# Computational Tools for Additive Manufacture of Tailored Microstructure & Properties

*High Performance Materials - Crosscutting Research and Advanced Energy Systems Project Review Meeting*

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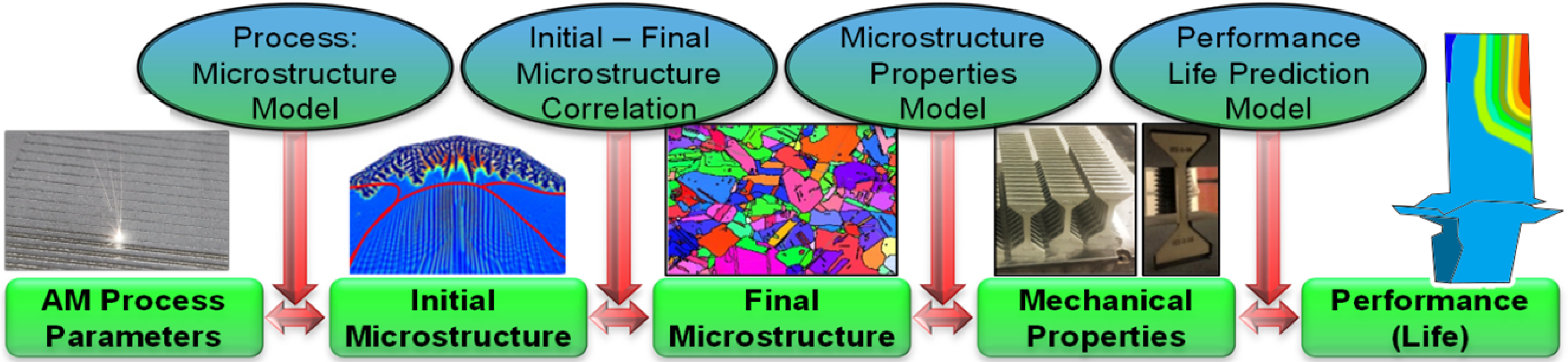
# Background & Introduction

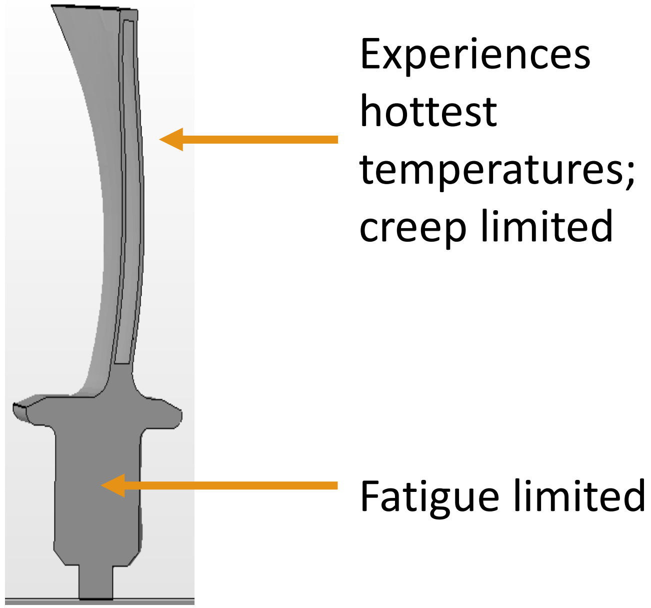
Purpose: *Establish computational tools to link AM parameters to material properties to enable parts with spatially varying microstructure for enhanced performance*

- **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



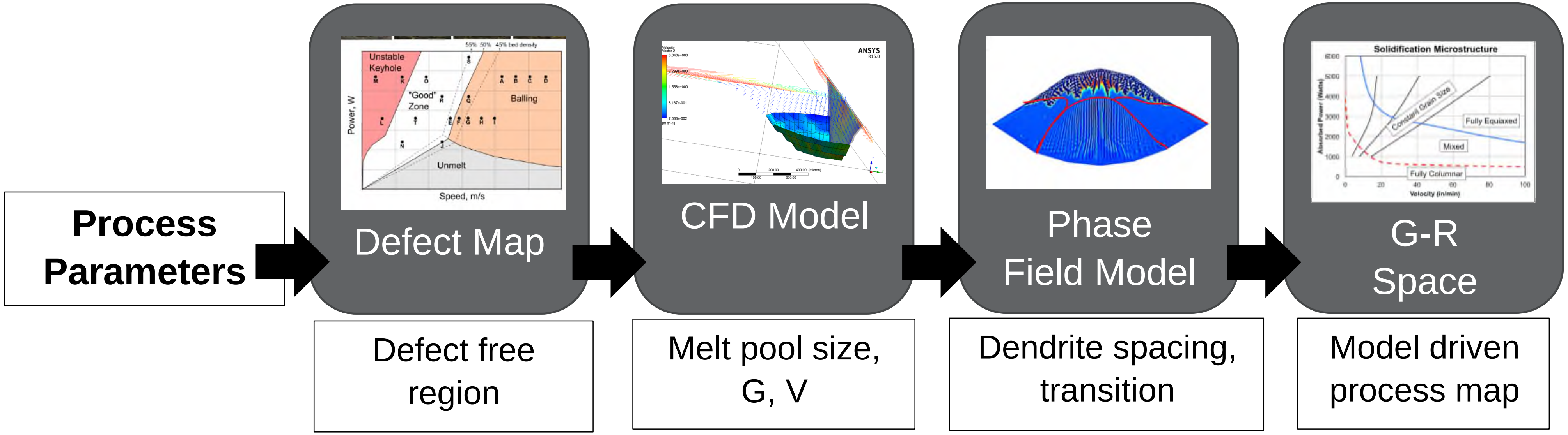
# Motivating / Target Case Study for the Program

- AM of a turbine blade with coarse grains in the airfoil and fine grains at the root
- Platform: standard off-the-shelf laser powder bed system
- Material: IN718, Ni-superalloy



# Linking AM Parameters to Microstructure

***Microstructure influenced by thermal history of the melt pool***




Approaches to control melt pool solidification

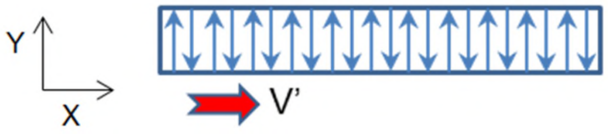
1. Increase layer thickness → requires sufficient laser power
2. Laser scan path → need control over scan strategy

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.

