Computational, Analytical Needs in AM

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Questions

(1) Computational methods and approaches for simulating materials processing, properties and performance relationships for materials design using additive manufacturing as well as key process parameter identification and process mechanics.

(2) How to leverage high performance computing spanning scientific discovery to ensembles of engineering solutions?

(3) How to integrate topological design loops with additive manufacturing processes and mechanics within a computational framework?

(4) How can AM benefit from fundamental advances in verification, validation and uncertainty quantification methodologies? (Prelude to In-Situ Monitoring & Diagnostics theme)

(5) What analytical, experimental, and software tools, are needed?

(6) How can these be integrated to impact adoption of AM? (Transition to scalability theme)

(7) What opportunities exist for high performance computing, in order to provide fundamental scientific discovery of the process-properties-performance relationship, relevant to AM?

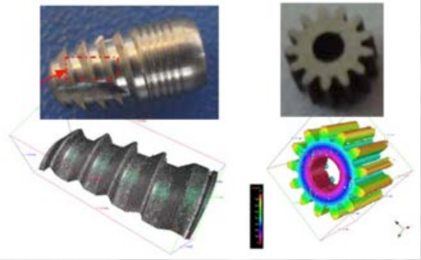
(8) What are those drivers and what fundamental advancements are needed for computational methods and optimization techniques?

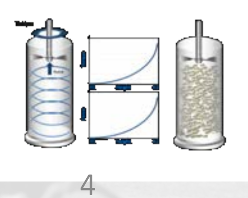
(9) [ADDED] Is there sufficient funding in the US for fundamental research and development (TRL1 through TRL3) for additive manufacturing?

(10) [ADDED] Most US academic institutions house their additive manufacturing programs in mechanical engineering departments, and materials departments remain largely disengaged. How can we better involve our top-tier MS&E students and faculty in additive manufacturing?

CMU NextManufacturing Facility

- Metals
  - **(2) Arcam S12 Electron Beam Metal Machines**, fully upgraded with the multi-beam option
  - **EOS M290 Laser Sintering Metal Machine**, with all available material parameter sets
- Polymers
  - Objet350 Connex Multi-Material 3-D Printer
  - (2) Stratasys Dimension Elite FDM Machines
  - Multiple Cube Pro Maker Machines
- Metrology
  - Freeman Tech Powder Rheometer
  - Infinite Focus G4 with Real 3D Surface Measurement
  - GF Machining Solutions AC Progress VP3 Wire EDM Machine



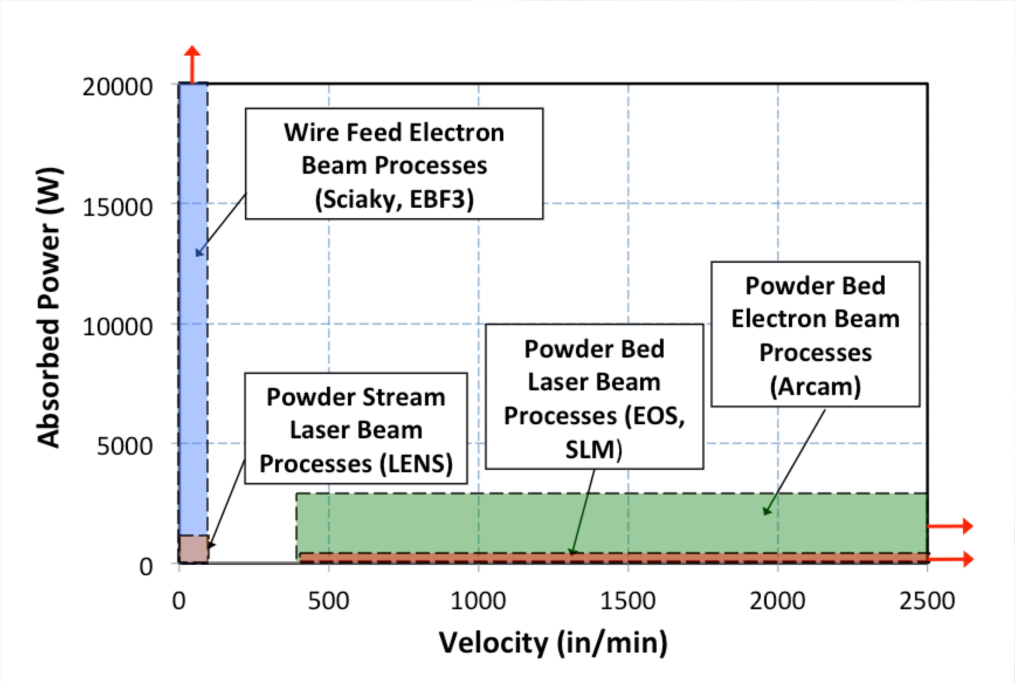


We encourage Industrial Partners to use our equipment on a fee basis; also training on AM equipment

State of the Art for Direct Metal AM

- You can print most 3-D shapes directly out of metals
  - Close to 100% dense, features down to 200 microns
  - Build Volumes Approx. 10”x10”x8”
  - Parts can take 4-8-24 hours (or more) to build
  - AM is for Real: GE fuel nozzle and other AM-fabricated parts are going into commercial jet engines
- Current processes were developed to allow shapes to be built
  - Other process outcomes are important when making components
  - Microstructures differ (strongly) from conventional processing; non-equilibrium
  - High residual stress as-built
  - Quality depends on service conditions
  - Certification is non-trivial

Direct Metal AM Processes in P-V Space



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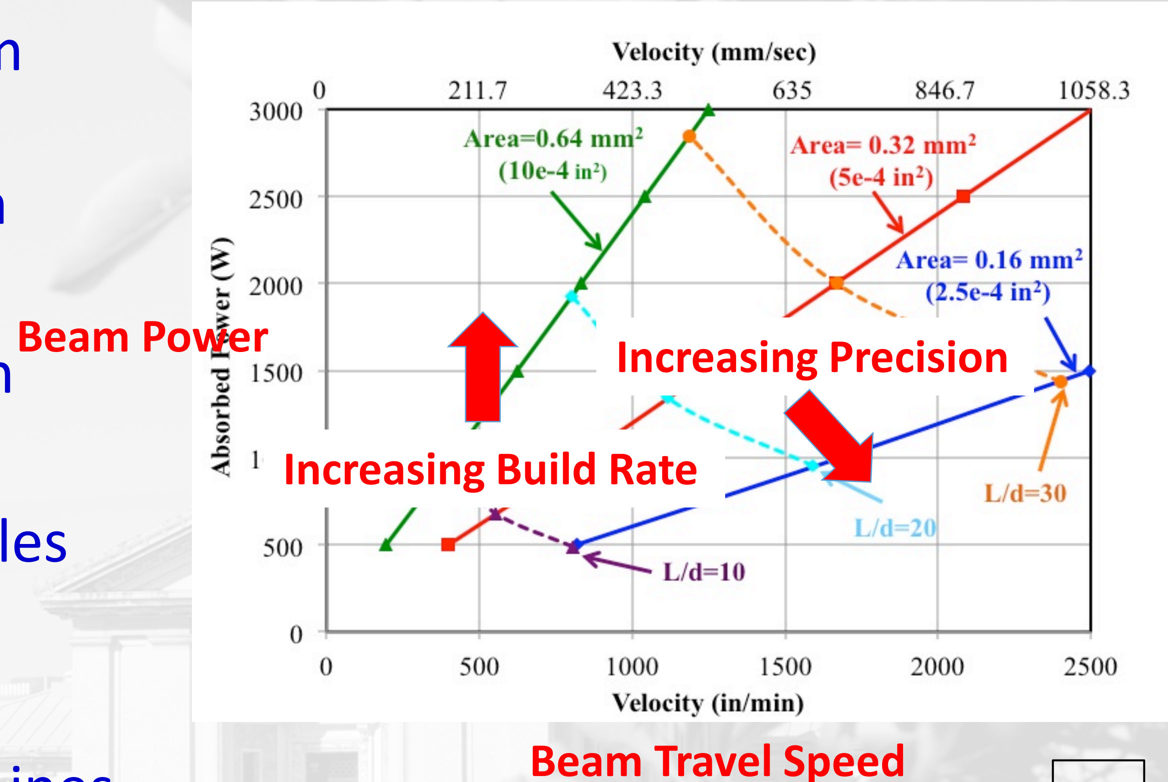
- CMU is mapping all direct metal processes across 6 alloy systems
  - Approach is the same, results are different (mainly because of varying thermal properties) but many results are analogous
  - CMU work can help any direct metal AM machine user get the most out of their substantial investment in machine, maintenance, tech support, etc.

Process Map Impact on Early Decision-Making for Adopting AM

- Almost all manufacturers who use (or make) metals are now looking closely at direct metal AM
  - How to identify components as good or bad for AM (need to map part specifications to AM process technical capabilities)
  - Complication: AM benefits come from re-design specifically for AM
- Time to get up to speed
  - 6-12 months is typical
- Manipulating or changing the process
  - Quantitative predictions are important, but just knowing which direction to move in processing space is a huge benefit
- **Physically-based process modeling can impact all of these**

Build Rate vs. Precision

- Beam Power vs. Beam Travel Speed Map for Arcam Electron Beam Process
- Build Rate Scales with Power
- Process Precision Scales with Melt Pool Size (Straight Lines)
- Can Stay on Straight Lines while Increasing Power to Maintain Precision and Increase Build Rate



- Adding information about melt pool geometry in relation to successive tracks can, e.g., define risk of incomplete melting

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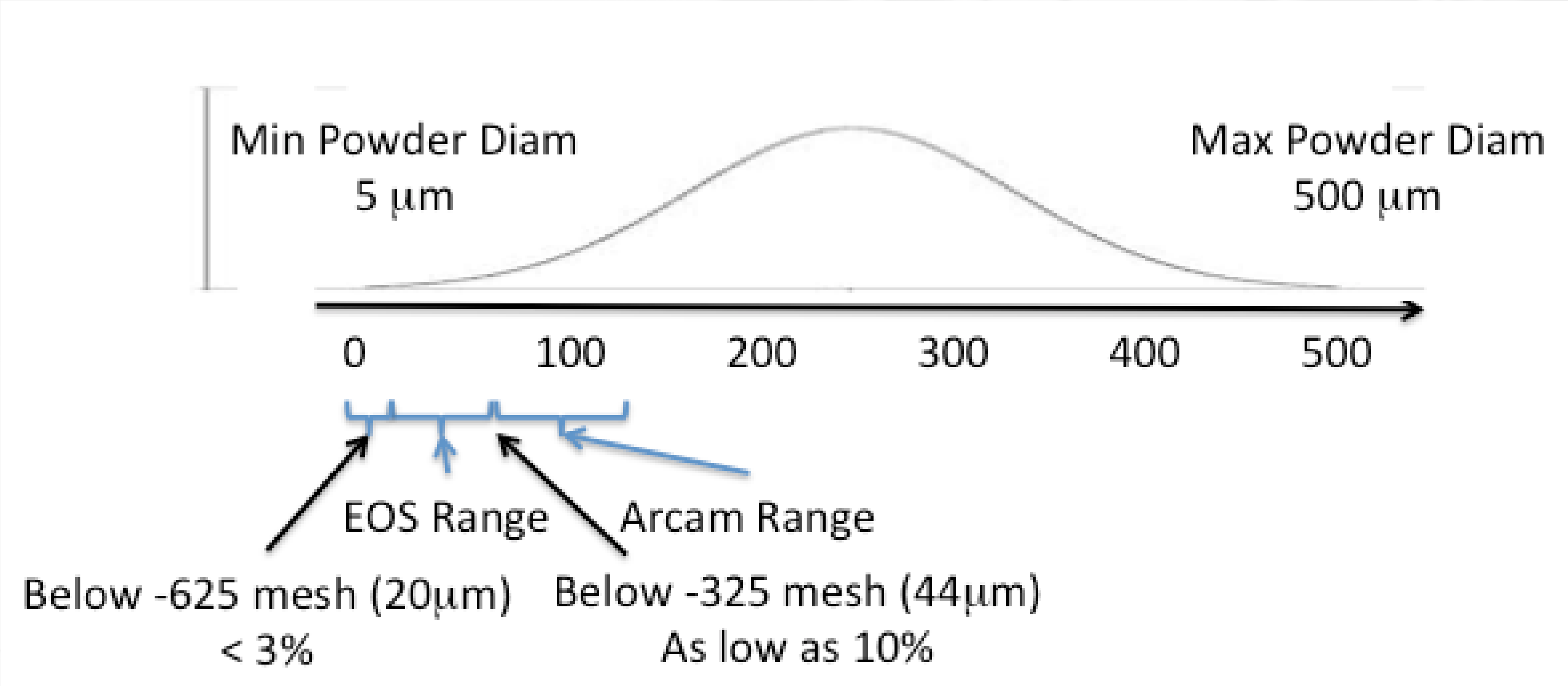
AM Powders



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- Only use a fraction of the powder produced: **need better understanding of fluid flow to optimize production of small powders**
- Ti-6-4 Powder Costs: Arcam: $255/kg EOS: $617/kg
- Unused powder may be recycled <u>or scrapped</u> – problem with Oxygen content
- Powder particles commonly have voids: these may lead to porosity in parts
- We are working to allow some use of **larger size powders** if an application allows **rougher surfaces** – can substantially decrease cost

