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Center for Advanced Non-Ferrous Structural Alloys
An Industry/University Cooperative Research Center

Project 52-L: Data Driven Qualification (DDQ) Framework for Metals Additive Manufacturing (AM)

Semi-annual Spring Meeting
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Sponsor: National Center for Defense Manufacturing and Machining (NCDMM)

NCDMM
NATIONAL CENTER FOR DEFENSE MANUFACTURING AND MACHINING

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- Student: Charles Smith (Mines)
- Advisor: Jonah Klemm-Toole (Mines)
- Co-Advisor: Amy Clarke (Mines)

Project Duration
M.S. January 2021 to December 2022

- Problem: The range of equipment suppliers that use their own proprietary feedstock and process parameters makes each AM system and qualification protocol unique.
- Objective: Use a data driven qualification approach to form relationships across platforms and alloy systems using intelligent machine learning algorithms and physics-based modeling.
- Benefit: Accelerated qualification and adoption of AM parts into military vehicles.

Recent Progress

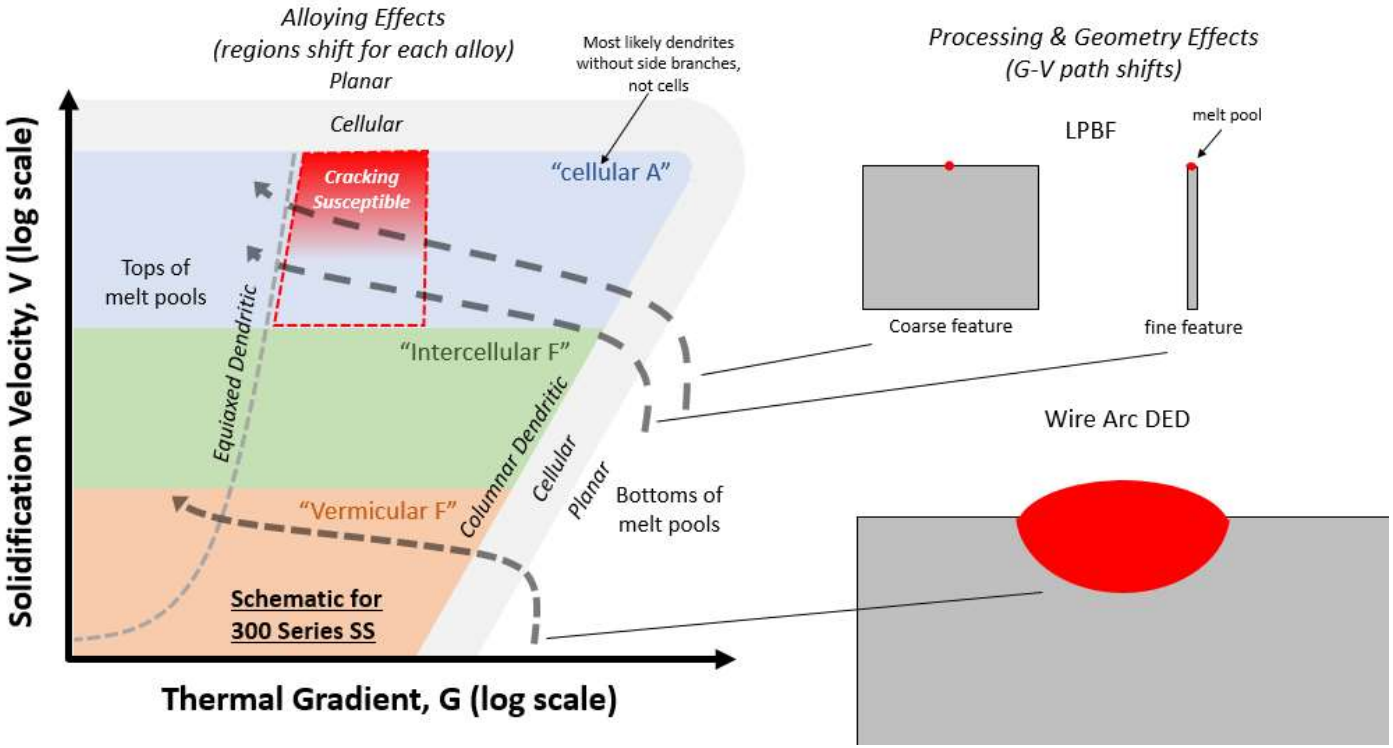
- Completed first draft of analytical solidification model.
- Simulation are finished to model thermal gradients and heating characteristics.
- Experimental results to validate solidification model has begun.

Metrics		
Description	**% Complete**	**Status**
1. Literature review	75%	●
2. Preliminary thermodynamic modeling/simulations	85%	●
3. Development of G (temperature gradient) and V (solidification velocity) diagram	70%	●
4. Microstructural characterization of AM builds	10%	●
5. Validation with different AM builds	5%	●

Overview

- Project background and approach
- Predictive solidification microstructure map
  - Methodology
  - Models
  - Results
- Heat transfer simulation
  - Methodology
  - Predictive results
- Comparison between predictive microstructure to experimental results

Approach



J. Klemm-Toole, unpublished, 2020

The map can predict the resulting microstructure (solidification + solid state transformation) if the solidification velocity and thermal gradient are known for a process.

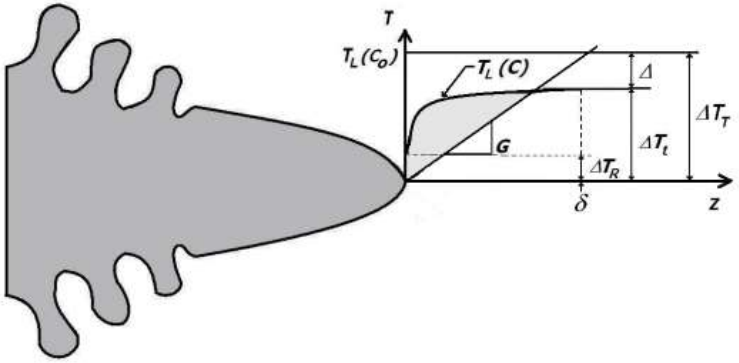
Alloy

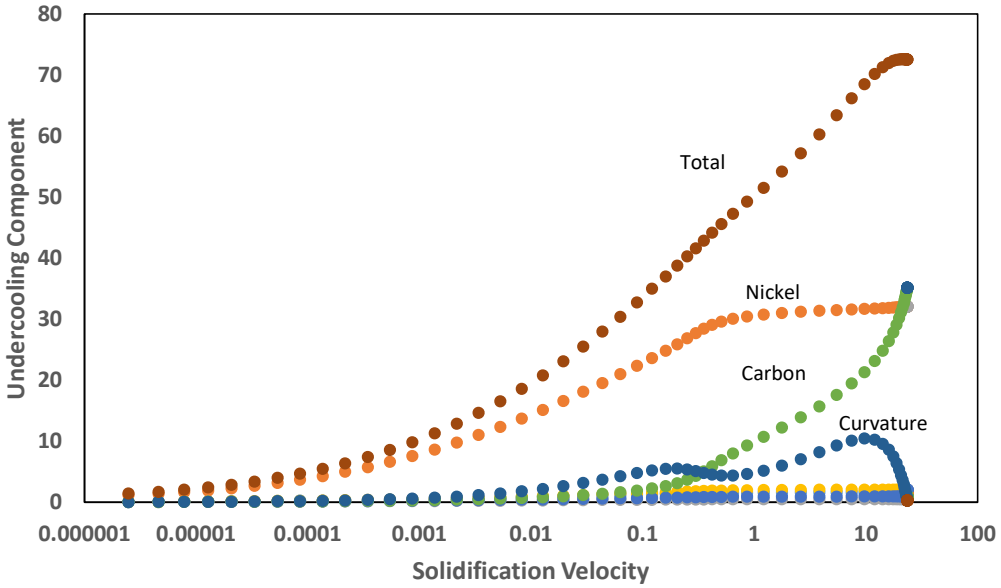
- 316L Stainless Steel was used for the solidification model in both the LPBF and WAAM simulation.
- Exact composition varies between processes.
- Composition used in this model was measured from powder samples from before and after the LPBF print.

Element	wt%
Cr	17.91
Ni	12.22
Mo	2.5628
Mn	1.1086
Si	0.6947
C	0.03714
Fe	Balanced

Ivanstov Marginal Stability (IMS) Model

- Models the stability of dendrites by calculating solute distribution ahead of the dendrite tip.
- Uses partitioning coefficients, liquidus slope, and diffusion coefficient to predict dendrite undercooling, dendrite tip radius, and solidification velocity.





McFadden and Browne, Computational Materials Science, 2012

The IMS model provides the framework for the solidification model by observing the effects of undercooling and dendrite tip radius as a function of solidification velocity.

