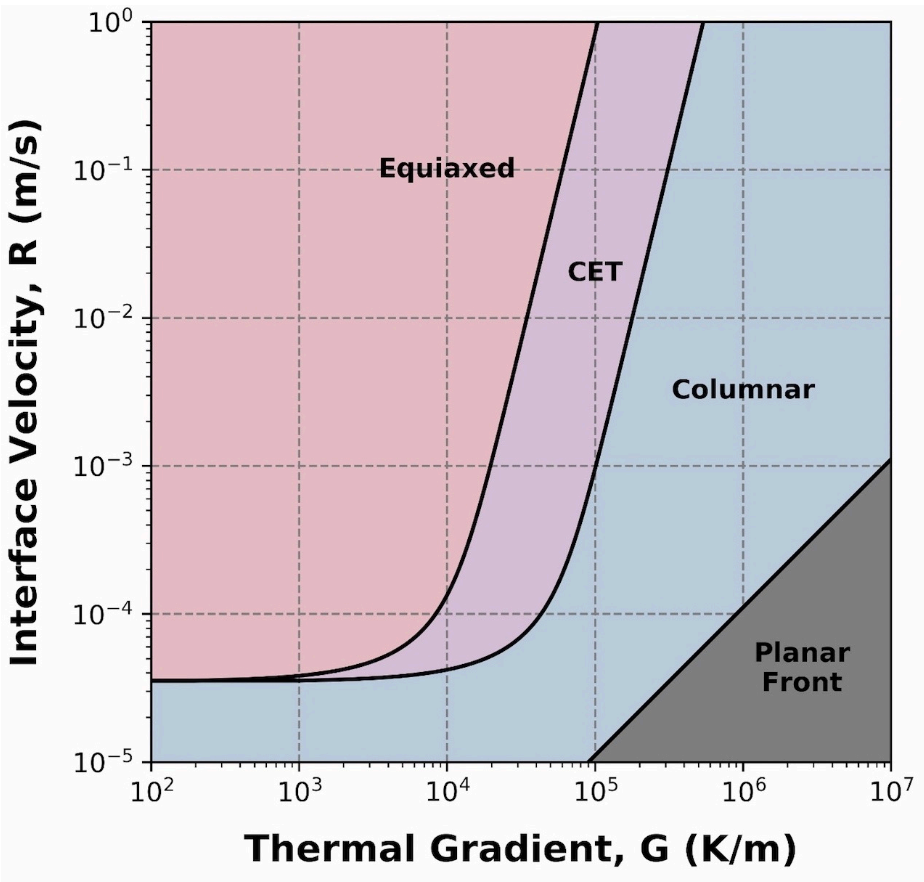
Local microstructure control relies on understanding solidification conditions

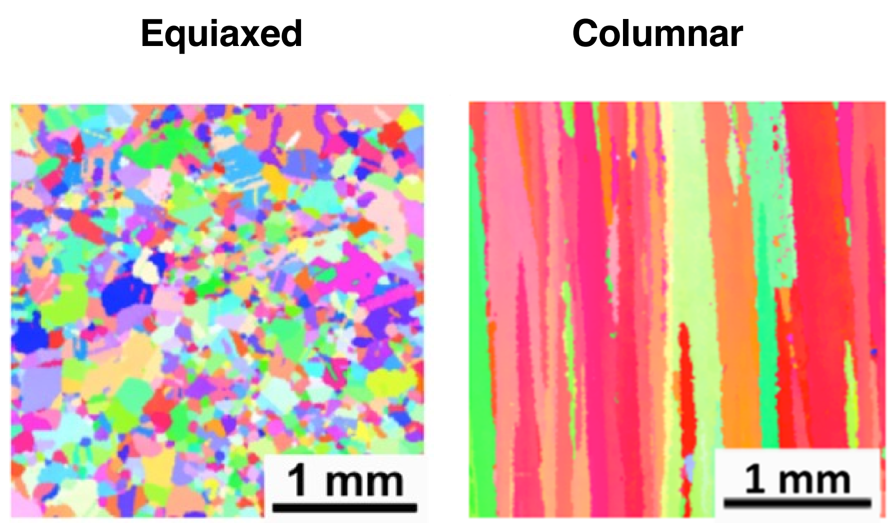
- Processing maps help predict microstructure



Local microstructure control relies on understanding solidification conditions

- Processing maps help predict microstructure

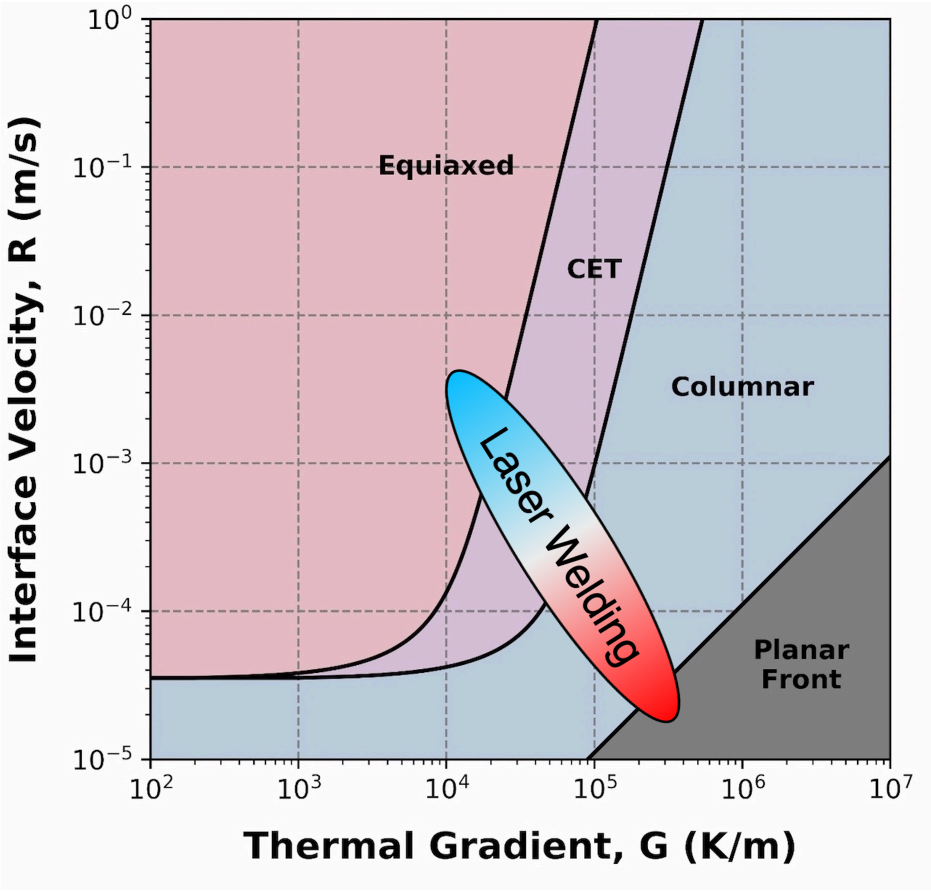




MM Kirka, Y Lee, DA Greely, A Okello, MJ Goin, MT Pearce, and RR Dehoff, *JOM*, 2017

Local microstructure control relies on understanding solidification conditions

- Solidification conditions are not static



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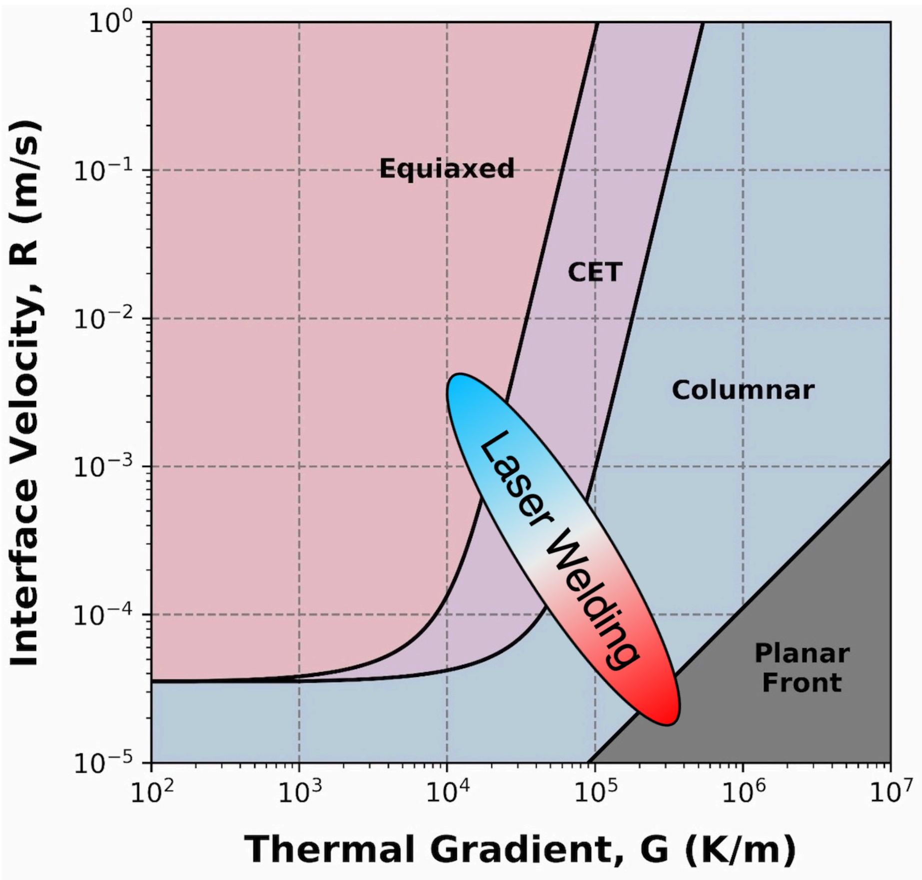

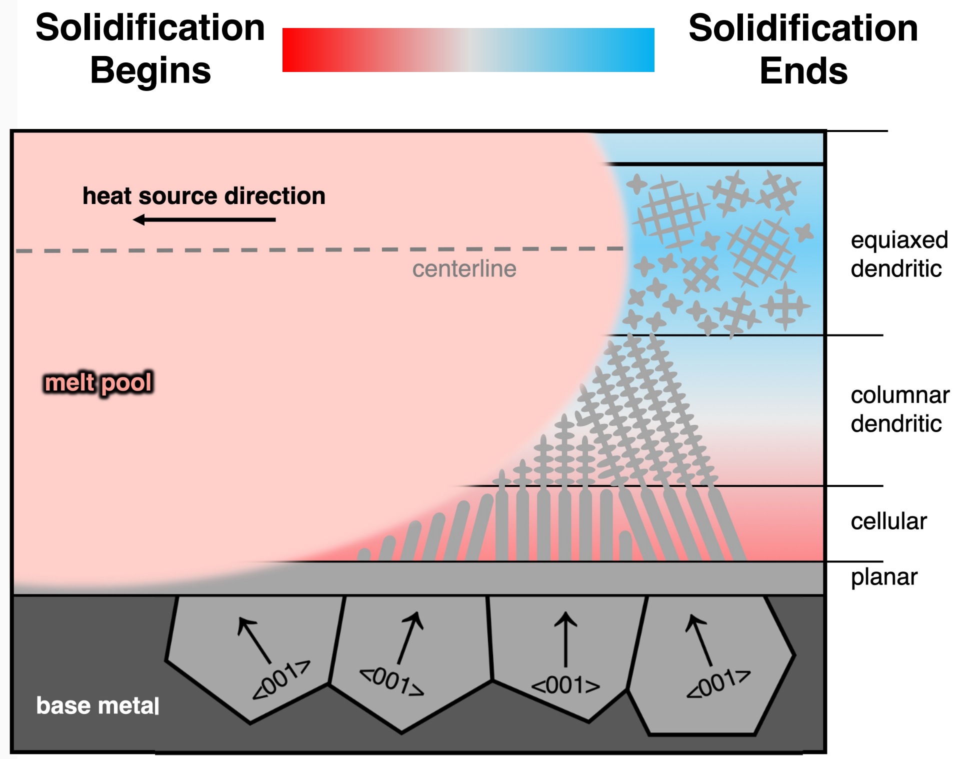

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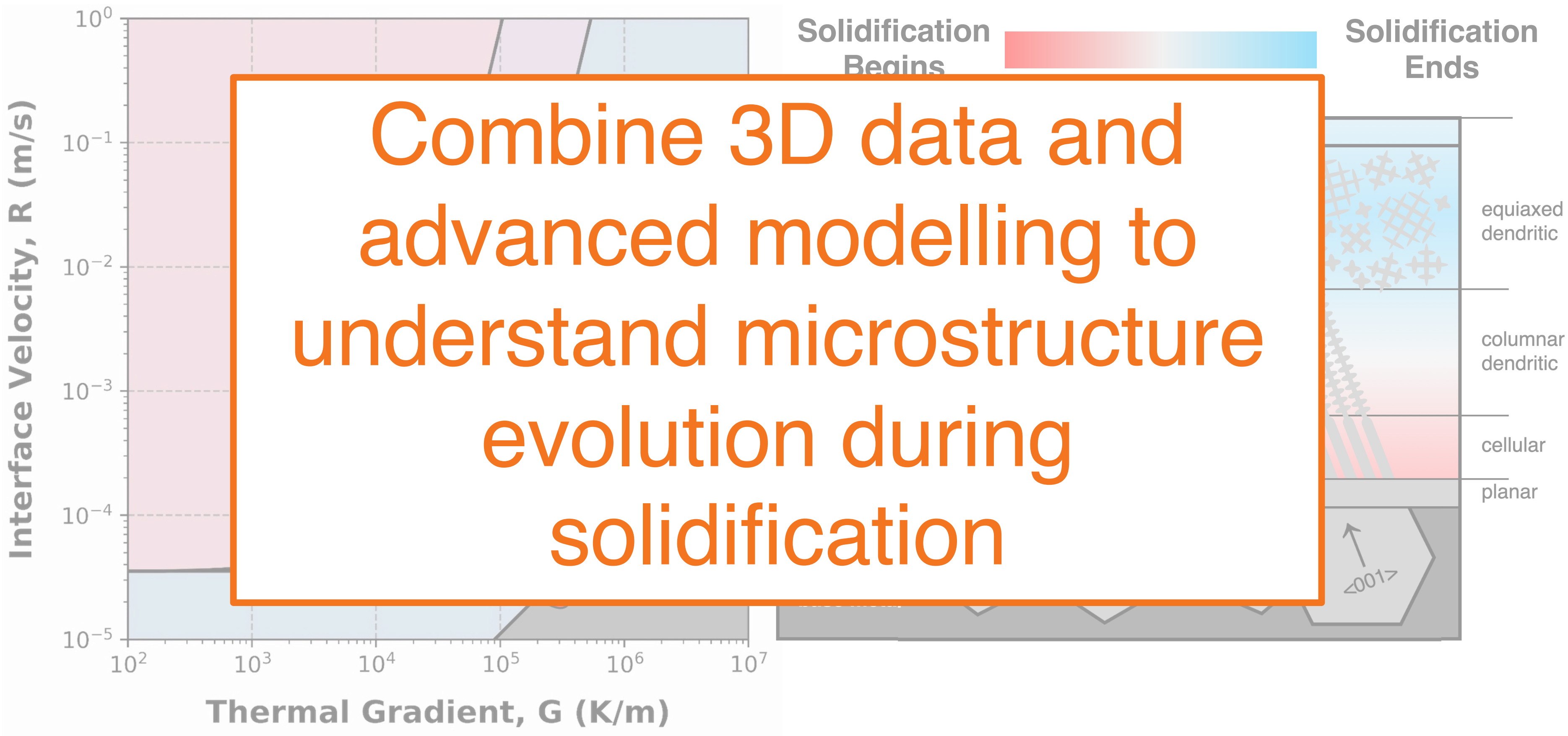

Combine 3D data and advanced modelling to understand microstructure evolution during solidification