Relating Powder Characteristics to Flow Behavior

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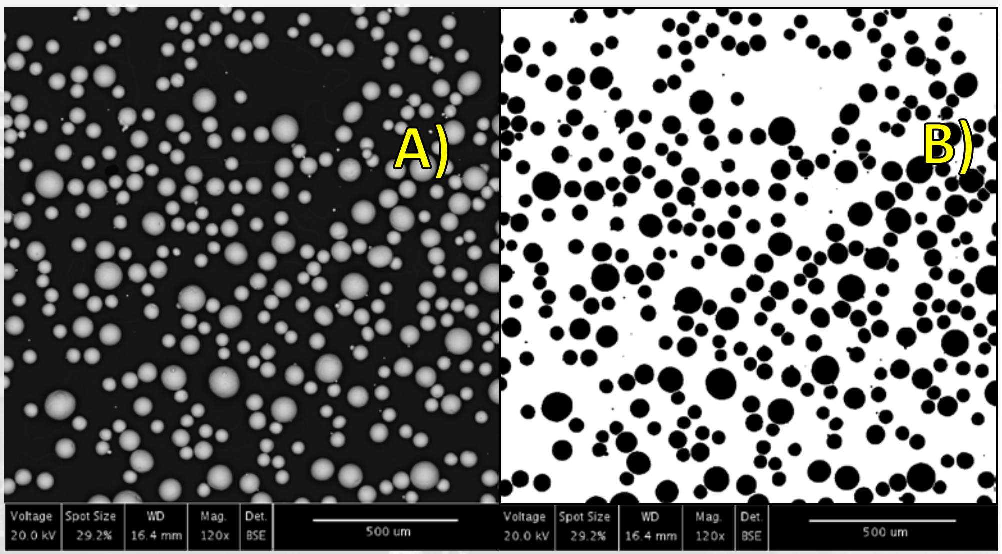
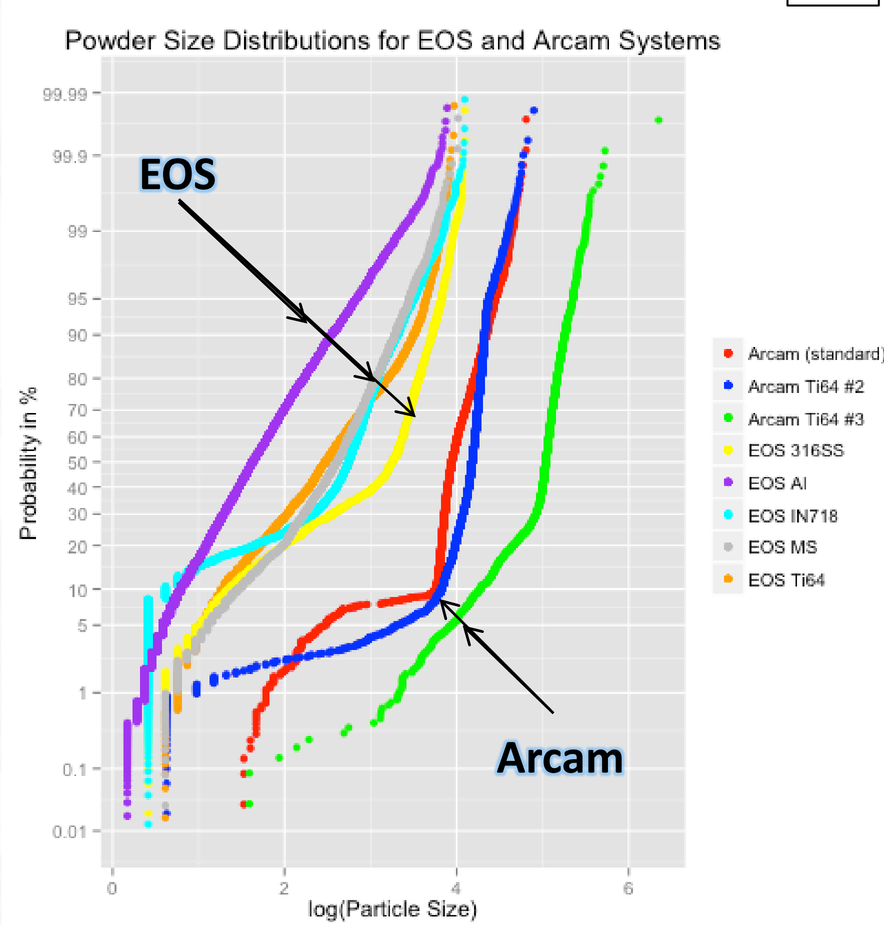
- Characterize powder via SEM and image analysis software (ImageJ)
- Relate powder properties to rheological behavior from Freeman FT4 Rheometer (Higgs)



(A) SEM image of Arcam Ti-6-4 powder.
(B) Thresholded image for analysis (ImageJ).



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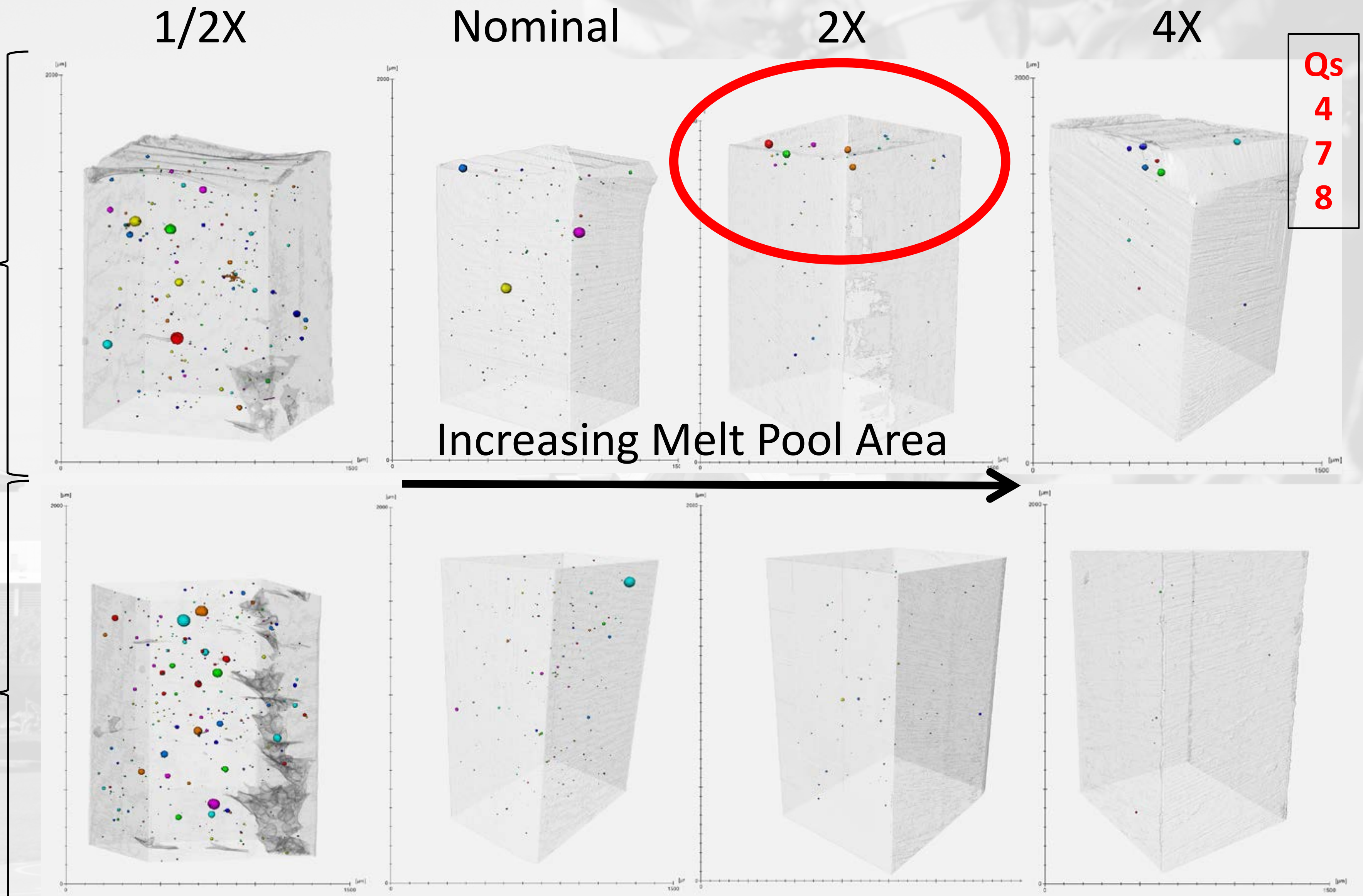
Computed Tomography, Ti64, Pores

Advanced Photon Source
Argonne National Laboratory



Pores: voids in particles, keyhole defects, incomplete fusion

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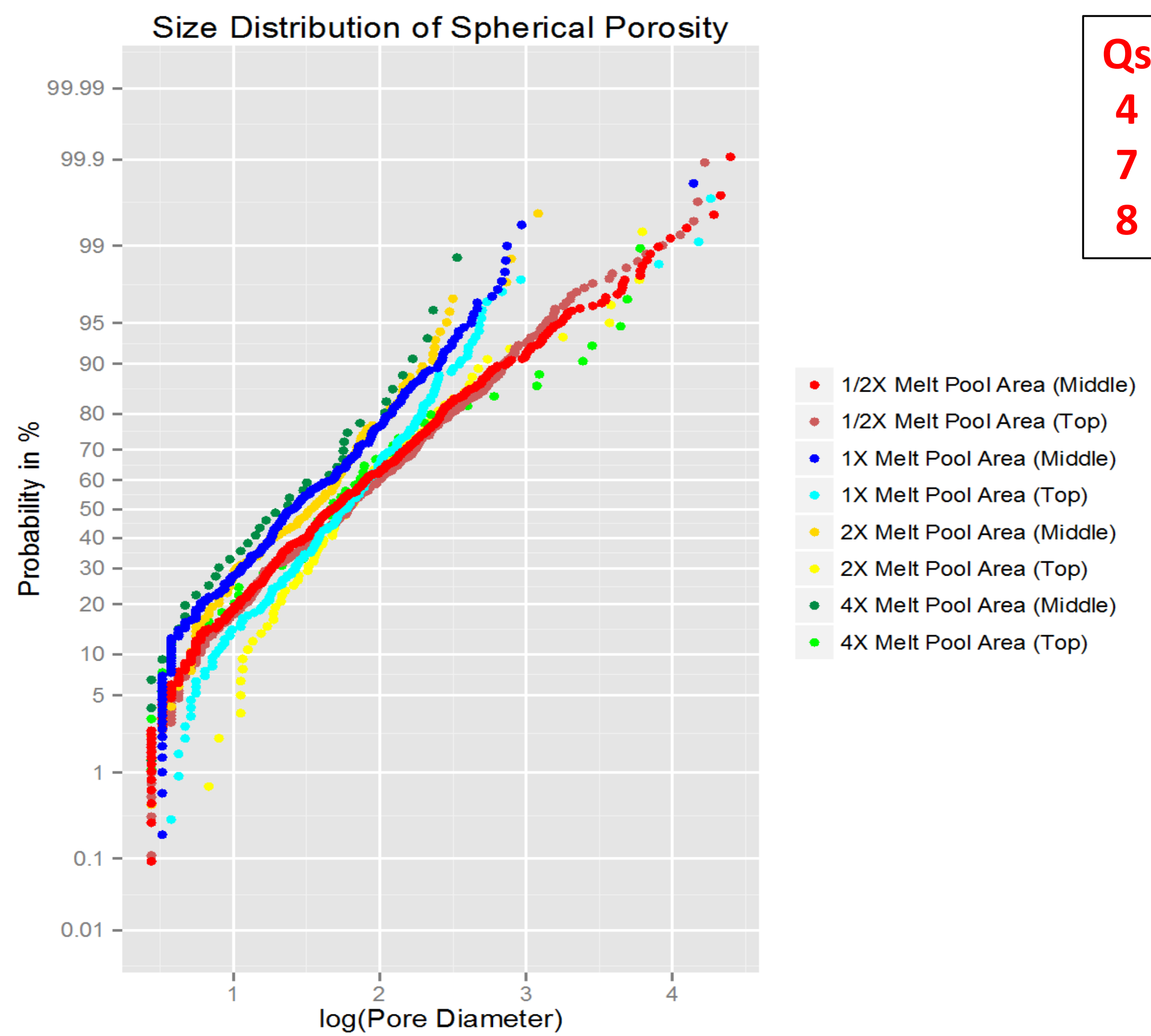
Pore Size Distributions