Planer, Cellular, and Dendritic Growth

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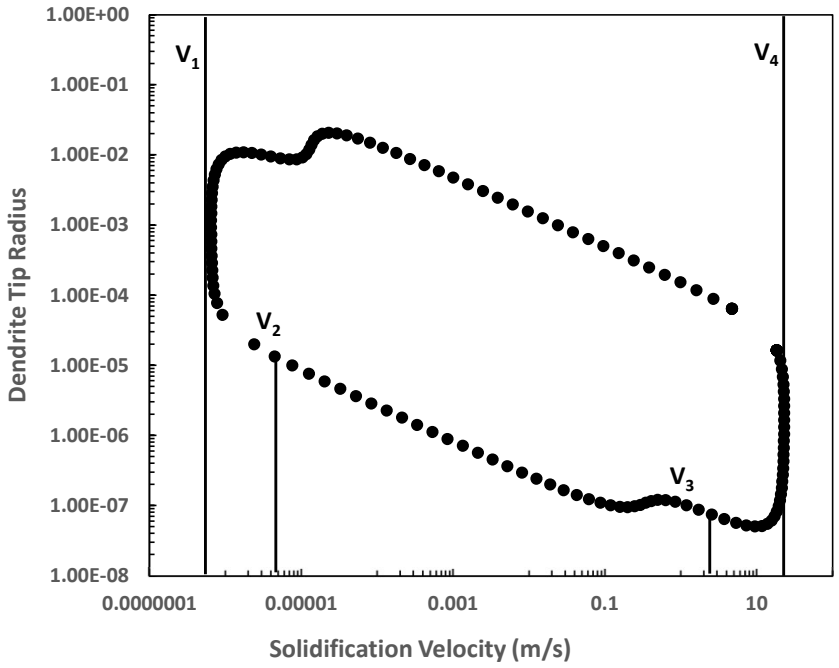
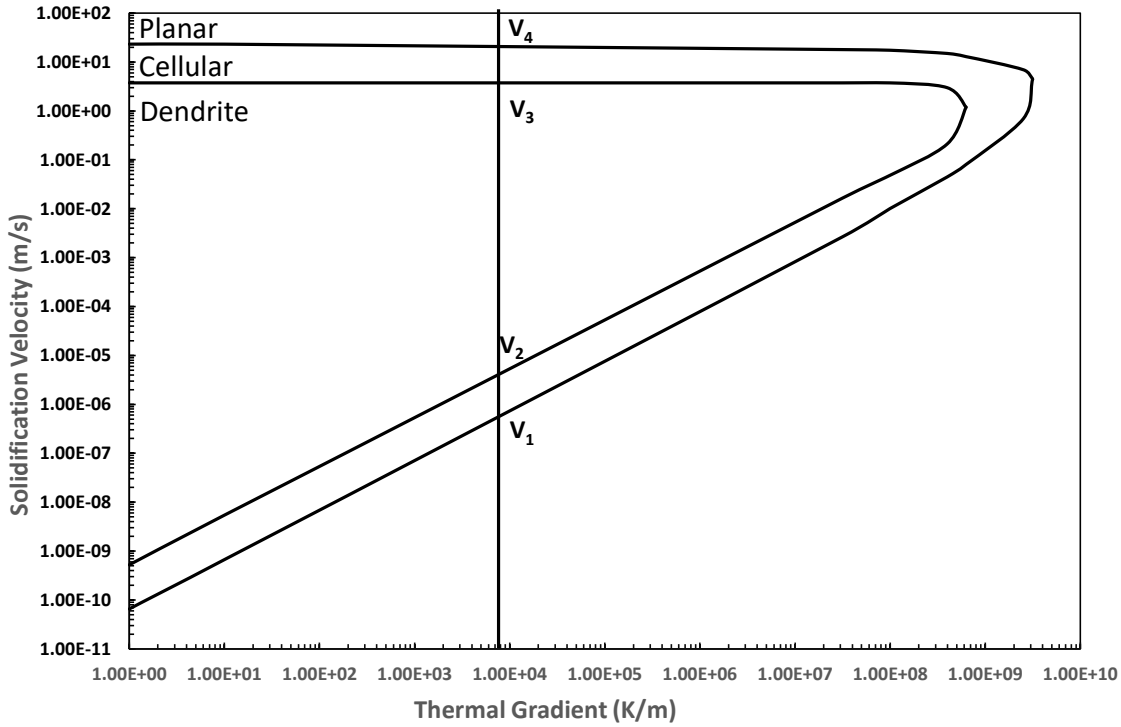
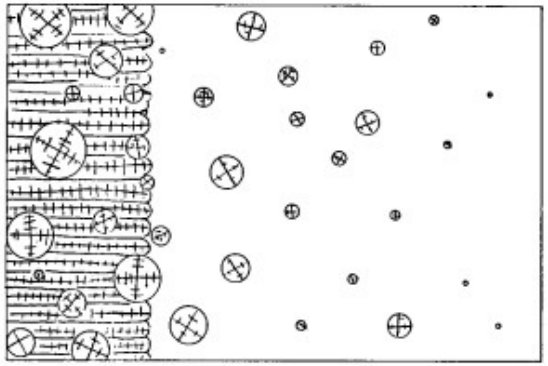
Thermal Gradient: 10^4 K/m

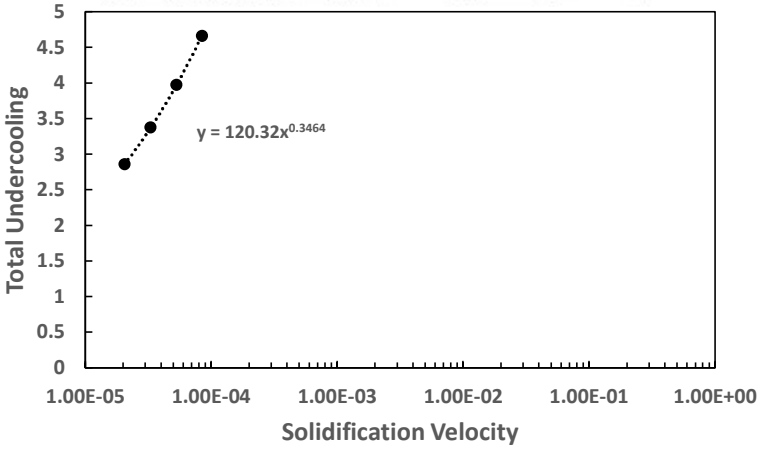




Changes in solidification behavior can be predicted by observing the evolution of dendrite tip radius with changes in solidification velocity at a given thermal gradient.

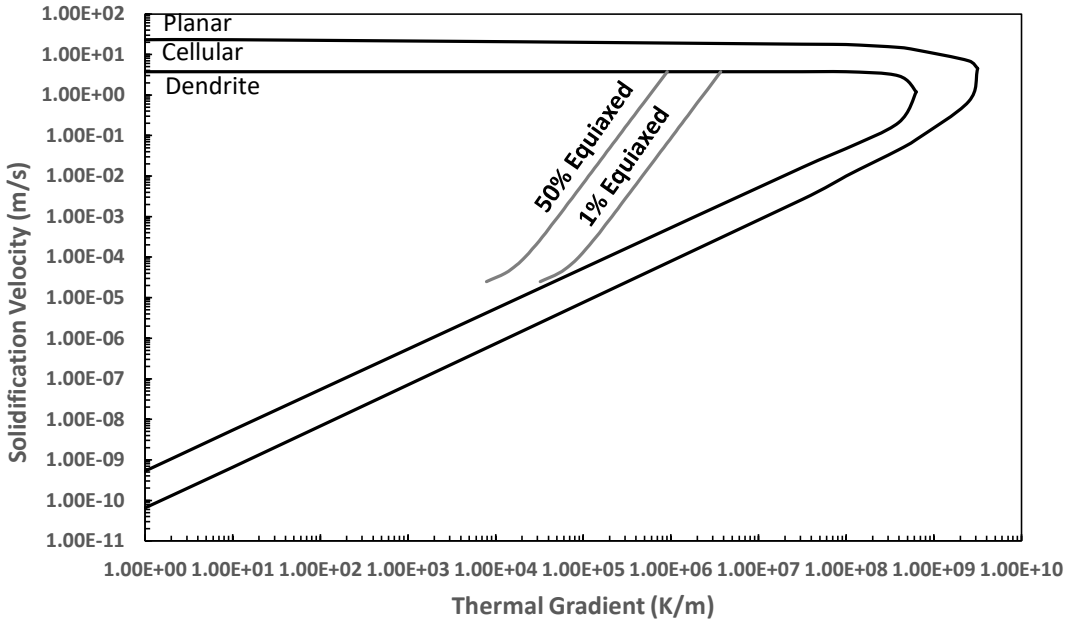
Columnar to Equiaxed Transition (CET)





J. D. Hunt, Materials Science and Engineering, 1984

- $a = \alpha^{\beta}, n = \frac{1}{\beta}$
- $\Delta T = (aV)^{\frac{1}{n}}$
- $G = \frac{1}{n+1}\sqrt[3]{-\frac{4\pi N_o}{3\ln(1-\phi)}}\Delta T\left(1-\frac{\Delta T_N^{n+1}}{\Delta T^{n+1}}\right)$

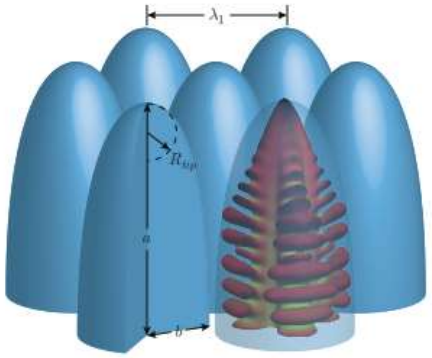


Using a power law fit of total undercooling vs solidification velocity from the IMS model, the range at which the transition from columnar to equiaxed dendrites occurs can be plotted as lines of partial transition.

