Computational Tools for Additive Manufacture of Tailored Microstructure & Properties

Annual Project Meeting Presentation: Simulation Based Engineering

Raytheon Technologies Research Center

Team: Ranadip Acharya, Paul Attridge, Luke Borkowski, Brian Fisher, John Sharon, Alex Staroselsky, & Anthony Ventura

This material is based upon work supported by the Department of Energy under Award Number **DE-FE0031642**.

Background & Introduction

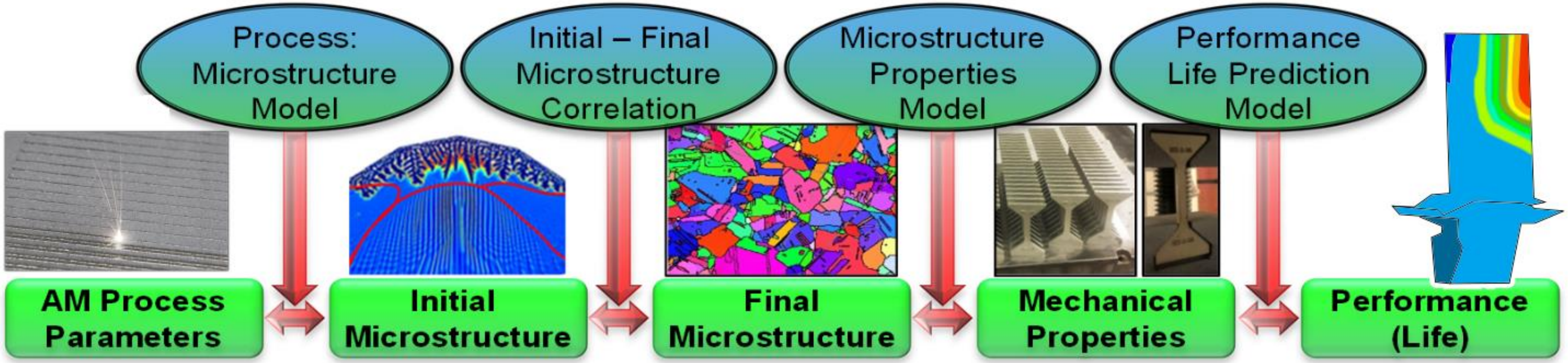
Purpose: ***Establish computational tools to link AM parameters to material properties to enable parts with spatially varying microstructure for enhanced performance***

Project seeks to demonstrate the application of computational methods & tools on microstructure evolution and prediction of mechanical behavior for nickel based superalloy parts.

Current State: use "standard parameters" to print parts with a homogenous microstructure; limited control over grain size, morphology, etc.

Desired State: a predictive thread of AM input parameters through to tailored property placement

Challenge: AM parts go through multiple steps, each with strong impact on finished part



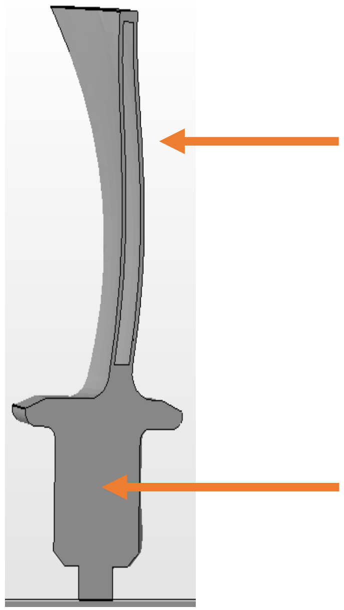
Core Questions

Successful implementation of thread that links AM process parameters through to part performance requires answers to the following:

- What AM process parameters can be readily be controlled & modeled to manipulate deposit microstructure?
- Do differences in as-deposited microstructure get erased with post processing thermal treatments (e.g. stress relief)?

Motivating / Target Case Study for the Program

- AM of a turbine blade with coarse grains in the air foil and fine grains at the root
- Platform: Laser Powder Bed Fusion
- Material: IN718, Ni-superalloy