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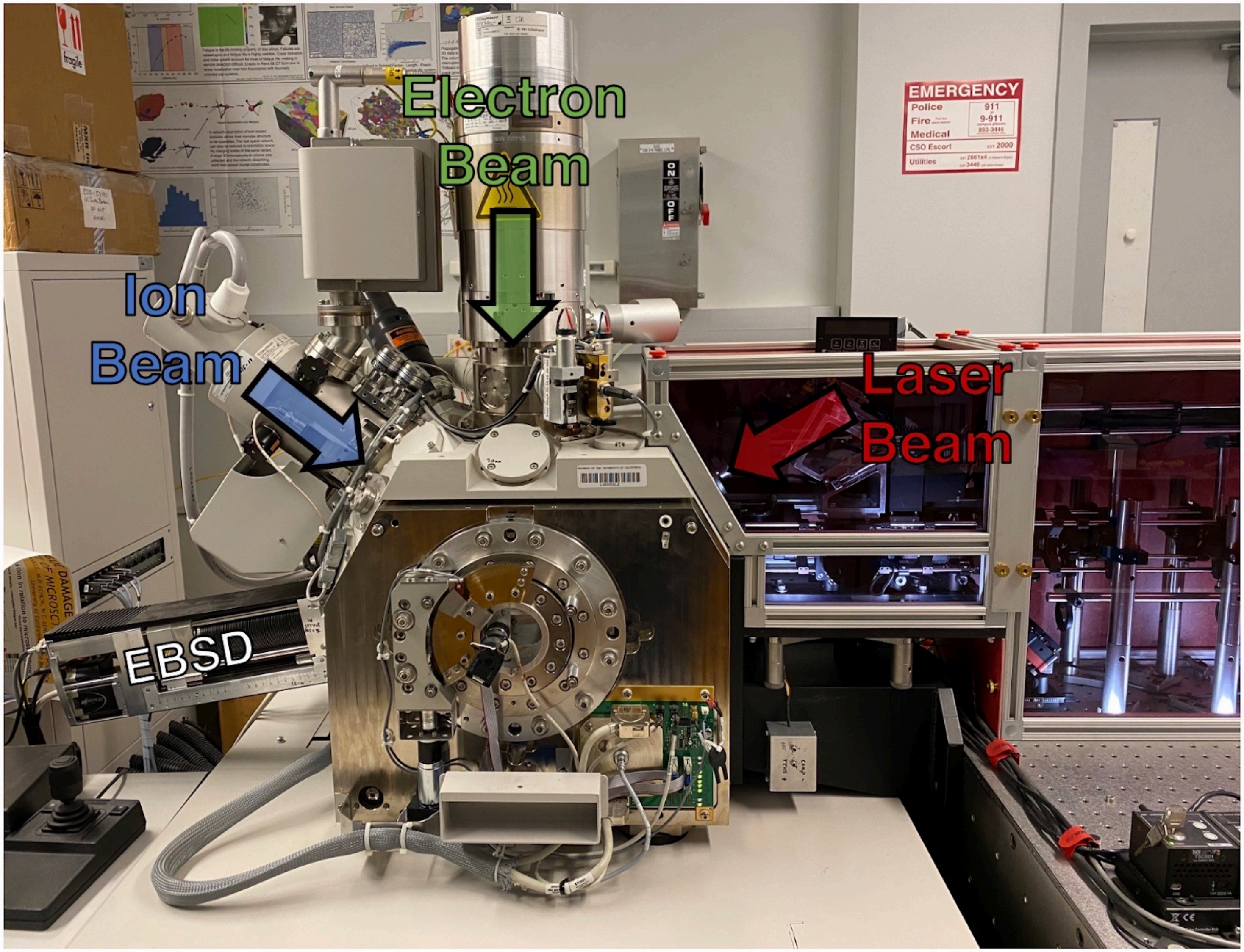
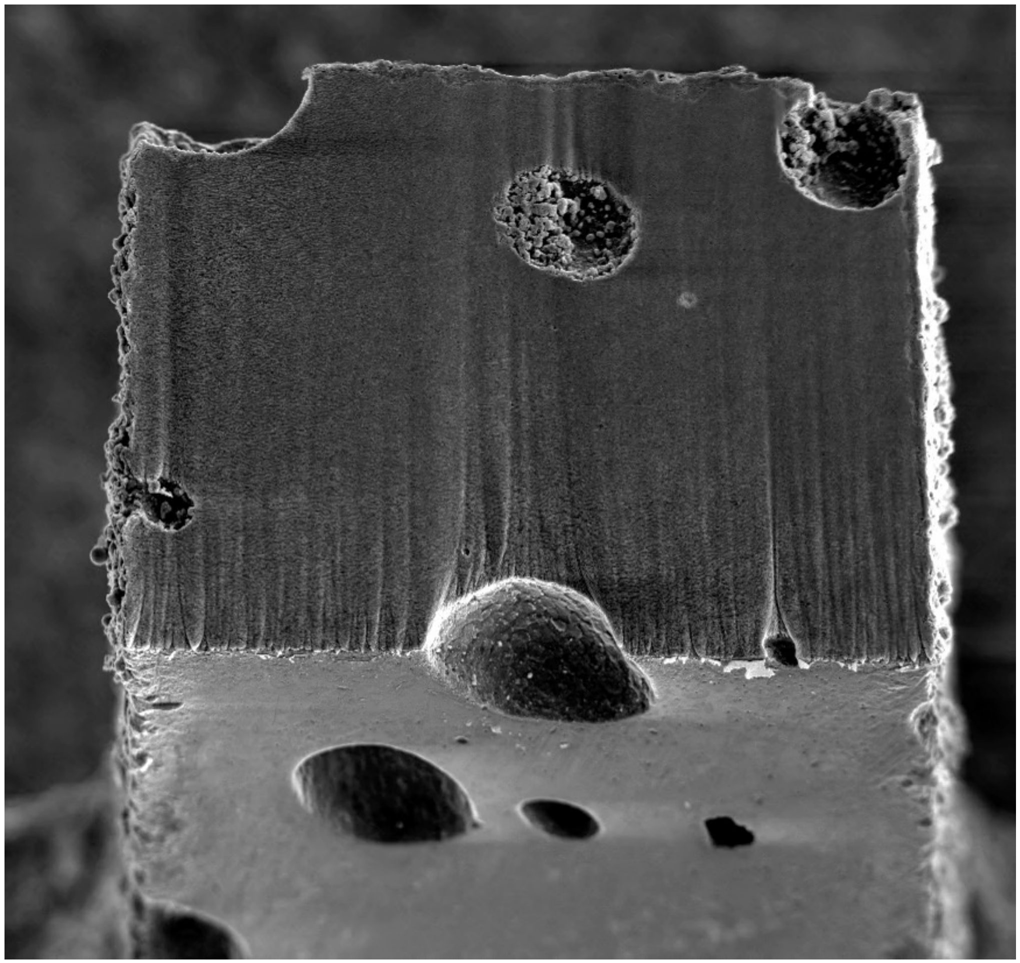
The TriBeam collects rich multi-modal datasets in three dimensions



TriBeam tomography generates data in a set of slices

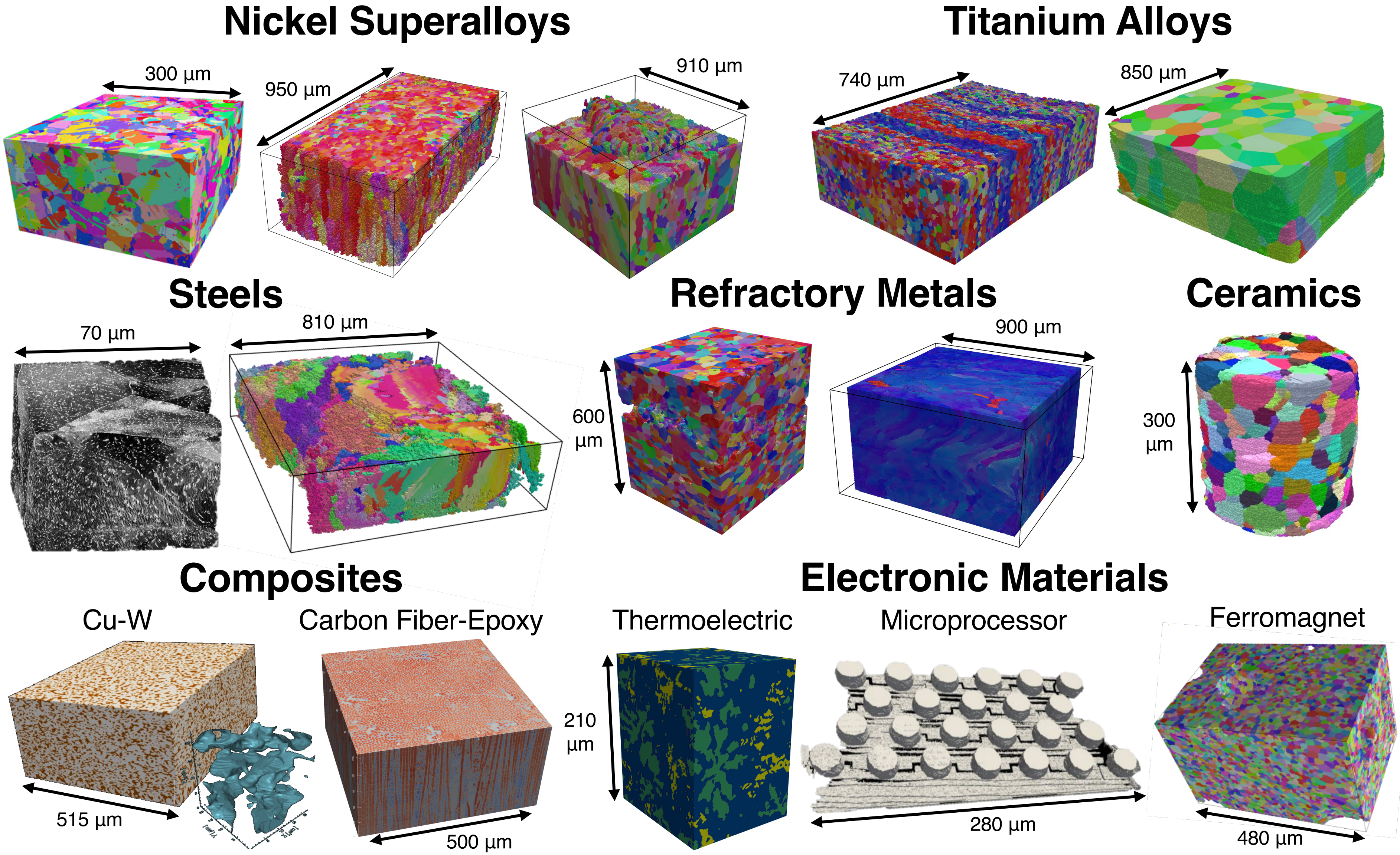
- Secondary electron images taken after laser machining*



250 µm

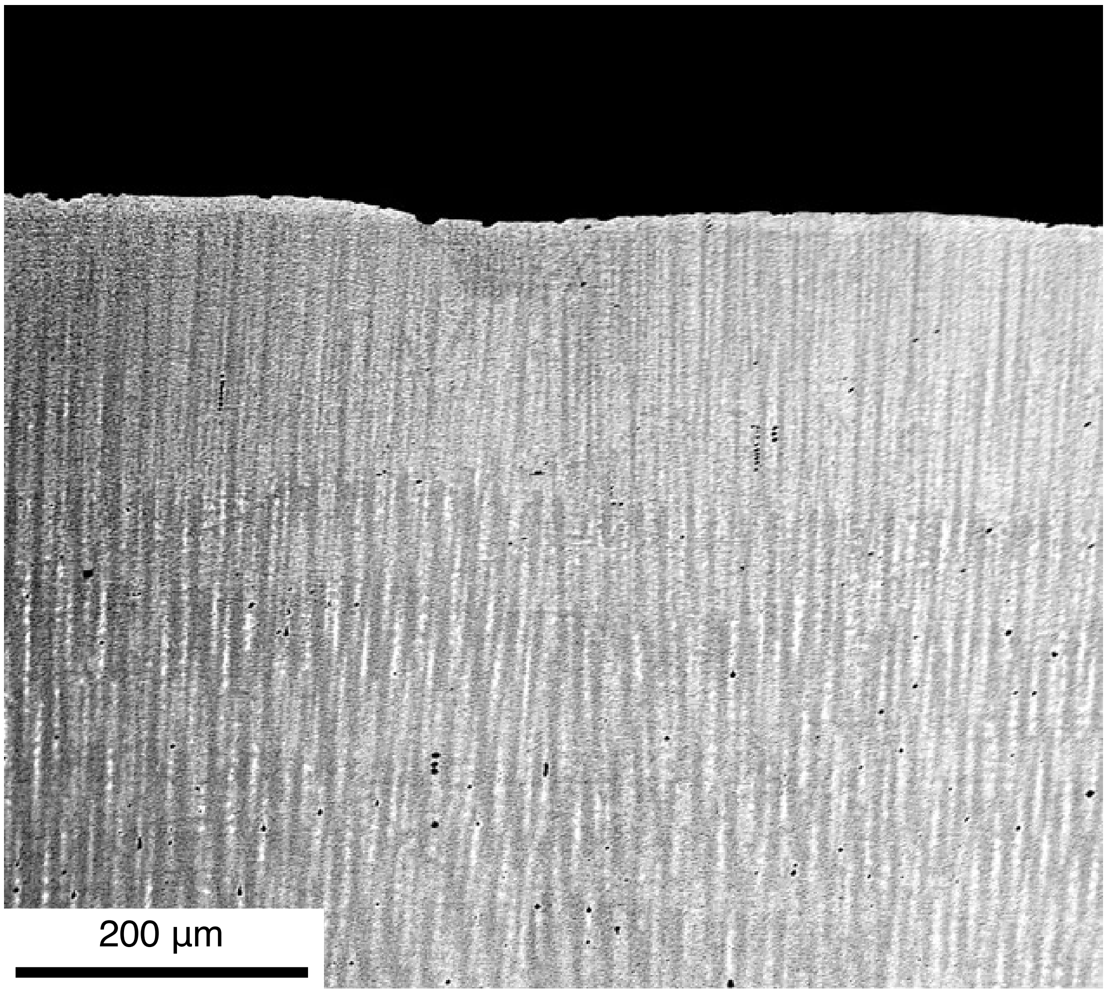
*Additively Manufactured AlNiCo magnet

Femtosecond laser ablation makes the TriBeam material agnostic

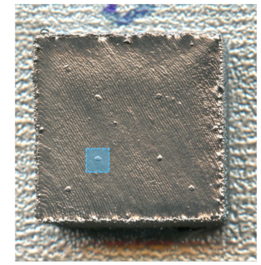


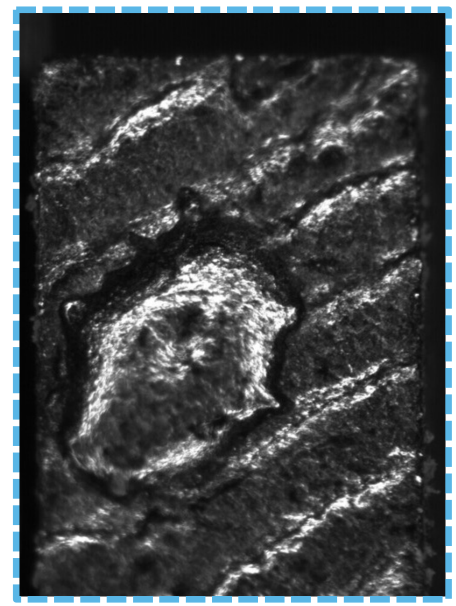
Isolated melt pool on a bulk raster block

Build Direction



Raster Melt

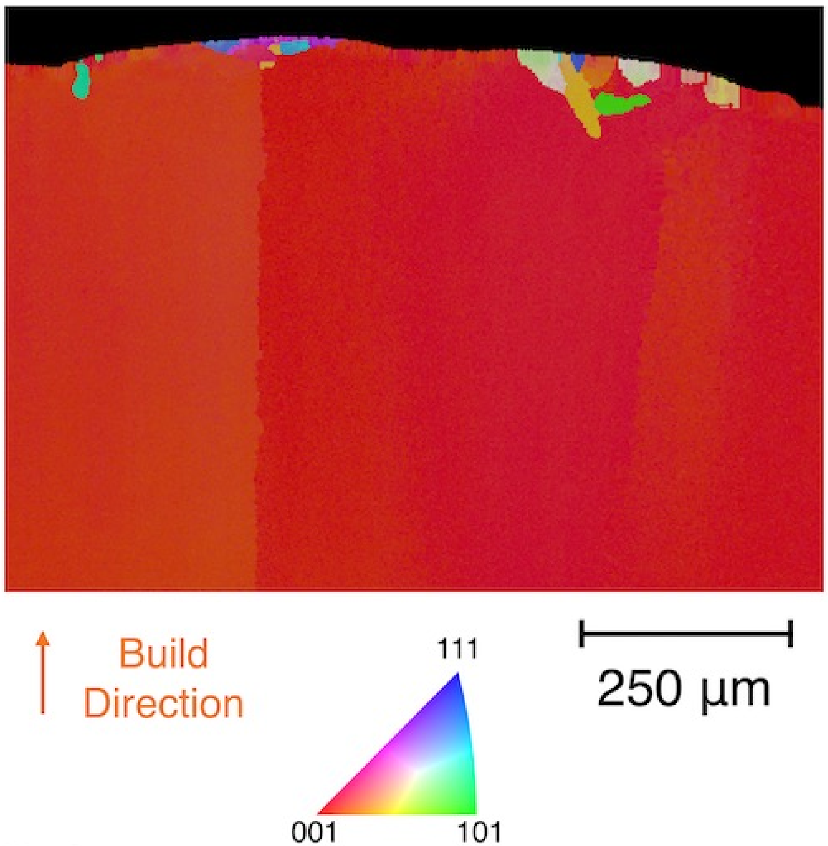


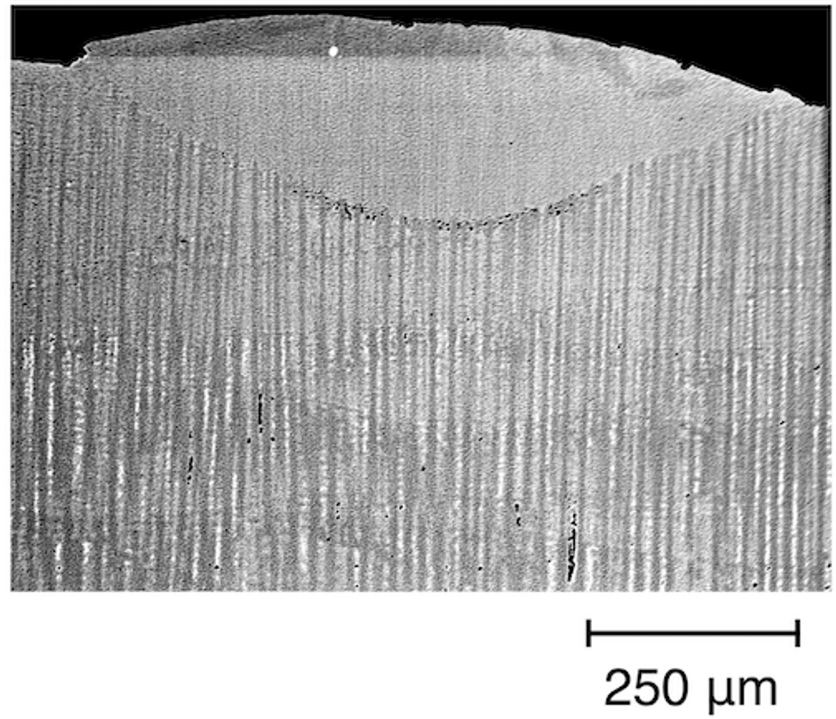


Build Direction

EBSD data shows nucleated grains, BSE data shows melt pool boundary

- Can fuse data modalities using TPS algorithm in 3D
- Also removes any distortions in EBSD data