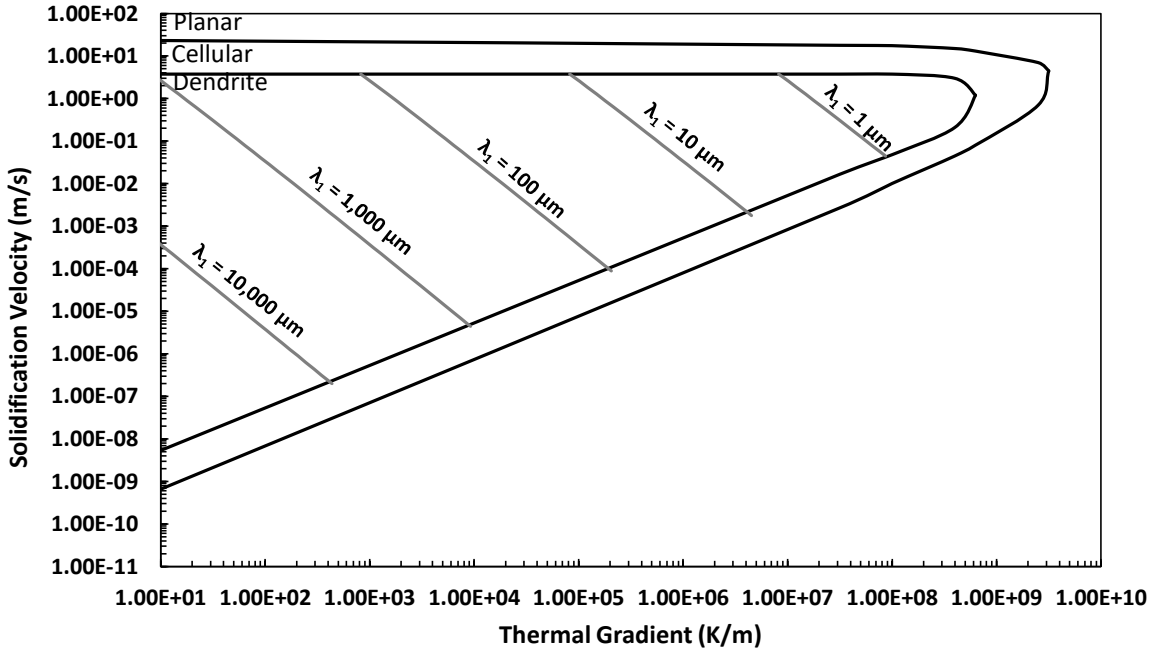
Primary Dendrite Arm Spacing (PDAS)

- PDAS prediction are only valid for columnar dendrites
- Uses the coefficients and exponents of a power law fit for tip radius and solidification velocity and for total undercooling vs solidification velocity

$$\lambda_1 = \sqrt{\frac{3\left(\alpha_1 V^{\beta_1}\right)\left(\left(T_L - \alpha_2 V_2^{\beta_2}\right) - T_{base}\right)}{G}}$$



J. A. Dantzig and M. Rappaz, Solidification, 2016



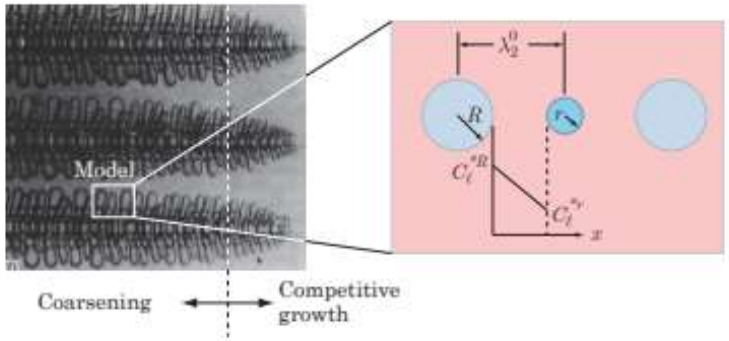
PDAS is only dependent on solidification velocity, thermal gradient, dendrite tip and base temperature and independent of time.

Secondary Dendrite Arm Spacing (SDAS)

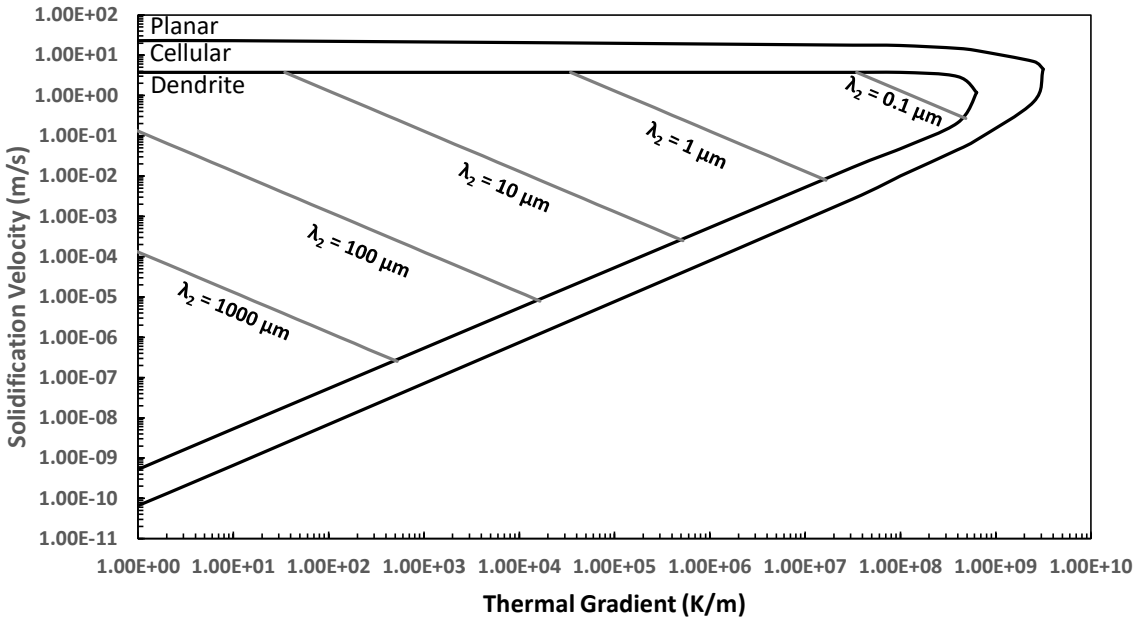
- SDAS changes with time due to elimination of smaller side branches and the growth of larger ones.
- The process is called coarsening and is where the length scale of the microstructure increases over time.
- Dependent on liquidus and solidus temperatures, liquidus concentration at solidification, liquidus slope, partition coefficient, diffusion coefficient.

$$\lambda_2 = 5.5 M^{\frac{1}{3}} t_f^{\frac{1}{3}}$$

$$M = \frac{-\Gamma}{\sum \frac{m_j(1-k_j)(c_{f,j}-c_{0,j})}{D_j}} * \ln\left(\frac{\sum \frac{m_j(1-k_j)c_{f,j}}{D_j}}{\sum \frac{m_j(1-k_j)c_{0,j}}{D_j}}\right)$$



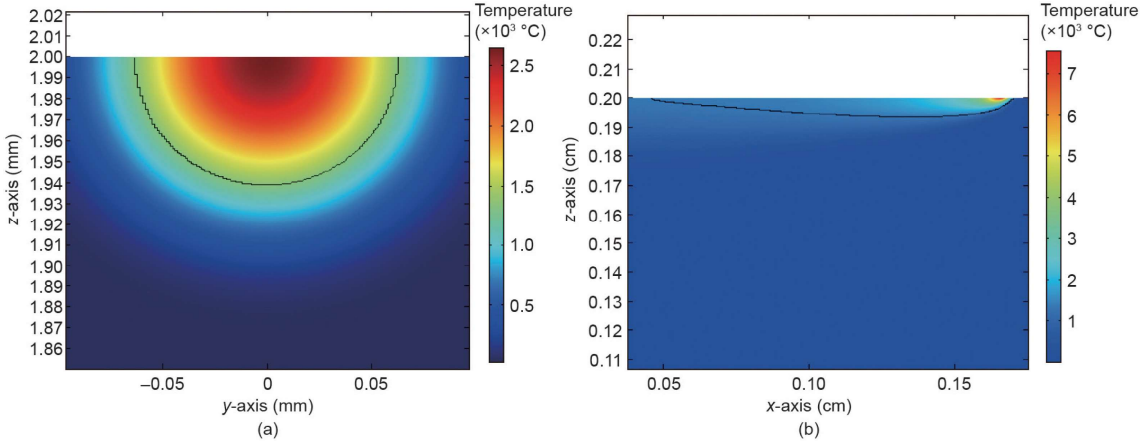
J. A. Dantzig and M. Rappaz, Solidification, 2016



SDAS is related to local solidification time but also changes after solidification due to coarsening.