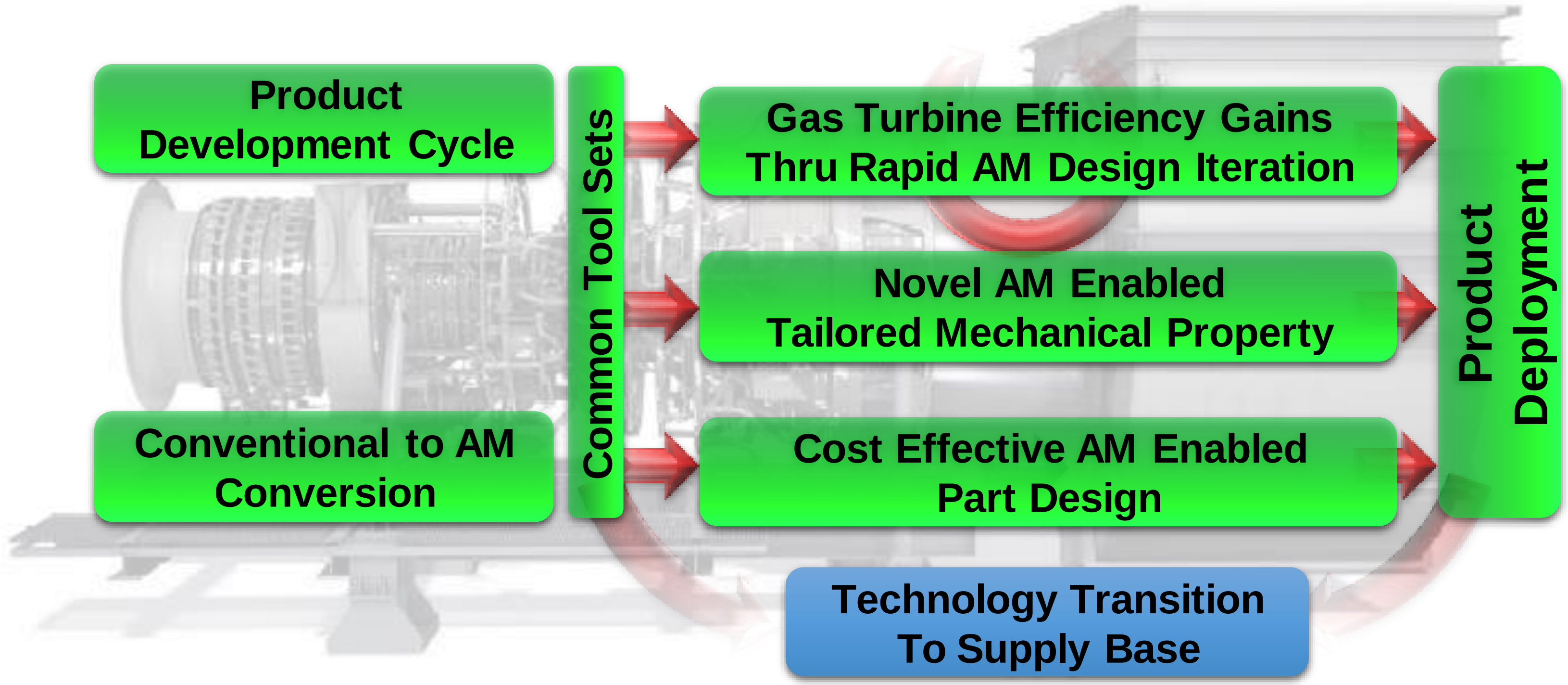
Experiences hottest temperatures; creep limited

Fatigue limited

Fossil Energy Impact

Revolutionize hardware via additive manufacturing (AM)

- Process efficiency gains through new component design can be gained by rapid concept iteration as casting development cycle times are erased.
- Enhanced part lifetime/performance through AM enabled spatially varying microstructures.
- Upend part replacement supply chains with new processing developments impacting a large existing base including F-Class turbines.
- AM applicable to all Industrial Gas Turbines as well as derivative power generation systems such as aerospace turbines.



Project Outline & Status

Key Tasks & Progress

A. Models to link AM Process Parameters to As-Deposited Microstructure ☑

B. Initial to Final Microstructure Evolution Correlation (Post Processing Effects) ☑

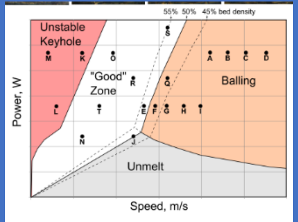
C. Microstructure-Properties-Performance Model *In Progress*

D. Demonstration of Spatially Varied Microstructure Via AM ☑

Update: Link AM Parameters to Microstructure

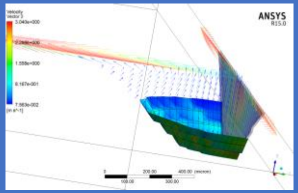
Microstructure influenced by thermal history of the melt pool

Process Parameters → Defect Map → CFD Model → Phase Field Model → G-R Space



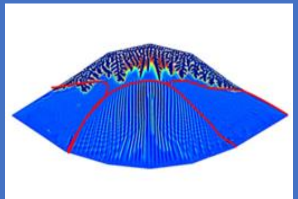
Defect Map

Defect free region



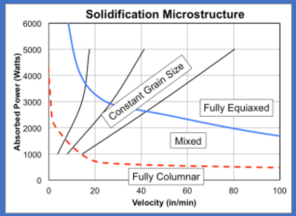
CFD Model

Melt pool size, G, V



Phase Field Model

Dendrite spacing, transition



G-R Space

Model driven process map

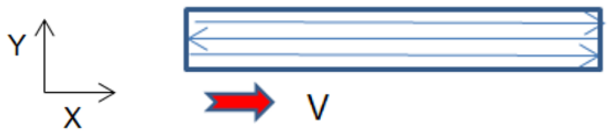
Approaches to control melt pool solidification

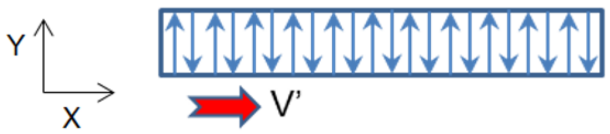
1. Increase layer thickness → requires sufficient laser power
2. Laser scan path → need control over scan strategy

RTRC's COTS powder bed systems are too limited in laser power to take advantage of Approach 1 so focus was placed on manipulating laser scan vectors.

