QuesTek Innovations—Application of ICME to the Design and Development of New High-Performance Materials for AM

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Session 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

- Highlight of my talk
- Computational thermodynamics, Mechanistic property modeling

#2 - How can these be integrated to impact adoption of AM?

- Materials and process design
- ICME-based Qualification

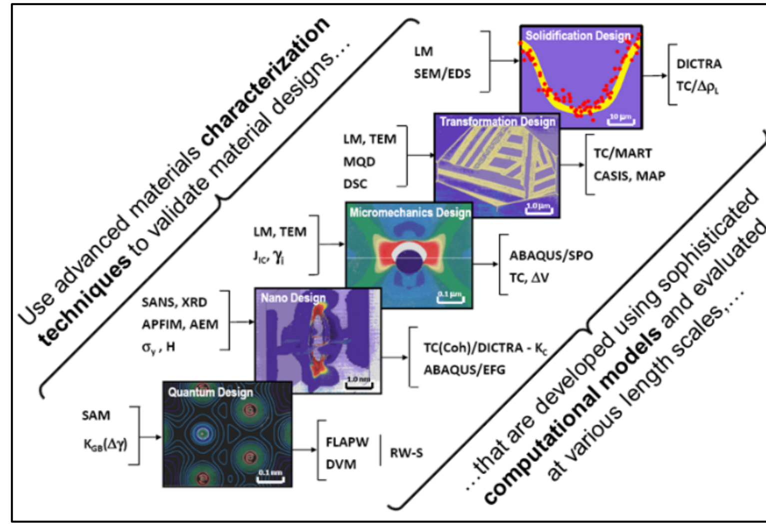
Outline

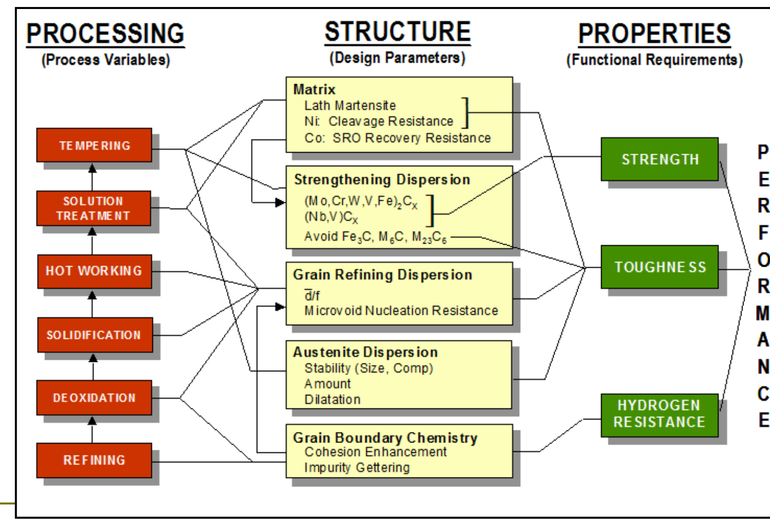
- Overview of AM Computational Materials Design
- Case Studies from Current Research (focus on metals)
  - Key AM-specific material responses
    - *Unique Recrystallization response central to AM*
    - Identifying key computational methods to address these critical factors
- Accelerated Insertion of Materials (AIM) methodology
  - Accelerating qualification cycle by using ICME tools to project property minima from process uncertainty
    - *For AM, this is more about Part qualification more than just Material qualification*
- Perspective on Industrial need for computational approaches to AM

Computational Thermodynamics

CALPHAD-based thermodynamics, coupled with computational models to simulate:

- Phase transformations
  - Solidification
  - Solid-state (precipitation, recrystallization)
- Microstructural constituents
  - Strengthening phases
  - Impurities (dispersoids – size and fraction)
  - Evolution during complex thermal cycling, post-processing (PrecipiCalc)