Data fusion can be achieved via the Thin Plate Spline Algorithm (TPS)*

Distorted frame is a function of the reference frame
$$(\mathbf{X}, \mathbf{Y}, \mathbf{Z}) = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$$

$$(X, Y, Z) = f(x, y, z) = \underbrace{a_1 + a_x x + a_y y + a_z z}_{\text{Affine Portion}} + \underbrace{\sum_{i=1}^{n} w_i U(|P_i - (x, y, z)|)}_{\text{Bending Portion}}$$

- Radial basis function:

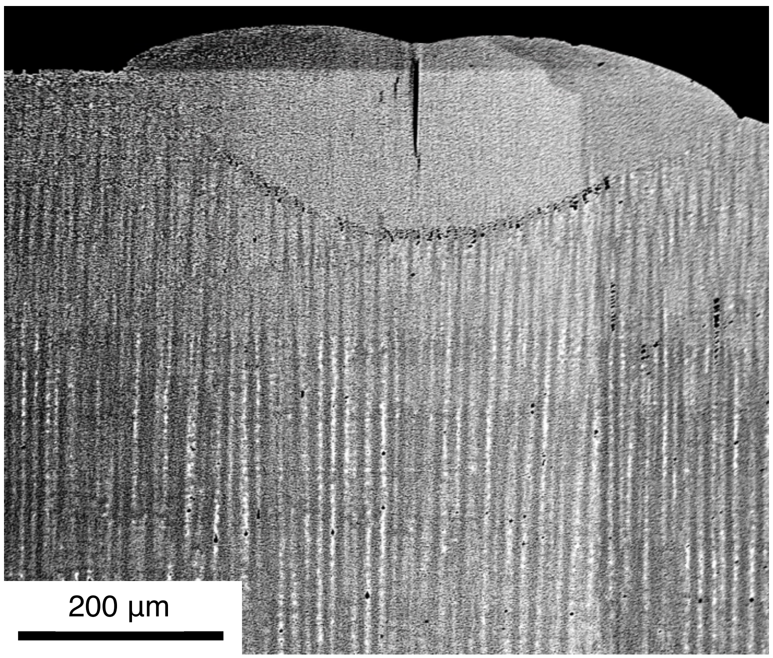
$$U(r) = r^2 log(r^2)$$

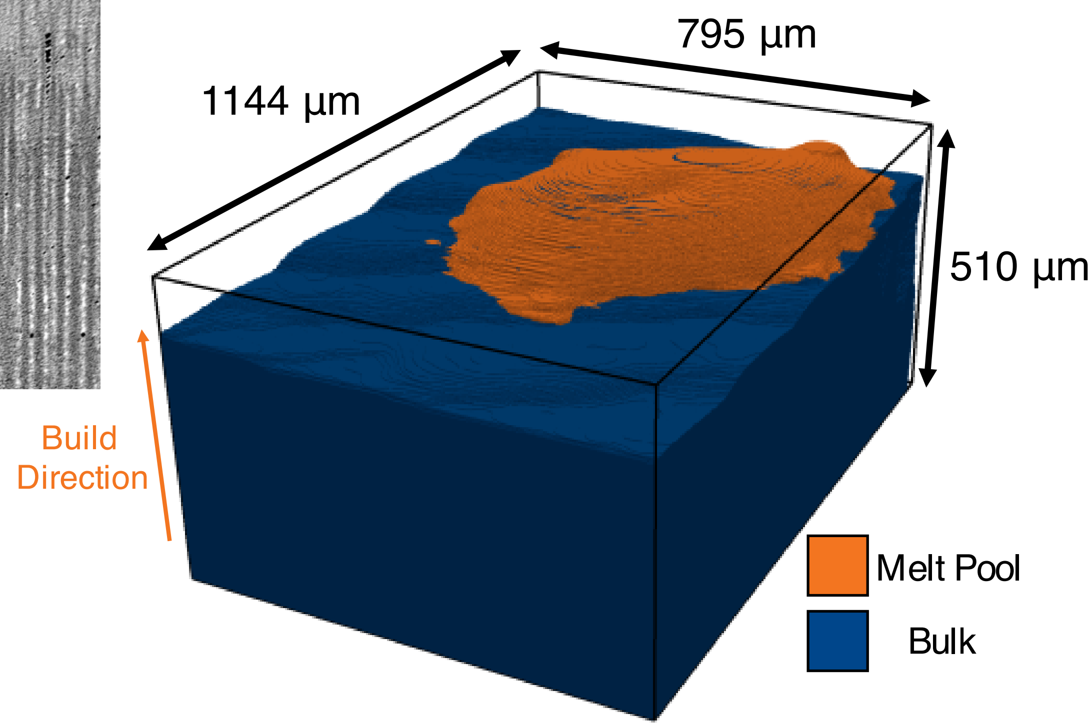
- Solve for weighting coefficients w_i and a_1, a_x, a_y, and a_z using n control points (CP) to create a system of $n+4$ equations
    - CPs are shared locations in distorted (X_i, Y_i, Z_i) and reference (x_i, y_i, z_i) images
        - Triple points, voids, precipitates, sample edges

*Extended to 3D using 2D form described in Y. B. Zhang, A Elbrond, F. X. Lin, *Materials Characterization* (2014)

EBSD aligned with BS imaging using TPS, allowing melt pool segmentation

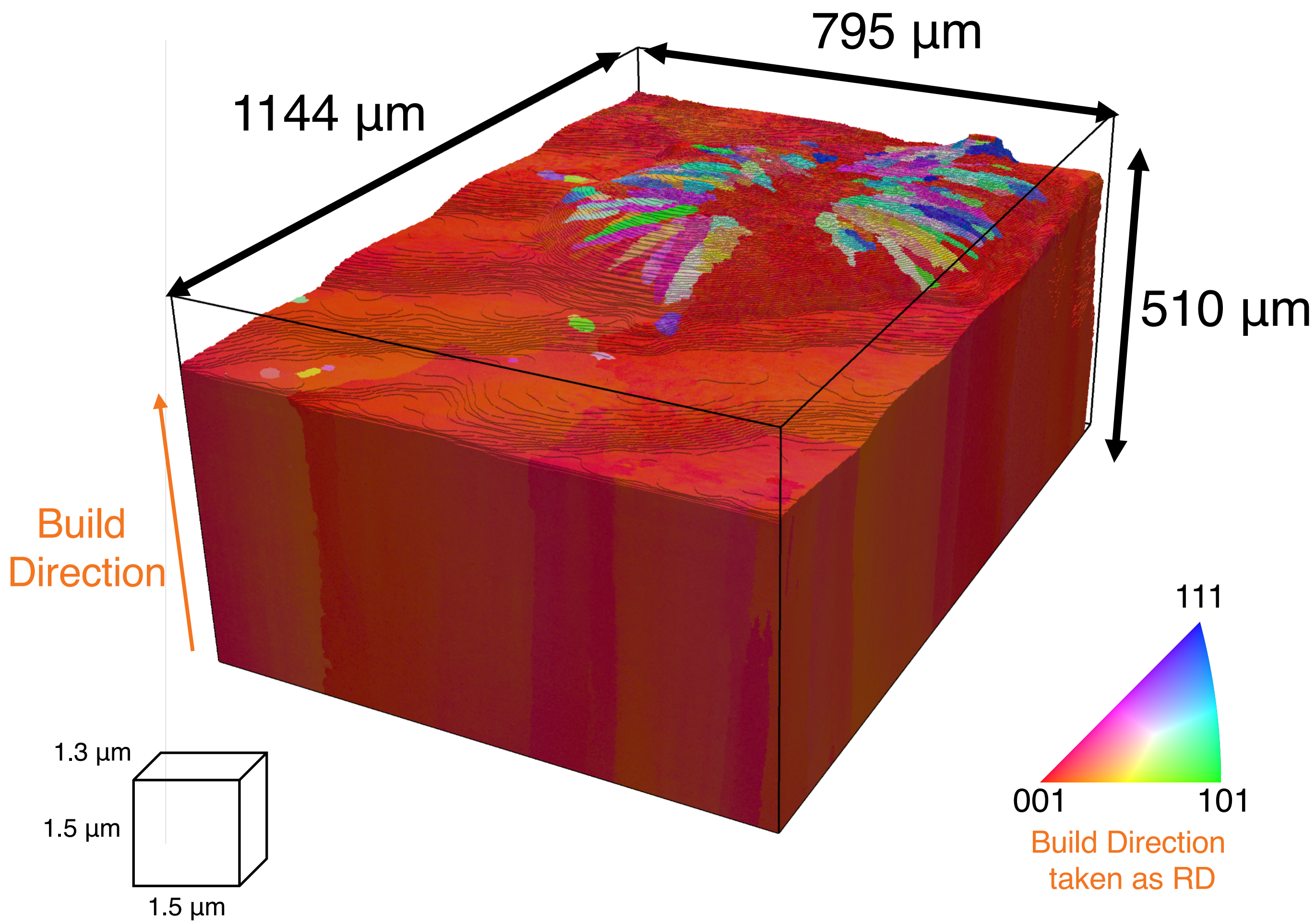
- 3894 control points used for thin plate spline algorithm



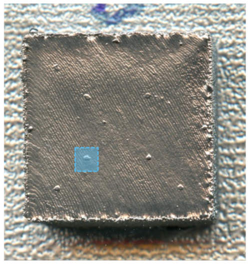


Reconstruction of isolated melt pool on a bulk raster block

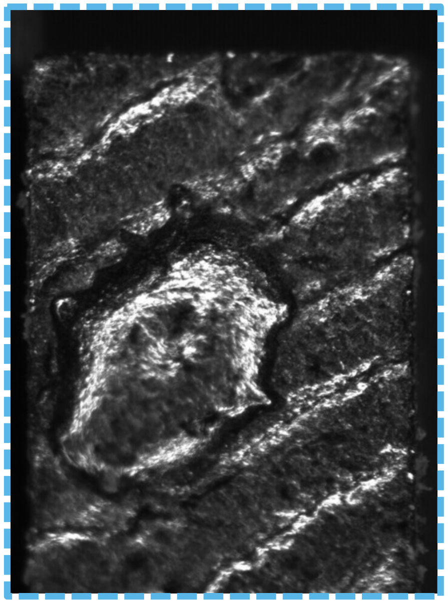
- 878 slices collected (~20 minutes per slice)
  - 3.6 TB of data



Raster Melt



10 mm



0.5 mm

Build Direction

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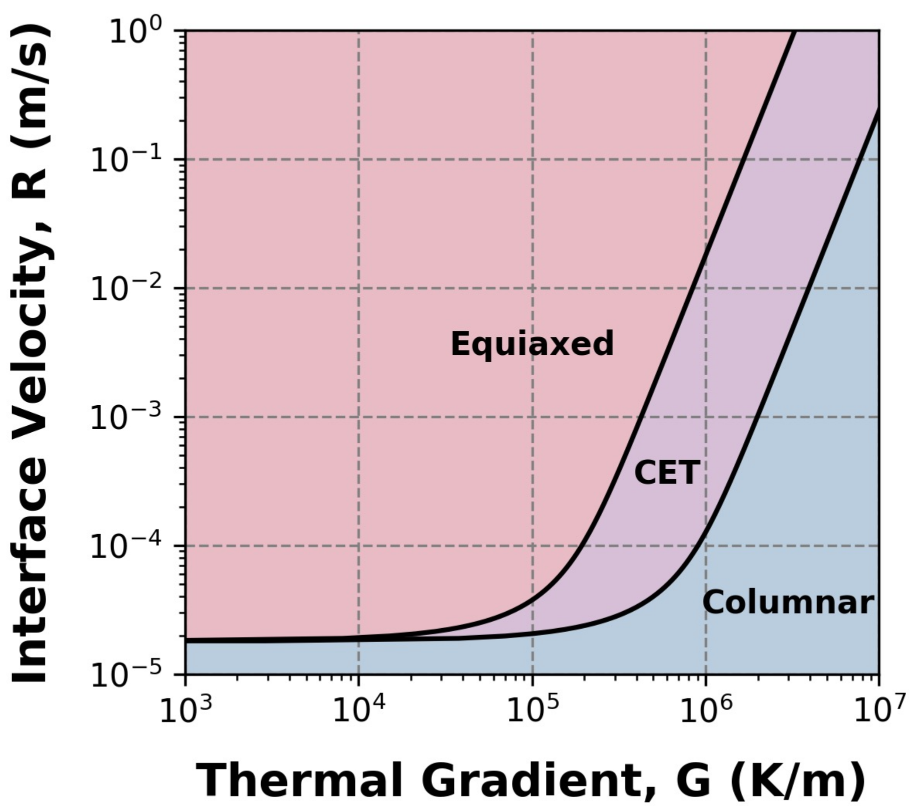
Need to accurately predict the columnar to equiaxed transition (CET)

$$G = \frac{1}{n+1}\sqrt[3]{\frac{-4\pi N_0}{3\ln\left[1-\phi\right]}}\cdot\left(1-\frac{{\Delta T_n}^{n+1}}{(a\cdot R)^{(n+1)/n}}\right)\cdot(a\cdot R)^{1/n}$$

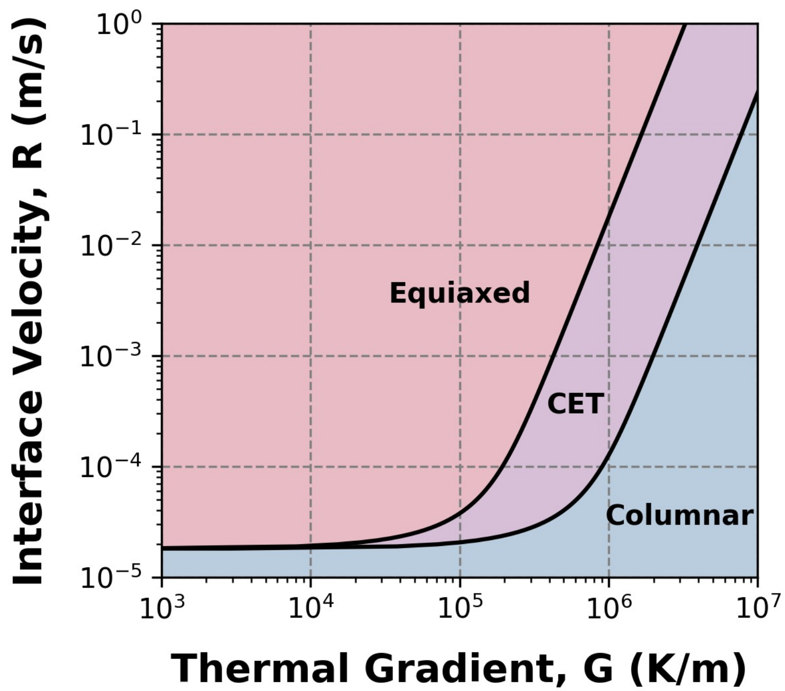


Video Courtesty HKDH Bahdeshia

Need to accurately predict the columnar to equiaxed transition (CET)

- Gäumann's modification of Hunt's CET model at high G
  - Developed for laser deposition on single-crystal Ni superalloys

$$\frac{G^n}{R} = a\left\{\sqrt[3]{\frac{-4\pi N_0}{3\ln[1-\phi]}}\frac{1}{n+1}\right\}^n$$



G = Thermal Gradient

R = Interface Velocity

N_0 = Nuclei density

a, n = Material constants

ϕ = Probability of grain nucleation ahead of interface

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$$\frac{G^n}{R} = a\left\{\sqrt[3]{\frac{-4\pi N_0}{3\ln[1-\phi]}}\frac{1}{n+1}\right\}^n$$

Rearrange to yield:

$$\phi = 1 - exp\left\{\frac{-4\pi N_0 a^{3/n}}{3(n+1)^3}\left(\frac{R}{G^n}\right)^{3/n}\right\}$$