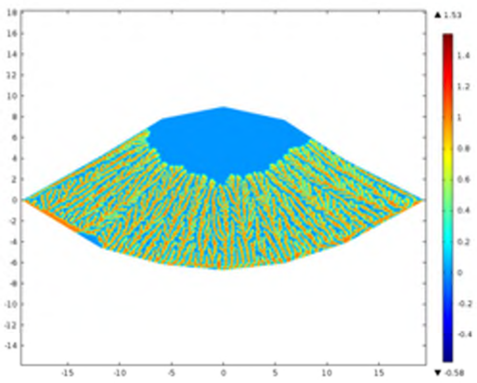
# Linking AM Parameters to Microstructure

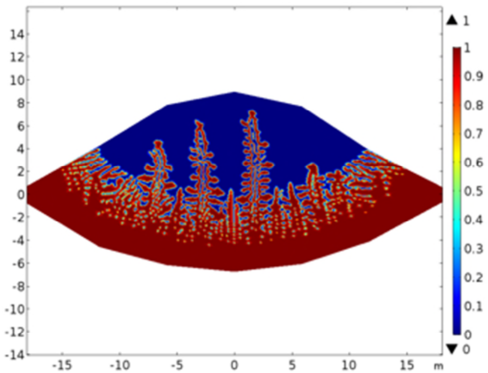
***Use an "Active Melt Pool" scan whereby the melt pool is active for longer time thus lowering cooling rate & making a flatter pool to promote a 2D microstructure for larger columnar grains***

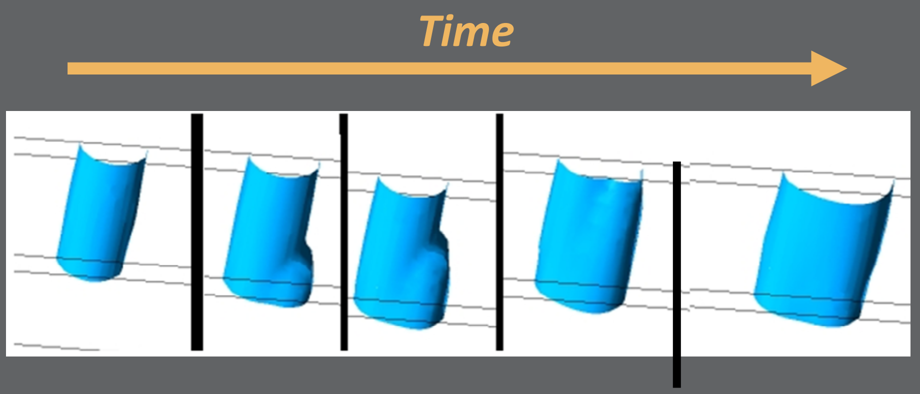

**Standard or default scan strategy**




**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

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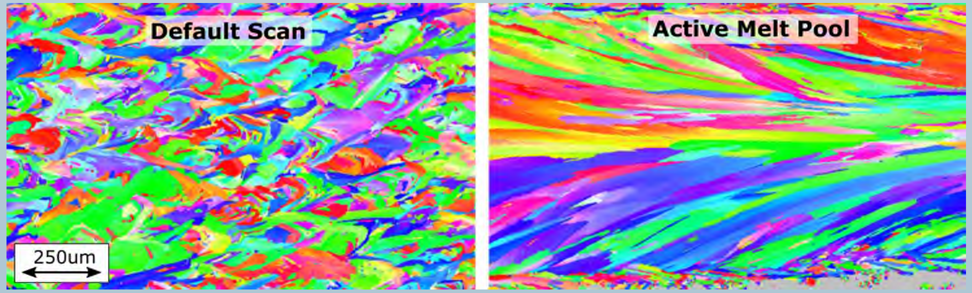
# Linking AM Parameters to Microstructure

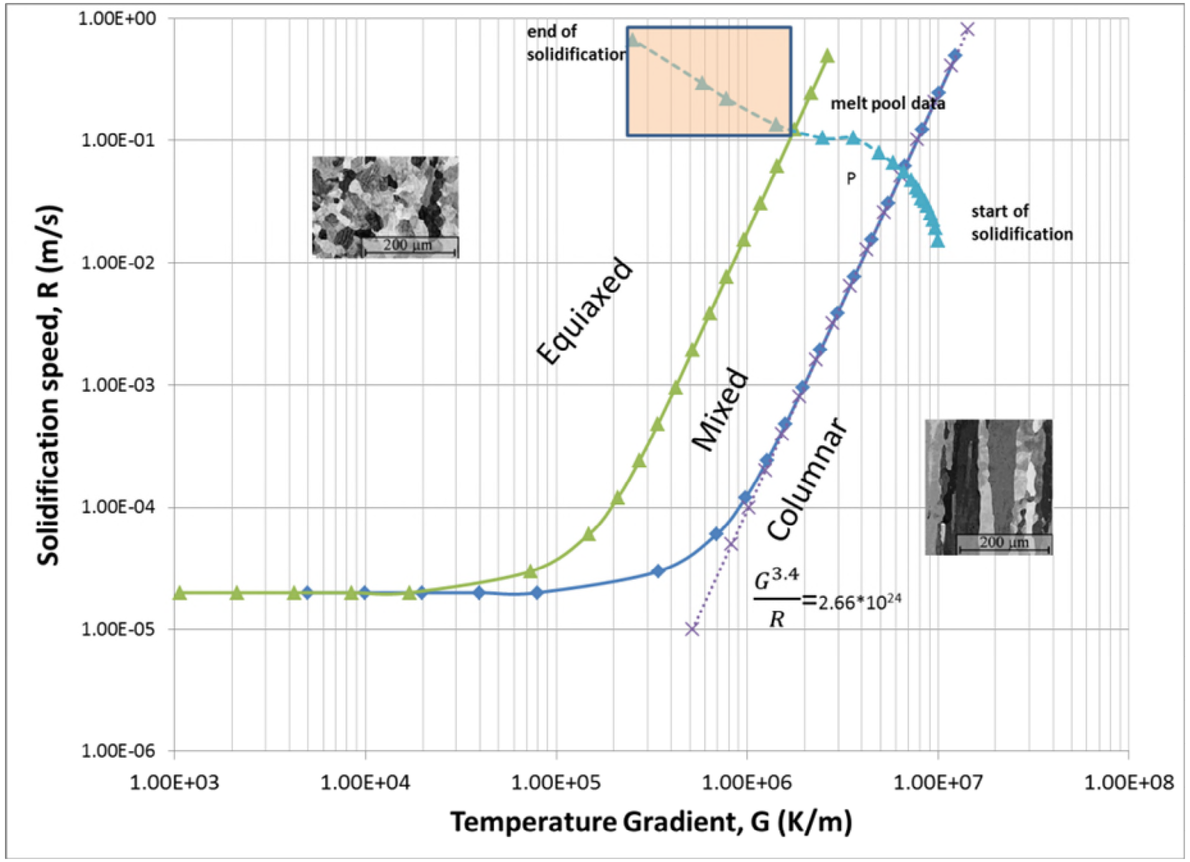
Active melt pool technique experimentally validated to result in larger, more columnar like, grains

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.