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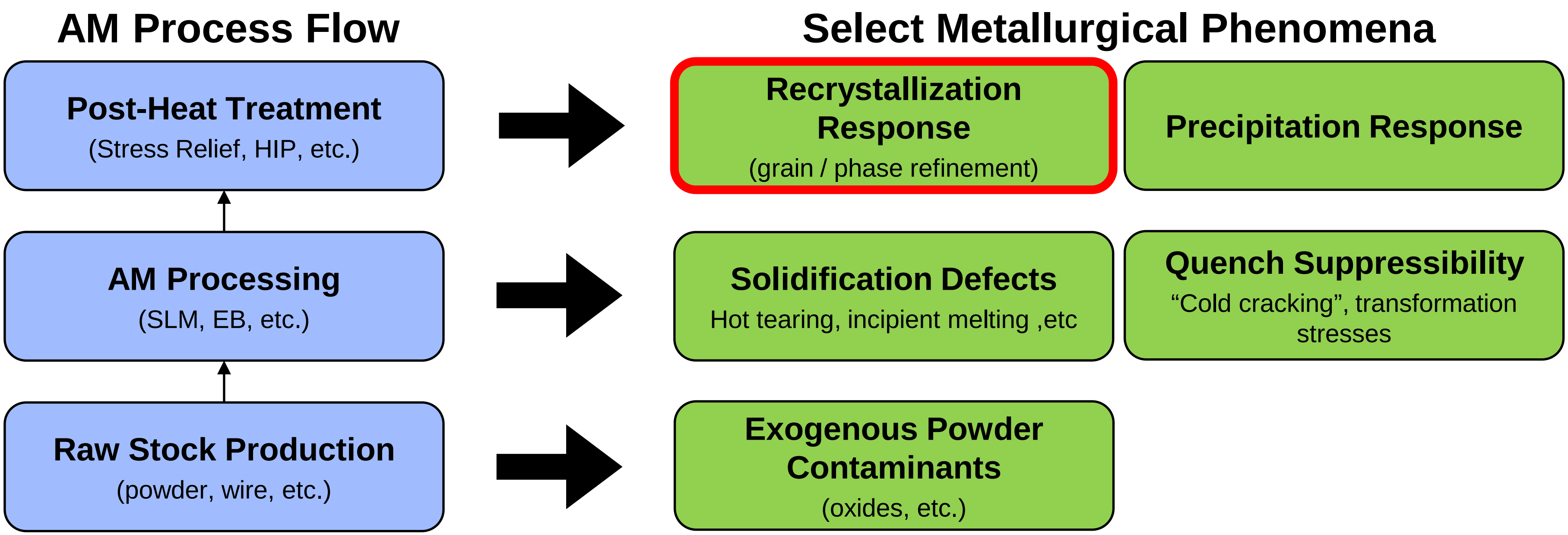
Select AM-specific Metallurgy

- AM materials respond differently to processing than their conventionally processed counterparts
- Unique microstructures in both as-built and post-processed conditions
- Post-processing responses are driven largely by:
  - Complexity of thermal history
  - Magnitude of residual stresses generated by process

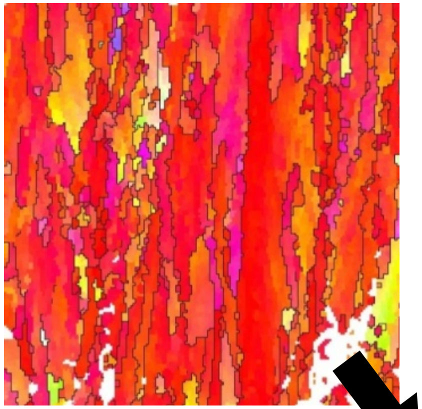


Existing alloys and post-process conditions not optimized for AM-specific behaviors, resulting in complex microstructures and unreliable AM performance