Heat Transfer Model

- Rosenthal Model
  - Assumptions
    - Thermophysical properties are temperature independent.
    - Scanning speed and power input are constant.
    - Point heat source
    - The heat transfer is governed purely by conduction.

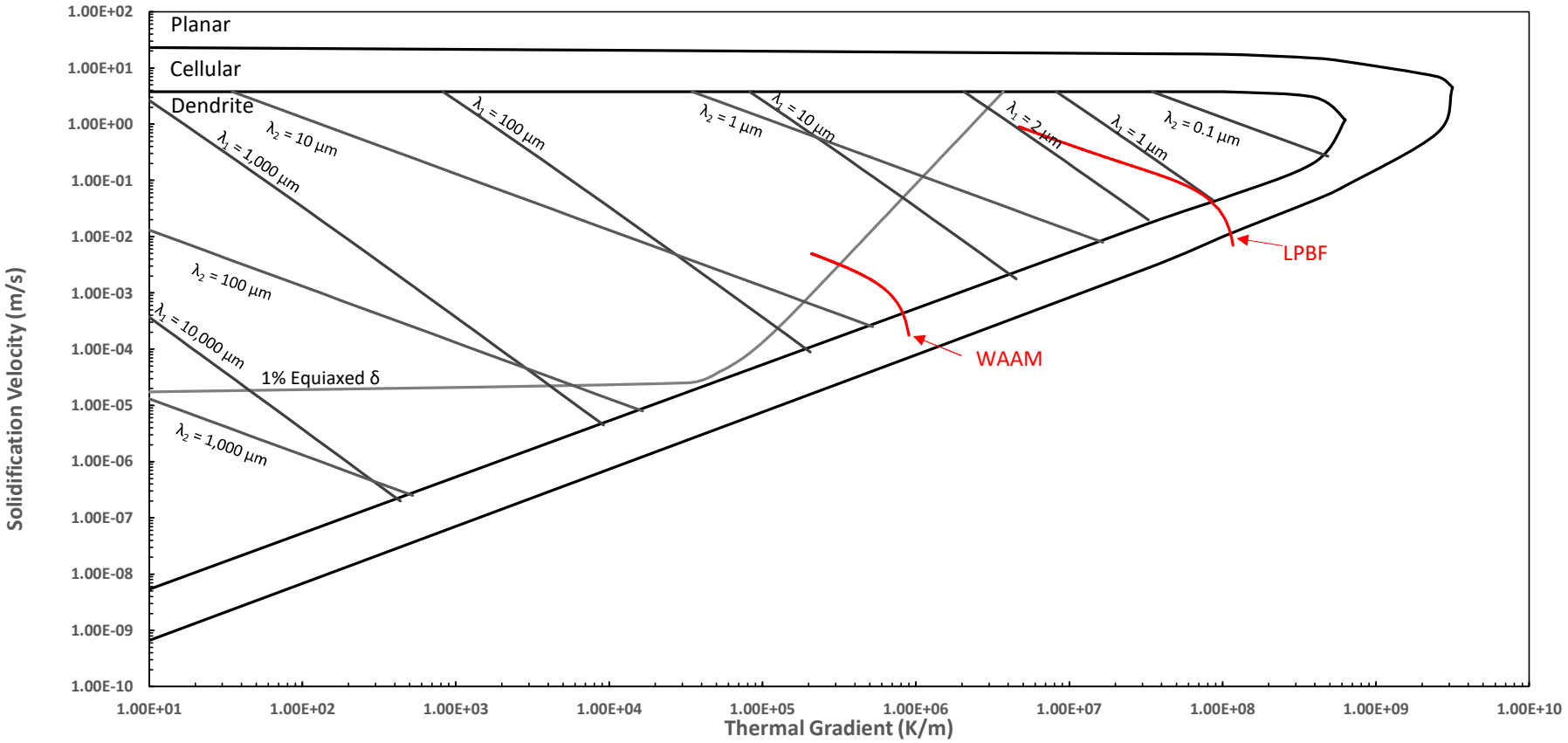


$$T = T_o + \frac{\lambda P}{2\pi k r} \exp\left[-\frac{V(r+\xi)}{2\alpha}\right]$$

P. Promoppatum et al, Engineering, 2017

The Rosenthal model predicts semi-circular melt pool cross-sections whose depths and widths are deeper and narrower respectively compared to many additive manufacturing techniques.

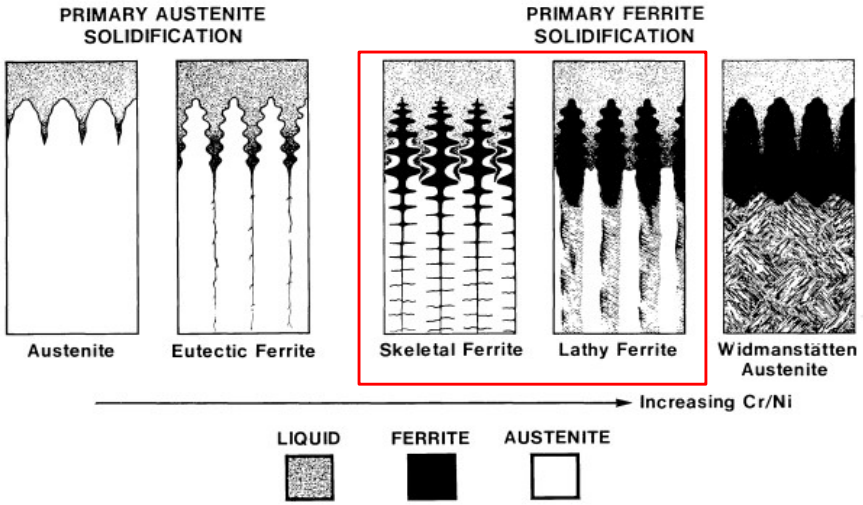
Analytical Microstructure Map

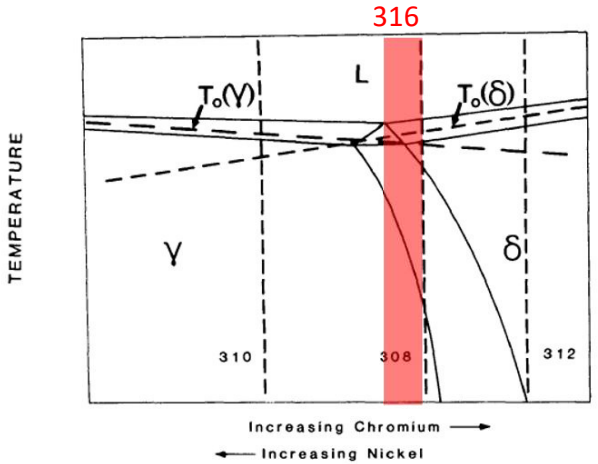


The analytical microstructure map shows lines of constant PDAS and SDAS. A Rosenthal model of a LPBF and WAAM process is plotted to show general areas at which these processes occur.

Primary Ferrite and Primary Austenite Solidification

- At high enough solidification velocities and undercooling, the primary solidification transitions from primary ferrite solidification to primary austenite formation.
- The primary solidifying phase change is assumed when the temperature of an austenite dendrite tip is higher than a ferrite dendrite tip.