Update: Link AM Parameters to Microstructure

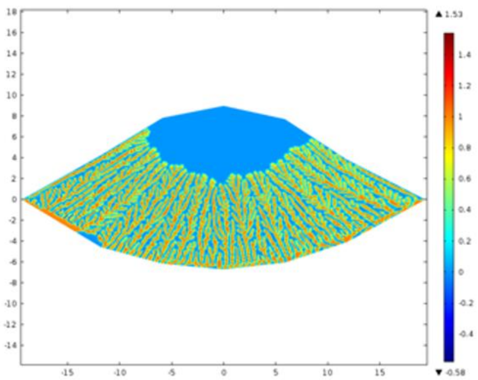
Use an "Active Melt Pool" scan whereby the melt pool is active for longer time thus lowering cooling rate & making a flatter pool to promote a 2D microstructure for larger columnar grains

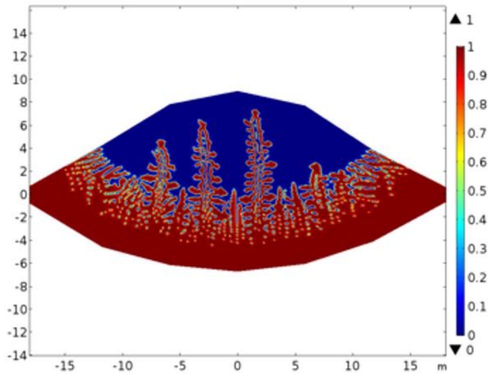


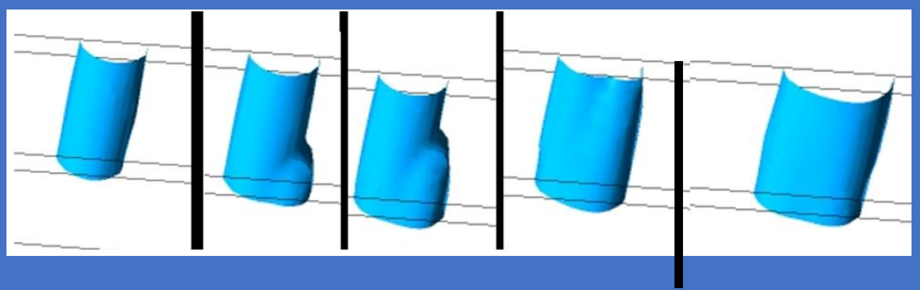


Standard or default scan strategy

Active melt pool scan strategy







CFD simulation of active melt pool shows that this scan strategy results in a wide and flat melt pool

Phase field simulations indicate active melt pool results in larger dendrites

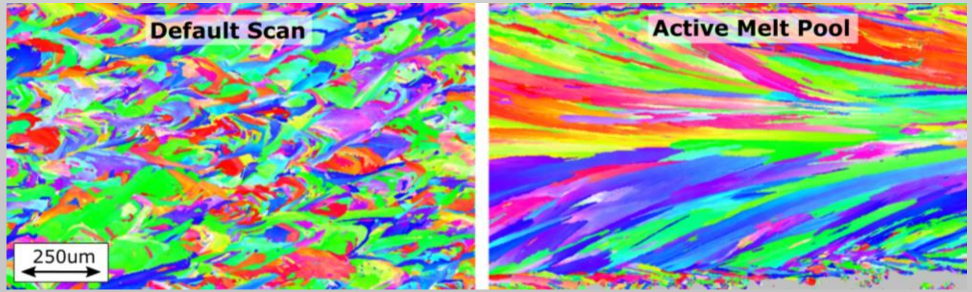
Update: Link AM Parameters to Microstructure