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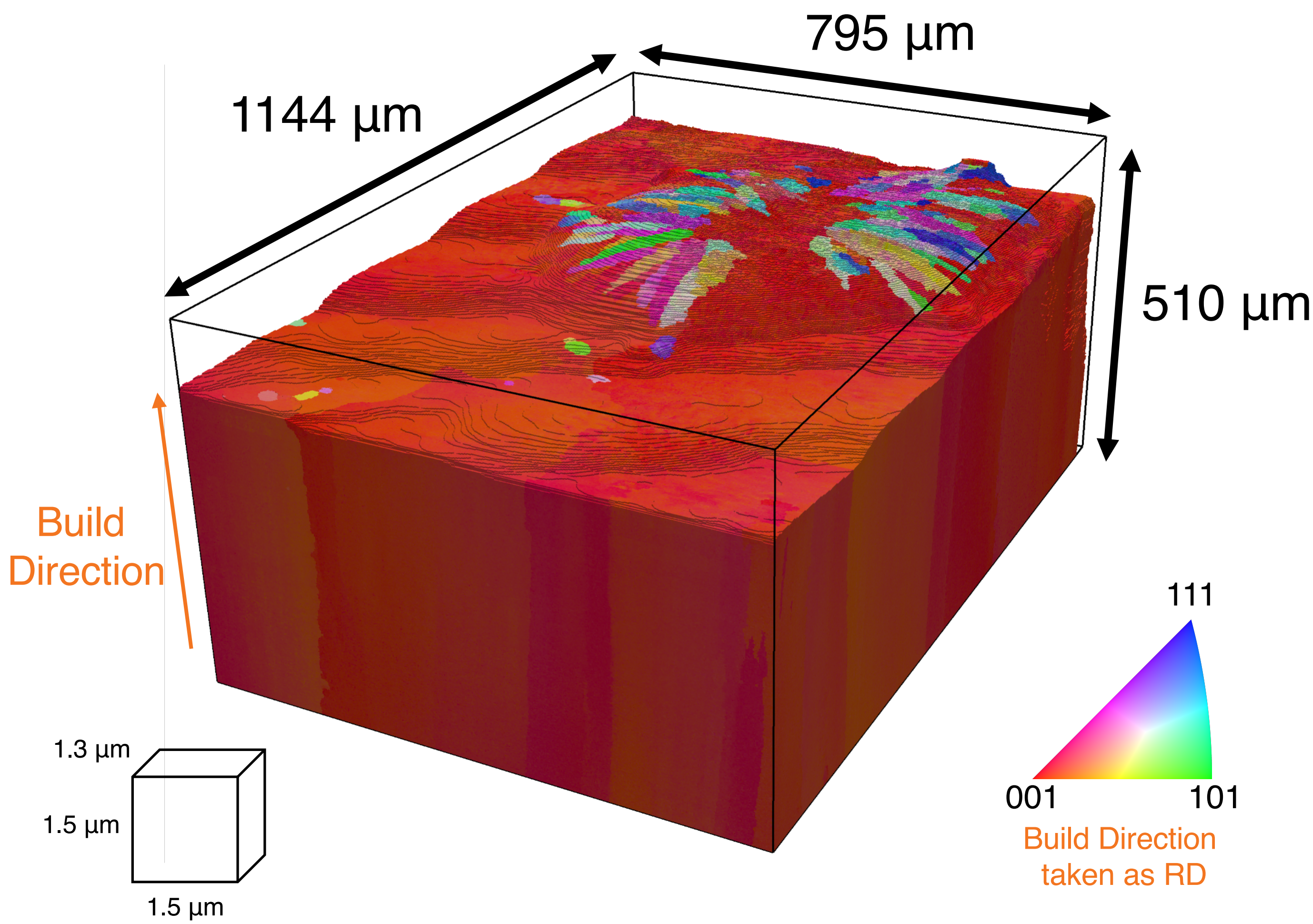
Apply model to isolated melt pool on top of raster melt block



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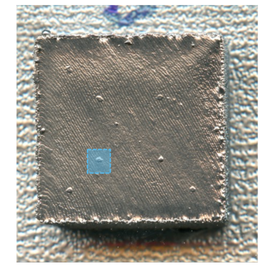

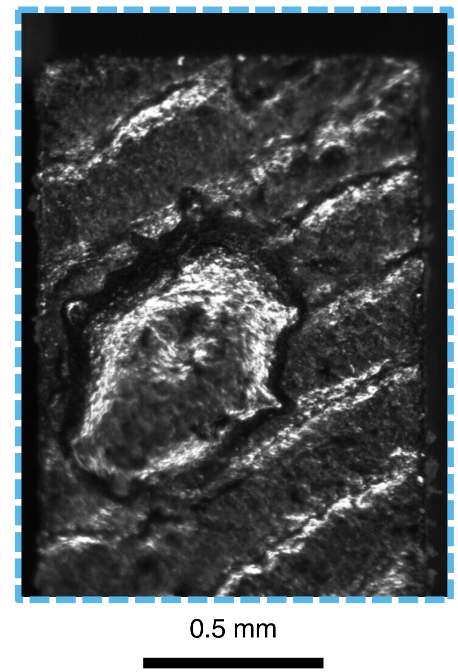

G and R can be calculated for this solidification event using TRUCHAS

- Want to predict the formation of nucleated grains

$$\phi = 1 - exp\left\{\frac{-4\pi N_0 a^{3/n}}{3(n+1)^3}\left(\frac{R}{G^n}\right)^{3/n}\right\}$$

TRUCHAS
- ☐ G = Thermal Gradient
- ☐ R = Interface Velocity
- ☐ N_0 = Nuclei density
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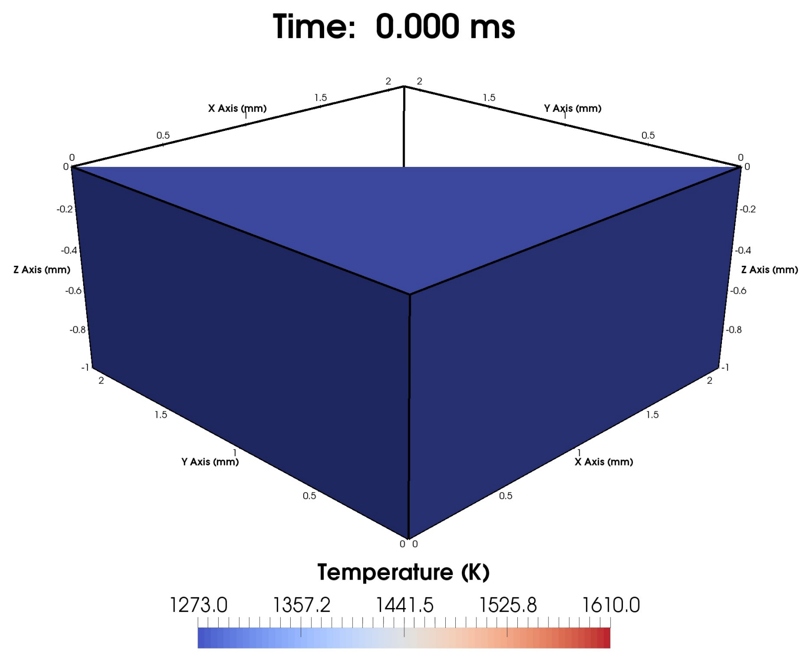
- ϕ = Probability of grain nucleation ahead of interface

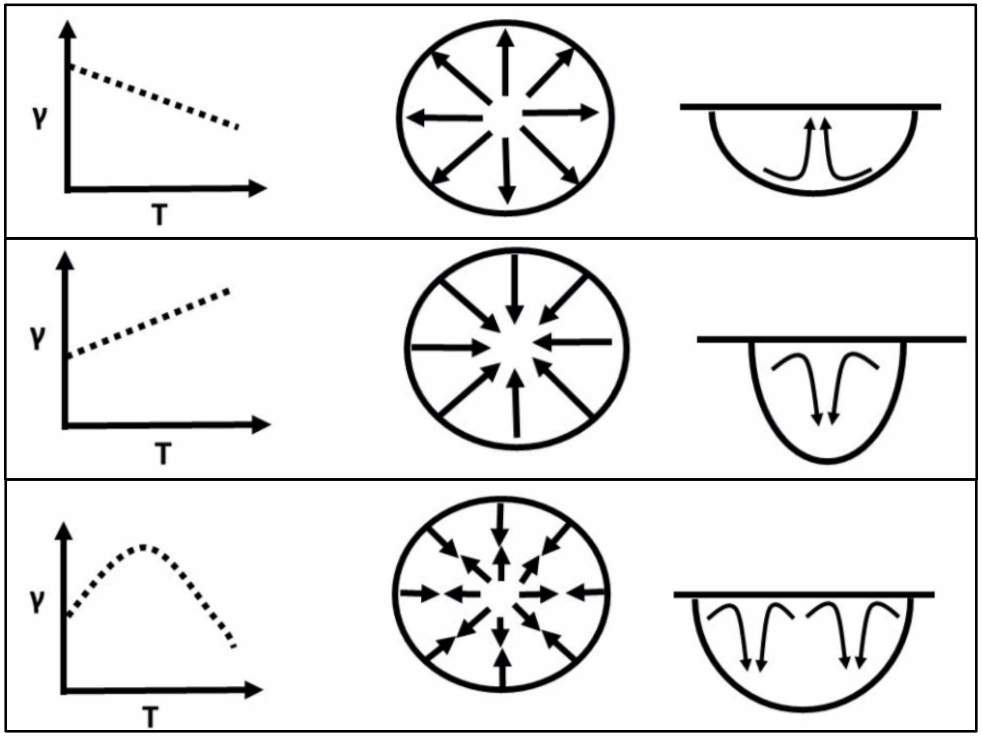
Can use TRUCHAS to model differences in temperature profile during solidification

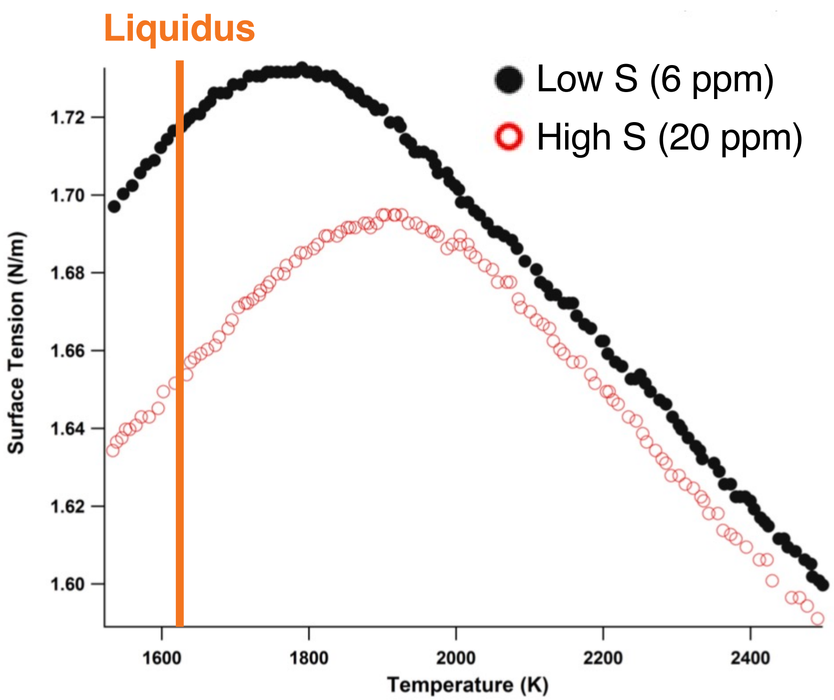
- Can model heat transfer and fluid flow
  - Designed for casting, so does not currently consider powder-beam interactions or multiple melt layers
- Enables 3D calculation of thermal gradient and solid-liquid interface velocity on µm and ms scales
  - Inaccessible to in-situ monitoring
- Code has been validated against Abaqus and that of Debroy et al.



TRUCHAS Simulations performed with and without fluid flow

- Performed simulations with relevant beam settings
  - 10 mA 0.5 ms dwell, 1273 K preheat
  - All simulations with heat transfer, two also include fluid flow
    - Fluid flow incorporates temperature dependence of surface tension (ɣ)





N Raghavan, PhD dissertation, 2017
Adapted from PD Lee, PN Quested, and M Mclean, *Phil. Trans. R. Soc. Lond.*, 1998

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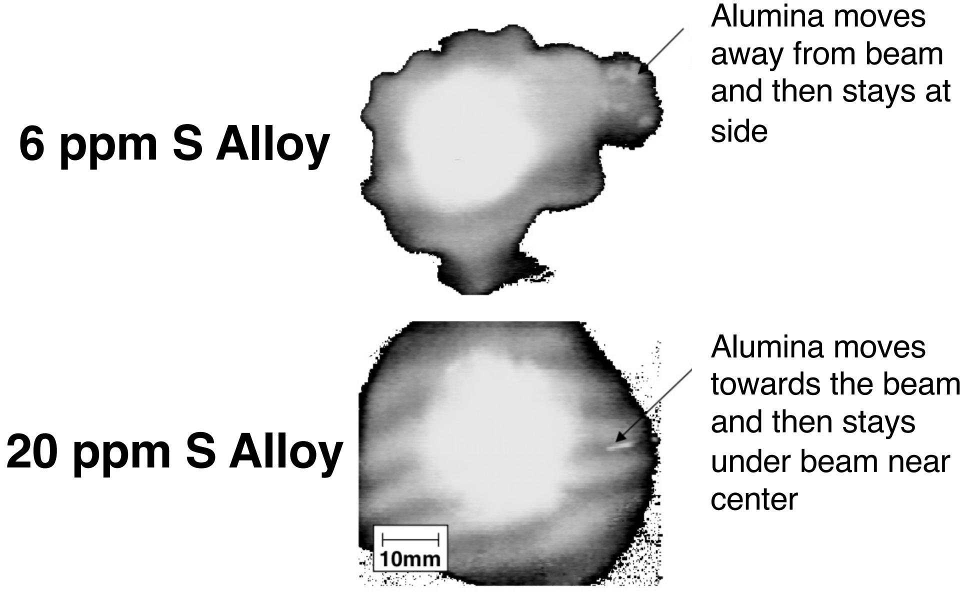

