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ASC Additive Manufacturing

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and
Marianne Francois, ASC AM Team Lead

June 8, 2015

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LANL ASC Additive Manufacturing Efforts

- LANL ASC AM ($1600k)
- Marianne Francois
  - ASC AM Team Lead
  - Process to Performance Modeling Integrator
- ASC IC Truchas Project ($800k)
  - Neil Carlson, Project Leader
  - Process Modeling
    - Ondrej Certik, Computational Physics and Methods (CCS-2)
    - John Gibbs, Metallurgy (MST-6)
    - Scott Runnels, Methods and Algorithms (XCP-4)
  - Solidification and Microstructure
    - Chris Newman, Fluid Dynamics and Solid Mechanics (T-3)
    - Terry Haut, Computational Physics and Methods (CCS-2)
- ASC PEM Materials Project ($800k)
  - Dean Preston, Project Leader
  - Materials Performance Modeling
    - Curt Bronkhorst, Fluid Dynamics and Solid Mechanics (T-3)
    - Veronica Livescu, Materials Science in Radiation and Dynamic Extremes (MST-8)
  - Reduced-Order Model
    - Scott Vander Wiel, Statistical Sciences (CCS-6)

Vision: Process-Aware Additive Manufacturing through Modeling and Simulation

Los Alamos
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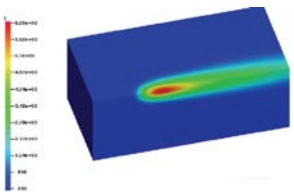
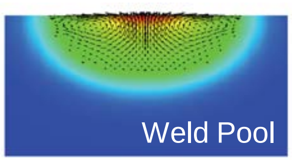
Process Modeling ⟷ Microstructure Modeling ⟷ Properties Modeling ⟷ Performance Modeling

Liquid/solid phase change

3D multi-physics microstructure-aware solidification capability

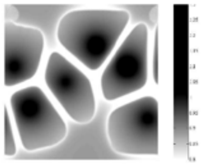


Moving heat source



Direct numerical simulation of grain growth

Initial grain distribution (nucleation site)

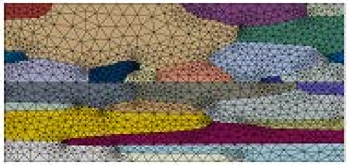


Final grain shape and composition

Solid/solid phase transformation

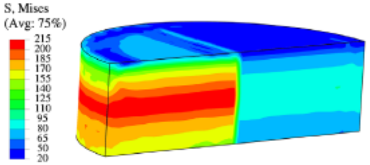
Polycrystal models to determine elastic, plastic, and damage properties

Polycrystal and grain boundary properties



AM specific interface properties

Thermal-mechanical models to predict elastic, plastic, damage, and failure processes



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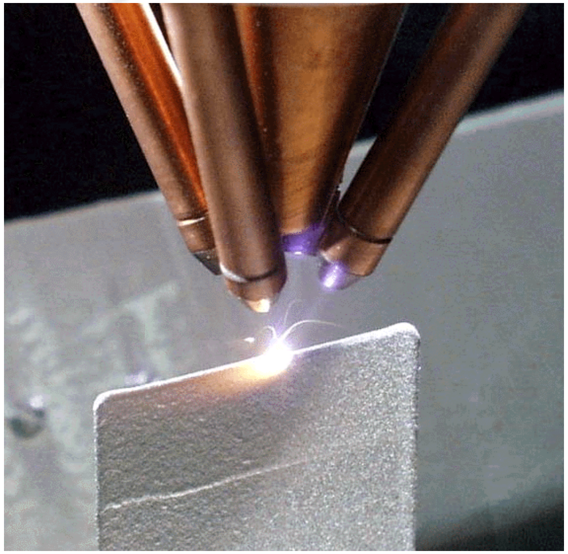
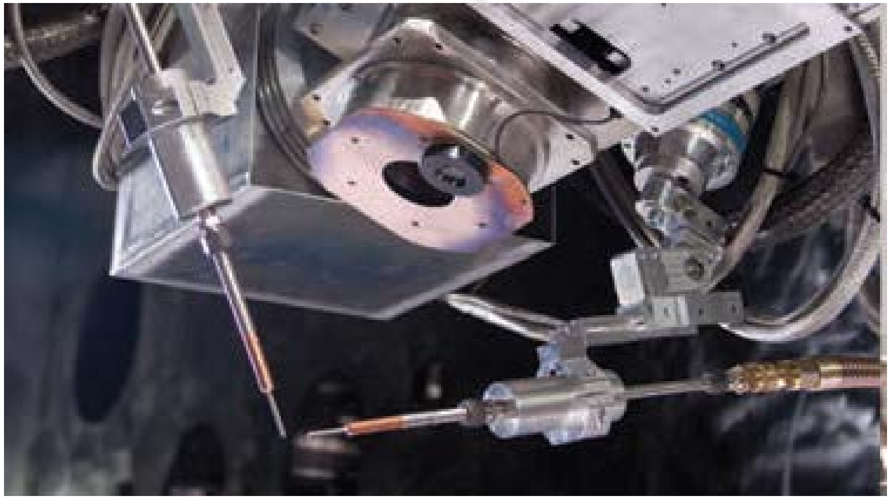
Focus on Directed Energy Deposition Technology