NATIONAL ENERGY TECHNOLOGY LABORATORY

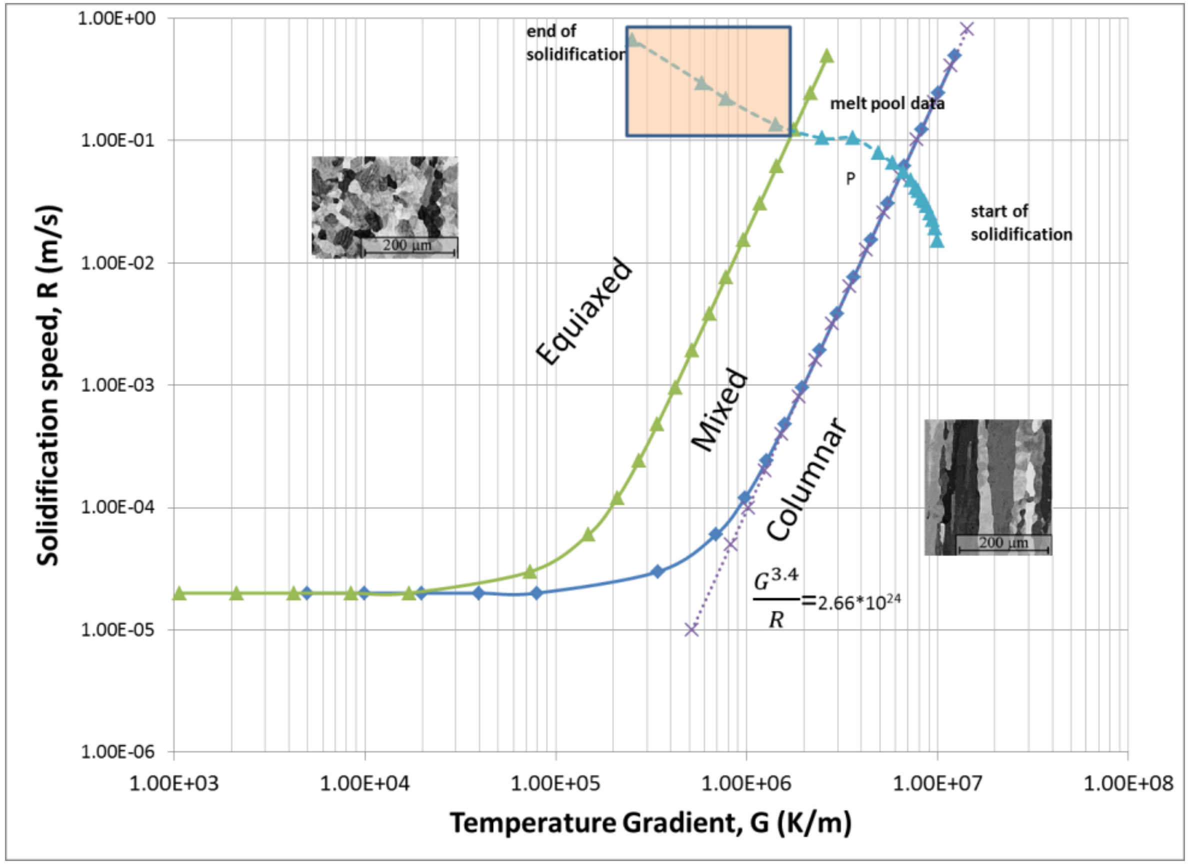
Active melt pool technique experimentally validated to result in larger, more columnar like, grains

CFD simulation provides thermal gradient G, & solidification speed (R) that can be plotted on a microstructure solidification map.

Validation



EBSD scans of IN718 additive coupons made with default and active melt pool scan strategy

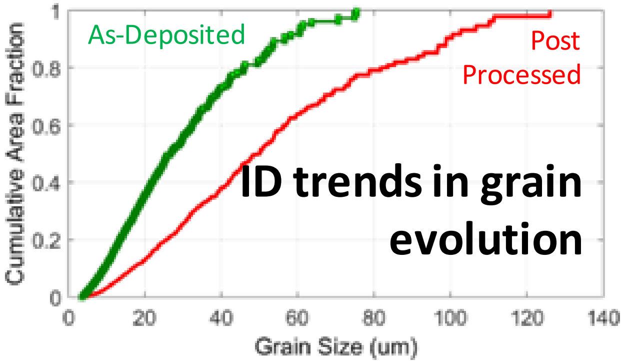


Active melt pool solidification primarily in the columnar zone. The top of the melt pool (orange zone) may be equiaxed but this is erased when the next layer during AM is processed.

Update: Microstructure Evolution Trends

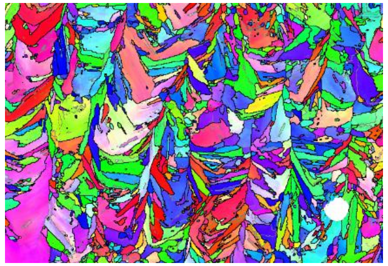
Insights for Microstructural Evolution

While custom heat treatments could be employed to influence grain structure evolution, this work follows industry standard post-processing thermal treatments.



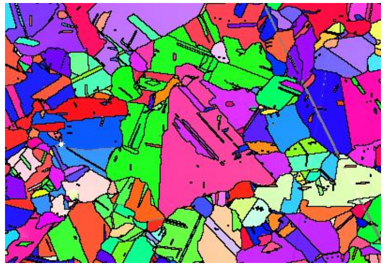
Track trends in the evolution of ***grain size***, ***shape***, and ***orientation distribution*** that are key inputs to the microstructure sensitive performance model.