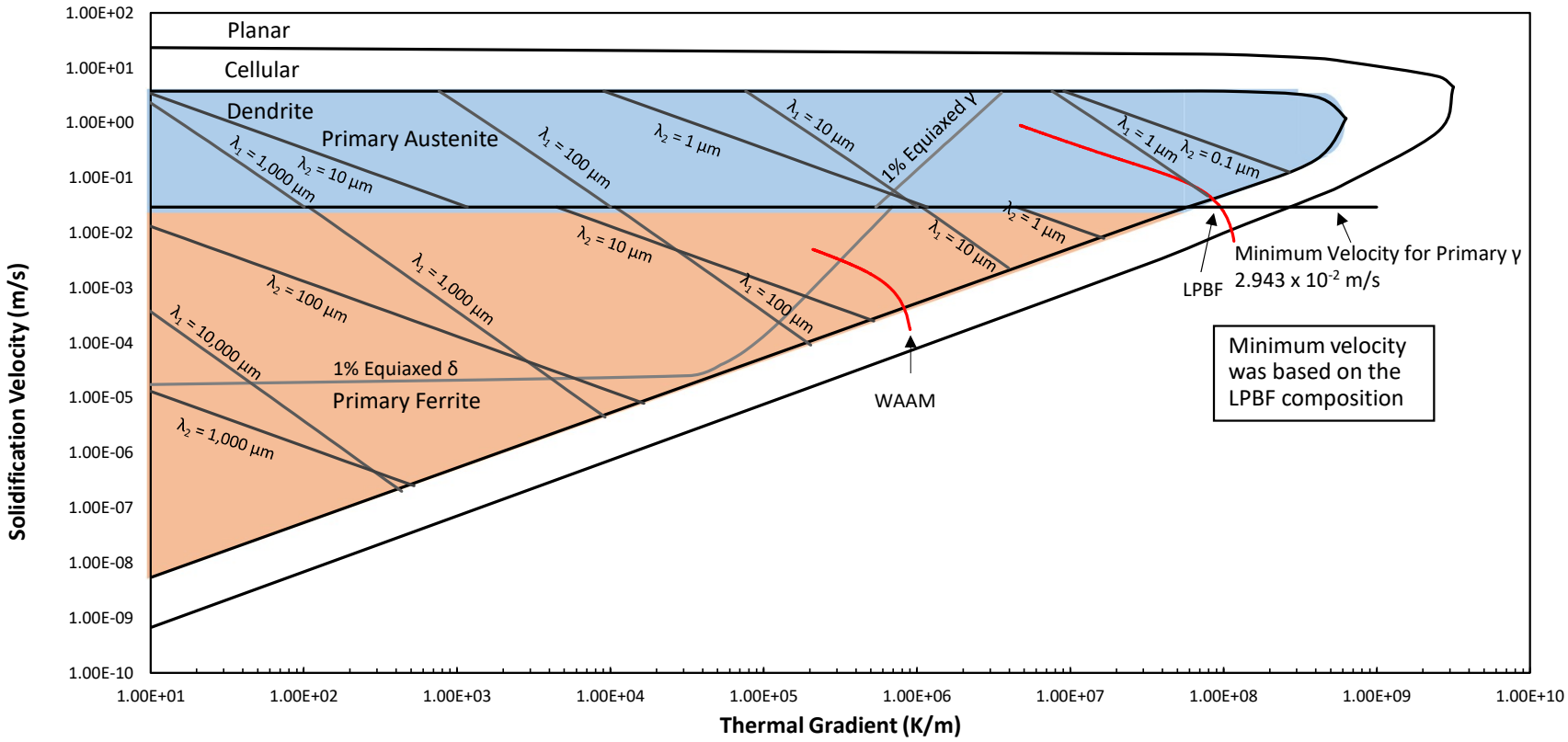




S.A. David et al, ORNL/TM-10487, 1987
J. A. Brooks et al, International Materials Reviews, 1991

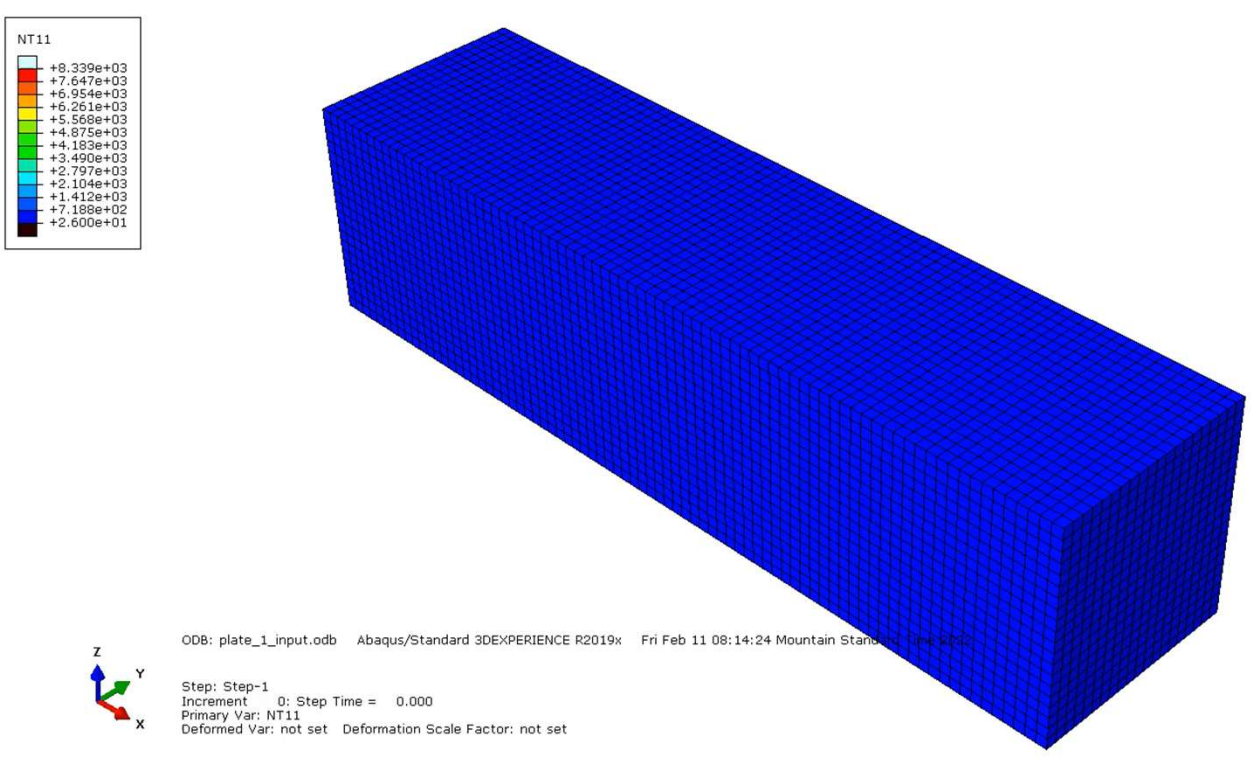
With increasing solidification velocities, the dendrite tip temperature decreases and can transition from primary ferrite to primary austenite solidification.

Primary Ferrite and Primary Austenite Solidification



The analytical microstructure map shows lines of constant PDAS and SDAS with regions of primary ferrite solidification and primary austenite solidification shaded.