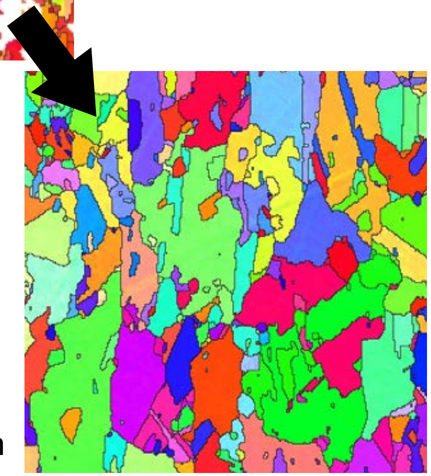
Case Studies from Current Research – Ni Superalloys

- AM residual stresses can drive recrystallization during post-processing
- If properly utilized, possible to mitigate many deleterious effects of AM
  - *Residual stress, anisotropy, property debits relative to wrought counterparts*
  - *Phenomenon exemplified in SLM of Ni superalloys*
- **Issue**: established materials and processes are not optimized for AM-specific recrystallization response
- **Opportunity**:
  - Linking process modeling (residual stress) with post-process modeling to optimize for this AM-specific response
  - Alloy and processing design to tailor behavior for AM

Residual Stresses can drive recrystallization during post-processing



As-built microstructure
- Heavily anisotropic



Stress-relieved
- Isotropic, fine grain

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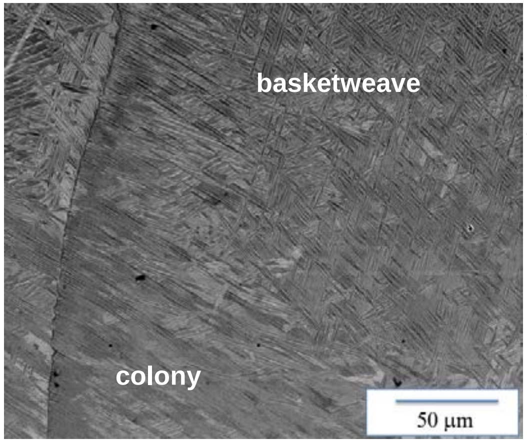
Case Studies from Current Research – Titanium

- Current Ti (e.g. Ti-64) rely on equiaxed, uniform microstructures for ductility
  - *Alloys optimized for wrought processing*
  - *AM-unique microstructures (cooling-rate driven - variable within build)*

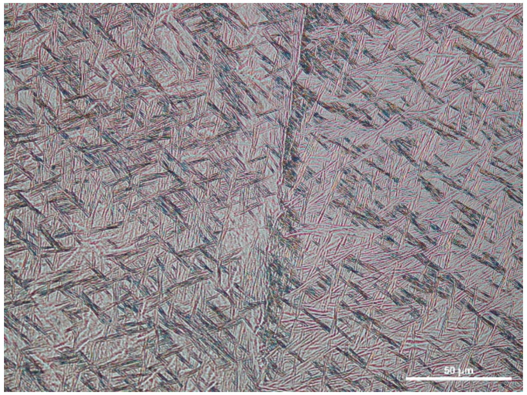
- **Issue:** Research showing this is not achievable in AM – resulting in severely limited performance in current EB Ti-64

- **Opportunity**: Computationally-driven alloy design to reduce cooling rate sensitivity
  - Circumvent need for recrystallization
  - Design goal: achieve uniform basketweave microstructure for EB process
  - Combined high strength+ductility, minimized anisotropy