As-deposited Microstructure → **Post Processing** → **Final Microstructure**



Quantify grain size with EBSD

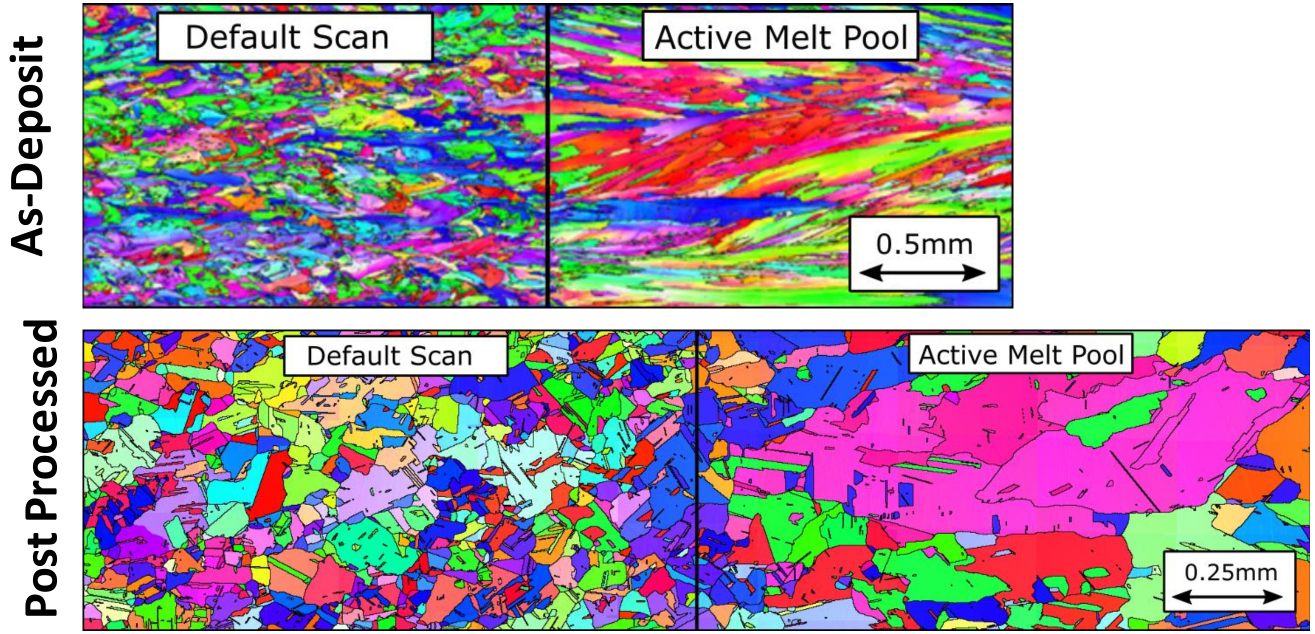
- Stress Relief (*ASTM F3055)*
- HIP (*ASTM F3055)*
- Solution + Age (AMS 5663M)

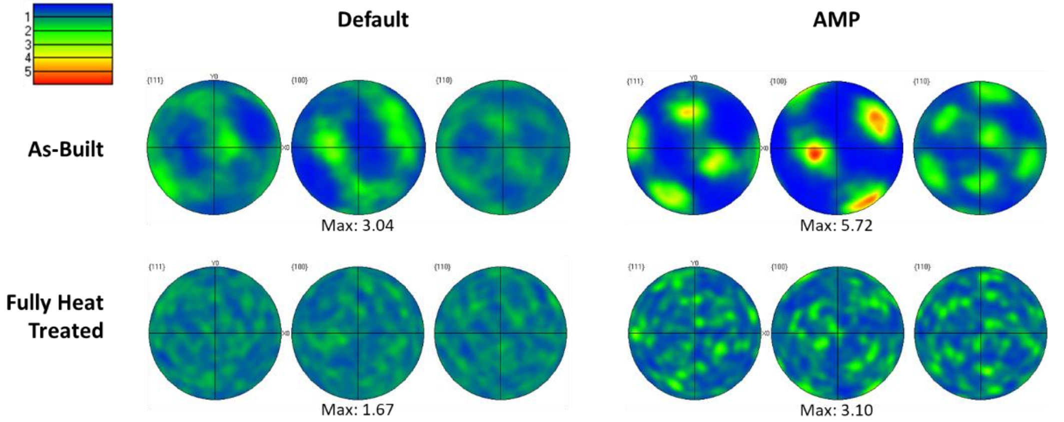


Quantify final grain size with EBSD

Update: Microstructure Evolution Trends

Larger grains from active melt pool approach retained through post processing.





Overall, texture is random for both default & active melt pool (AMP) deposits in post processed state