LPBF Heat Transfer Simulations

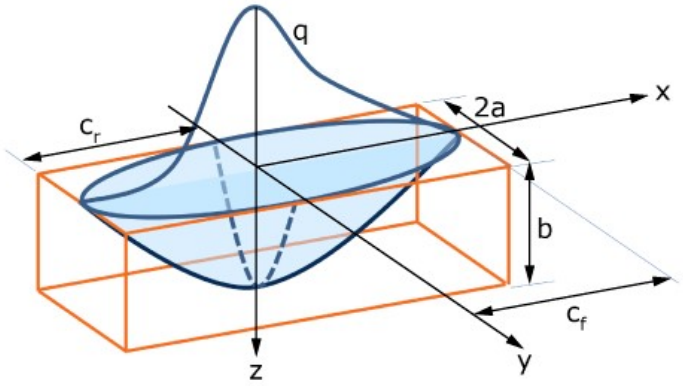


- Power = 200W
- Scanning speed = 1400mm/s

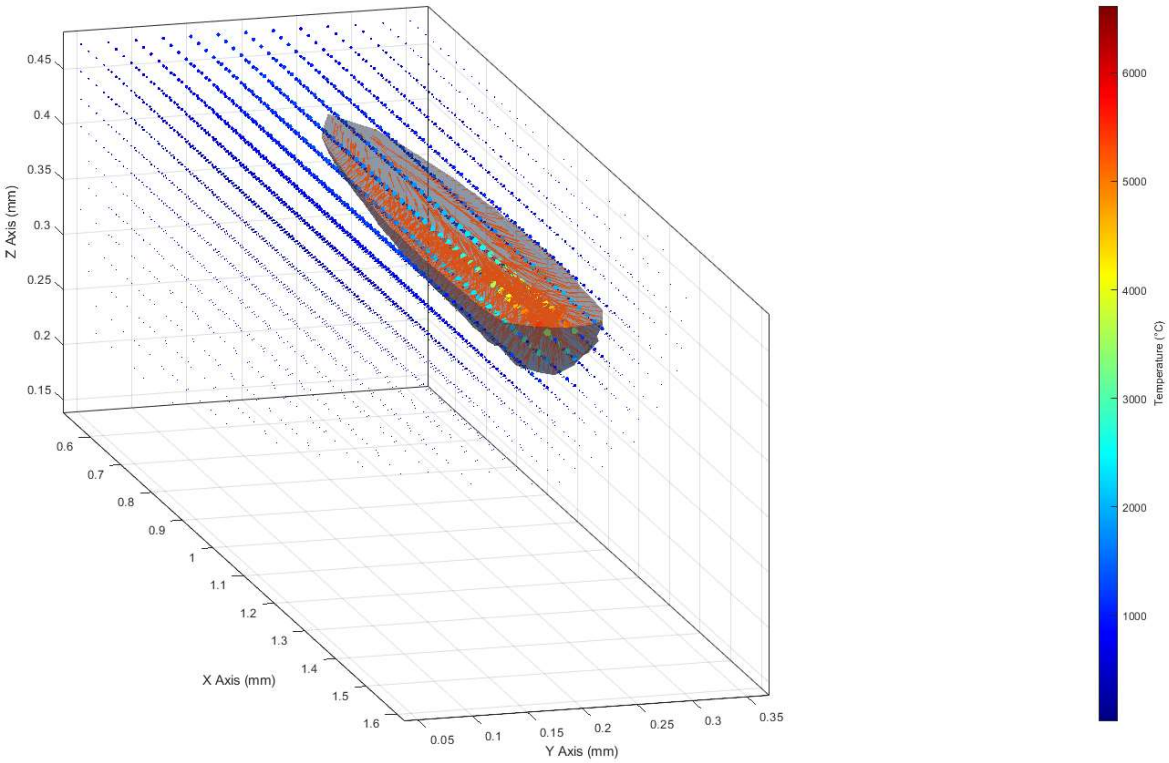
Abaqus simulations are used to model a double pass build and can be used to predict the thermal gradients (G) and solidification velocities (V).

GV Calculations and Results

- The Abaqus simulations are modeled to match the melt pool geometry of an experimental result.
- Goldak heat distribution
- Normal vectors are plotted along the melt pool boundary and the magnitude of these vectors are the thermal gradient.

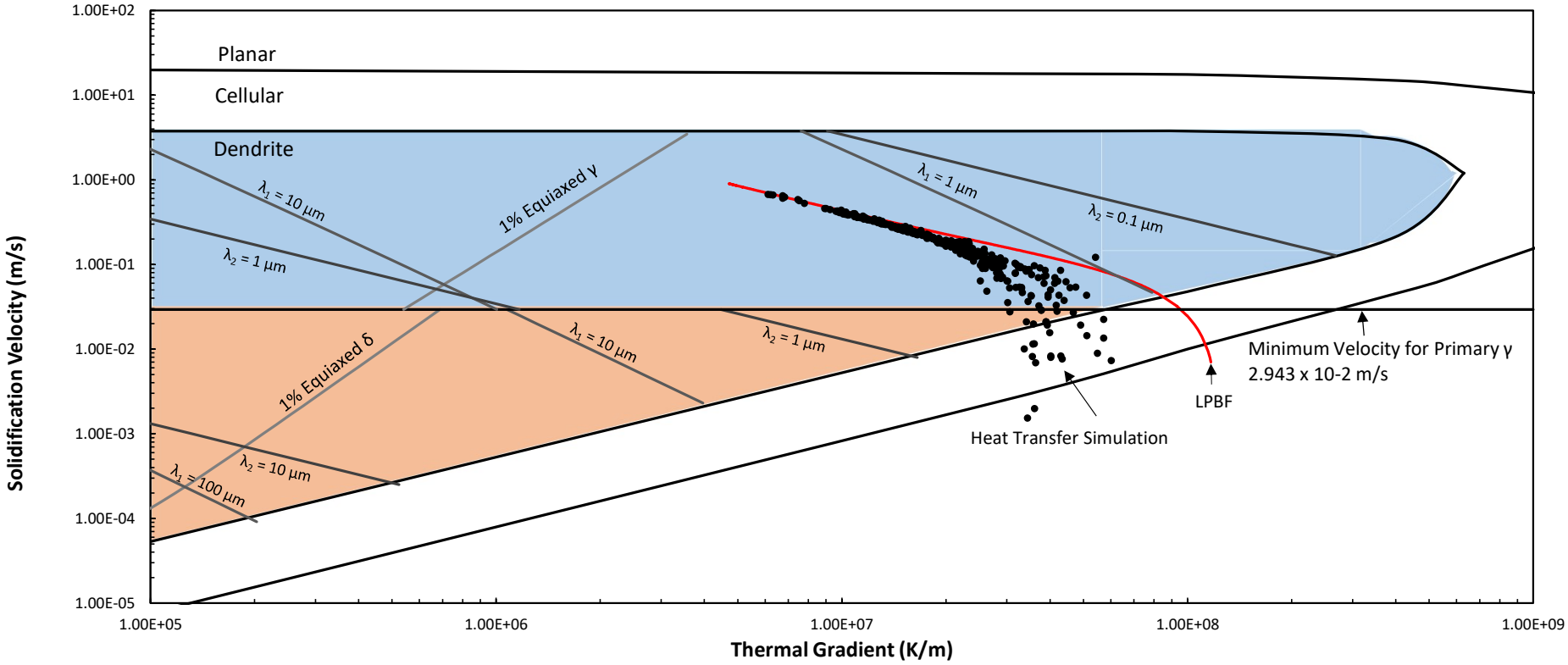


Abaqus software documentation



The Abaqus simulations are modeled to have similar melt pool geometries to an experimental build and the thermal gradients, cooling rates, and solidification velocities are calculated from the model.

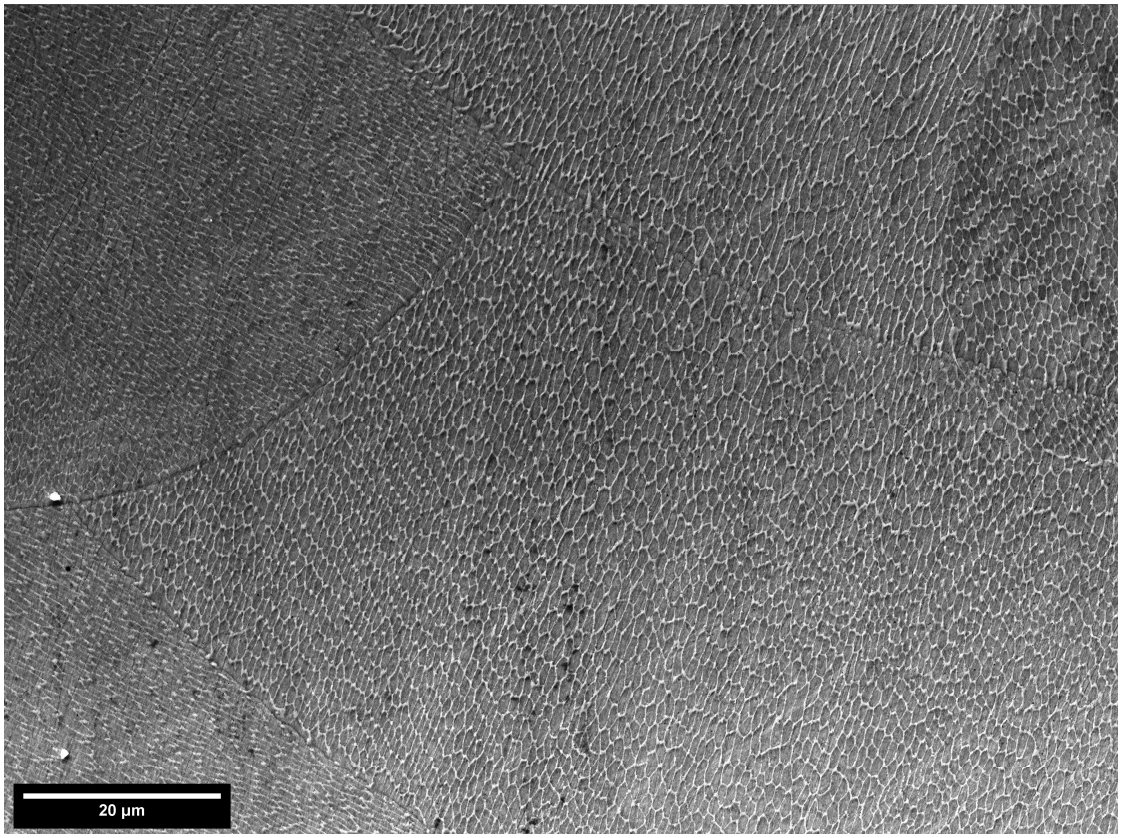
Abaqus GV Path



Predicted PDAS values should be around 1-2 µm with the majority of the microstructure being primary austenite and mostly columnar dendrites.