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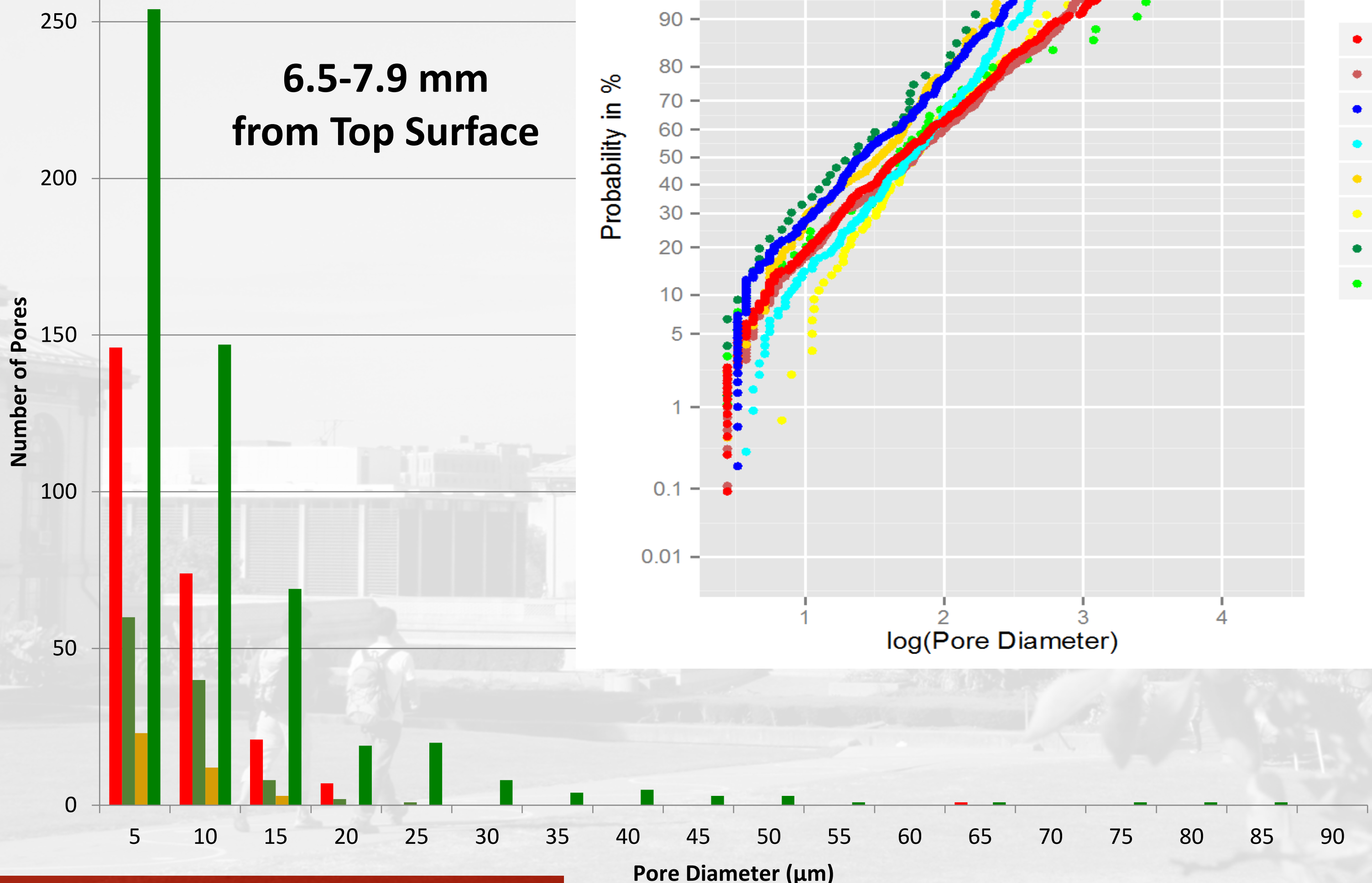

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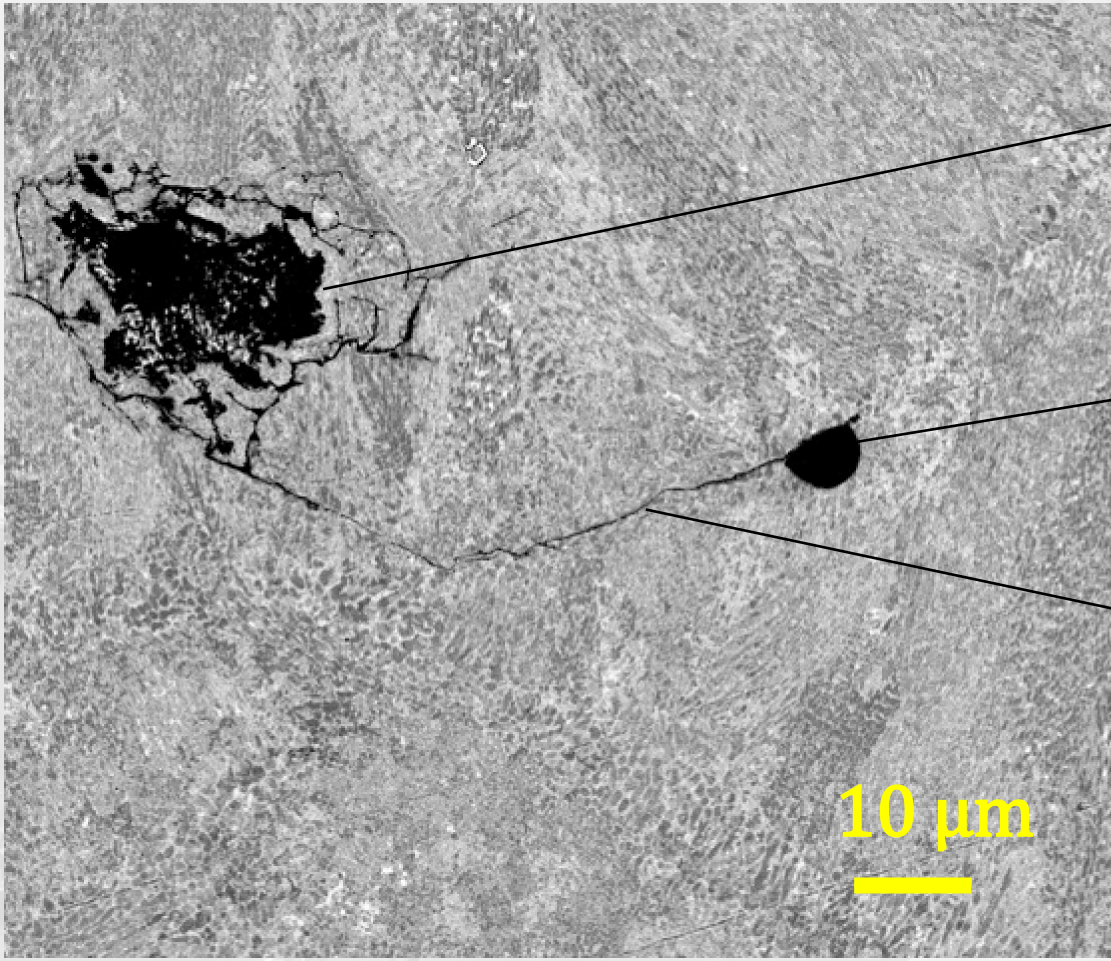
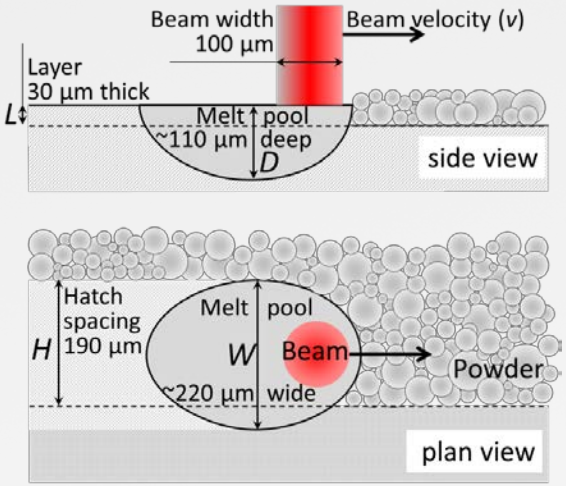
Lack-of-fusion defect in Al-10Si-1Mg – scanning electron microscopy



Backscattered electron image

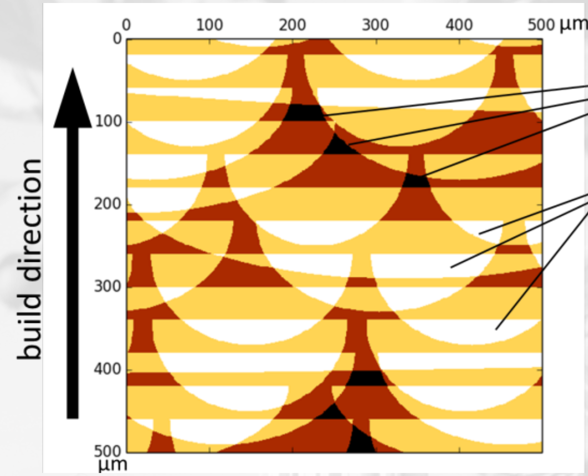
Magnusen *et al*. (1997). Analysis and prediction of microstructural effects on long-term fatigue performance of an aluminum aerospace alloy. *Intl. J Fatigue*, **19** (Supp. 1), S275-S283.

Porosity/Density Prediction



Melt pool geometry

Note relevance of Marangoni effect



Melt pool overlap across layers

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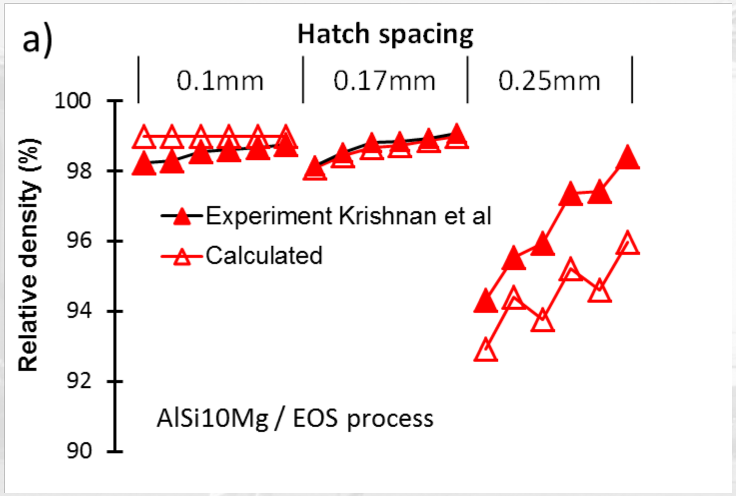
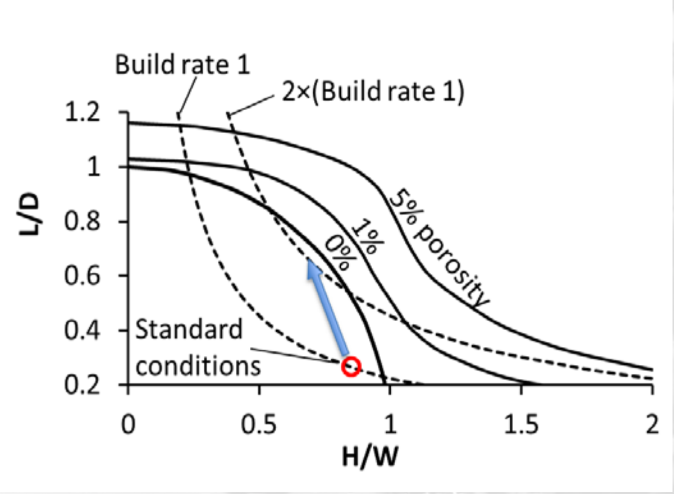


Comparison of model with literature data



Comparison with standard operating point

Ming Tang, Chris Pistorius

Variability

- There are many sources of variability: e.g., local part geometry; e.g., melt pool size and shape
- This variability matters to porosity, reproducibility etc.
- Known issue in the welding community