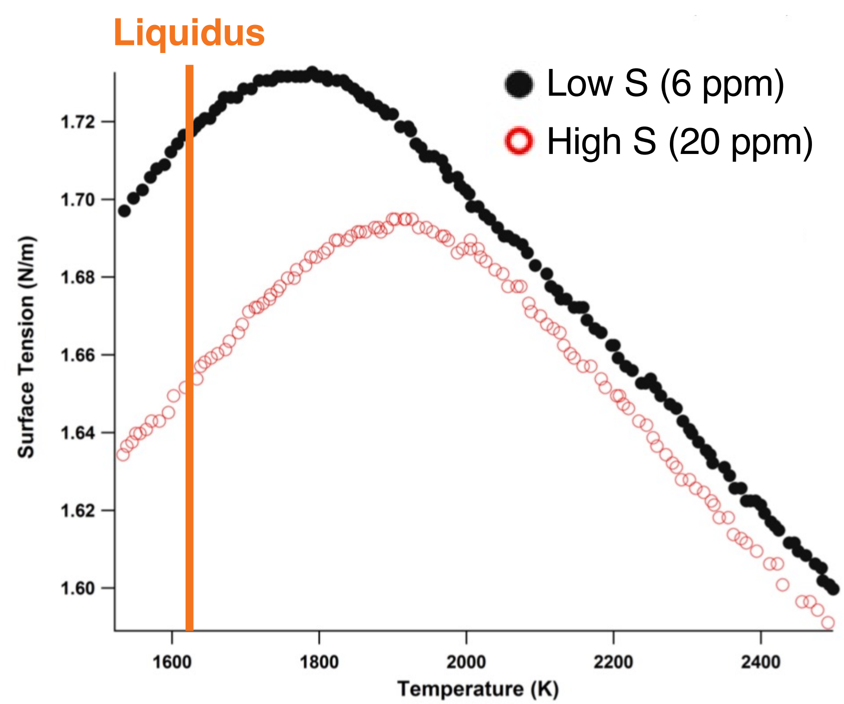

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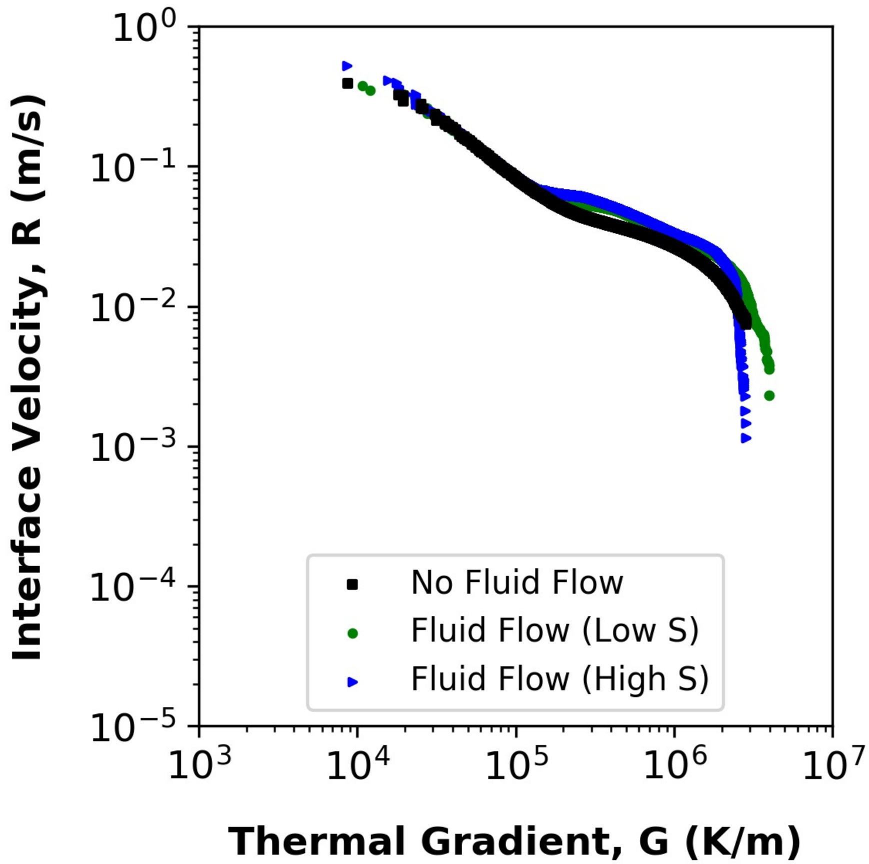
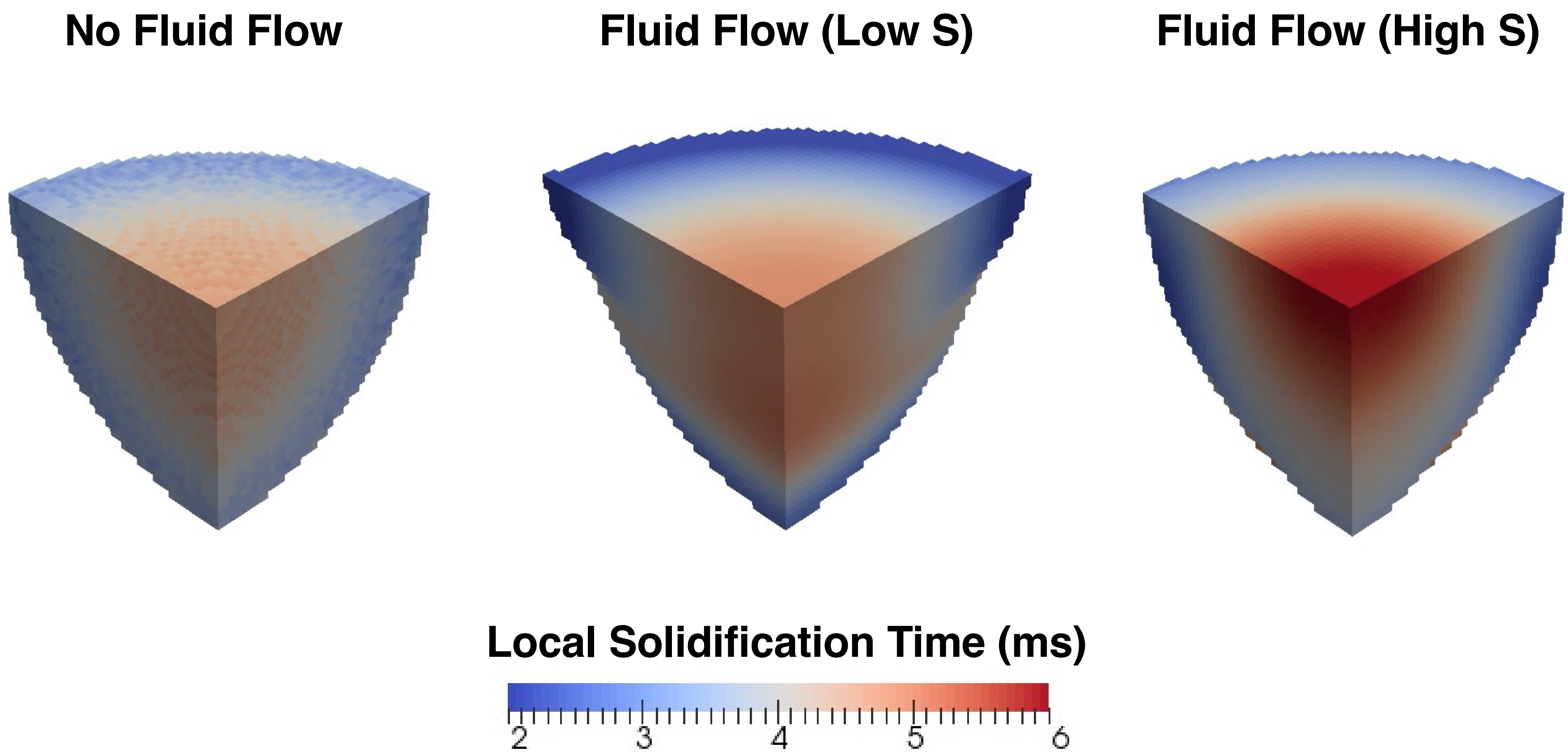
Results of TRUCHAS simulations

- Incorporation of fluid flow increases interface velocity in middle stages of solidification

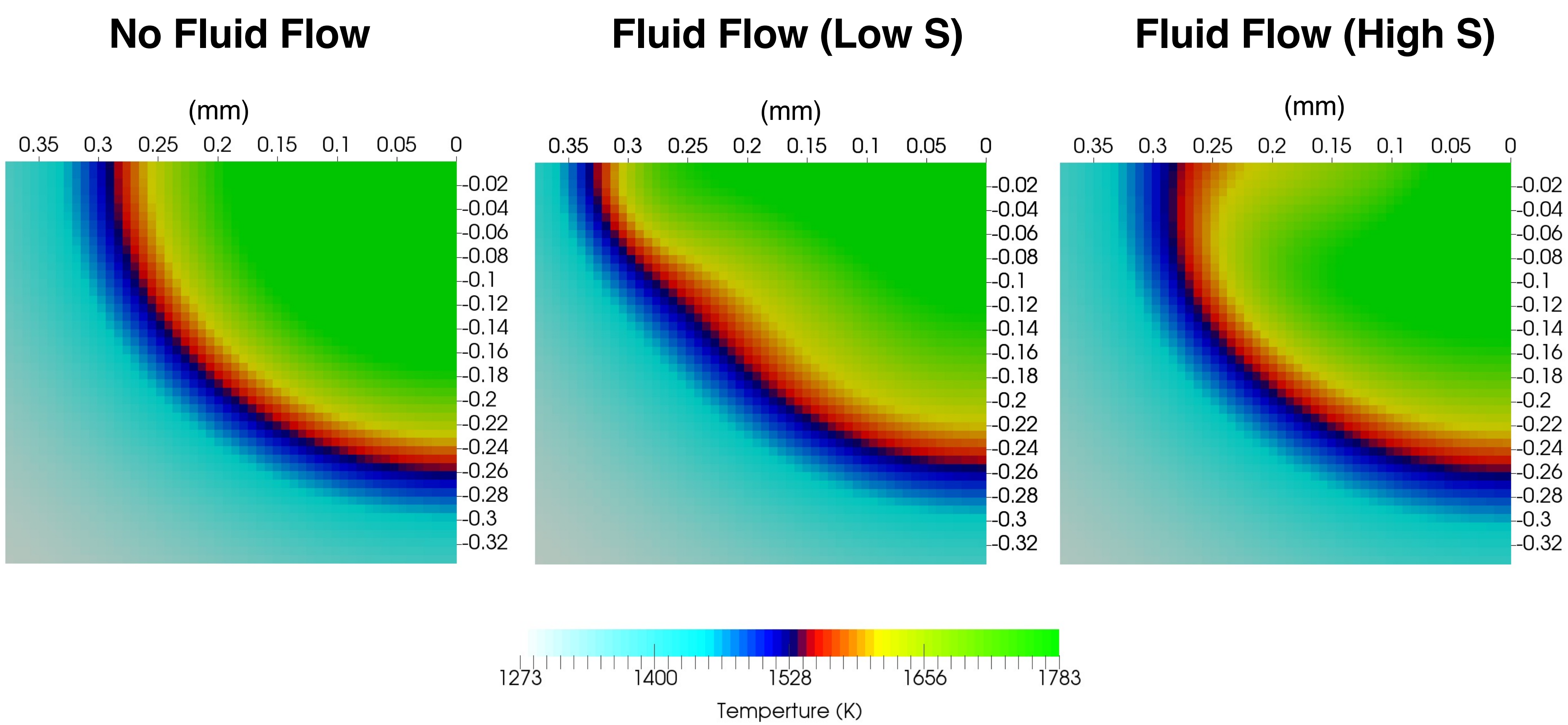


Higher S content increases local solidification time



Pool spreads more with lower S content, which is also seen in 304 steel welds

- Fully Solid, Mushy Zone, and Fully Liquid
- Maximum extent of melt pool at t ≈ 3 ms