- E-beam or Laser as Heat Source
- Wire or Powder as Feedstock
- Sciaky (E-beam/Wire), Optomec (Laser/Powder)

Available Products

- Sciaky (US)
  - E-beam/wire
  - Maximum build volume
  - Decreased hazards
  - 4x higher deposition rate

- Optomec (US)
  - Laser/powder
  - Real time alloying
  - Minimized need for structural supports
  - Existing NDA

Material	Ultimate Tensile Strength (MPa)	Yield Strength (MPa)	Elongation (%)
LENS 316 Stainless Steel	799	500	50
316 SS Anneal bar	591	243	50
LENS Inconel® 625	938	584	38
IN 625 Annealed bar	841	403	30
LENS Ti-6Al-4V	1077	973	11
Ti-6Al-4V Annealed Bar	973	834	10

Long-Term Project Objectives

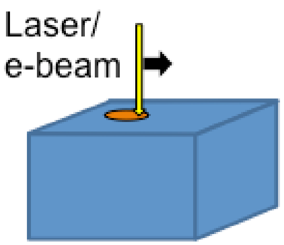
- Expansion of LANL existing modeling and simulation capabilities to direct energy deposition AM processes
- Integration of processing and performance modeling through microstructure prediction
- Validation with experimental testing as part of our methodology towards prediction and control
- Process modeling with Truchas: towards microstructure-aware process modeling
- Prediction of properties and performance of additively manufacturing parts

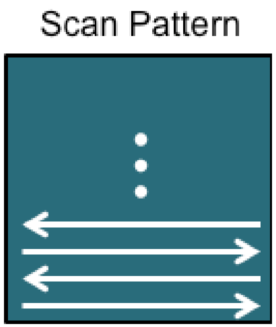
FY15 ASC Work Scope

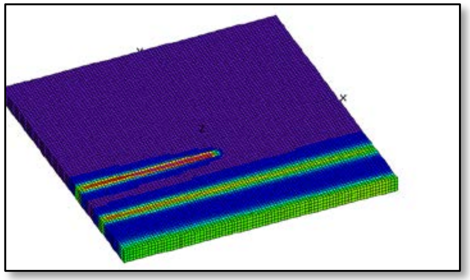
- Capability to model energy deposition in Truchas
- Evaluation and identification of high priority Truchas capability needs to model melt pool dynamics, residual stress and distortion for directed energy AM processes
- Preliminary capability of microstructure growth models applicable during the solidification process
- Capability to model single crystal stainless steel (SS)
- Thermo-mechanical studies of single deposited layer of SS and first estimate of polycrystal internal stress state
- Scoping studies of the development of fast-running emulators of slow running physics-based models for predicting properties of additively manufactured parts

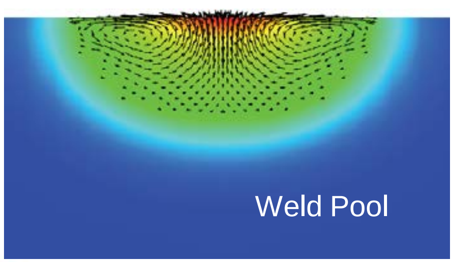
Truchas Process Modeling
Runnels, Gibbs, Carlson, Francois