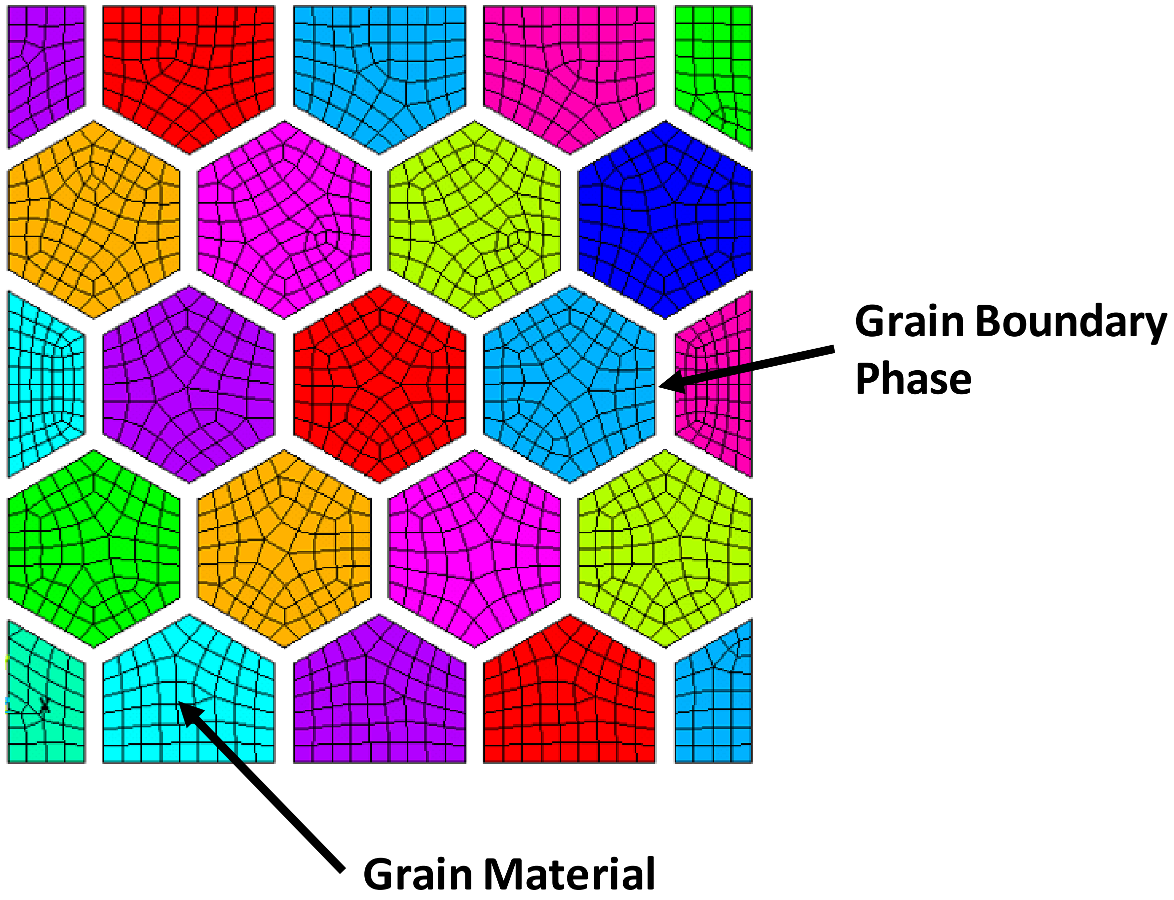
Scan Strategy	Grain Size (μm)		Trends
	As-deposit	Post Processed	
Default	27	70	~2.5X increase in grain size, more equi-axed
Active Melt Pool	44	365	~8X increase in grain size, elongated grains

Update: Microstructure Performance Models

Grain-scale simulations to predict global creep behavior governed by bulk grain & grain boundary mechanisms

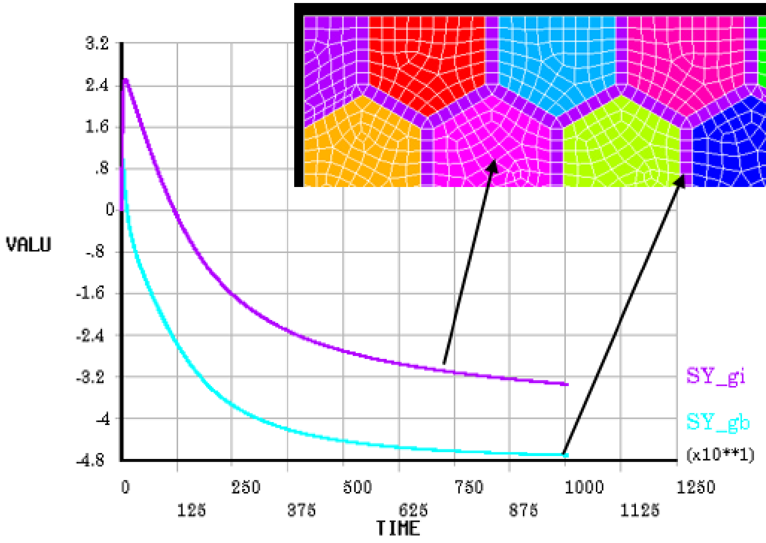
- Additive IN718 modeled as a connected 2 phase system
    1. Grain Material modeled with crystal plasticity
    2. Grain Boundary Phase modeled by Norton's Law

- Microstructure sensitivity → smaller grains means more grain boundary phase influence in the material response.