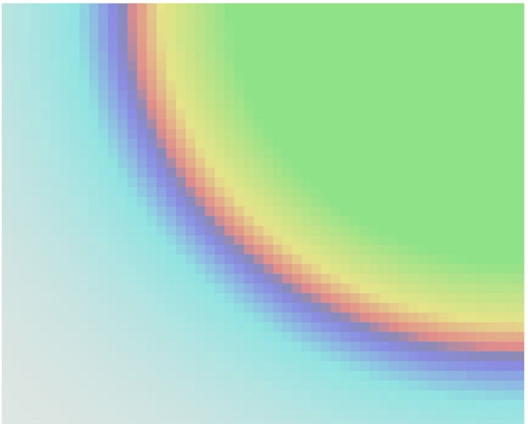
Visualizing fluid flow

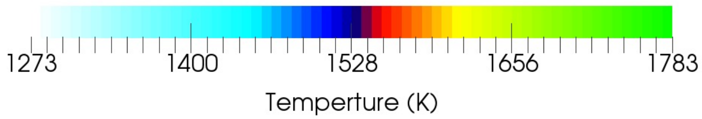
Time: 2.014583

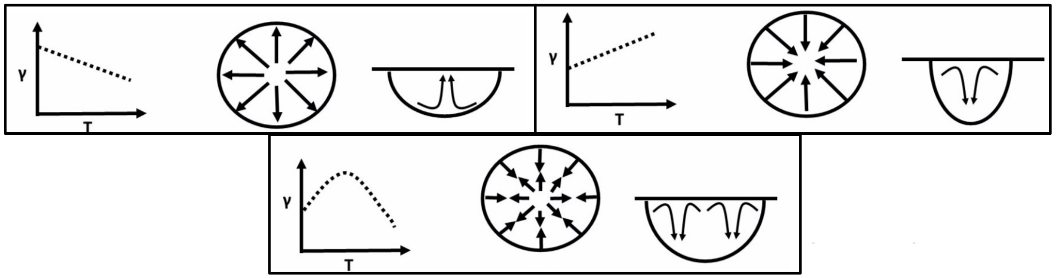
Low S Fluid Flow

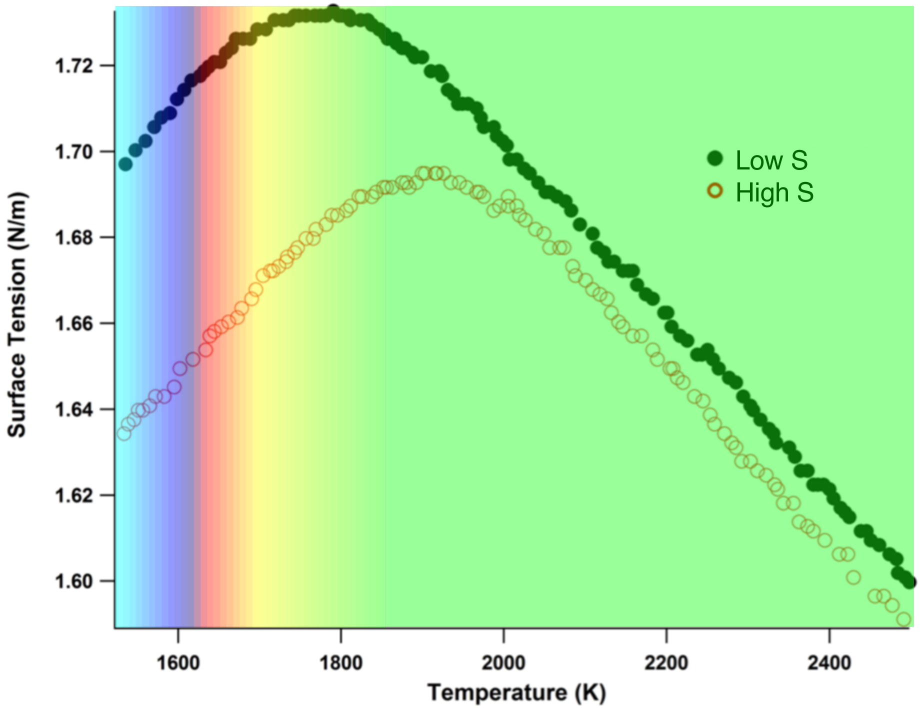
Time: 2.014583

High S Fluid Flow



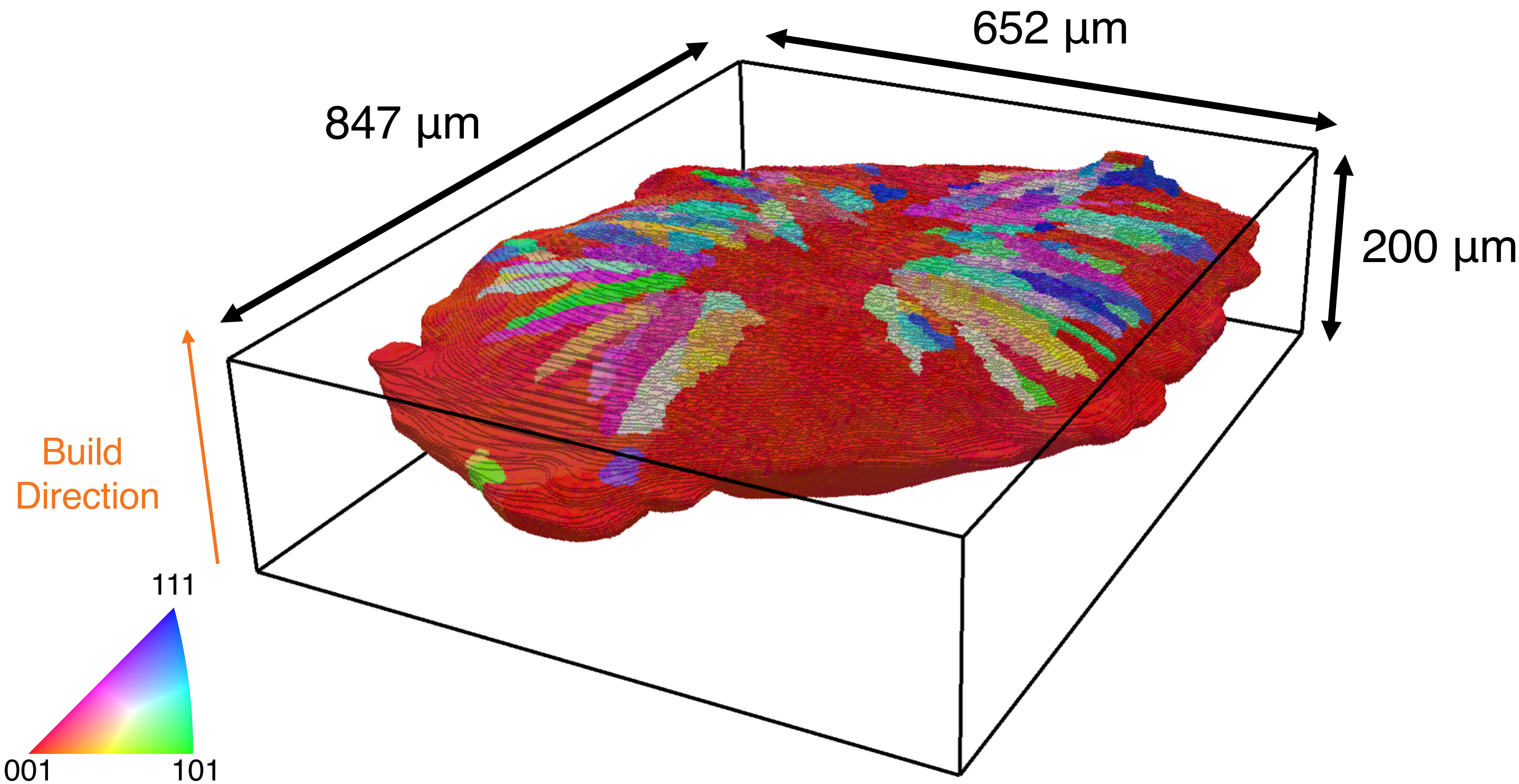






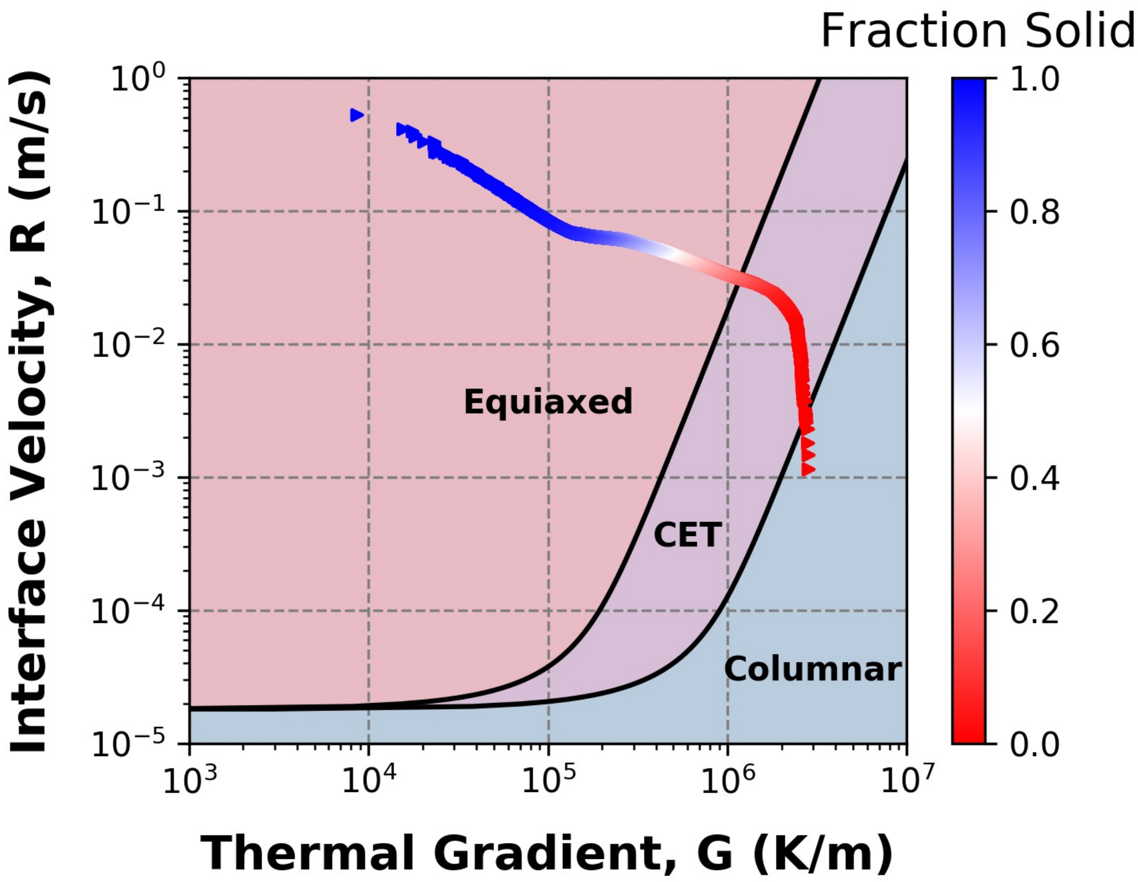
Isolated melt pool from full dataset

- Nucleated grains form radially around center of pool



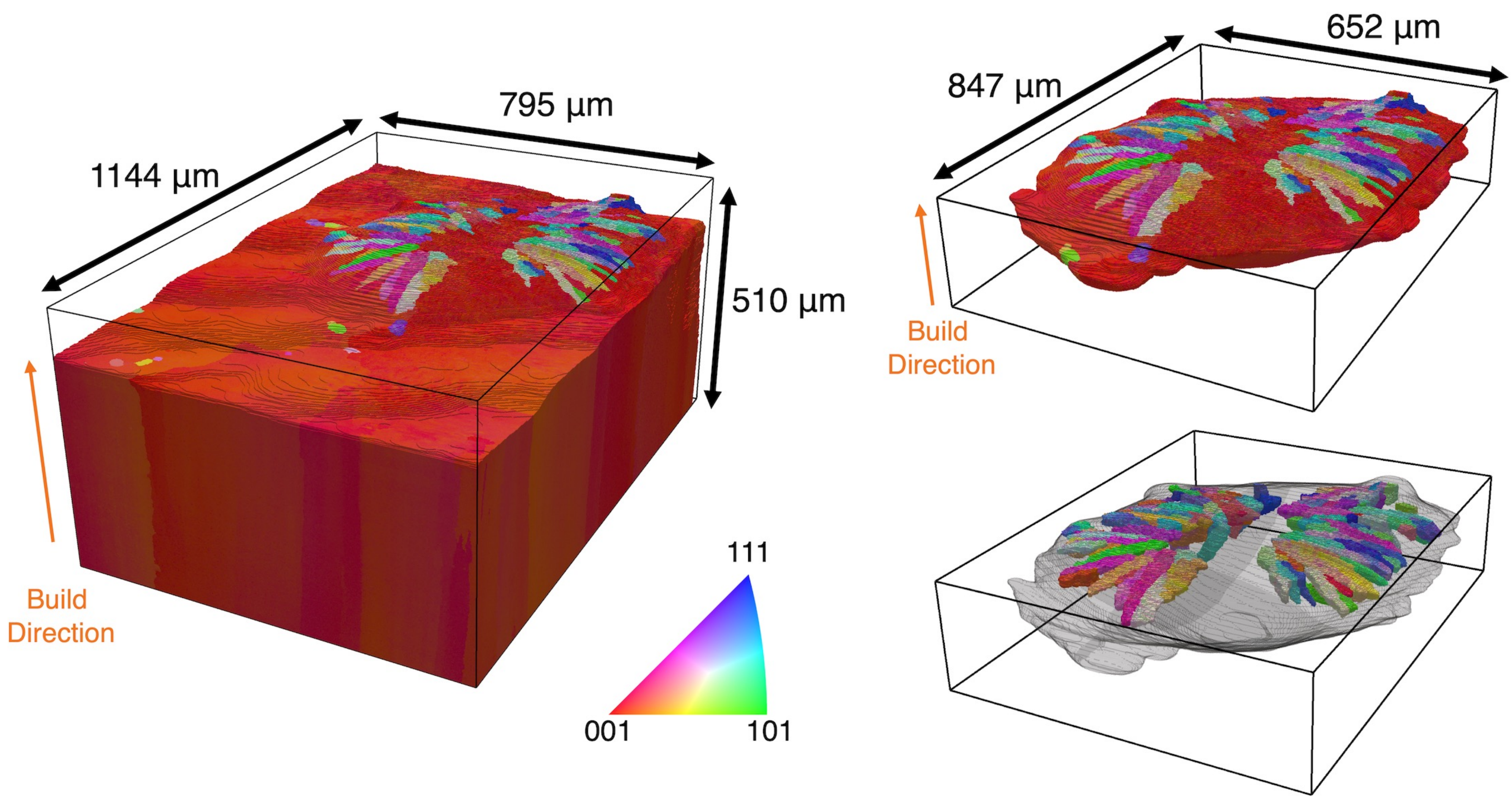
Results of TRUCHAS simulations

- Predicts nucleated grain fraction (Φ) of **80.8%**



Results of TRUCHAS simulations

- Predicted nucleated grain fraction (Φ) of **80.8%**
- Measured nucleated grain fraction (Φ) of **11.4%**



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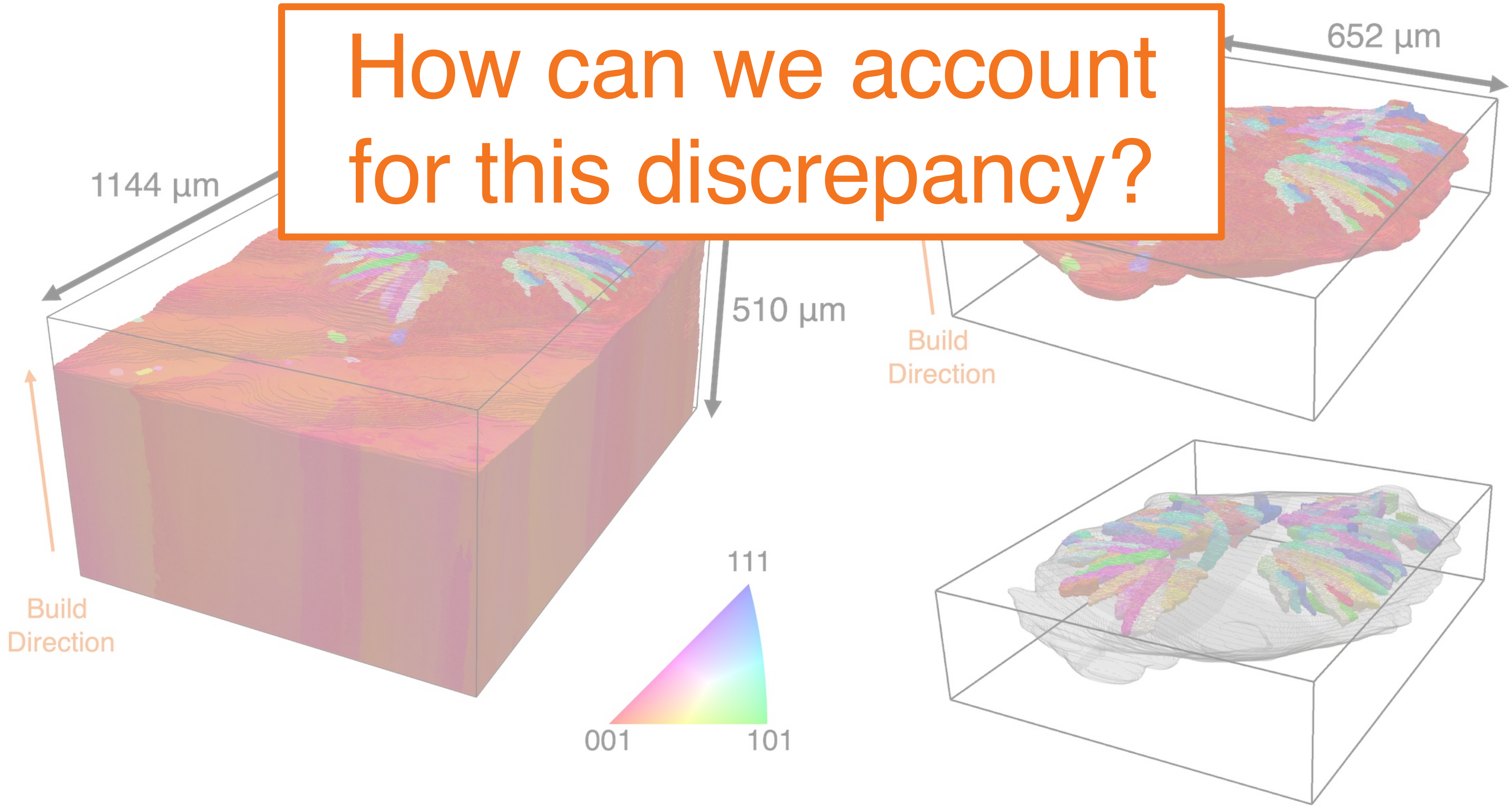

How can we account for this discrepancy?

Checklist for Columnar to Equiaxed Transition (CET) Model

- Want to predict the formation of nucleated grains

$$\phi = 1 - exp\left\{\frac{-4\pi N_0 a^{3/n}}{3(n+1)^3}\left(\frac{R}{G^n}\right)^{3/n}\right\}$$

TRUCHAS

- ☑ G = Thermal Gradient
- ☑ R = Interface Velocity
- ☐ N_0 = Nuclei density
- ☐ a, n = Material constants

ϕ = Probability of grain nucleation ahead of interface

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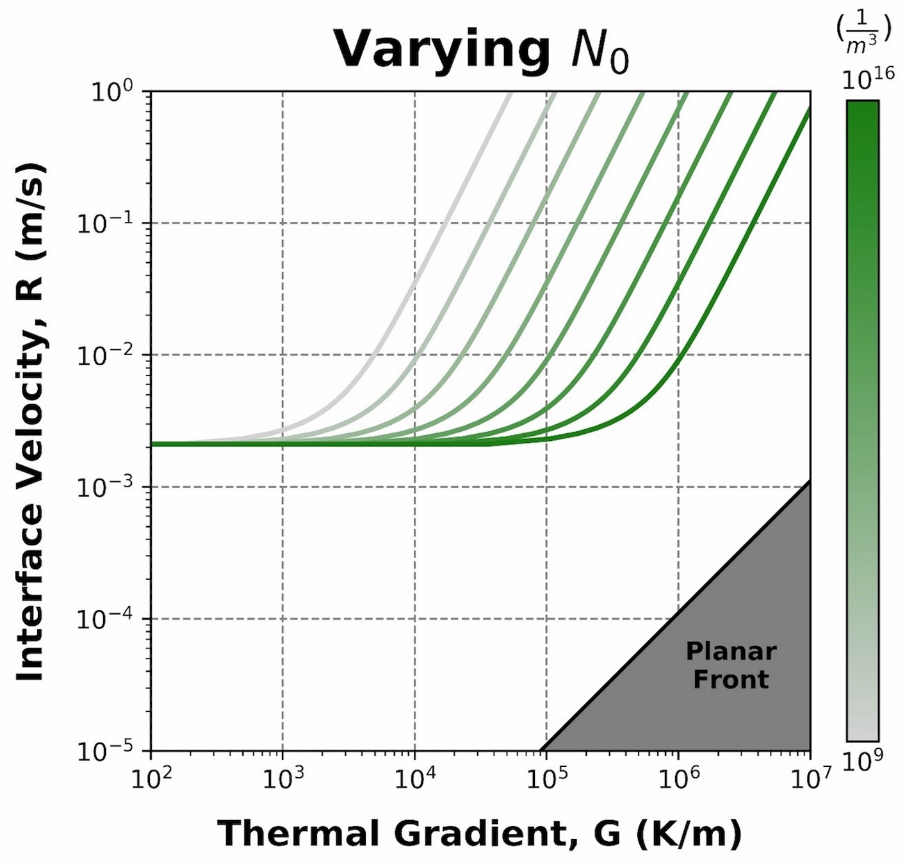

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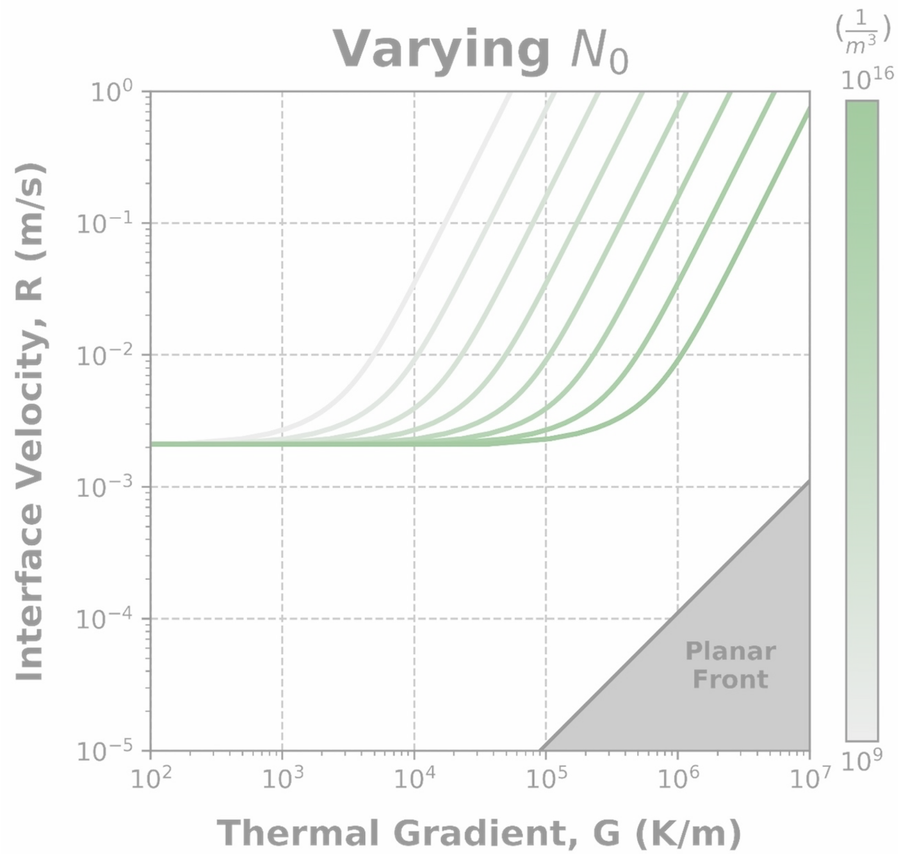

3D data shows N_0 is three orders of magnitude lower

$2{\times}10^{15} \rightarrow 5.3{\times}10^{12}\ m^{-3}$

ahead of interface

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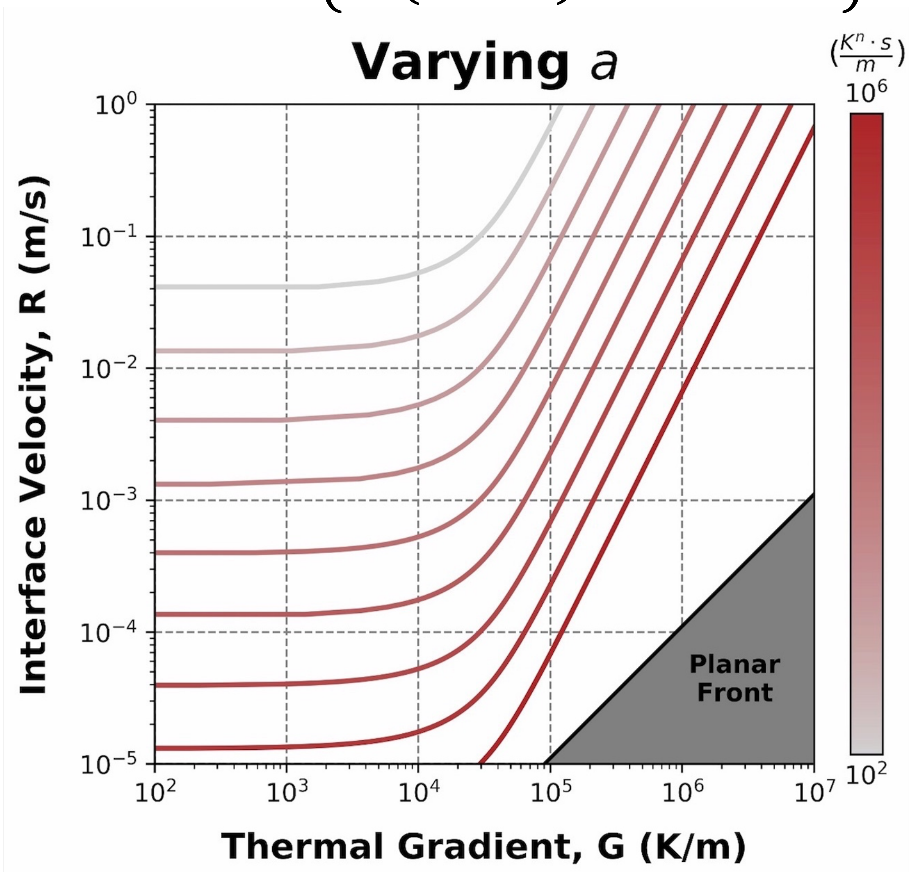
Checklist for Columnar to Equiaxed Transition (CET) Model