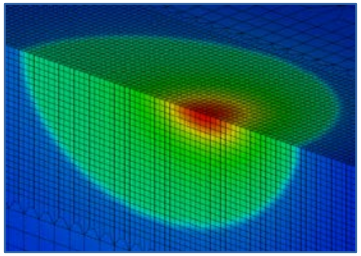
- Established a basic moving heat source scannir capability in Truchas; both volumetric and surfac flux forms.
- Developed coupled 3D heat transfer with phase change models in Truchas for 316 SS.
- Currently reestablishing and evaluating earlier Marangoni-driven weld pool flow dynamics.
- Started evaluation of Truchas models of residual stress and distortion.
- Working closely with AMIT team to determine built parameters

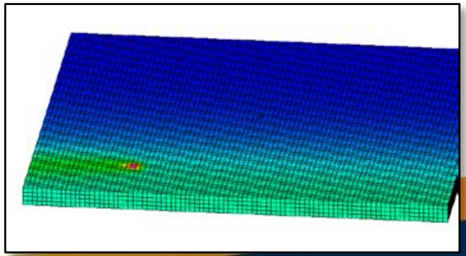












Solidification and Emulation

Developing a preliminary capability to predict microstructure evolution during the solidification and melting processes

Newman, Francois

- Developed advanced numerical methods for phase field
  - 2^{nd}-order time implicit integration methods resulting in gain in accuracy and computational time compared to explicit method
  - Structured and unstructured meshes
- Validated for single crystal growth

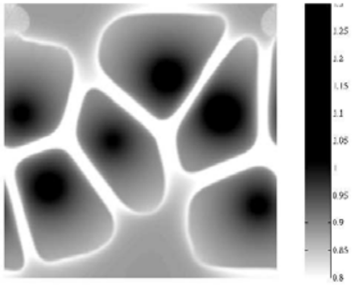
Fast Emulators of Slow Running Physics-Based Models to Predict Material Properties

Vander Wiel, Bronkhorst

- Identified physics to emulate and defined problem scope

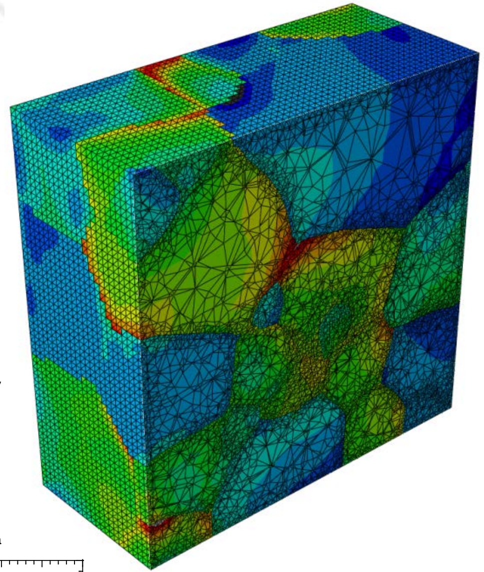
Initial grain distribution (nucleation sites)

Final grain shape and composition

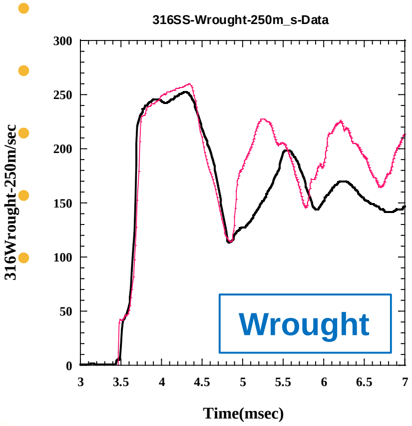


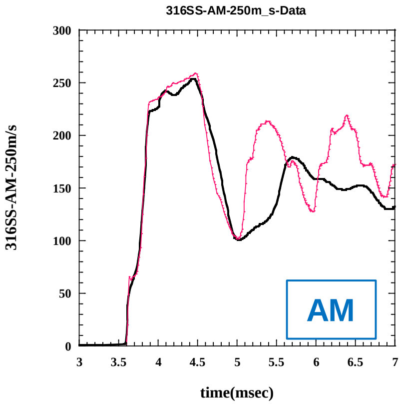
Material Perf. Modeling: Dynamic Response
Bronkhorst, Livescu, Vander Wiel