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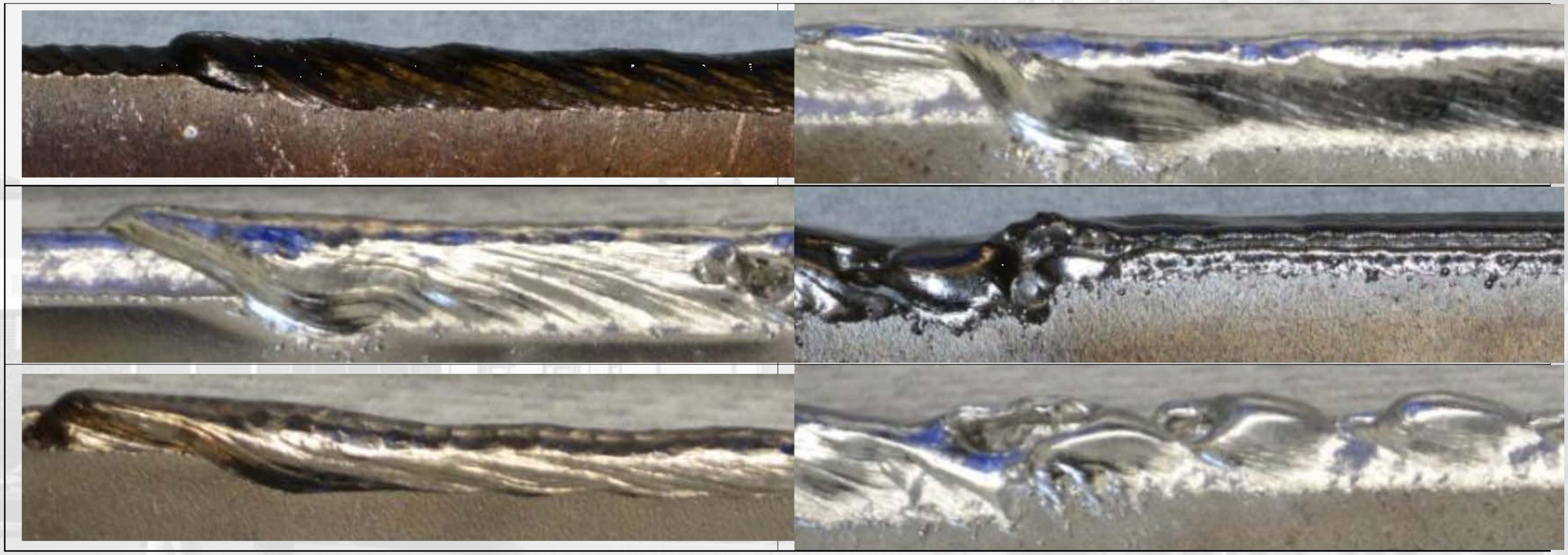
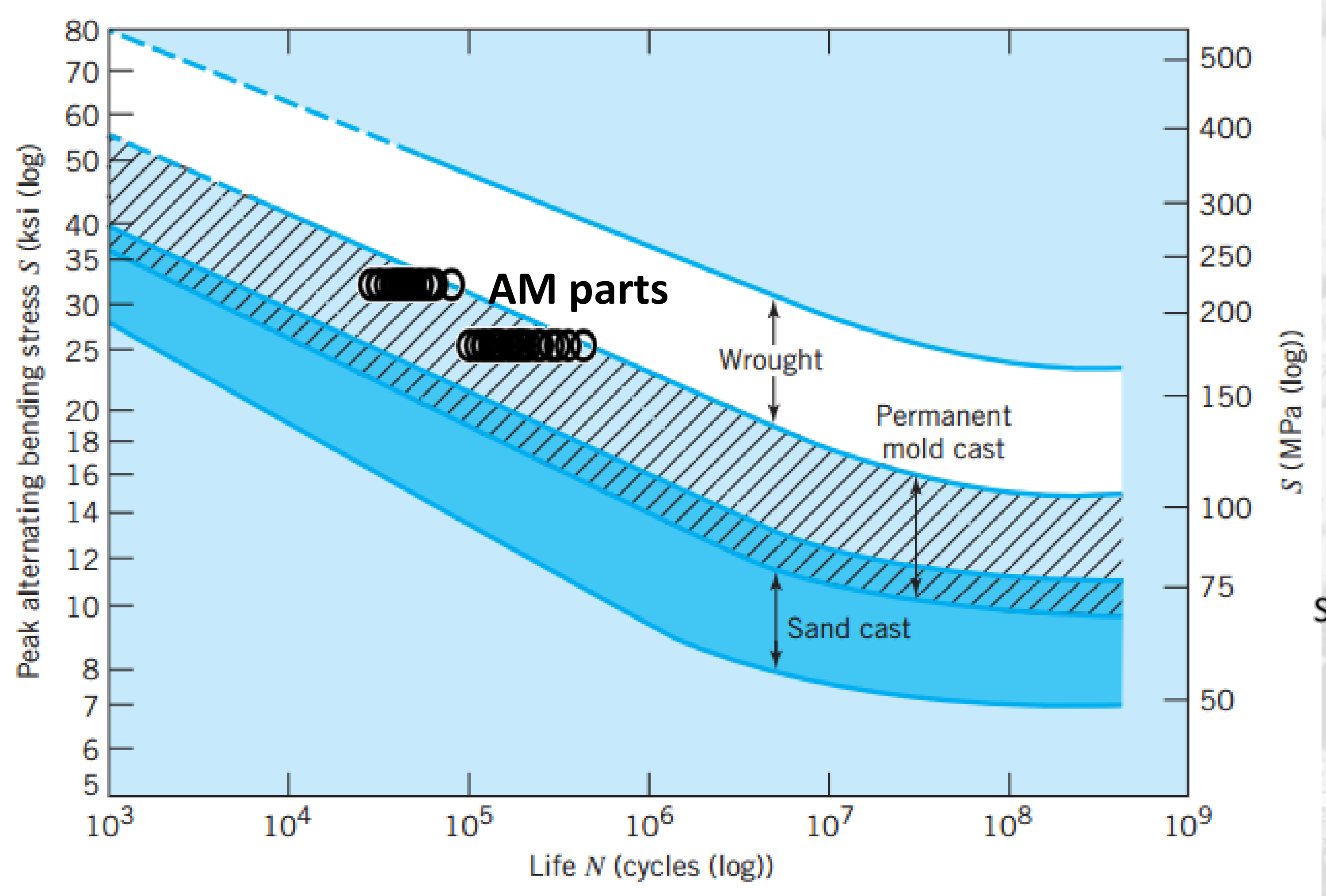
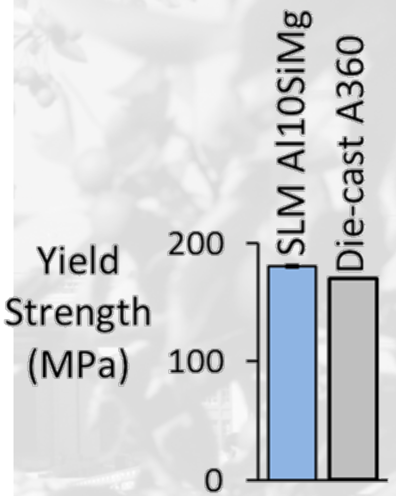


Weld beads in Ti-6-4; courtesy of J. Fox, CMU

Fatigue resistance and strength compared with Al parts produced by <u>traditional manufacturing</u>

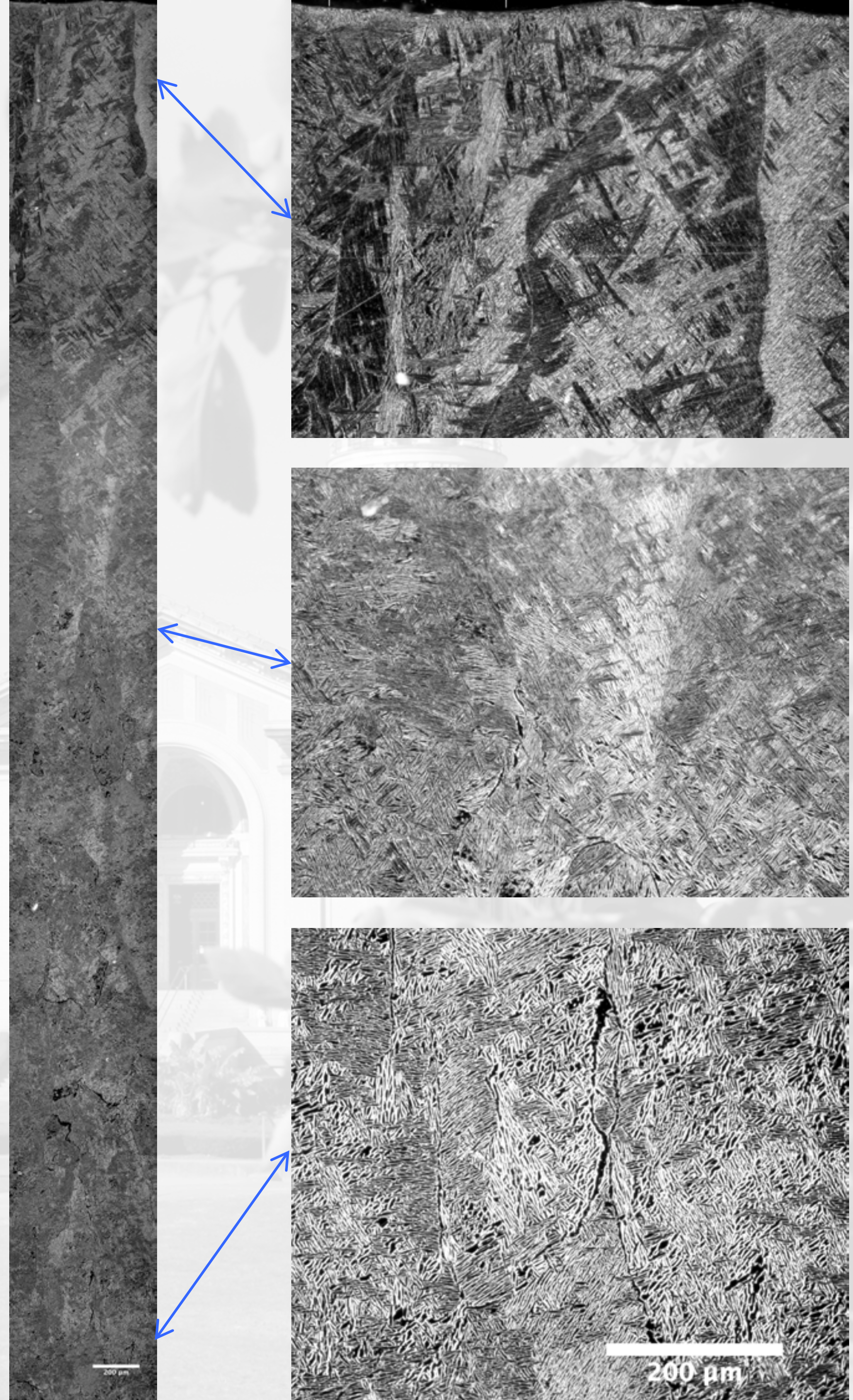




R.C. Juvinall & K.M. Marshek. *Fundamentals of machine component design*. Vol. 83. New York: John Wiley & Sons, 2006, p. 318

Ti-6Al-4V

- Standard microstructures are based on heat treatment in the two-phase range; this gives a mix of primary α and Widmanstatten $\alpha+\beta$.
- Despite the high cooling rate (~10^6 /s), the β structure is columnar and the transformation gives either martensite or acicular α.
- Variations in thermal history can give rise to significant transitions in microstructure. This example documents the variation in a Ti-6Al-4V build, which shows a martensitic microstructure near the top and a basketweave microstructure (or tempered martensite) towards the base.



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2-PHASE AM REPRESENTATIVE TI STRUCTURES

Effect of Microstructural Features on Mechanical Behavior

How do the microstructural features such as the β-grain size, α-colony size and the relative volume fractions affect the overall mechanical response of Ti alloys?

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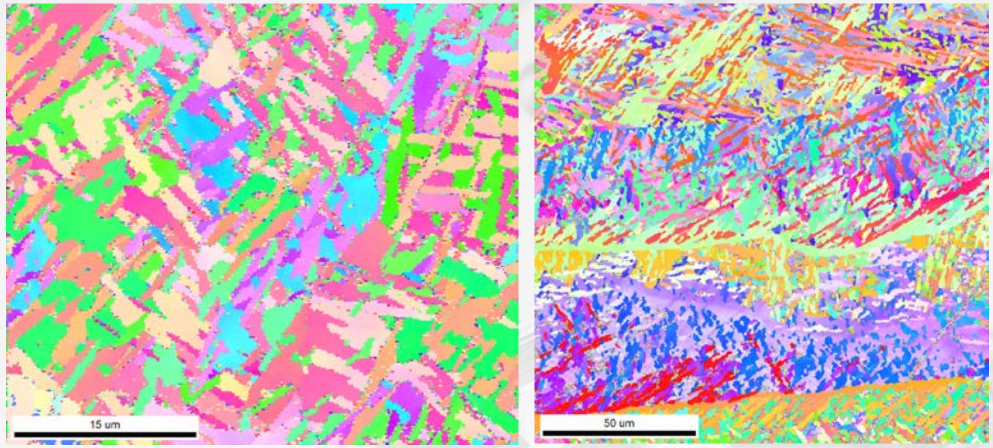


EBSD orientation maps of an additively manufactured near α Ti alloy (same sample, different scaling). Average β size is 100 microns and average α size is few microns.

- Based on the sensitivity study and the EBSD maps, 225^3 statistically representative microstructures are created with varying β (BCC) size-morphology and α (HCP) fractions.
- α particles → higher hardening parameters
- BCC to HCP transformation in Ti alloys (Burgers OR)