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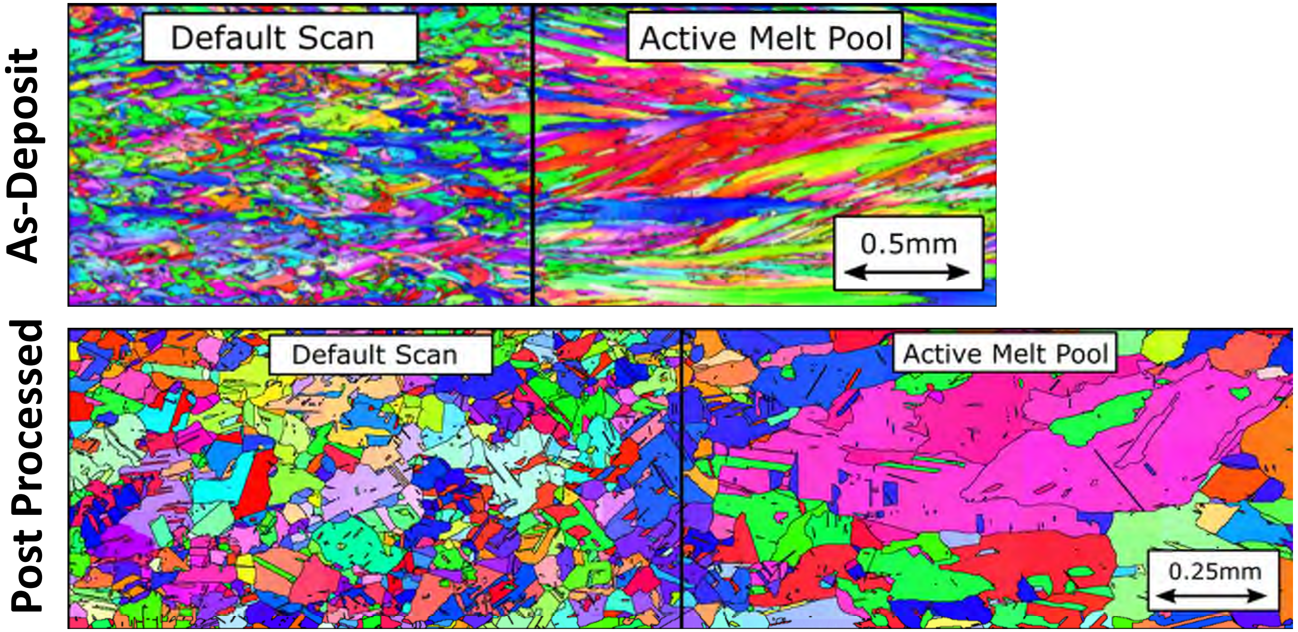
# Microstructure Evolution Trends

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




- Follow industry standard post-processing thermal treatments
  - Stress Relief (*ASTM F3055)*
  - HIP (*ASTM F3055)*
  - Solution + Age  (AMS 5663M)

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

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# Spatially Varied Microstructure Demo

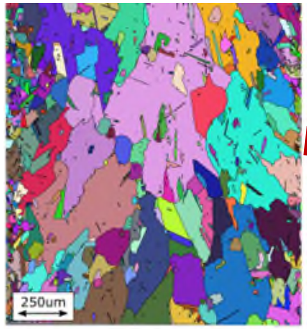
**Successfully printed a turbine blade surrogate with coarse grains in the air foil (creep resistance) and fine grains at the root (fatigue resistance)**