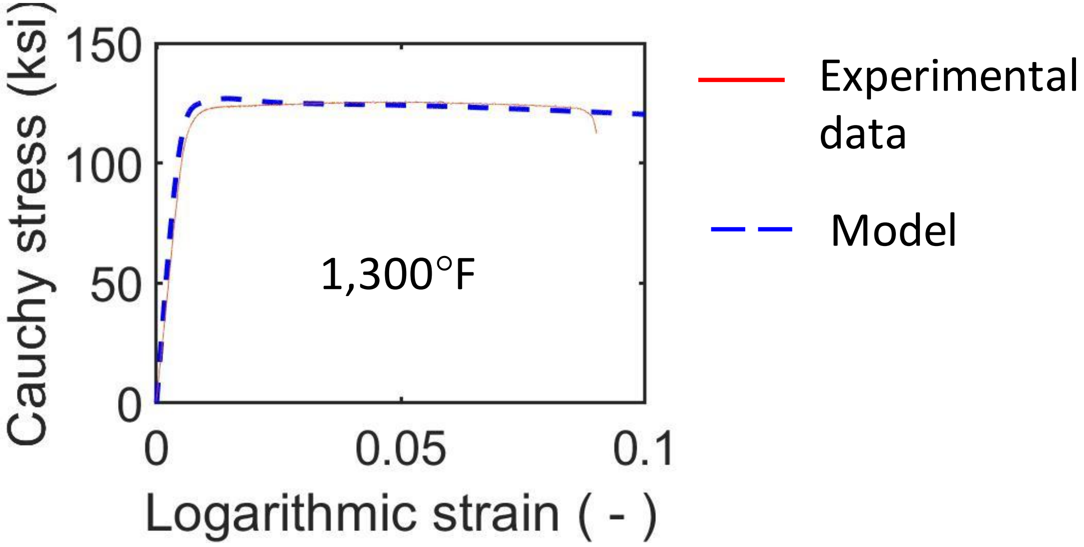


Work In Progress

- Model is de-bugged and operational with surrogate material calibration factors



- Model calibrated for time independent quasi-static tensile/compressive behavior



- Collection of time-dependent creep data for additively manufactured coarse grain and fine grain deposits are in progress & required for model calibration to predict creep performance.

Update: Spatially Varied Microstructure Demo

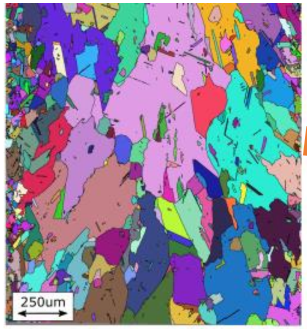
Successfully printed a turbine blade surrogate with coarse grains in the air foil (creep resistance) and fine grains at the root (fatigue resistance)

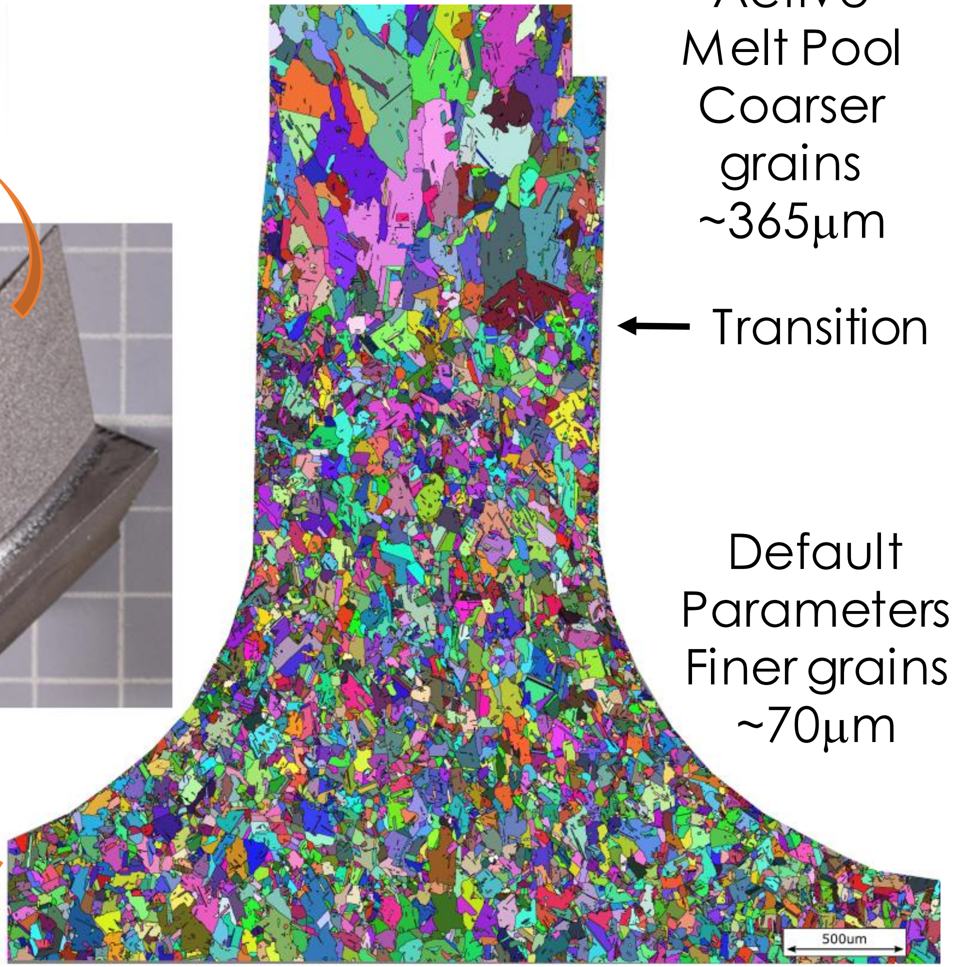
Strategy

- Print blade using powder bed system with "default" parameters in the root & active melt pool scan strategy for the airfoil.