Proper design of microstructures critical to predictability, reliability



EB Ti-64*
- Mixed microstructure
- Anisotropic



AM-designed EB-Ti
- Uniformly basketweave
- Isotropic and ductile

*P. Collins et.al, JOM 66(7) (2014) 1299-1309

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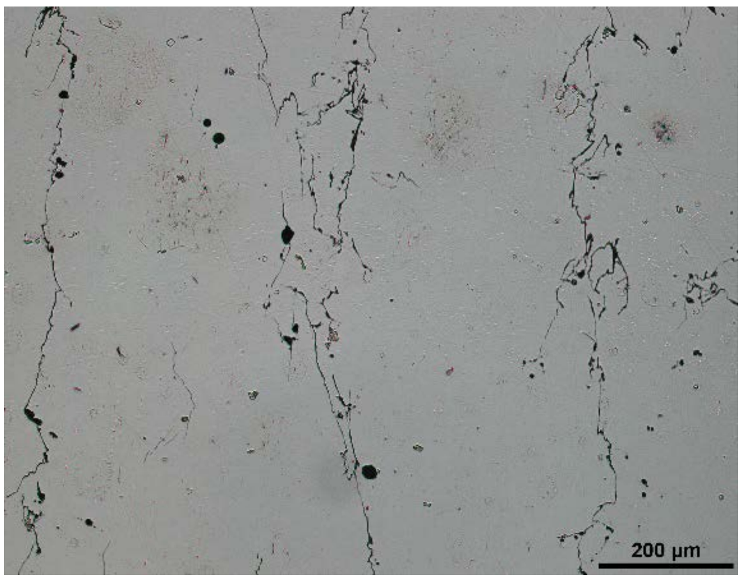
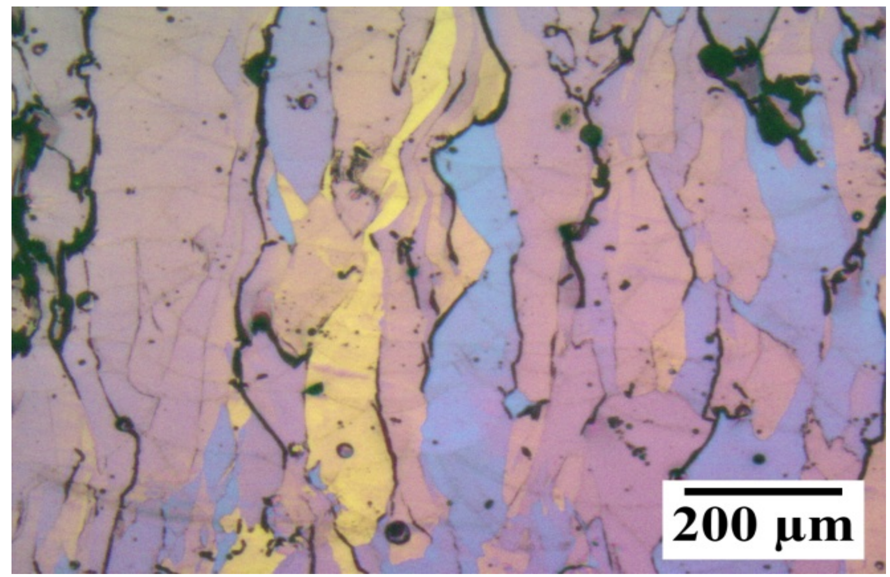
Case Studies from Current Research - Aluminum

- AM of high-strength Aluminum currently limited by *Hot Tearing* phenomenon
  - *Driven by high residual stress, sub-optimal solidification behavior*
- **Opportunity:**
  - *Integration of residual stress prediction with solidification theory (thermodynamics)*
  - *Design of new AM-specific alloys that address crack susceptibility*