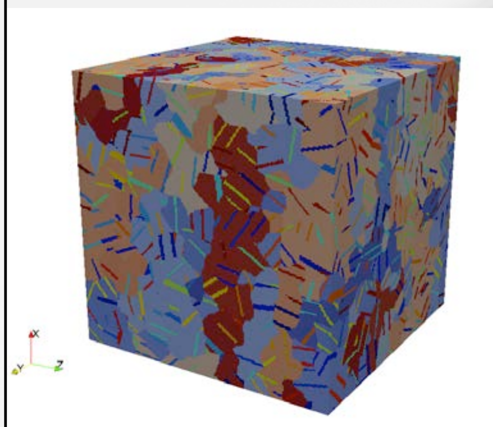
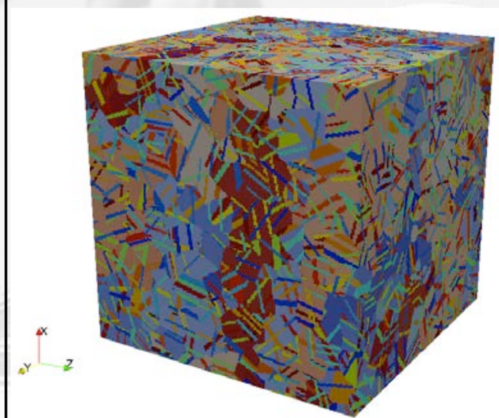
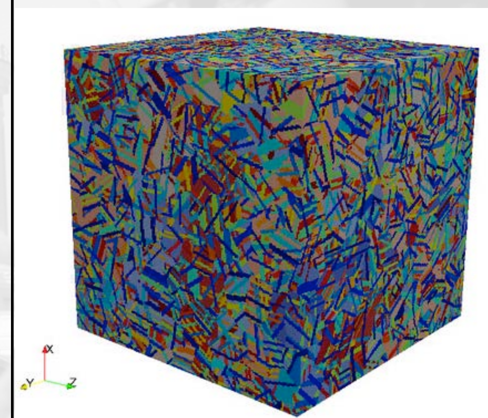
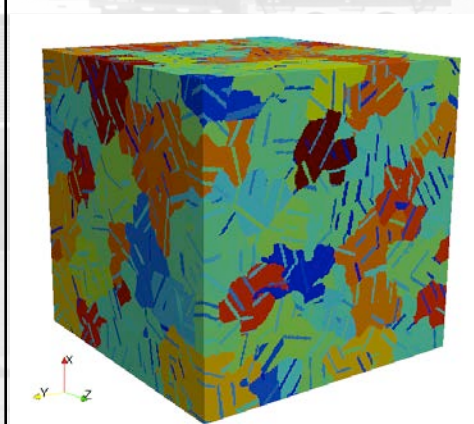
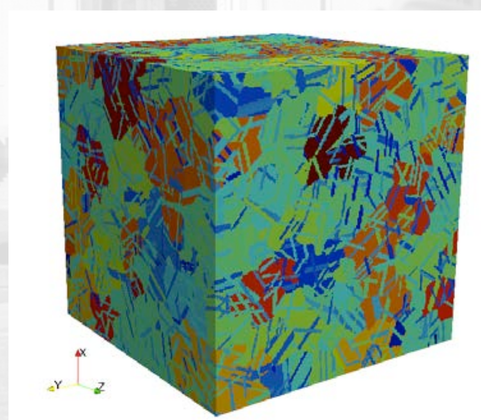
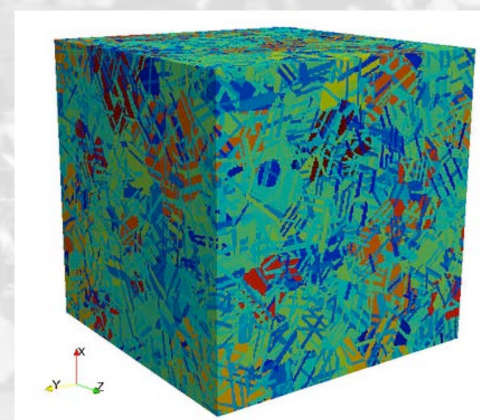
$$(0001)hcp \,||\, \{011\}bcc$$

$$[1120]hcp \,||\langle 111\rangle bcc$$

Variant number	BCC plane // to $(0001)_\alpha$	BCC direction // to $[11\bar{2}0]_\alpha$
1	(110)	$[\bar{1}1\bar{1}]$
2	(110)	$[1\bar{1}\bar{1}]$
3	$(1\bar{1}0)$	$[11\bar{1}]$
4	$(1\bar{1}0)$	$[111]$
5	(011)	$[11\bar{1}]$
6	(011)	$[\bar{1}1\bar{1}]$
7	$(01\bar{1})$	$[\bar{1}11]$
8	$(01\bar{1})$	$[111]$
9	(101)	$[\bar{1}11]$
10	(101)	$[11\bar{1}]$
11	$(\bar{1}01)$	$[1\bar{1}1]$
12	$(\bar{1}01)$	$[111]$

Tugce Ozturk

Synthetic microstructures via Dream.3D*

	15% Alpha	40% Alpha	65% Alpha
Columnar beta matrix			
Equiaxed beta matrix			

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* dream3d.bluequartz.net [open source]

FFT Simul.

Effect of Alpha Fraction, Columnar Beta, Strain Along z*

Effect of Beta Morphology, Strain Along z*

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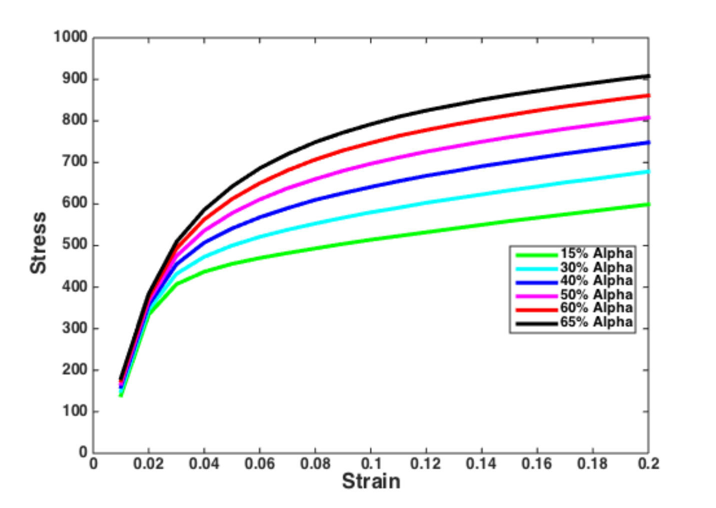
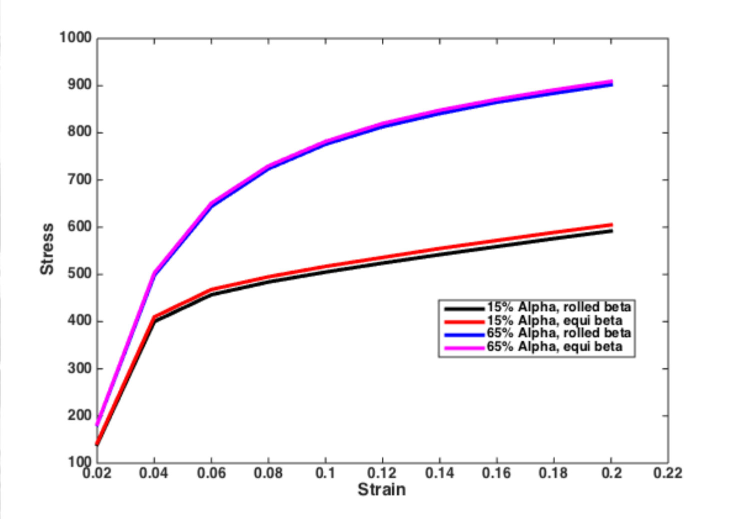


Effect of Alpha Fraction

As the alpha fraction increases, so does the overall strength.



Effect of Beta Morphology

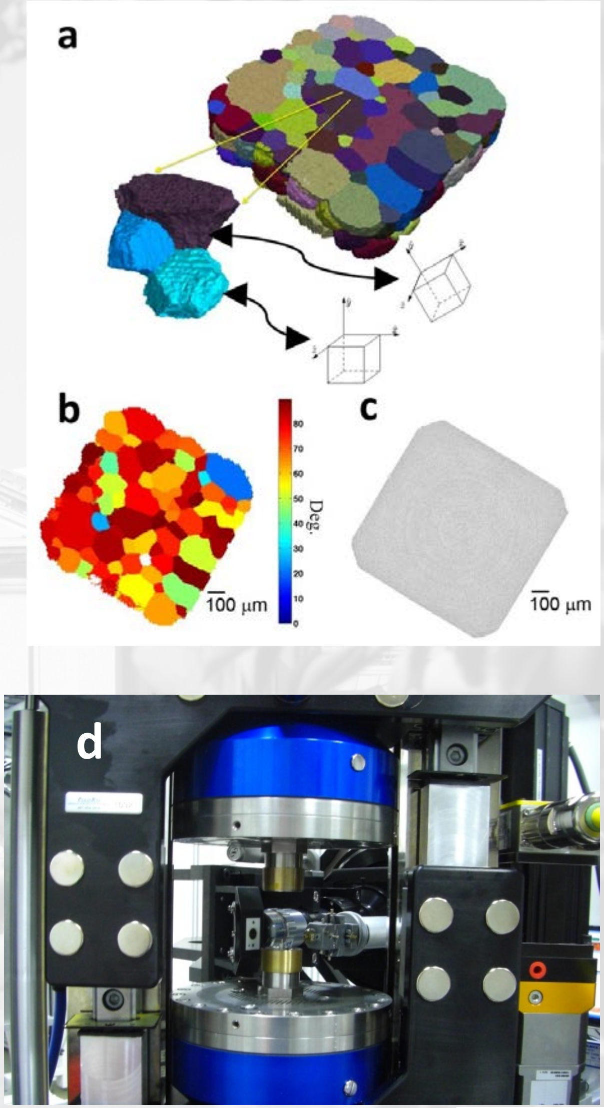
As the alpha fraction increases, β morphology effect diminishes for random textured β matrix.

Tugce Ozturk

*Viscoplastic-FFT: Lebensohn, *Acta Mater.* (2001) **49** 2723

Advanced Synchrotron Capabilities: CT+HEDM

- Recently completed High Energy Diffraction Microscopy (HEDM) experiment at 1-ID on AM Ti-6-4
- 3D microstructure and orientation information with Near-Field mode
- 3D residual stress distribution via Far-Field mode
- Capability for in situ loading during CT, NF and FF; RAMS loading system developed by AFRL; software by CMU, LLNL, others
- **All such experiments require supercomputer resources for data reduction, reconstruction and analysis**



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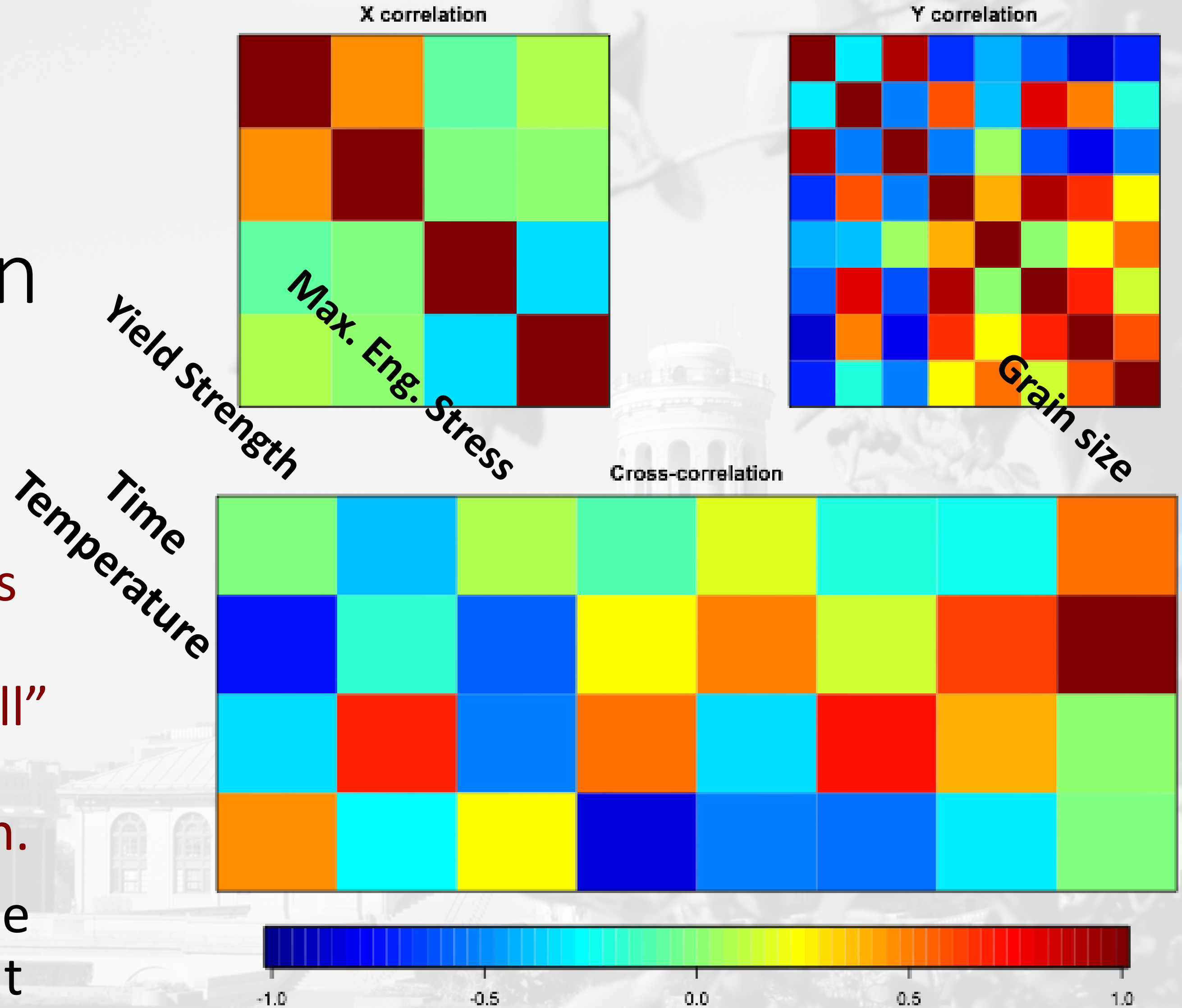
Tugce Ozturk, Robert Suter et al.

Plot from Canonical Correlation Analysis



- Packages such as “R” facilitate analysis of “small” data, e.g., via cross-correlation.
- Separation of the input and output variables; shows the cross-correlation.

```
> allvars = read_excel(“data_file”)
> invars<-allvars[,1:4]
> outvars=allvars[,5:12]
> simpleCorr=matcor(invars, outvars)
> img.matcor(simpleCorr, type=2)
```

Questions

(1) Computational methods and approaches for simulating materials processing, properties and performance relationships for materials design using a

stress-strain ir

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Examples avai

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manufacturing? Research $, of course; also internships, scholarships directed at AM.