- Want to predict the formation of nucleated grains

$$\phi = 1 - exp\left\{\frac{-4\pi N_0 a^{3/n}}{3(n+1)^3}\left(\frac{R}{G^n}\right)^{3/n}\right\}$$



- ☑ G = Thermal Gradient
- ☑ R = Interface Velocity
- ☑ N_0 = Nuclei density
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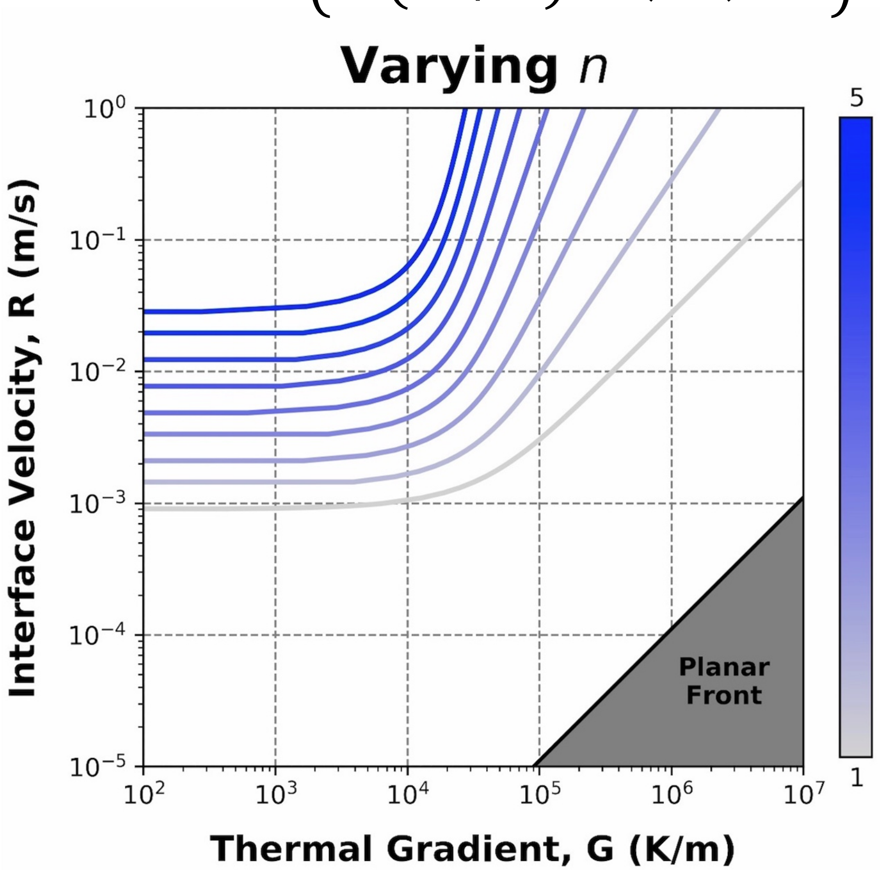

☑ G = Thermal Gradient

☑ R = Interface Velocity

☑ N_0 = Nuclei density

☐ a, n = Material constants

ϕ = Probability of grain nucleation ahead of interface

Material constants are alloy dependent, but can be determined using KGT model

- Want to predict the formation of nucleated grains

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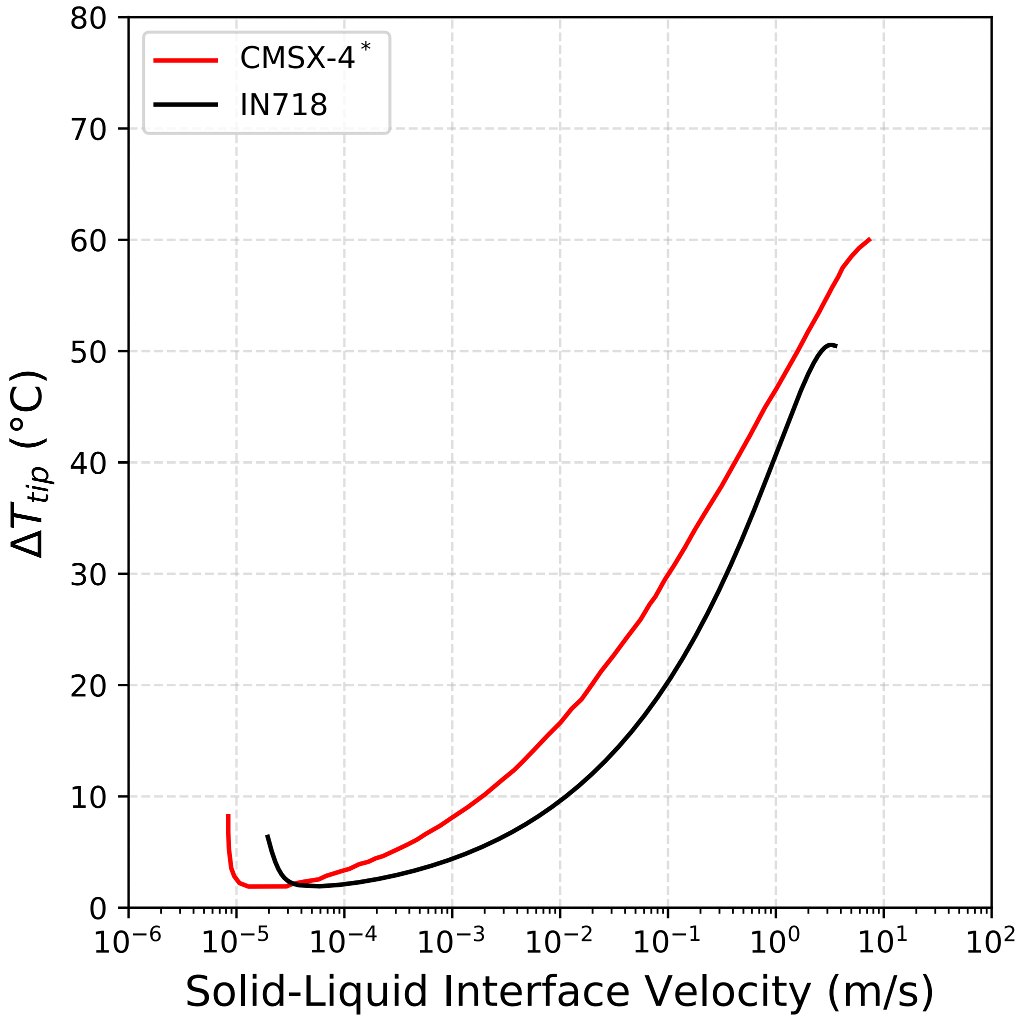
TRUCHAS → ☑ G = Thermal Gradient; ☑ R = Interface Velocity

3D Data ← ☑ N_0 = Nuclei density

KGT Model ← ☐ a, n = Material constants

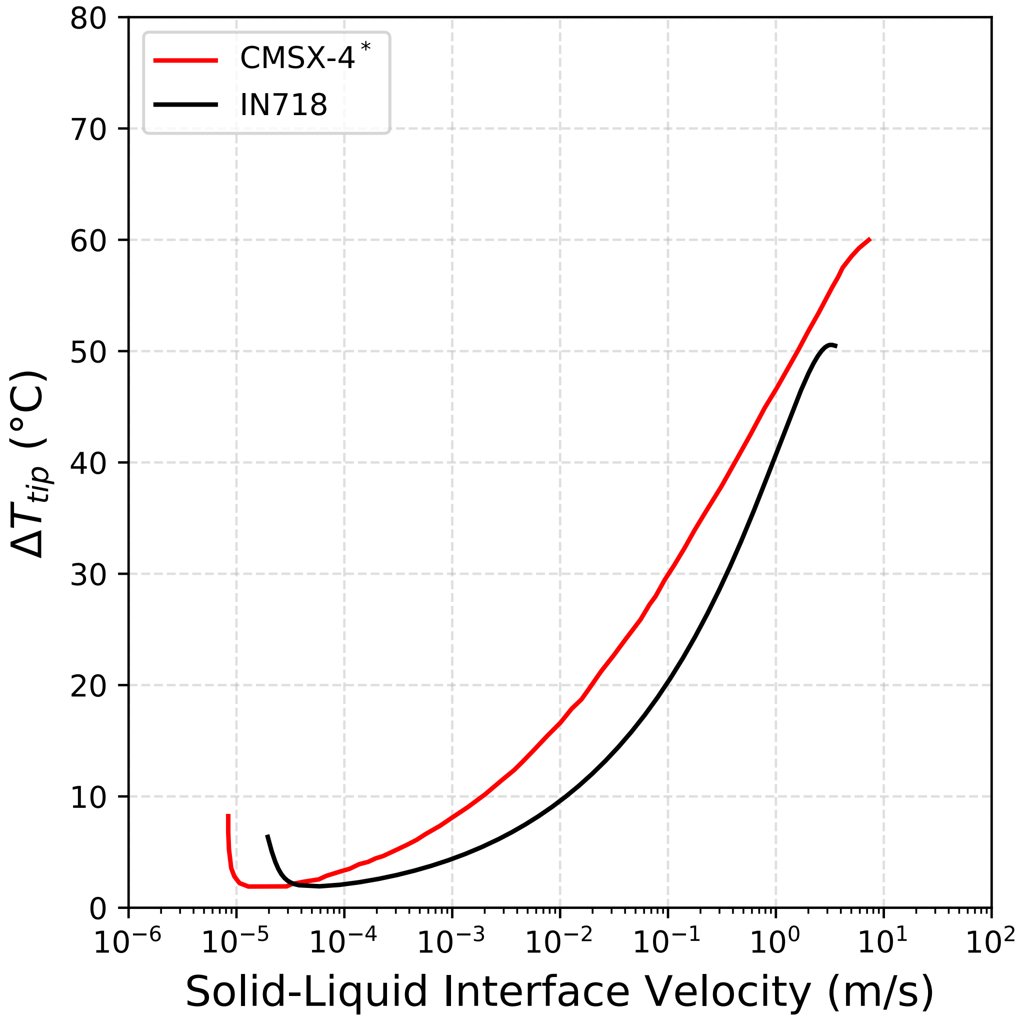
ϕ = Probability of grain nucleation ahead of interface

Kurz Giovanola Trivedi (KGT) model predicts undercooling at the dendrite tip



Kurz Giovanola Trivedi (KGT) model predicts undercooling at the dendrite tip

$$\Delta T_{tip} = (a \cdot R)^{1/n}$$



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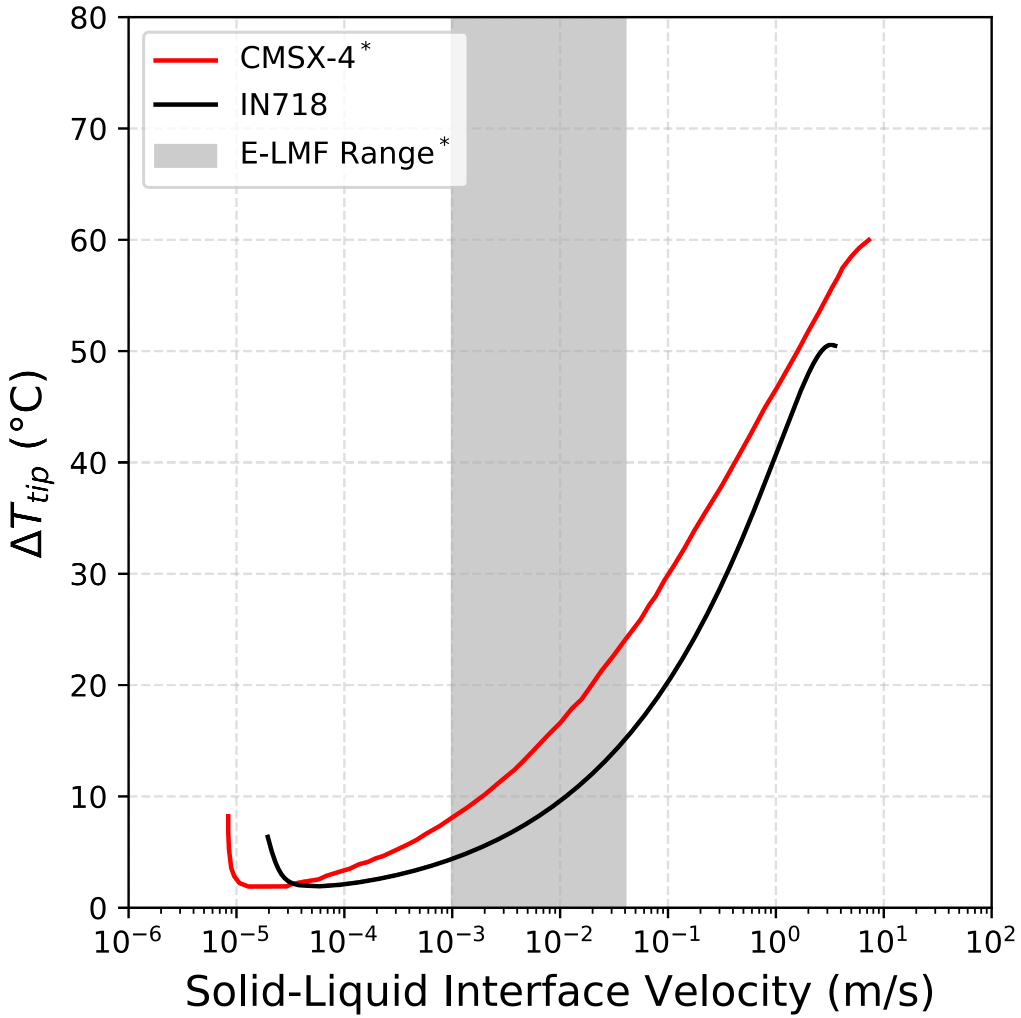

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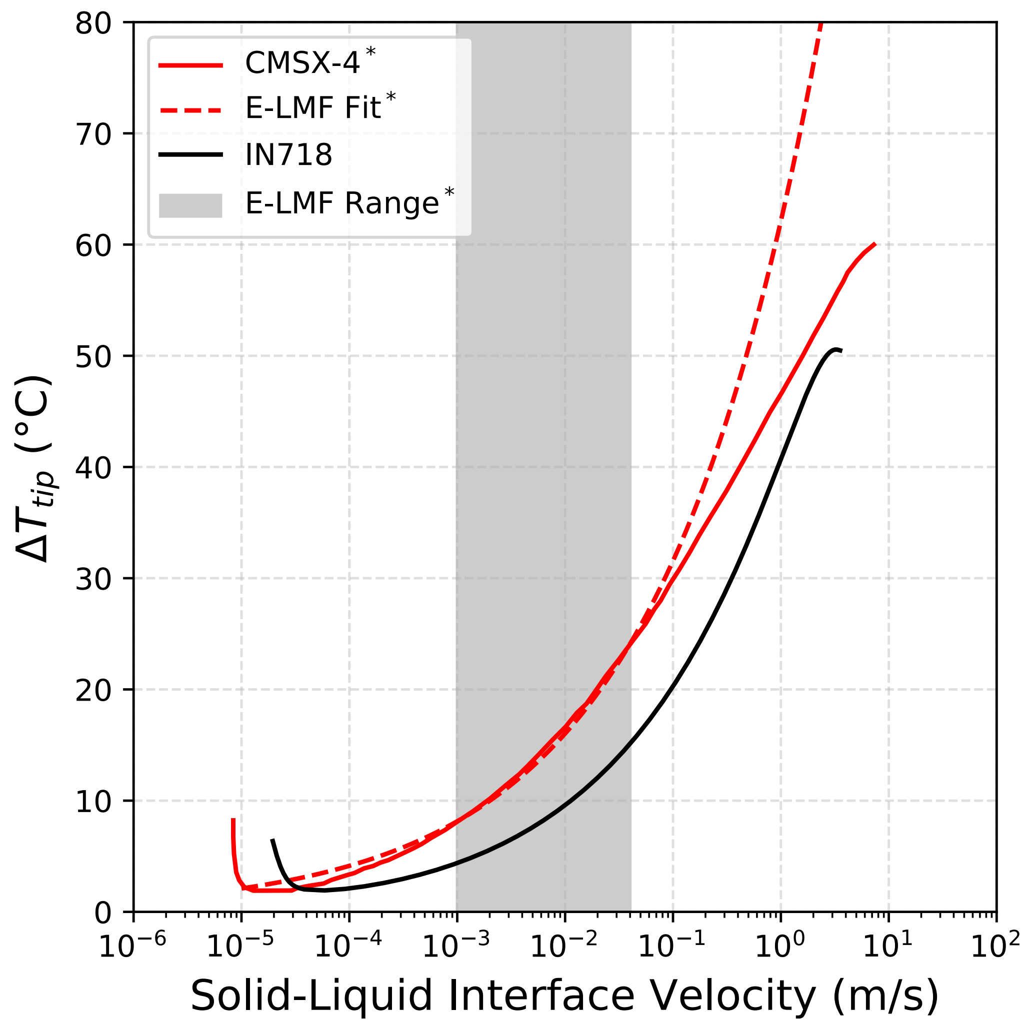