Hot tearing in aerospace grade Al-Mg processed by DMLS

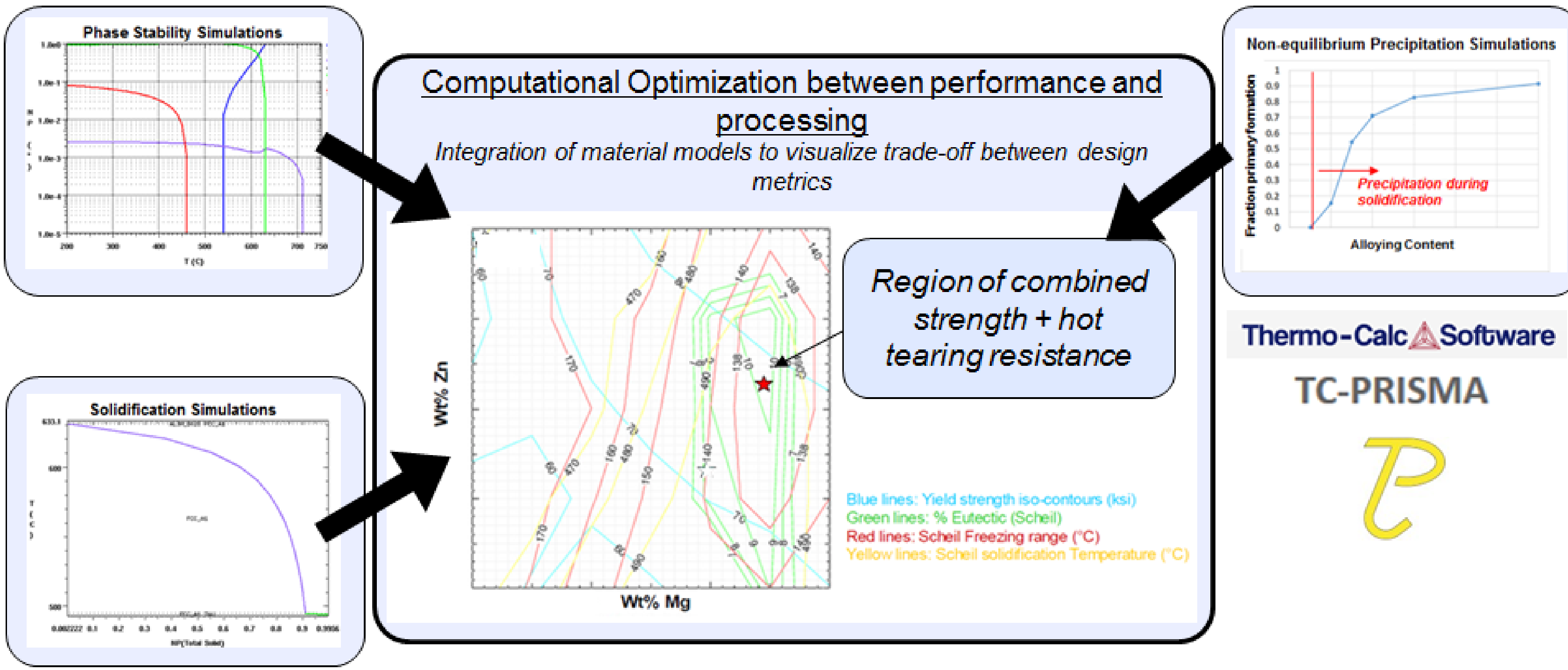


*Hot tearing in 6061 processed by DMLS**

*B. Fulcher et.al, SFF Symposium Proceedings, Aug 2014

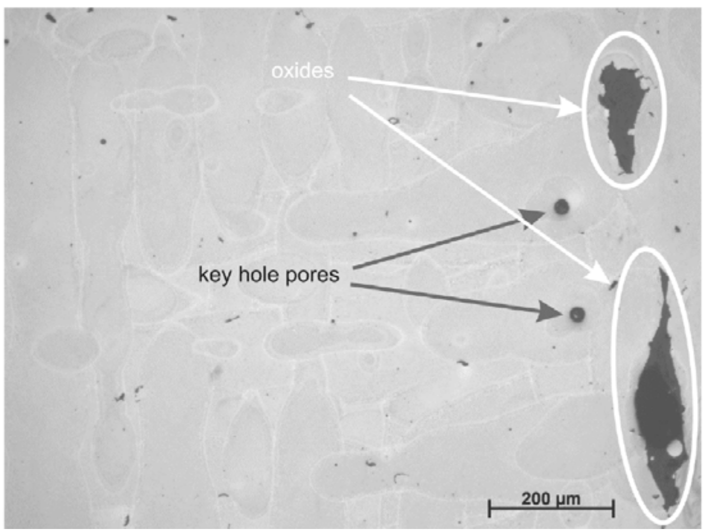
Example "Material Design for AM"