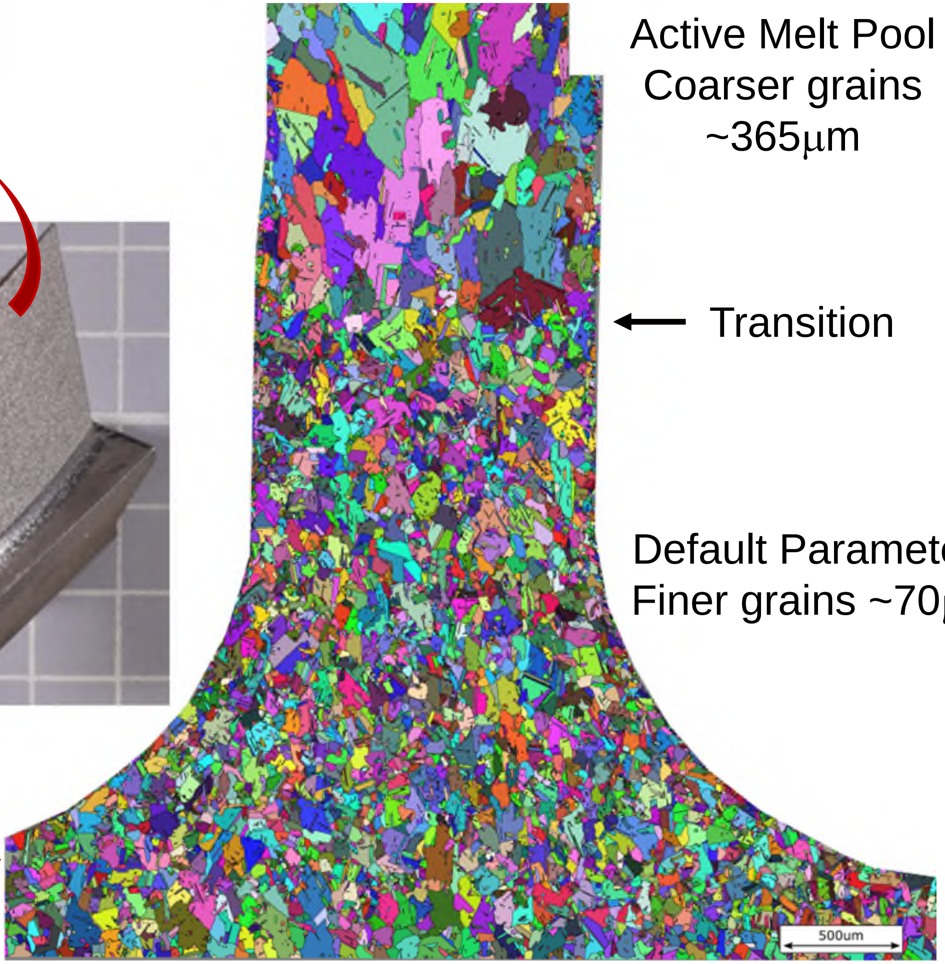
### Strategy

- 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
- No abnormal defects




*EBSD scan with random color assigned to individual grains*

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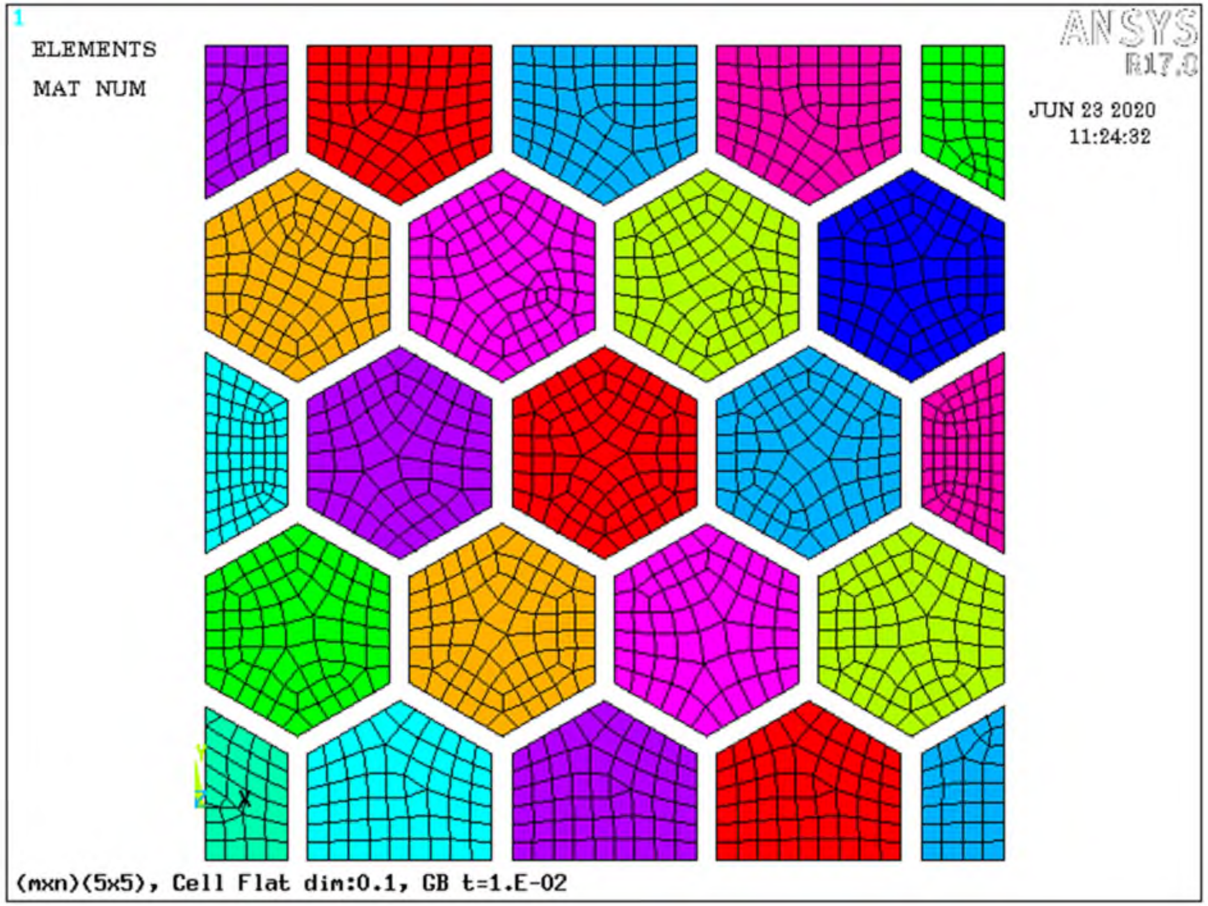
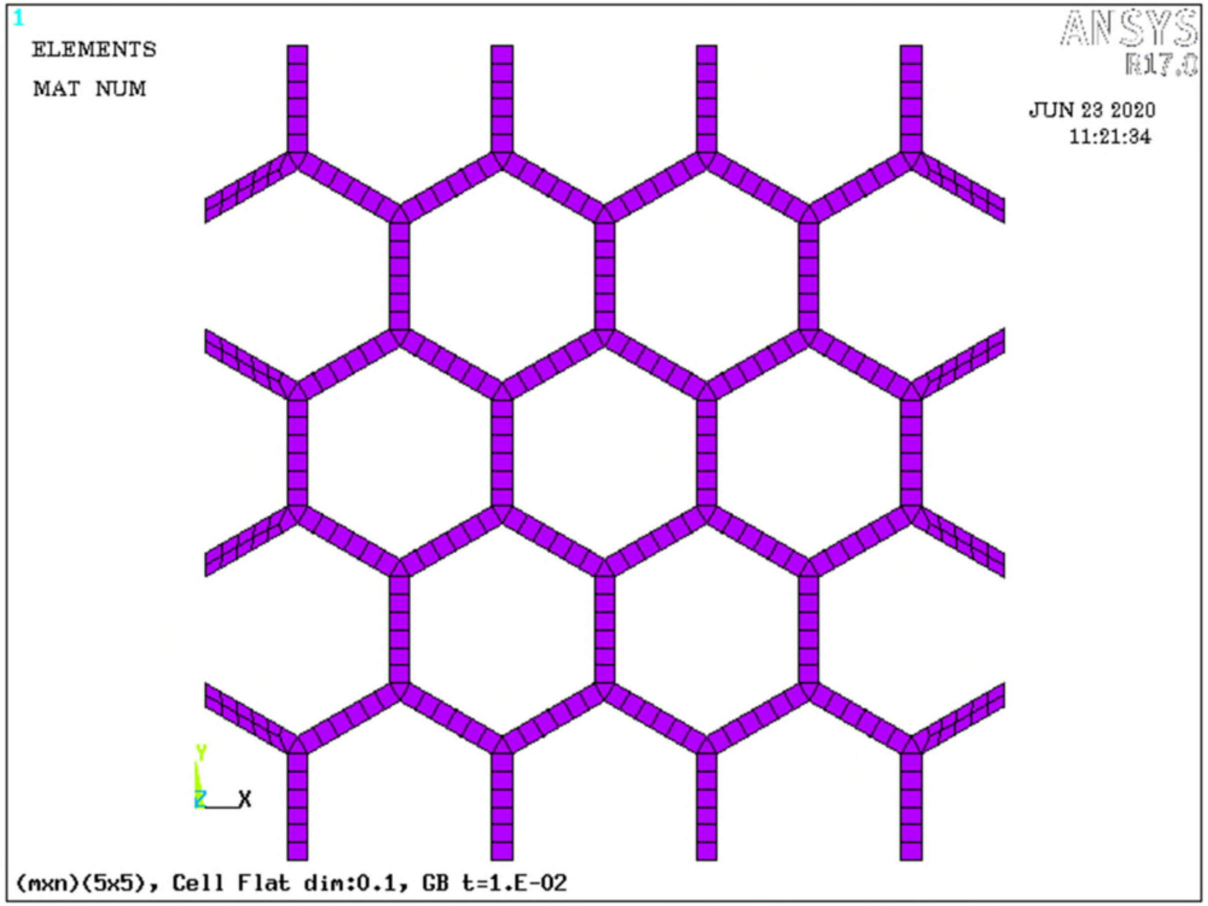
# Property model: Capturing Microstructure Effects

- Grain interior modeled using crystal plasticity code, grain boundary modeled through Norton law, both are linked together
- Porosity evolution captured using Rice and Needleman's model*




*Needleman, A., V. Tvergaard, and J. W. Hutchinson. 1992. 145-178.