Rollett's personal view:

- How to integrate/ scale up/ homogenize detailed modeling of heat+fluid+energy flows into reduced order models?
- How to set up data sharing that is useful for data analytics but also fair to the groups that contribute the data?
- How to support industry with basic research that impacts practical issues, e.g. powder manufacture, qualification?
- How to incorporate materials microstructure (including orientation, lattice strain) into continuum codes?
- How to exploit big data techniques to deepen the validation process, e.g. use reconstructed images, or the diffraction data itself?

Process Map Impact on Aerospace Qualification

Current Practice

Complex Mix of Inter-Related Process Variables

Trial and Error Experiments

1. High Cost – In Aerospace $Millions to Qualify One Process to Make One Part
2. Long Times: Years to Qualify a Process
3. Each Machine Can be Different

Final Goal

Process Outcomes

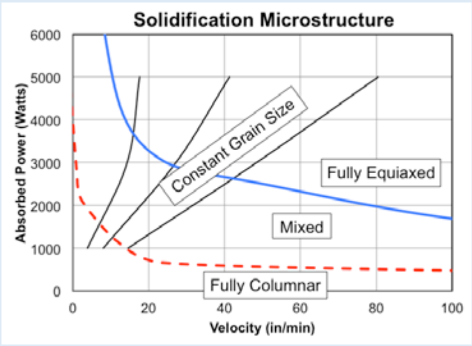
1. Part Geometry
2. Surface Finish
3. Microstructure and Properties
4. Flaws
5. Precision

Process Mapping

Identify Primary Process Variables

1. Beam Power
2. Beam Travel Speed
3. Material Feed Rate
4. Background Temperature
5. Local Geometry

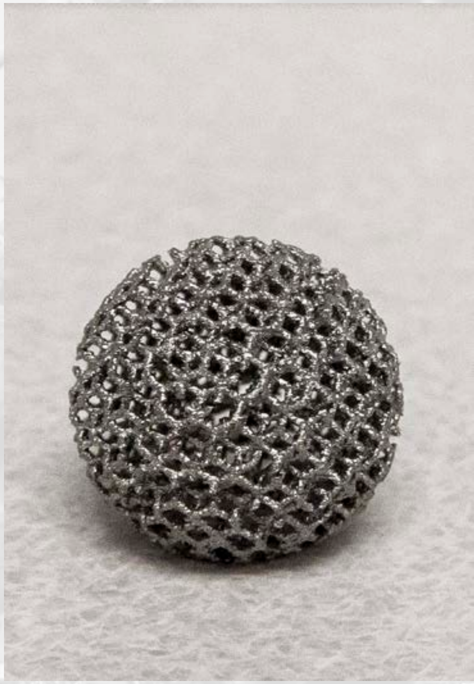
Map the Process



- Process Mapping Quickly Points Users to Optimal Process Variable Combinations
- Backed by 12 Fundamental and Tech Transfer Research Projects Funded by NSF, ONR, NIST, America Makes, the State of Pa and Others

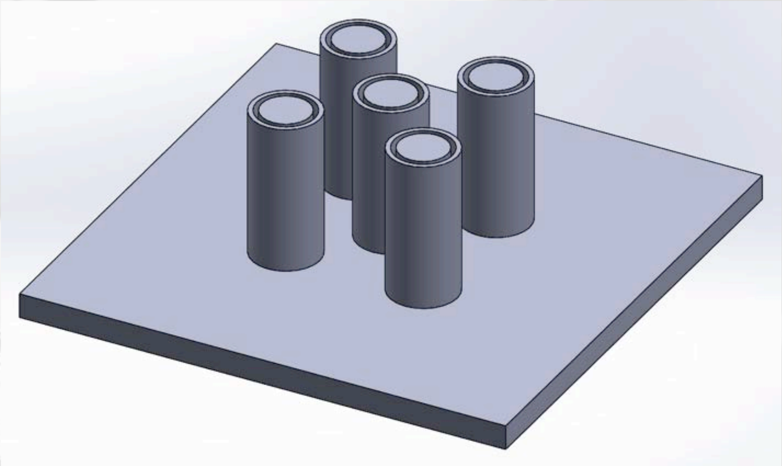
Our Research

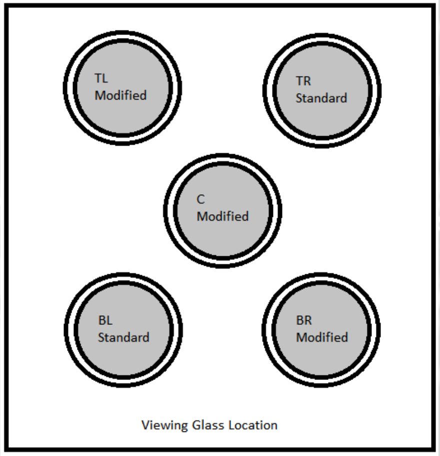
- Our Patent Pending *Process Mapping* Technology Uniquely Maps the Dependence of Process Outcomes *(deposition rate, porosity, microstructure, precision, surface finish etc.)* in terms of Identified Primary Process Variables *(beam power, travel speed, layer thickness, background temperature, local geometry)*
- Customers can develop their own "recipes" for part fabrication
- Step through a series of geometries from single beads to components to component features
- Can map modeling results or experiments – we are defining limited numbers of experiments to run to characterize a process



Real-Time Microstructure Control

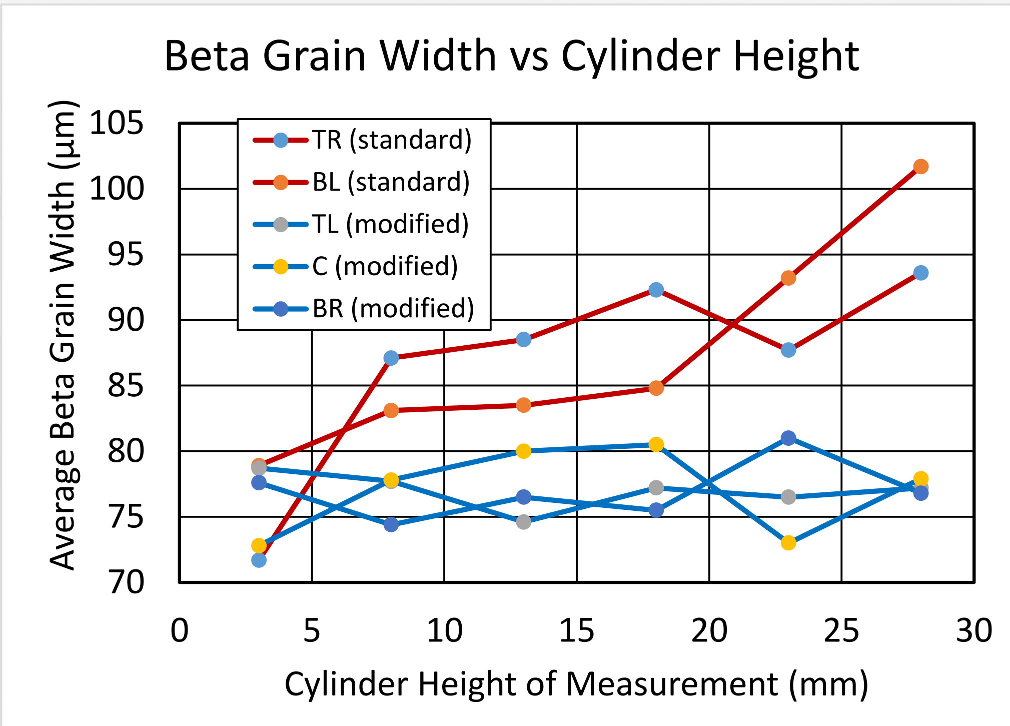
- Current Processes have Little or No Process Sensing and Control
- Arcam Process Typically Has Temperatures Drift Higher as a Part is Built
- This Causes Microstructural Features to Change from the Bottom to the Top of the Part
- Control Procedure
  - 5 Cylinder Builds, 3 Modified, 2 Standard, All 30mm Tall
  - Thermal Imaging at 5mm Increments used to Control Beam Power

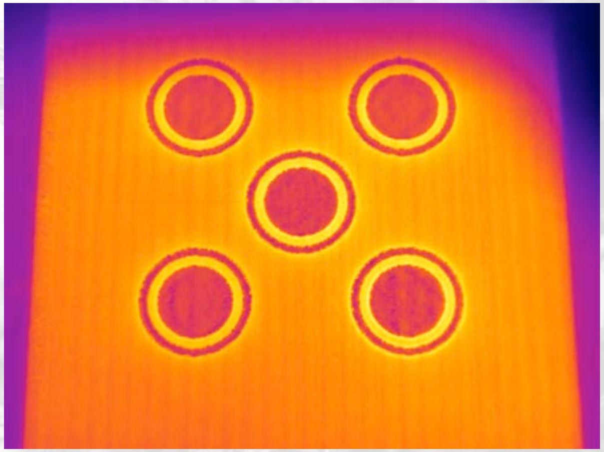




Real-Time Microstructure Control

- Standard Cylinders Both Show Steady Increases in Average Beta Grain Size with Part Height Location
- Modified (Controlled) Cylinders Show Essentially Constant Beta Grain Size Through the Height
- *A breakthrough result*





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Primary Process Variables

Beam Power

Beam Travel Speed

Layer Thickness

Local Part Temperature

Local Part Geometry (feature with potentially many geometric variables)

Process Maps

Developed from Models or Experiments

Process Outcomes

Build Rate

Process Precision

Surface Finish

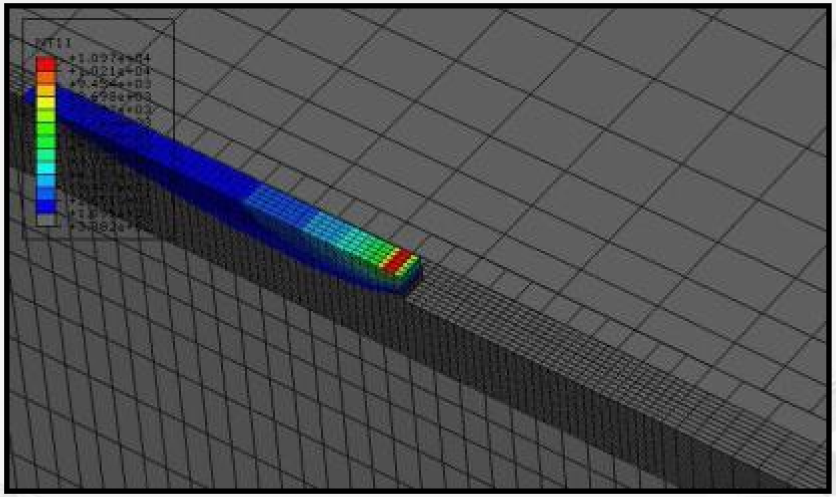
Porosity

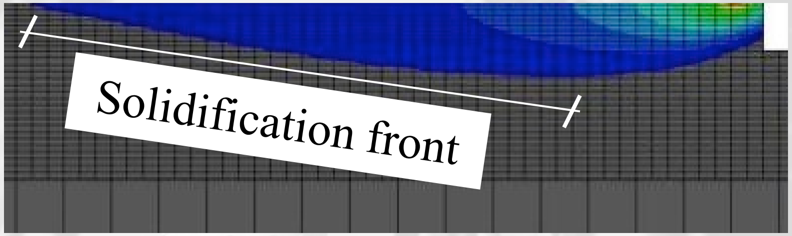
Microstructure (yield strength, fatigue strength, crack growth resistance, creep resistance)

Melt Pool Geometry

Finite Element Simulations of Single Beads

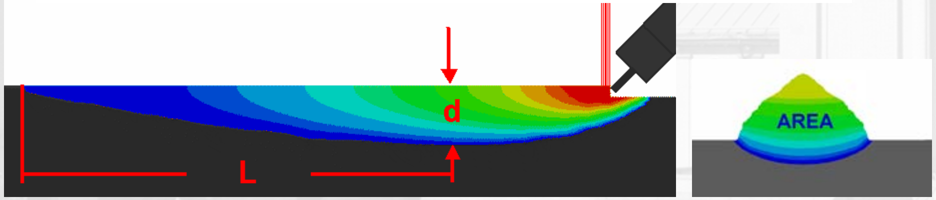
Single Bead (3D)





- Extract thermal conditions along the solidification front

Melt Pool Dimensions: A, L, d, L/d



Thermal Gradient

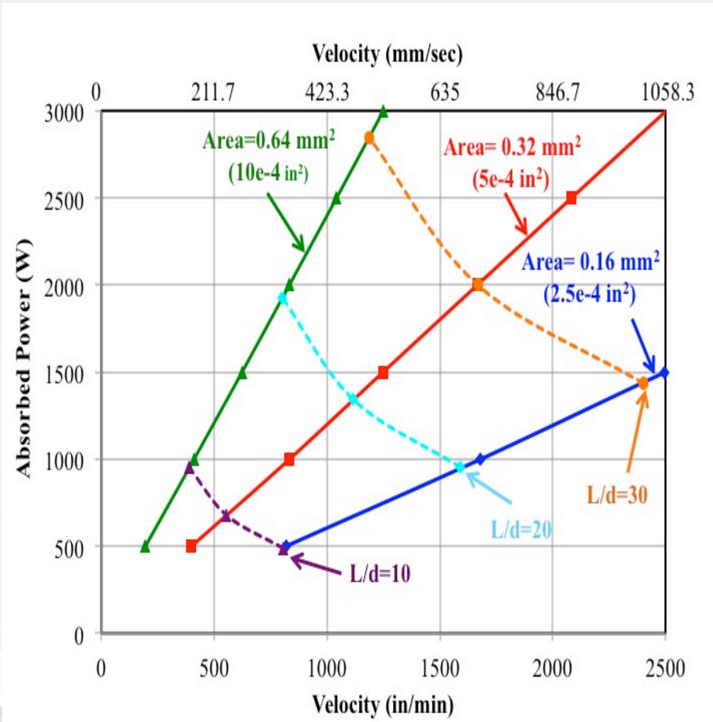
$$|\vec{\nabla} T| = \frac{|\vec{q}|}{k}$$