- Goal: Tailor a new 7xxx series (Al-Zn-type) to additive manufacturing:
  - Problem: Current AM Al-alloys (designed for casting) are low performance, and high-performance alloys (designed for forging) are not amenable to AM
  - Solution: Computational optimization between hot tearing susceptibility (processability) and precipitation strengthening (performance) for tailored material behavior



Other key AM-specific Material Responses

- Rare defects associated with exogenous powder contaminants expected to be a confounding factor for fatigue
  - ***Inclusions, contaminants, etc.***
  - *Hard lesson learned from PM+HIP superalloy technology*
- **Opportunity:**
  - *Process modeling accounting for exogenous defects (more than just porosity)*



Exogenous oxides in SLM Al*

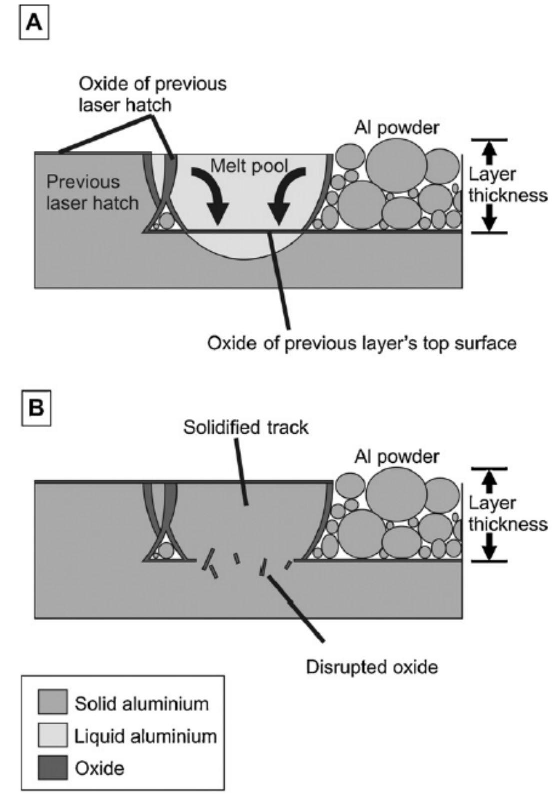


Fig. 19. (A) Marangoni convection in the melt pool. (B) Oxide disruption and solidification of the melt pool.

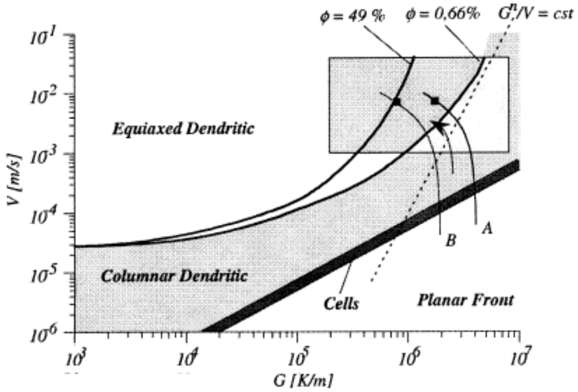
Theorized mechanism for oxide film entrapment in SLM Al**

**L. Thijs et.al, Acta Materialia 61 (2013) 1809-1819*
***E. Louvis et.al, J. Mater Proc Tech 211 (2011) 275-284*

Perspective on computational needs

- Some alloys (eg Ti64) highly sensitive to AM process, and so linkage between process and microstructure is critical
- Select Process-Microstructure modeling needs
  - Linkage between AM process models and solidification theory
    - *Columnar-to-equiaxed (CET) transition*
    - *Cellular-to-dendritic transition*
    - *Transformation kinetics (SDAS, 2nd-phase precipitation from liquid, etc.)*
  - Location-specific thermal history
    - *Input into solidification models, phase evolution models*
  - Residual stresses
    - *Input into recrystallization models*

- Better physical understanding of AM processes can drive targeted materials design for more predictable AM components