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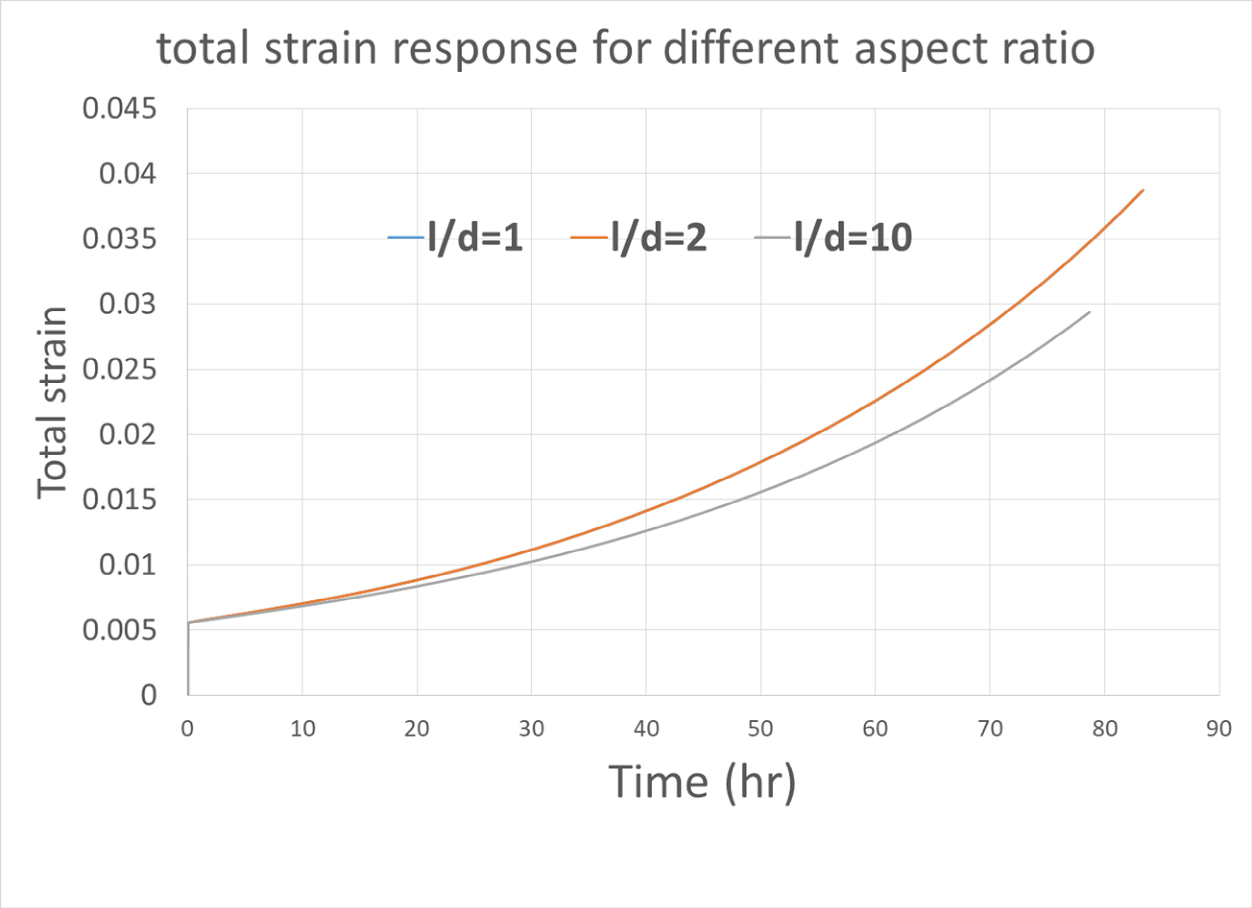
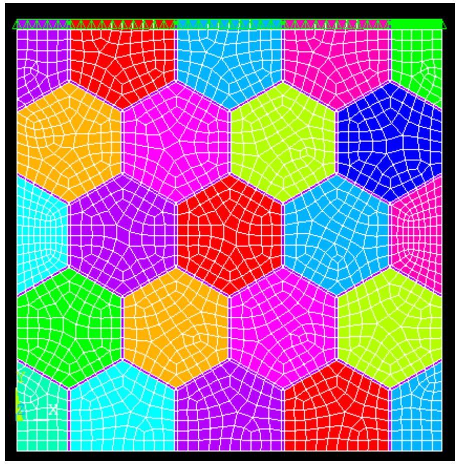
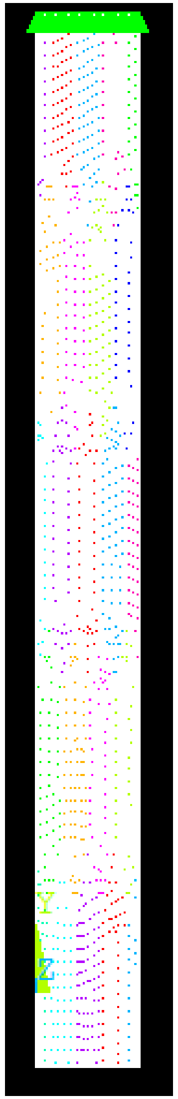
# Effect of Aspect Ratio on Creep

- Three sets of simulations were run with aspect ratio (l/d) at 1, 2 and 10.
- All simulations used random texture and a load of 600 MPa and at 650°C.
- Result indicates lower creep strain for higher aspect ratios, however they are not drastically different (which indicates the role of grain boundaries)



l/d=1
(equiaxed)



l/d=10
(columnar)



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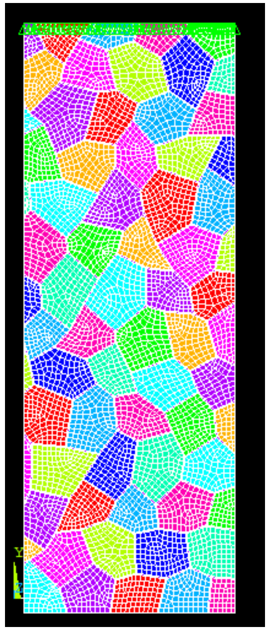
# Calibrating Creep Response with Literature Data

- The data shows near identical creep strain rate for equiaxed and columnar grains
- Columnar grains survived much longer compared to equiaxed grains
- The failures were associated with crack and void propagation in grain boundary region.
- The next set of simulations targeted simulating these conditions for random and directional texture as obtained from the publication.