Key Accomplishments

- Retention of spatially tailored microstructure after full post processing (Stress relief → HIP → Solution → Age thermal treatments).
- No egregious defects such as cracks, pores, etc.

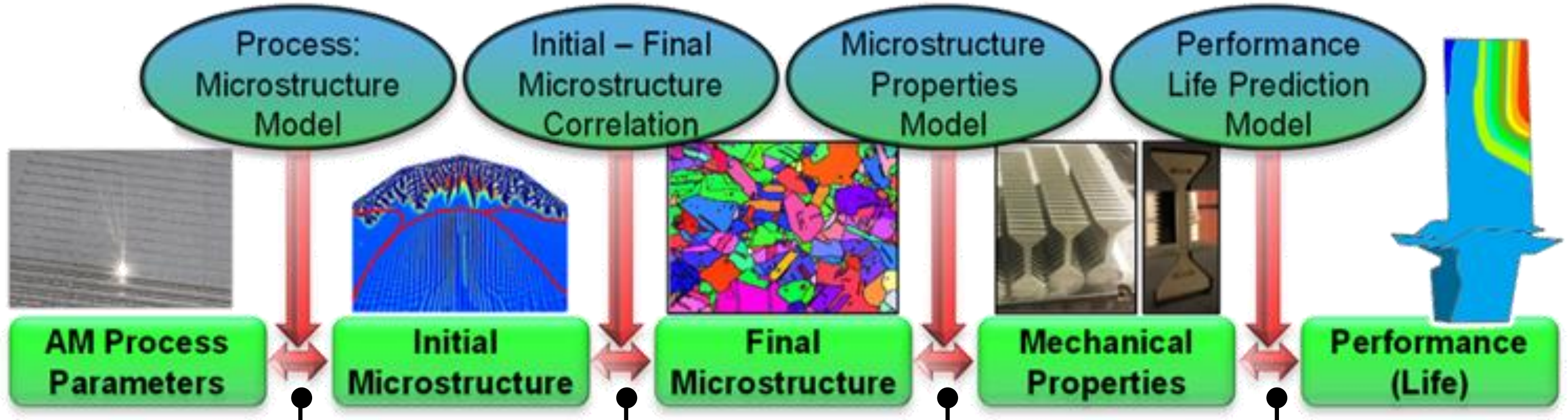




EBSD scan with random color assigned to individual grains

Preparing for Next Steps

Assembling the Full Framework Connecting Process-Structure-Properties-Performance



AM Process Parameters	Initial Microstructure	Mechanical Properties	Performance (Life)
Modeling Tool ANSYS, COMSOL, MATLAB	Correlation Empirical relation established using EBSD analysis.	Modeling Tool Crystal Plasticity – Standalone (Fortran)	Modeling Tool Crystal Plasticity - FEM (ANSYS)
Input(s) Process Parameter (Laser power, scan speed, hatch spacing, laser spot diameter, layer thickness)	Input(s) As-deposited grain size (area weighted average of equivalent circle diameter)	Input(s) Crystallographic texture Average grain size distribution	Input(s) Crystallographic texture Grain size distribution Mechanical properties Part geometry & loads
Output(s) Thermal Gradient, Solidification speed, Dendrite structure	Output(s) Post heat treat average grain size, crystallographic texture	Output(s) ODF crystallographic texture Creep behavior Crystal & grain boundary mechanical properties	Output(s) Location-specific creep rates

- Implementation with software packages common to industry

Directions Beyond the Program

Coordinate with AM platform providers to offer systems with features to enable more microstructural control

Methods to connect across the different models in the tool chain

Concluding Remarks

Summary

- Employed modeling to understand the impact of AM process parameters on the as-deposited microstructure → results in the ability to influence material properties & performance in 3D printed parts by intentionally adjusting scan vectors, laser power, speed, etc.
- Confirmation that spatially varied microstructure can be retained with post processing.
- Employed lessons learned to demonstrate AM of a turbine blade with spatially varying microstructure having coarse grains in the air foil for creep resistance and finer grains at the root for fatigue resistance.

Next Steps

- Finalize the microstructure sensitive property model for prediction of creep performance. Awaiting the collection of long duration (500+ hr) creep data for coarse and fine grain AM Ni-superalloy to use for model calibration.
- Complete program with documentation of all technical progress.

Acknowledgements

- This material is based upon work supported by the Department of Energy under Award Number DE-FE0031642.