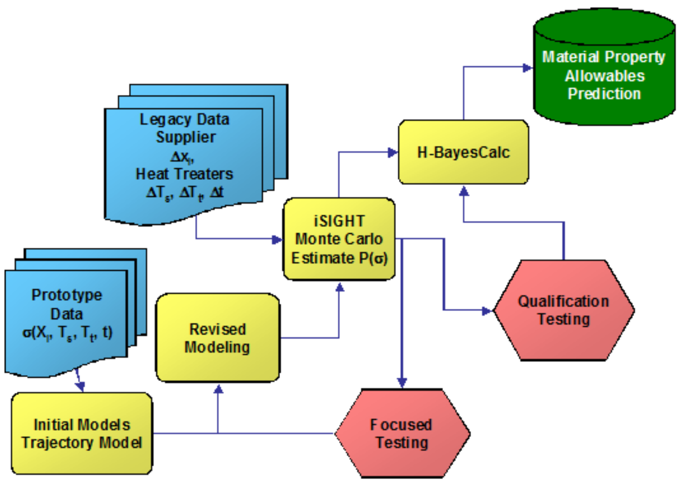


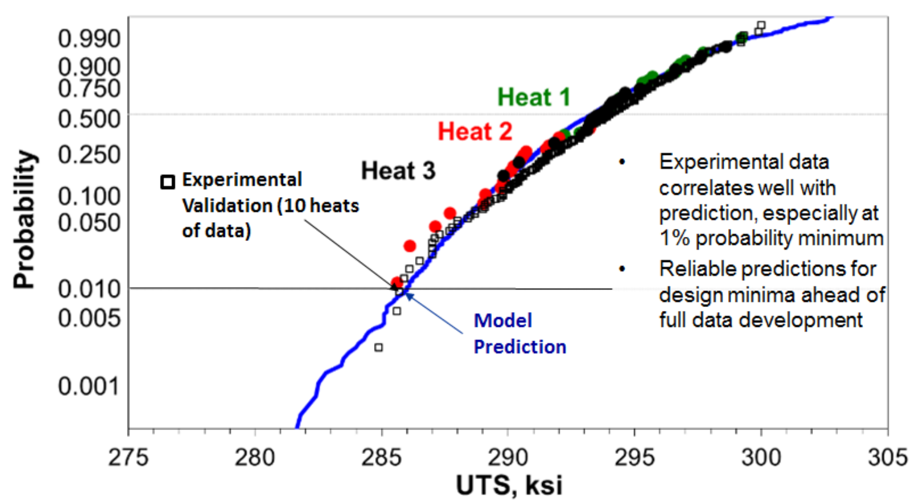
Example CET process map for CMSX-4*

**W. Kurz et.al, Sci Tech Adv Mater 2 (2001) 185-191*

ICME Qualification approach: "*Accelerated Insertion of Materials*"

- Current ICME approach to accelerated qualification of new material / processes
  - Coupling well calibrated, mechanistic property models with **predictable** sources of processing variation to project location-specific properties and design allowables
  - Currently extending AIM qualification framework into AM under DARPA Open Mfg (Honeywell)
    - Ni-superalloys





Case Study: AIM Qualification of Ferrium M54 UHS structural steel

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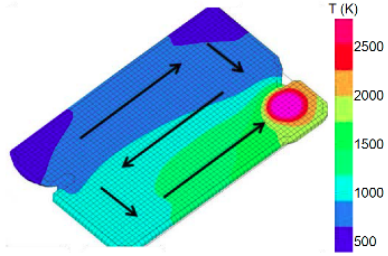
Process-microstructure-performance modeling for additive manufacturing

Direct Metal Laser Sintering (DMLS) Integrated Computational Materials Engineering (ICME) Framework

Finite difference physics process models predict location-specific thermal history of consolidated part:

- Gaussian moving heat source
- Melt pool with incorporated heat transfer, liquid radiation, and surface tension effects
- Cooling rate ~10^6 °C/s

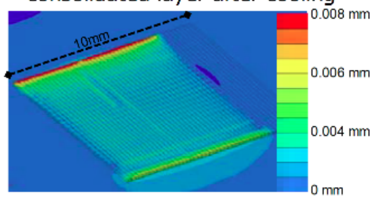
Temperature distribution from moving heat source during consolidation



