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)
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

AM Process Flow

- Raw Stock Production (powder, wire, etc.)
- AM Processing (SLM, EB, etc.)
- Post-Heat Treatment (Stress Relief, HIP, etc.)

Select Metallurgical Phenomena

- Recrystallization Response (grain / phase refinement)
- Solidification Defects: Hot tearing, incipient melting, etc.
- Precipitation Response
- Quench Suppressibility: “Cold cracking”, transformation stresses
- Exogenous Powder Contaminants (oxides, etc.)

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
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

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**Proper design of microstructures critical to predictability, reliability**

EB Ti-64*
- Mixed microstructure
- Anisotropic

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

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

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**Exogenous oxides in SLM Al**

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

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**Theorized mechanism for oxide film entrapment in SLM Al**


**E. Louvis et.al, J. Mater Proc Tech 211 (2011) 275-284*
Perspective on computational needs

- Some alloys (e.g., Ti64) are 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

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
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 $\sim 10^6 \degree C/s$

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

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?