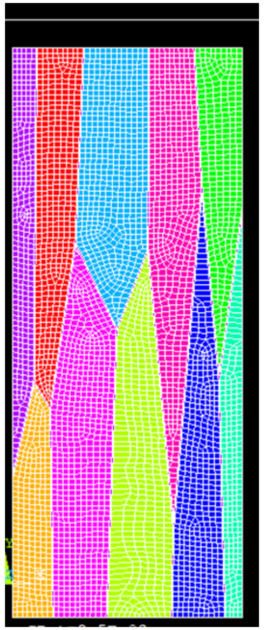
***E-beam additive IN718, post processed tested at 650°C and 600MPa***

| Condition | Min Creep Rate, $h^{-1}$ | Time to Rupture, h |
|---|---|---|
| Columnar Longitudinal | 1.1 E-06 | 4834 |
| Equiaxed Longitudinal | 1.9 E-06 | 922 |
| Columnar Transverse | 4.4 E-06 | 2736 |
| Equiaxed Transverse | 2.8 E-06 | 620 |

Shassere, Benjamin, et al. *Met Trans A* 49.10 (2018): 5107-5117.



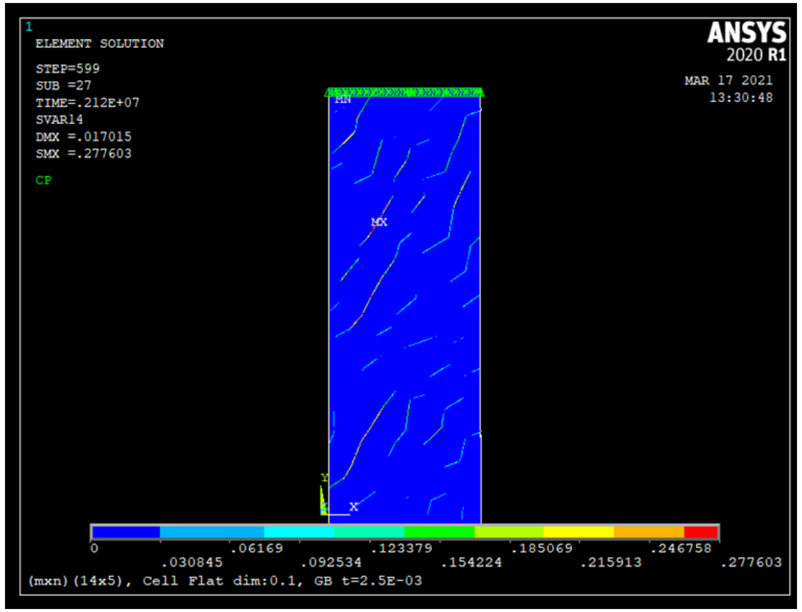
Equiaxed microstructure



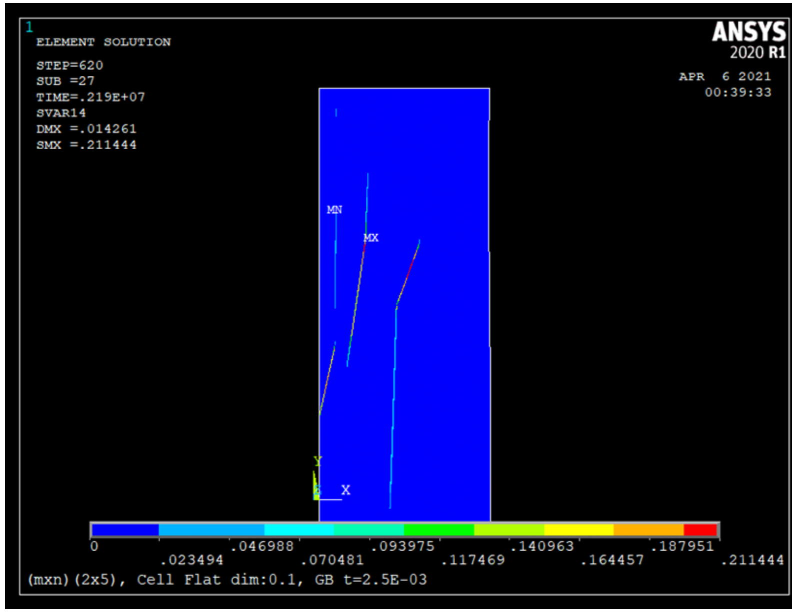
Columnar microstructure

# Comparison of void fraction at ~600 hours

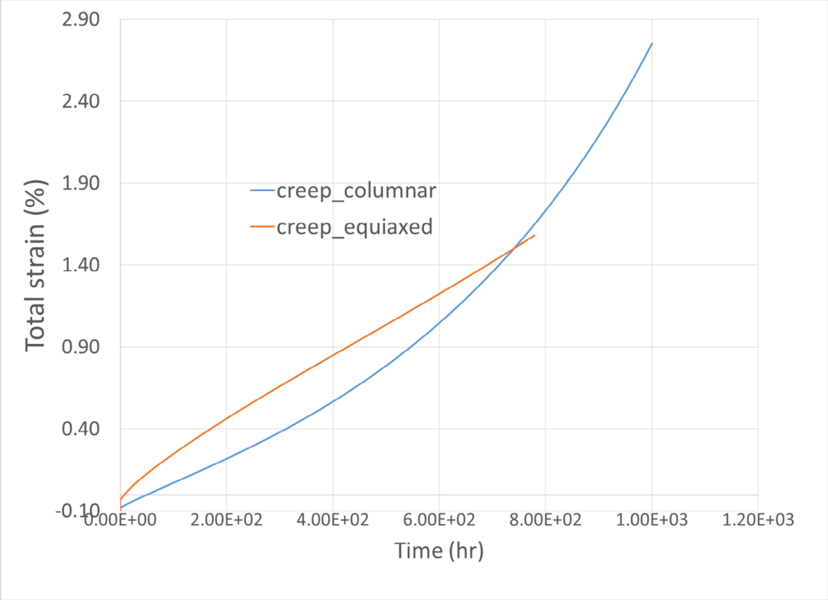
- Creep simulation at 1200F and at 600MPa showed lower void fraction for columnar grains with more directional texture
- The columnar grains survived 1000 hours of creep loading




Equiaxed grains at 589 hours




Columnar grains at 608 hours




Comparison of total strain results

- A critical volume fraction of 0.25-0.30 can be used to predict failure. Every third grid point indicates presence of void in grain boundary, thus having a very large chance of crack propagation.