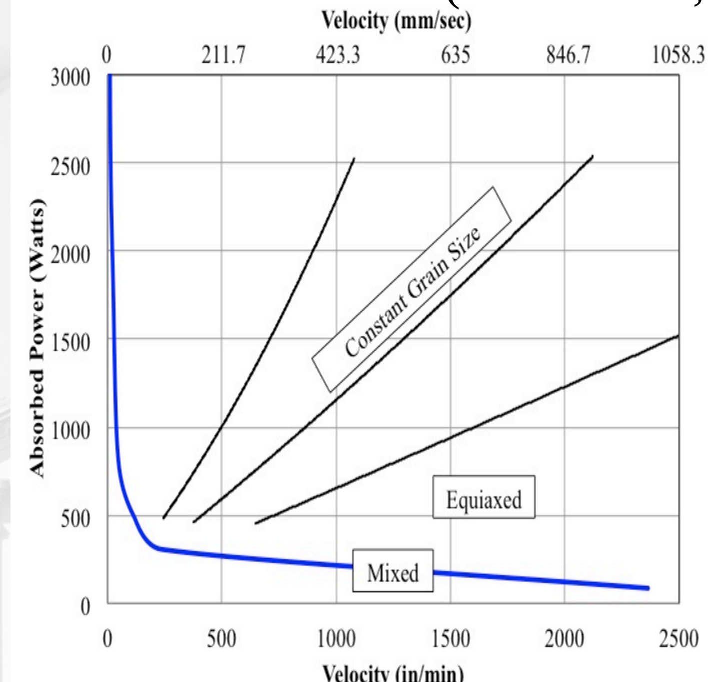
Cooling Rate

$$\frac{\partial T}{\partial t} = \left| \frac{T_S - T_L}{t_S - t_L} \right|$$

Integrated Solidification Microstructure and Melt Pool Dimension Control (Arcam) in Single Beads

(Gockel et.al, SFF 2014)

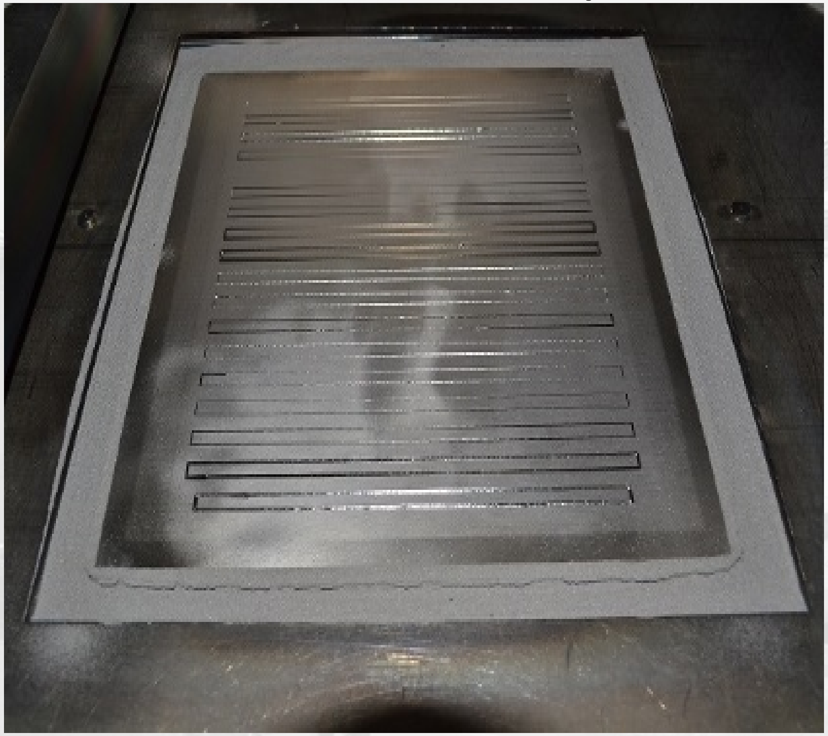


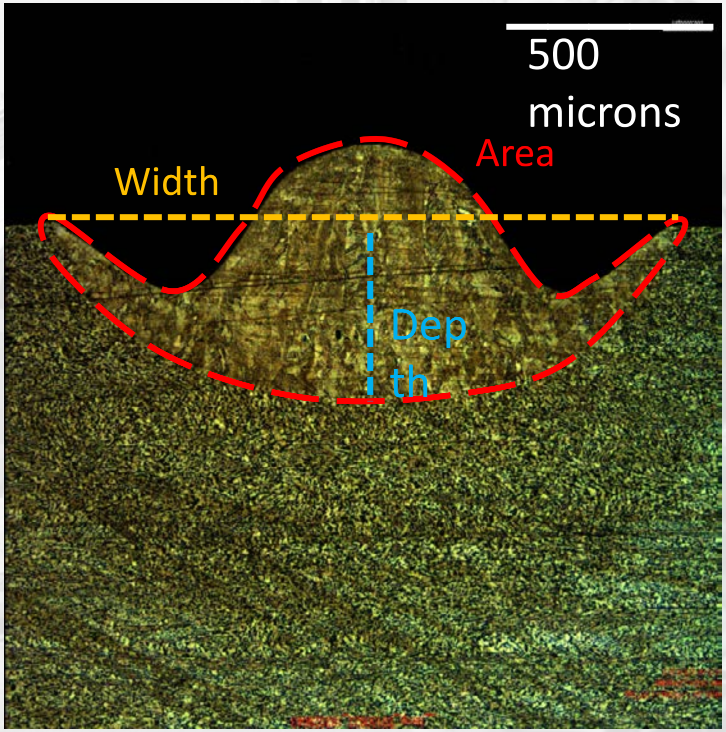


- Curves for a single geometry (single beads), background temperature and layer thickness
- Curves of constant area are curves of constant solidification cooling rate Same is true for curves of constant melt pool width
- ***Grain width should scale with melt pool width: This research applies this concept to grain size control using Arcam process variables***

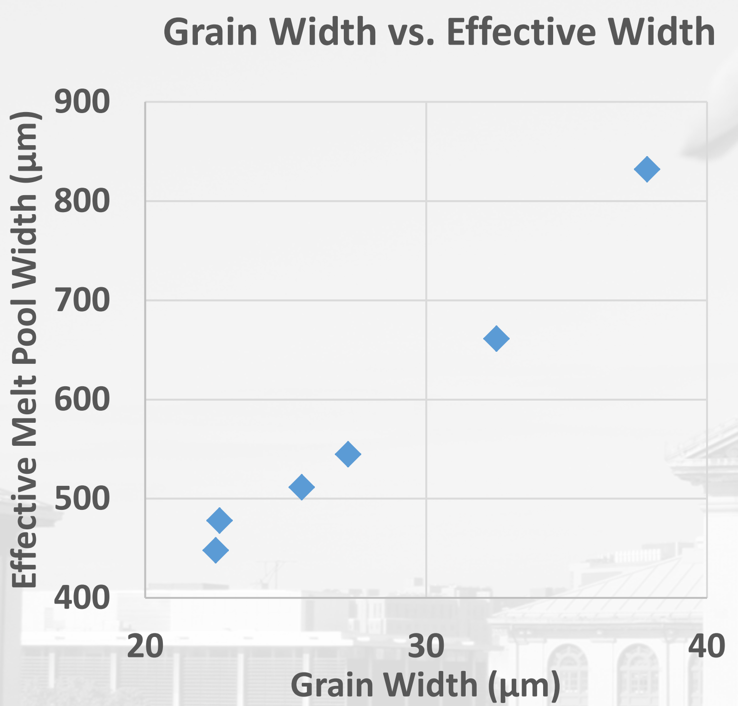
Single Bead Tests

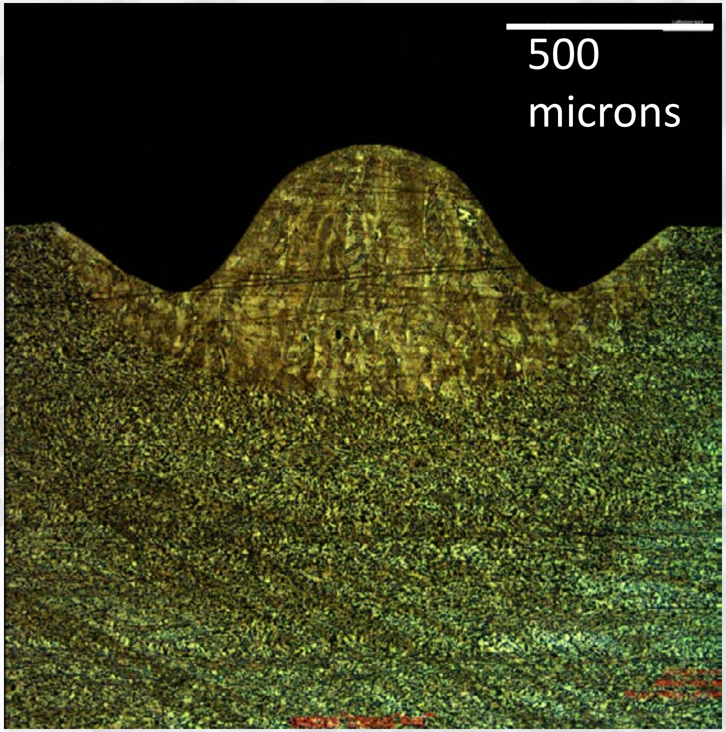
- Single bead tests were done on S12 machines at CMU
- Speed function is varied over a range of beam currents
- Cross-sections of the single beads are analyzed for melt pool area, width and depth





Grain Size Analysis in Single Beads

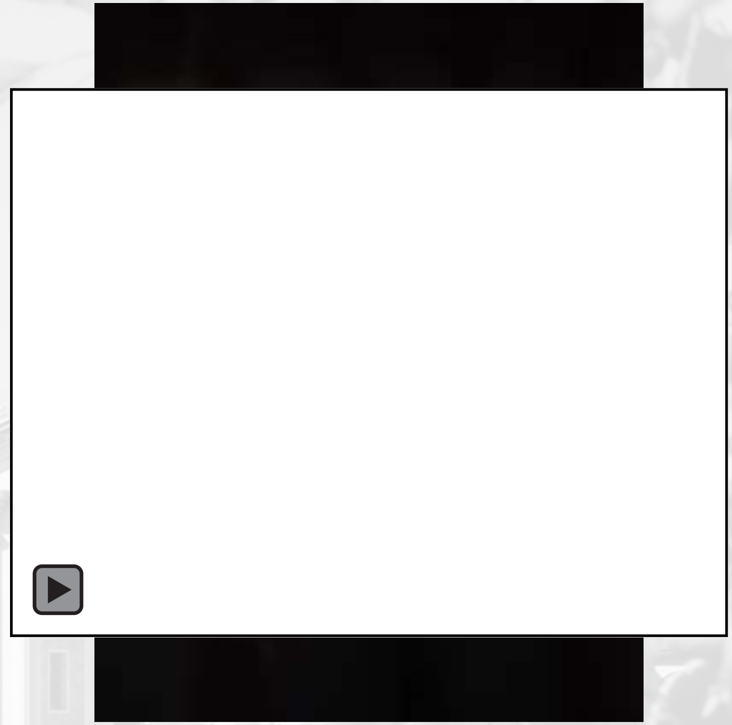




Grain size scales with Effective Width

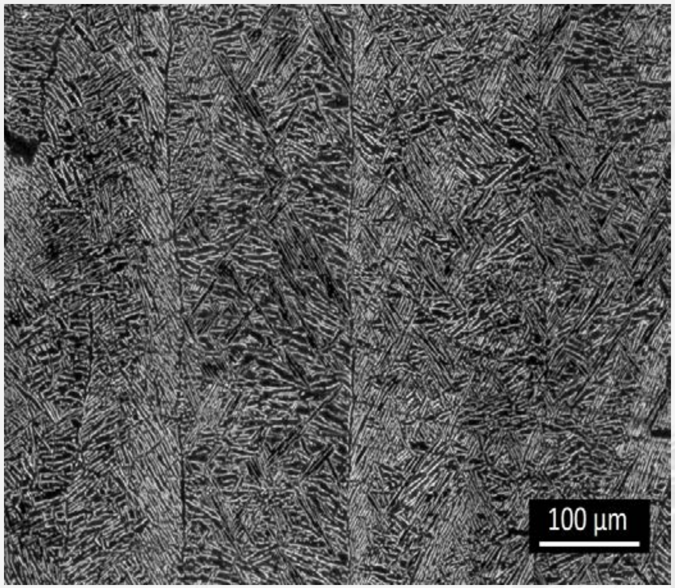
Number of grains per effective width is constant varying between 20-22