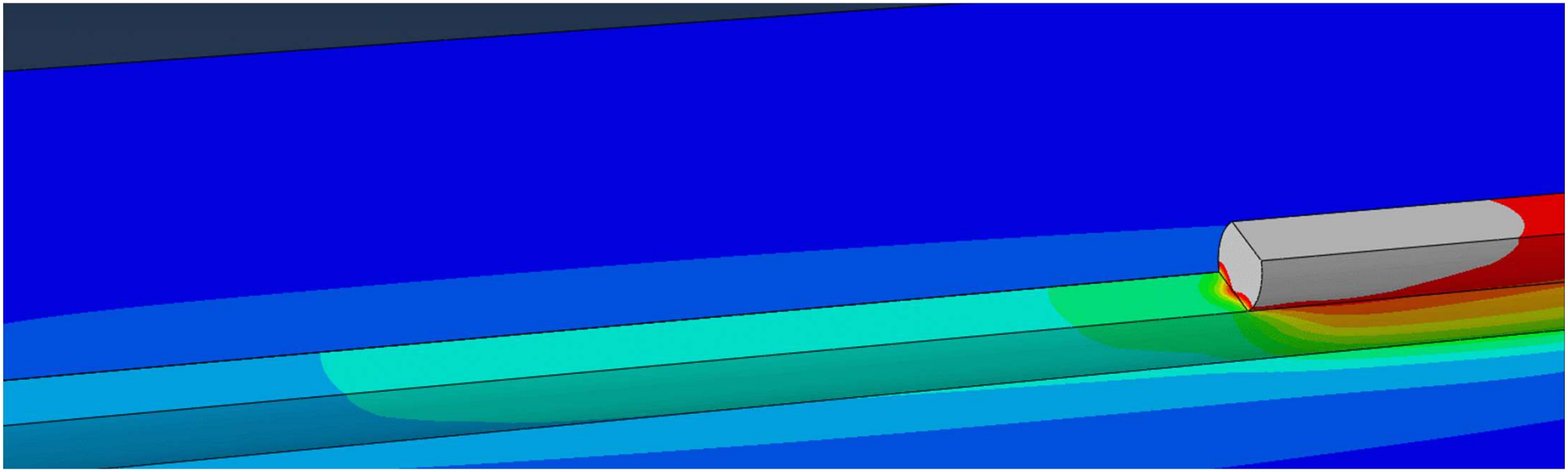
Predicted Microstructure vs. Experimental

- PDAS: average 1.85 µm
- Columnar dendrites with small amounts of equiaxed dendrites
- Primary austenite solidification



The measured PDAS is within the predicted measurements and the microstructure is similar to what is predicted from the model.

WAAM Heat Transfer Model



Courtesy of Dr. Anthony Petrella

Abaqus simulations are used to model a single pass with depositing material and can be used to predict the thermal gradients (G) and solidification velocities (V).

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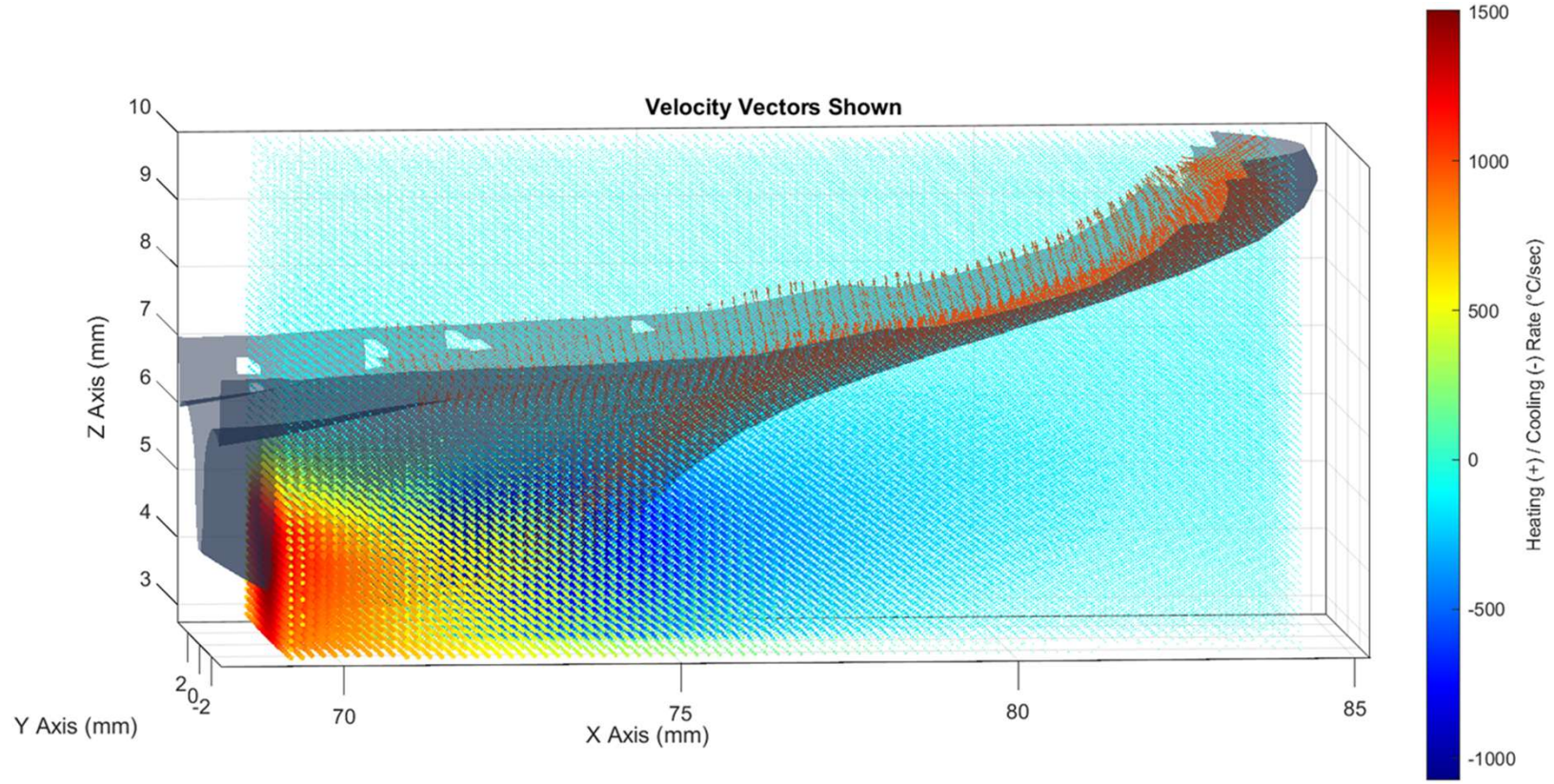
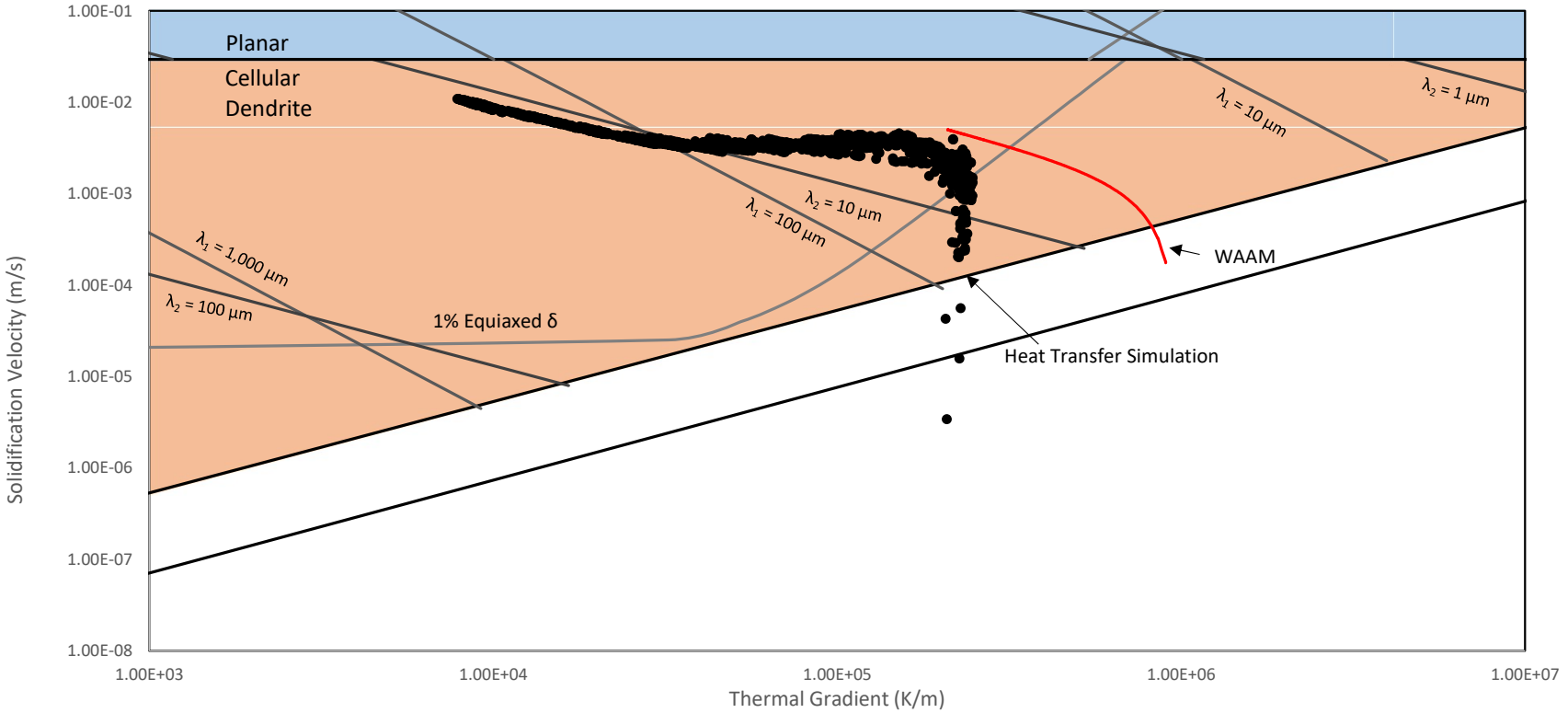
WAAM GV Calculations and Results