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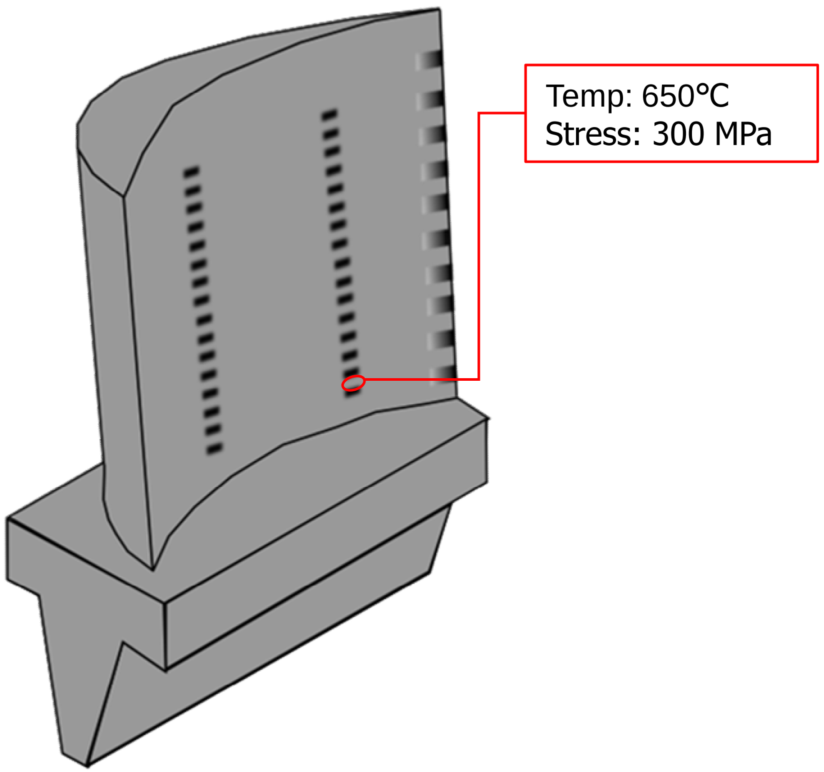
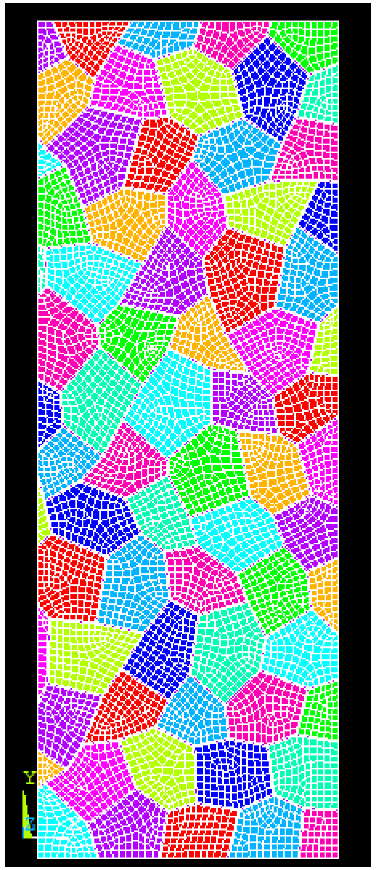
# Demo blade simulation

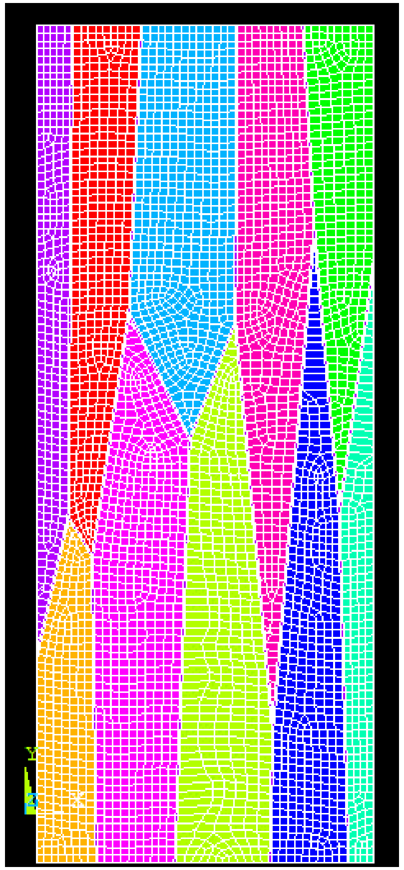
- Condition for creep simulation identified from literature as 650°C at 300 MPa
- Creep simulation for 50,000 hrs is carried out for representative equiaxed and columnar microstructure




Alstom GT13E2 turbine blade analyzed by Aminov et al.; *Optimal gas turbine inlet temperature for cyclic operation*; IOP Conf. Series: Journal of Physics: Conf. Series 1111 (2018)



Equiaxed microstructure



Columnar microstructure

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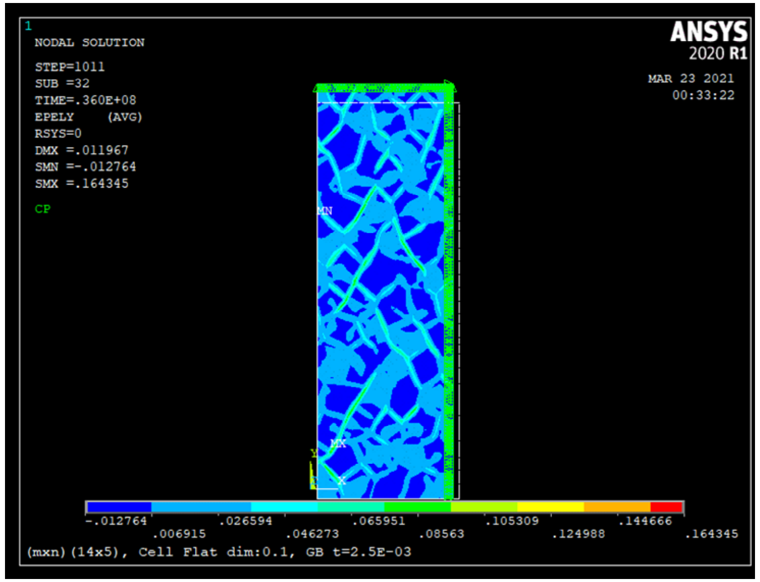
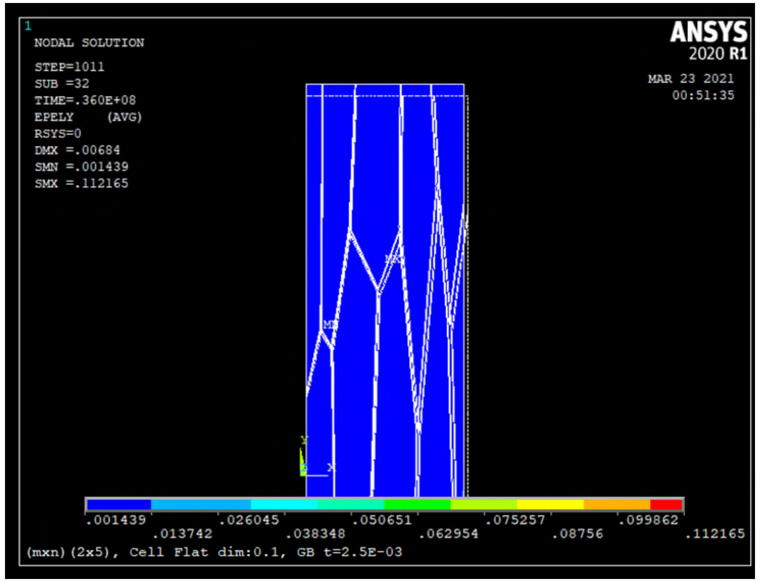
# Comparison of Columnar & Equiaxed Microstructure: Creep Response