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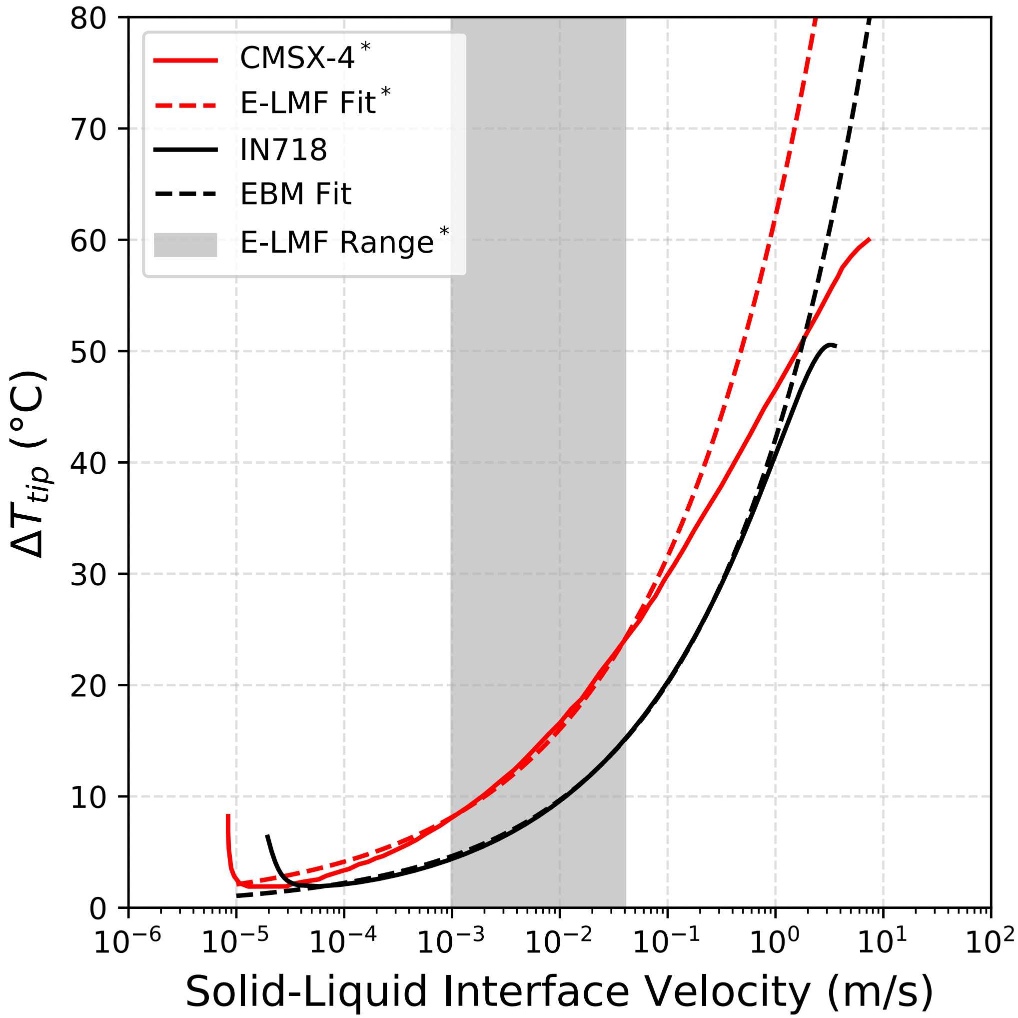


Kurz Giovanola Trivedi (KGT) model predicts undercooling at the dendrite tip

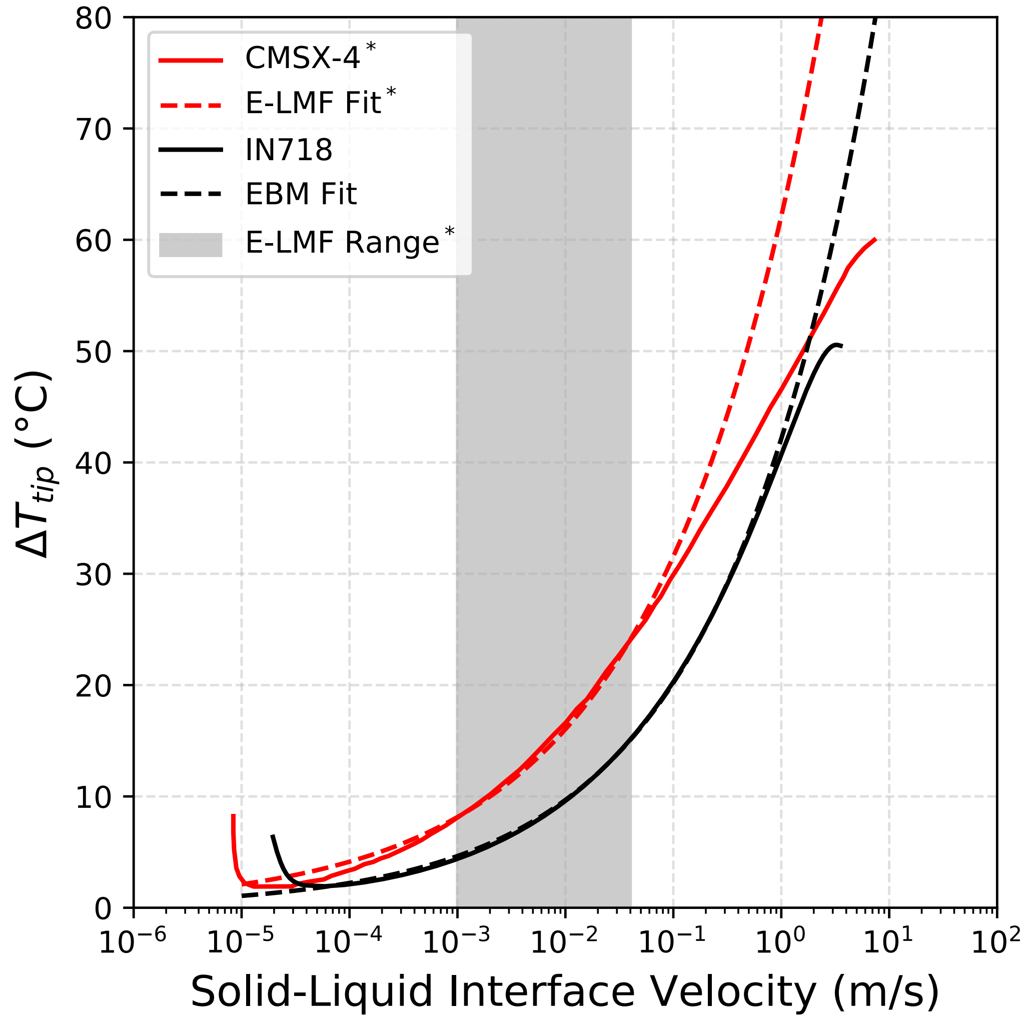
$$\Delta T_{tip} = (a \cdot R)^{1/n}$$

- *a* decreases by an order of magnitude (smaller equiaxed processing window)

  $1.25\times10^6 \rightarrow 1.23\times10^5$

- *n* decreases (larger equiaxed processing window)

  $3.4 \rightarrow 3.13$



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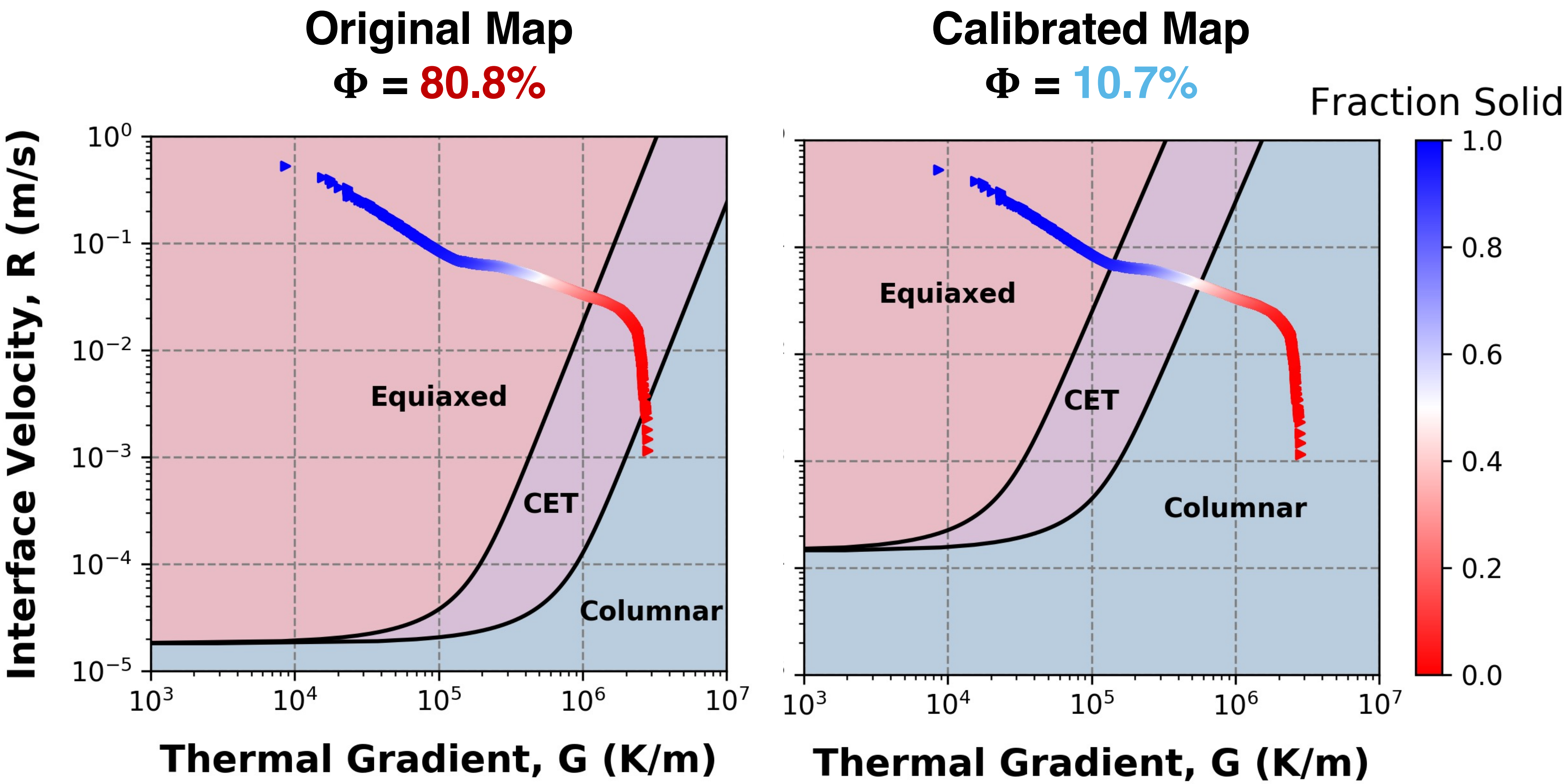
TRUCHAS	☑	G = Thermal Gradient
TRUCHAS	☑	R = Interface Velocity
3D Data ←	☑	N_0 = Nuclei density
KGT Model ←	☑	a, n = Material constants
		ϕ = Probability of grain nucleation ahead of interface

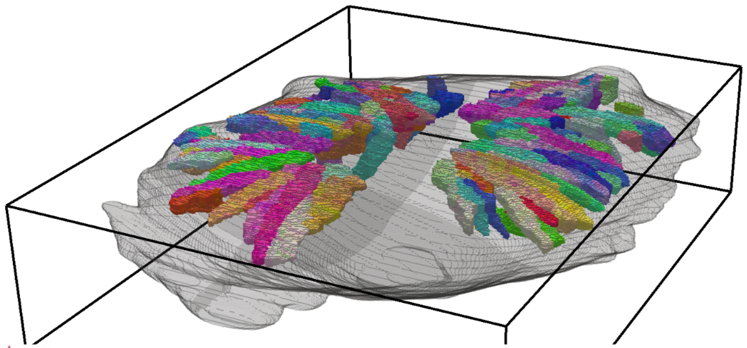
Calibrated processing map accurately predicts microstructure

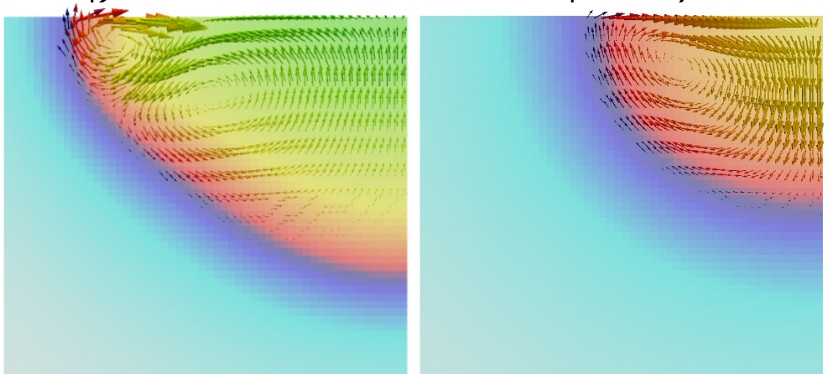
- Measured **Φ = 11.4%** from 3D data

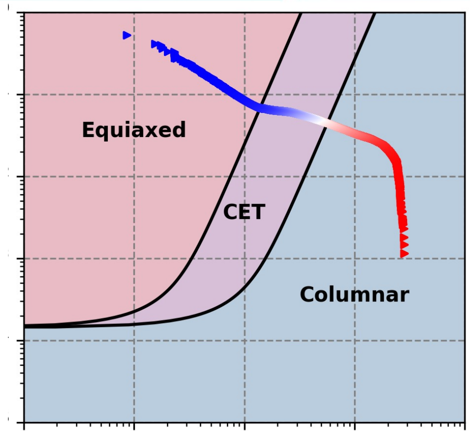


Summary

- 3D provides direct measurement of ground truth microstructures for calibration of processing maps
- Advanced simulations can provide insight to microstructure evolution during solidification
- Processing maps are alloy- and processing-dependent, and must be calibrated for the specific application of interest







Thanks!

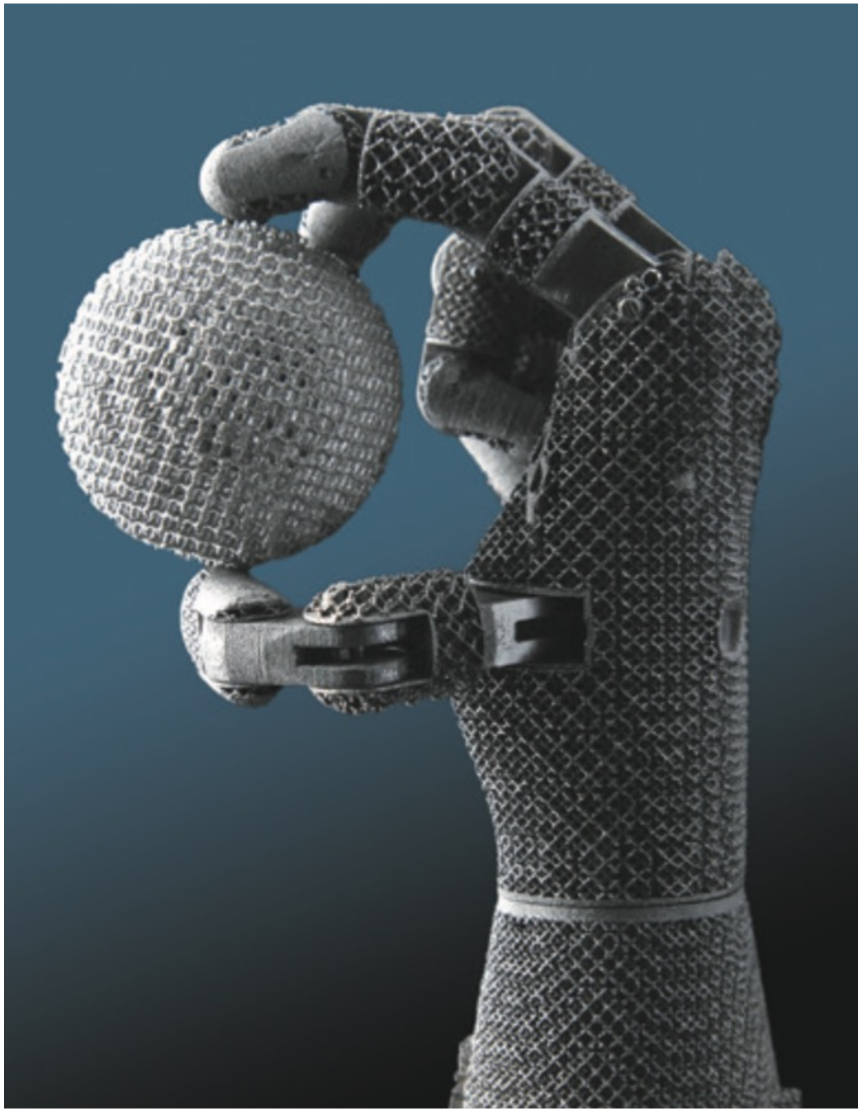


Image courtesy ORNL MDF