Abaqus simulations are used to models the solidification front of a WAAM process, this allows the G and V data to be extracted from the simulation.

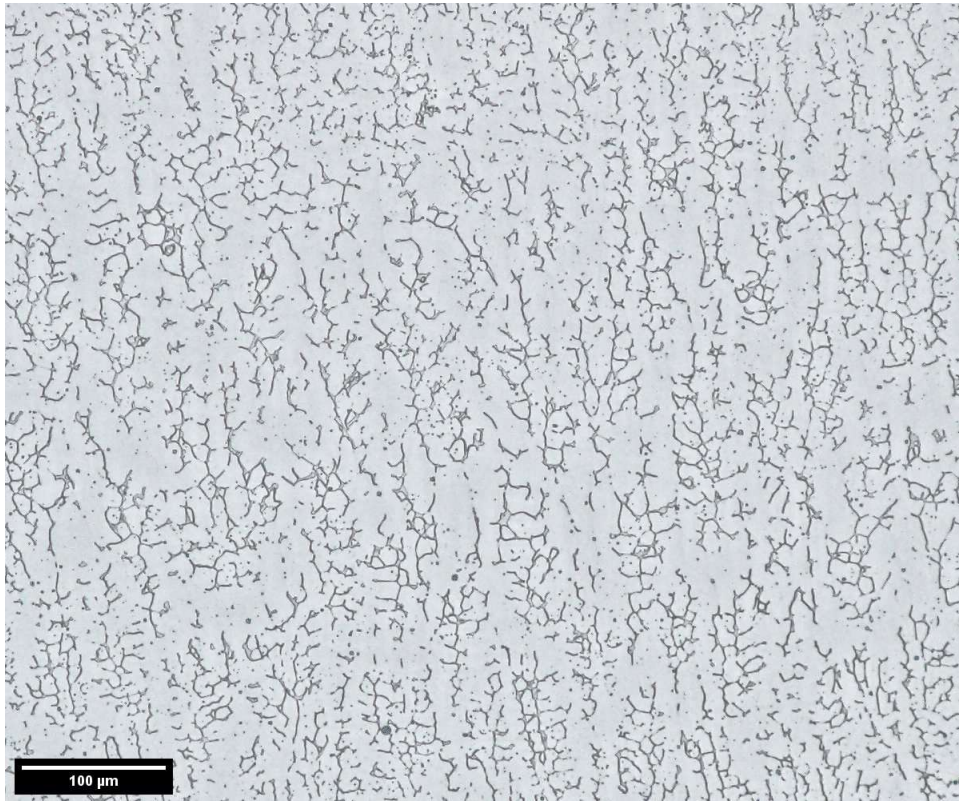
WAAM Heat Transfer Simulation and GV Calculations



Predicted PDAS values should be around 20 - 30 µm and SDAS values around 7-9 µm with majority of the microstructure showing columnar dendrites with equiaxed located at the top of the melt pool. The material should also have experienced primary ferrite formation.

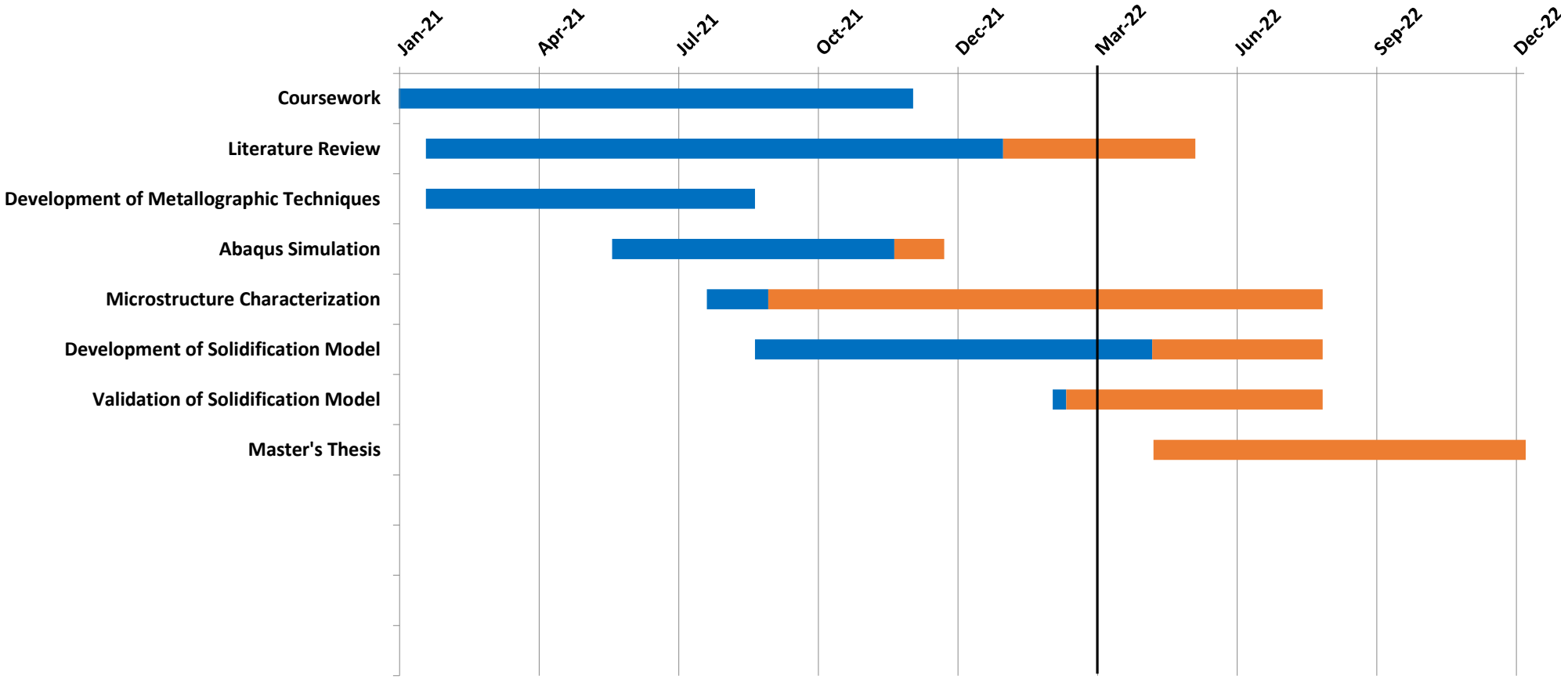
Predicted Microstructure vs Experimental

- PDAS: average 23.6 µm
- SDAS: average 7.2 µm
- Columnar dendrites with equiaxed located at the top of the melt pool
- Primary ferrite solidification



The measured PDAS and SDAS are within the predicted measurements and the microstructure is similar to what is predicted from the model.

Gantt Chart



Challenges, Opportunities & Next Steps

- The preliminary predictions of a LPBF and WAAM process seem to have similar PDAS and SDAS values and displays similar microstructure features to what is predicted by the model.
- Heat transfer simulations can provide thermal information to predict the microstructure of an AM build.
- The models and simulations that were performed are simple and can be adapted to different alloys given the thermal properties are known or can be measured.
- Perform validation of the solidification model using builds of different process parameters.

Thank you!

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