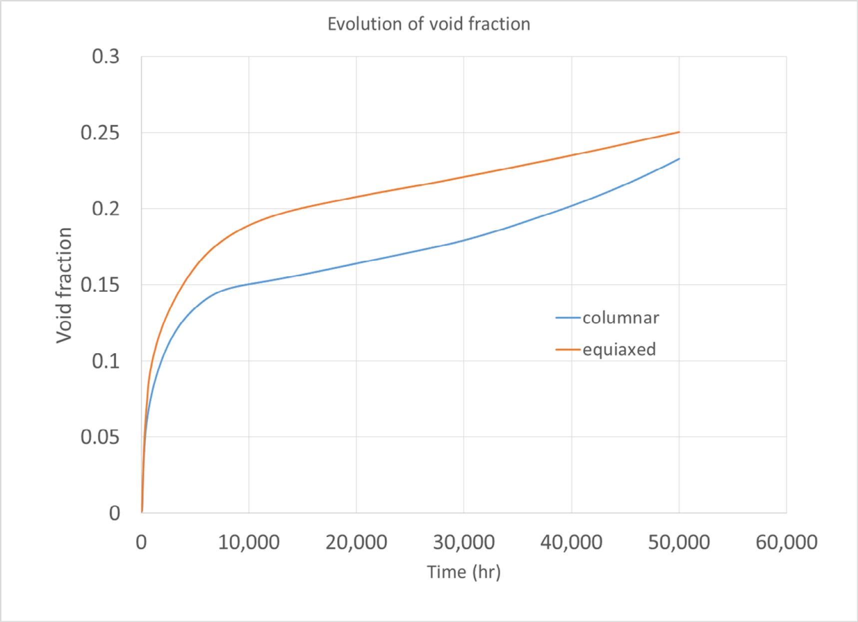
- Grain boundary is highly strained
- Strain is higher in grain interior for equiaxed microstructure as compared to columnar microstructure
- Void fraction is higher for equiaxed microstructure and close to critical void fraction value after 50,000 hours




Equiaxed microstructure



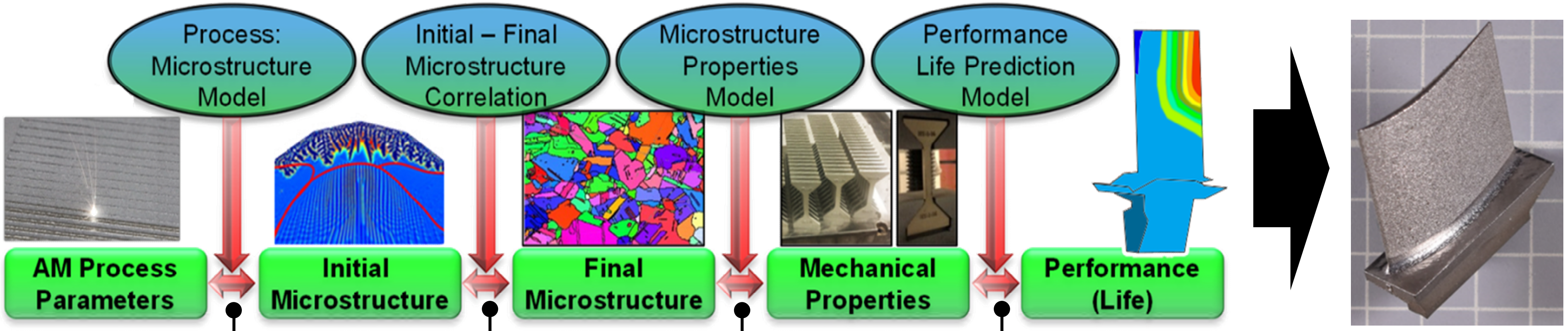

Columnar microstructure




Void fraction evolution

# Assembled Framework

***Connecting Process-Structure-Properties-Performance***




**Modeling Tool / AM Process Parameters**

<u>Modeling Tool</u>
ANSYS, COMSOL, MATLAB

<u>Input(s)</u>
Process Parameter (Laser power, scan speed, hatch spacing, laser spot diameter, layer thickness)

<u>Output(s)</u>
Thermal Gradient, Solidification speed, Dendrite structure

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<u>Correlation</u>
Empirical relation established using EBSD analysis.

<u>Input(s)</u>
As-deposited grain size (area weighted average of equivalent circle diameter)

<u>Output(s)</u>
Post heat treat average grain size, crystallographic texture

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<u>Modeling Tool</u>
Crystal Plasticity – Standalone (Fortran)

<u>Input(s)</u>
Crystallographic texture
Average grain size distribution

<u>Output(s)</u>
ODF crystallographic texture
Creep behavior
Crystal & grain boundary mechanical properties

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<u>Modeling Tool</u>
Crystal Plasticity - FEM (ANSYS)

<u>Input(s)</u>
Crystallographic texture
Grain size distribution
Mechanical properties
Part specific loads

<u>Output(s)</u>
Microstructure specific creep

# Summary & Conclusions

- Established an initial framework to model material evolution through each step of the additive process creating a link between AM process parameters and the resultant material properties/performance.
- Demonstrated AM of a turbine blade with spatially varying microstructure having coarse grains in the airfoil and finer grains at the root using an off-the-shelf laser powder bed system and standard post-processing treatments.
- Developed a microstructure sensitive creep model for IN718. Creep found to be more sensitive to grain morphology (boundary position relative to loading axis) as opposed to grain size. Understanding what the governing feature is will drive how to adjust the additive process to intentionally manipulate the resultant microstructure.

# Acknowledgements

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