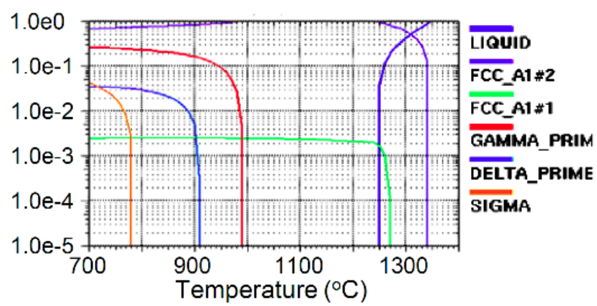
Microstructural models incorporate location-specific thermal history and predict

- Accumulated residual stresses
- Displacements
- strain hardening due to yielding
- Phase concentrations
- Grain size prediction dev underway

Displacement of single consolidated layer after cooling

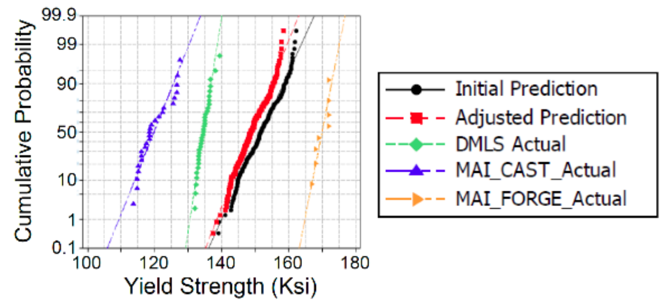


Phase concentration during cooling from melt



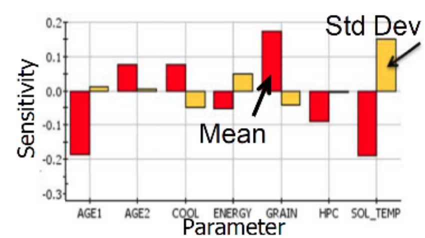
Yield strength prediction tool under development

- DMLS In718+ strengths significantly better than cast but much lower than forged
- Further incorporation of additive microstructural artifact effects needed



Qualification framework and uncertainty quantification indicates sensitivity for processing-property relationships

- Tensile properties are mostly driven by heat treatment (HIP, anneal, etc.)



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“Accelerated Insertion of Materials” (AIM) analysis to predict A-Basis Design Minima

- **Near-term issue: Process variables are well known in conventional processing, but not for AM!**
  - Need validated AM process models to provide input into true sources of AM-specific process variation, before such methods can see full utilization
  - Material dependent – driven by response to post-processing

- **Long-term issue: Qualification for additive manufacturing is really *Part* Qualification**
  - Qualification of material, process and component are linked
  - New qualification paradigm – *ICME approach uniquely suited*
  - Predictable materials are needed for predictable AM components

Perspective on Industrial need for computational advances in AM

- **Physical understanding of how material behaves during AM processing key to establish confidence for implementation**
  - Current adoption is being restricted by this lack of understanding
  - Fundamental modeling can shed light on physics of process to increase industry confidence
  - Modeling can help to down-select key variables for more targeted experimentation

- **Coupling in-process monitoring and modeling within an ICME framework critical for robust production**
  - Given the significant sources of variability in AM processes
  - Models that define select *quality metrics*, implemented with in-process monitoring to establish in-process *confidence intervals*

Long-term vision – AM-specific materials

Why do we need predictable materials?

- More reliable builds
- Reduced sensitivity to AM process variables
- Tailored microstructures
  - Mitigation of AM anisotropy
  - Design for AM-specific defects (e.g. inclusions)
  - Exploit AM-specific responses (e.g. rapid solidification and recrystallization)
  - *Existing materials are designed to do these things, why not AM-specific material specifications?*
- More predictable materials can simplify computational approaches

How to get there

- Materials design theories are there, what is missing is the **full** story of what makes any material "well-behaved" for AM
- Can process model insights facilitate AM materials design?