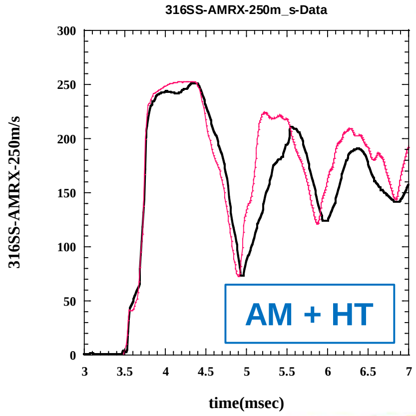
- Macro-scale analysis of 316L plate impact experiments are complete
- Experiments with AM materials with heat treatment (HT) to be redone with a new heat treatment schedule
- Developed polycrystal model to run through entire compression regime
- 316L metallography in progress (will guide modeling)
- Future polycrystal performance calculations for AM 316L will likely be 2D, with some 3D calculations for wrought materials and potentially for AM materials with heat treatment



Internal stress field







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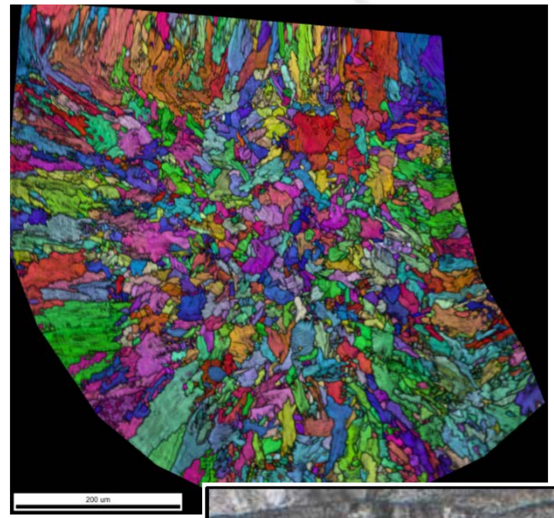
Material Perf. Modeling: Internal Stress
Bronkhorst, Livescu, Vander Wiel

- The microstructure within each of the weld beads suggests smaller and equi-axed grains in the center and elongated and larger grains around the perimeter
- Metallographically characterize grain morphology and crystallographic texture within single bead
- Develop a bead conforming 3D numerical model of an aggregate of weld beads
- Apply a Taylor model of the polycrystal within the model, which accounts for the number of grains and texture differences within bead
- Apply differing initial conditions to supply data for the reduced model



Weld bead microstructure

Weld bead aggregate

Integrated Additive Manufacturing Efforts

- LANL ASC Additive Manufacturing
  - ASC IC Truchas Project
  - ASC PEM Materials Project
  - Joint proposal written and submitted end of June to HQ
  - LLNL (lead), SNL, LANL and KCP
  - Funding direction announced in late September
    - LLNL $1.3M
    - SNL $1.3M
    - LANL $1.5M
    - KCP $150K
  - LLNL & SNL: powder bed system, design, and optimization
  - LANL: directed energy deposition
- Broad Integration
  - LANL Additive Manufacturing Implementation Team (AMIT): MST Division (D. Teter, D. Thoma, & G. Gray)
  - LANL-LLNL collaboration on thermo-physical data and material models
  - LLNL-KCP-LANL-SNL collaboration on:
    - Modeling the very early stages of melt-pool formation
    - Scoping studies on reduced-order models
    - End-to-end design vision: propagating the microstructural variability
    - Propagating the process variability into performance margins
    - Determining what is needed in terms of model predictability (e.g., residual stress and part distortion)
    - Where emulators are needed, and what is needed, in terms of simulation & experiments to support the building of emulators

Other Questions From HQ

- Importance to Mission
  - First coordinated attempt to ask the “process-to-performance” question
  - First activity pointed toward the 2024 Peg Post on Microstructure-Dependent Primary Performance
- Integration Efforts
  - See previous slide
- Impact
  - Progress being made
  - Deliverables are on target
  - But we are only six months into an informal project that begin with an abrupt start and continues with an uncertain future
- Challenges
  - An uncertain future
  - Appropriate budget for scope
  - Budget taken from existing scope, which necessitates the question, “What isn’t being done?”
  - Can process-aware, microstructure-dependent models be easily implemented in current or future ASC codes?

Questions?