Multi-layer Pad Tests

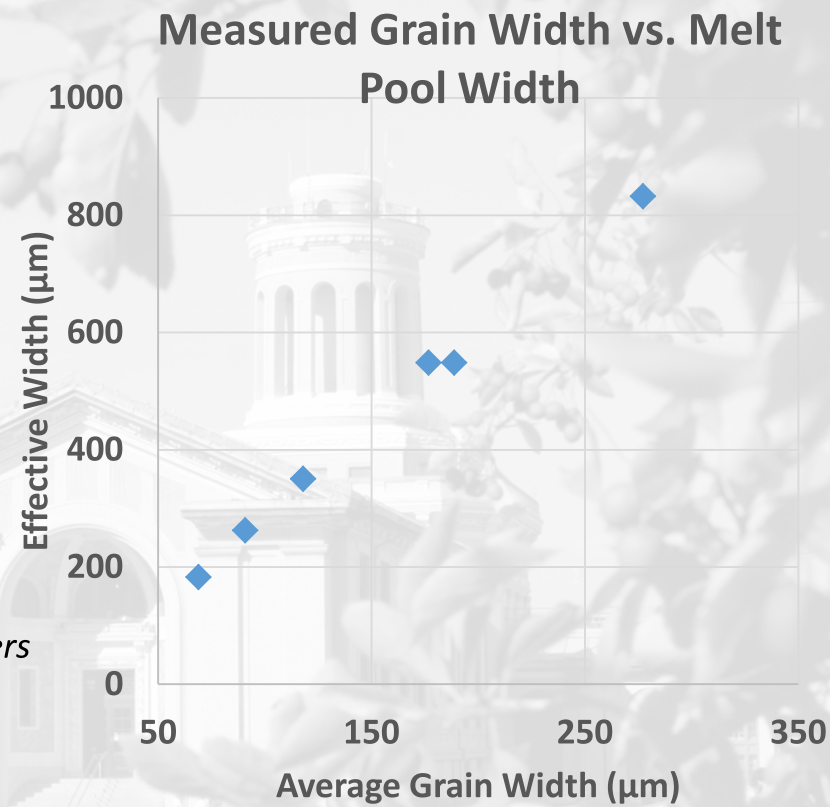


- Test blocks of size 30x30x20 mm are built with different beam currents and speed functions, one of them includes the nominal build parameters on Arcam S12

Prior Beta Grain Size – Pads (Solid Builds)

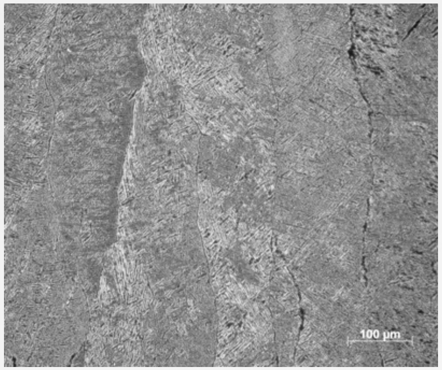


Cross-Section Micrograph of the block built with parameters yielding increased prior beta grain width

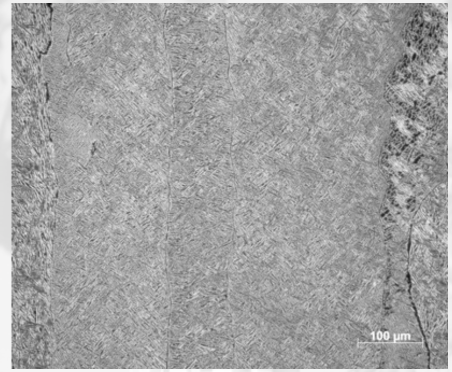


- *No trace of individual layers or individual melt pools in the final part*
- Columnar grains grow through layers and increase in width as build progresses
- Number of grains per effective width is ~ 3
- Decrease in number when compared to single beads – but still a constant!

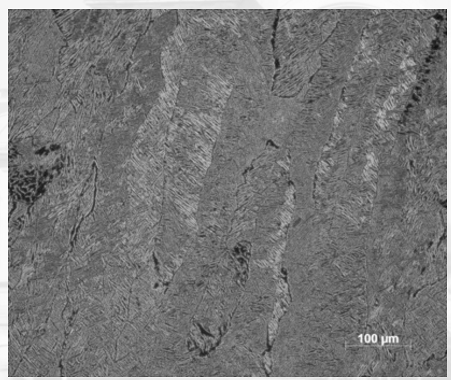
Ti64 Arcam Beta Grain Size Control (Cylinders)
(Beuth, Rollett, Cunningham, Harrysson)



Sample 1 Bulk Raster
Average β width = 117microns



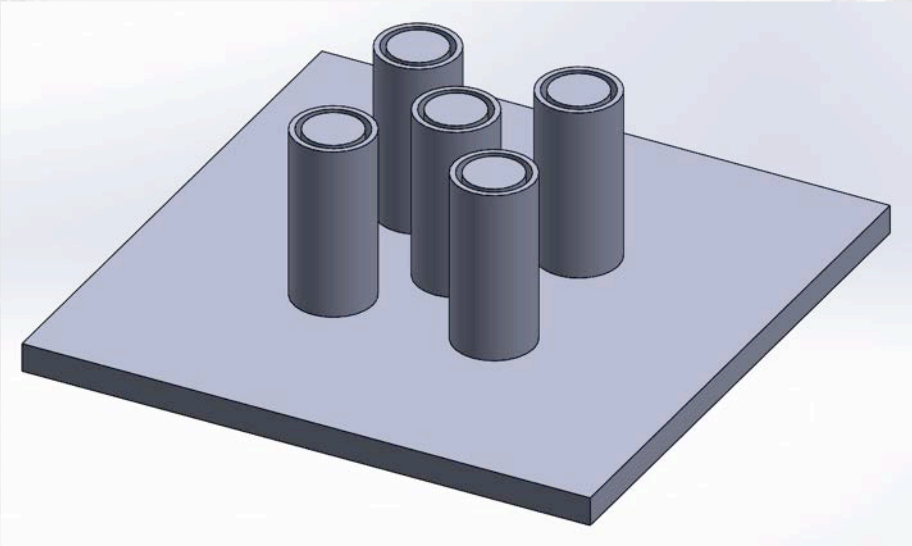
Sample 3 Bulk Raster
Average β width = 225microns

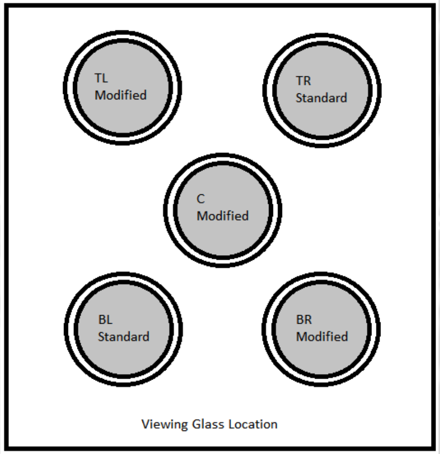


Sample 3 Contour
Average β width = 49microns

Experimental Procedure

- 5 Cylinder Builds, 3 Modified, 2 Standard, All 30mm Tall
- Thermal Imaging at 5mm Increments used to Control Beam Power (gives time to equilibrate temperatures, measure results, process them, then apply a new power value)
- 70μm layers, V=500mm/s, $P_{initial}$ =556W (500W Absorbed Power), $T_{preheat}$ = 760C





- Porosity Control

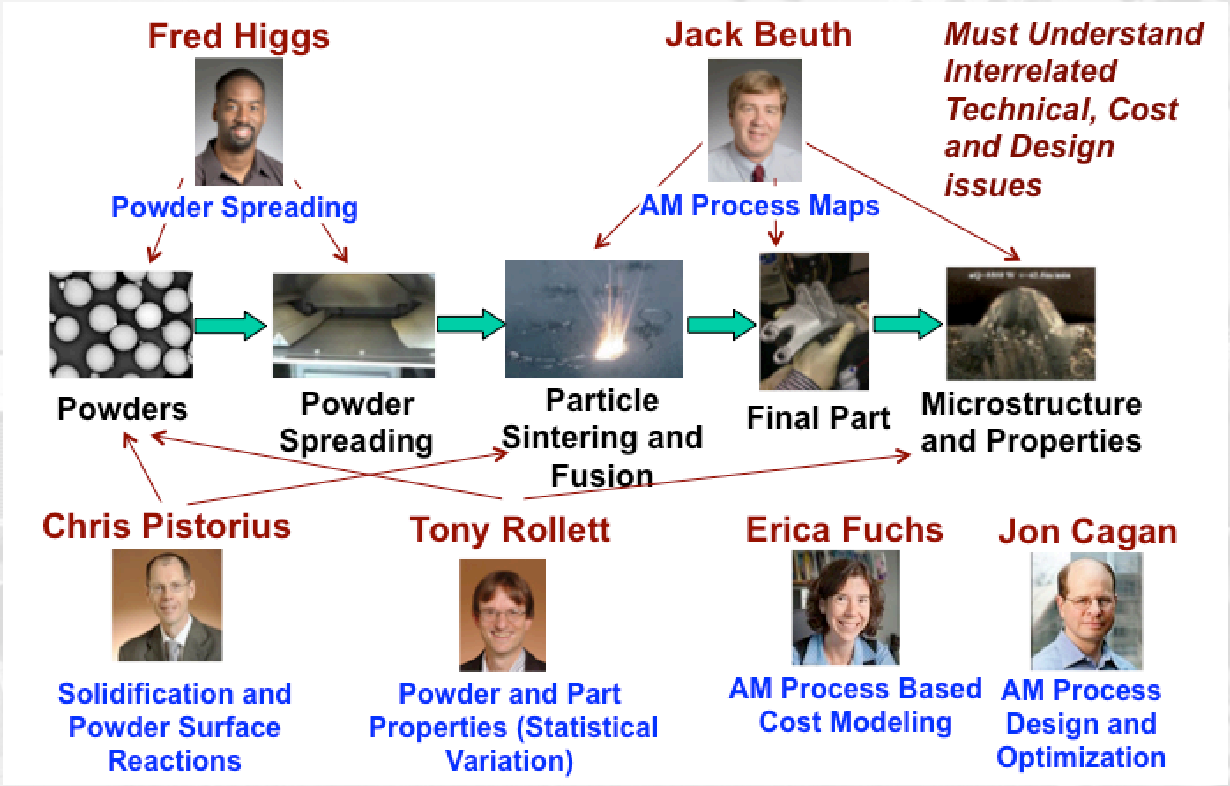
- Powders

CMU NextManufacturing Center

Exploring the manufacturing genome through additive processing

- Over 20 Faculty Across Campus
- AM is a *Testbed* for Developing New Methods for Advanced Manufacturing

Metals AM at Carnegie Mellon



AM Part Examples

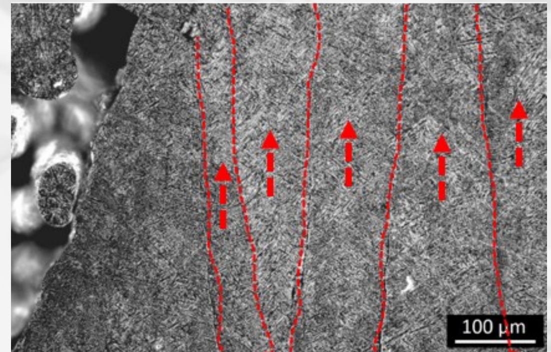
- GE External Engine Bracket

- Exoskeleton Component

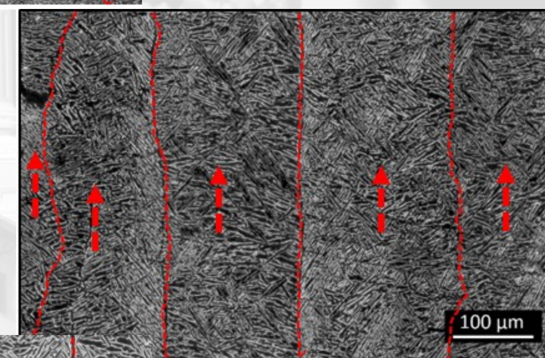
- CMU Meshed Sphere

Specifying Microstructure

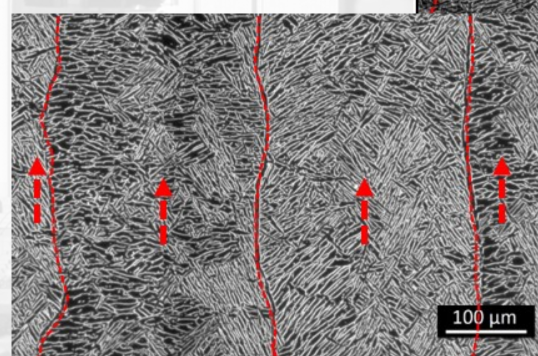
- Material Microstructure Determines Mechanical Properties
- Opportunity to Specify Microstructure and Properties on a Point-by-Point Basis in a Component
- We Understand How to Do This via Point-by-Point Changes in Process Variables
- Also Being Applied in Real-Time Control Systems



Bulk Raster
Average β width = 91 µm



Bulk Raster
Average β width = 177 µm



Bulk Raster
Average β width = 277 µm

Spatial Variation of Microstructure in Solid Builds

- As viewed from the top (sectioned and polished)
- Alternating Big and Small Grains
- Process Variables are Distinctly Changed within Ring and the Surrounding block
- Issue: What Spatial Resolution of Microstructure Changes is Achievable?