Workshop on Predictive Theoretical and Computational Approaches for Additive Manufacturing, October 7-9 2015, Washington D.C.

LA-UR-15-27758

Los Alamos NATIONAL LABORATORY EST.1943

Towards Modeling and Simulation of Additive Manufacturing of Metals at LANL

Session 1: Theoretical Understanding of Materials Science and Mechanics

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- G. Gray
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- D. Tourret
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Questions to be addressed

- Fundamental scientific (AM) issues ?
- Fundamental theoretical and computational approaches needs to fully understand AM ?
- Most important questions in materials and mechanics, engineering and mathematics ? Technical challenges for predictive theoretical and computational approaches in order to enable widespread adoption of AM ?
- Opportunities in R&D for theoretical and computational materials science, mechanics and multiscale computations
- **To address these questions, I will use LANL nascent effort in modeling and simulation of additive manufacturing of metals as example**

Fundamental AM issues

- How do we move toward a science-based qualification of AM metals ?
- How do we shorten qualification cycle ? (reduce cost)
- Currently, there is no Additive Manufacturing (AM) certified process, no standard, and there is a lot of variability
  - Multiple AM processes (powder-bed, directed energy deposition,…), various operating conditions and control parameters (power, scanning patterns,…), feedstock quality, post-processing (heat treatment)
- → **Need for fundamental understanding through scientific methodology integrating experiments with theoretical modeling and simulation.**

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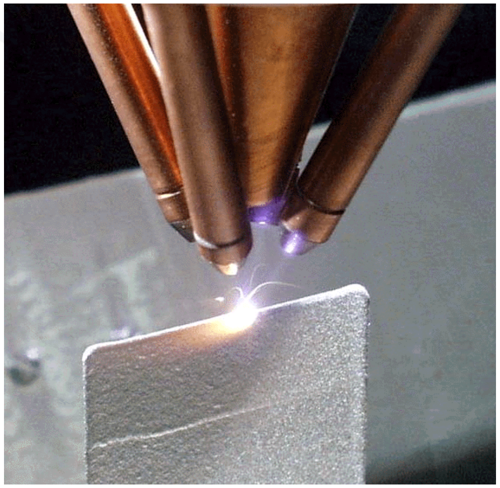
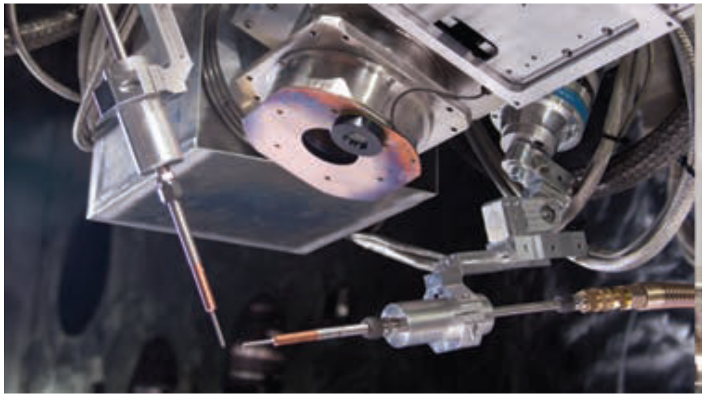
LANL Additive Manufacturing of Metals

- Part of multi-lab effort

(LLNL, SNL, LANL and NSC)

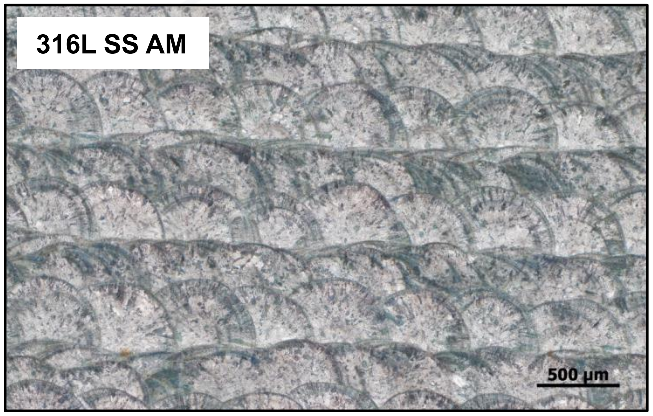
- LANL focuses on directed energy deposition system
  - Ebeam or laser as heat source
  - Powder or wire as feedstock
  - Optomec (laser/powder), Sciaky (e-beam/wire)

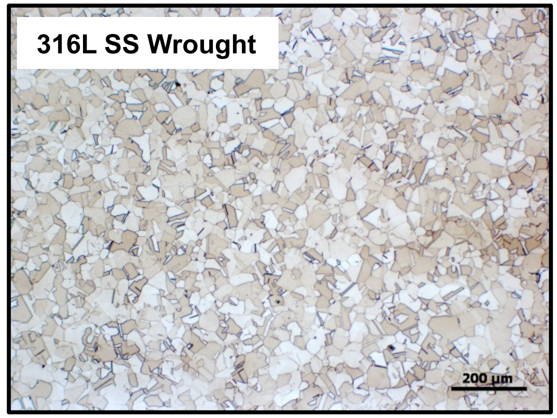


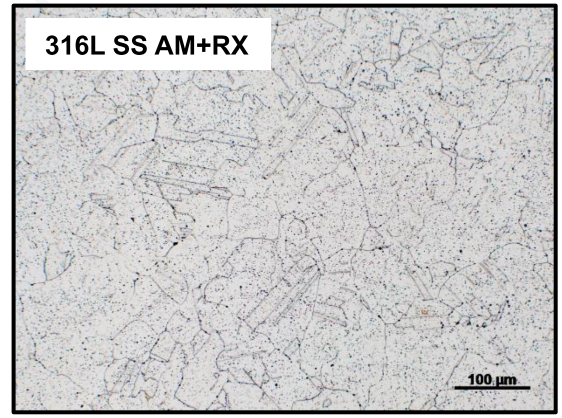


Fundamental scientific issues:
Same 316L SS material but different microstructures

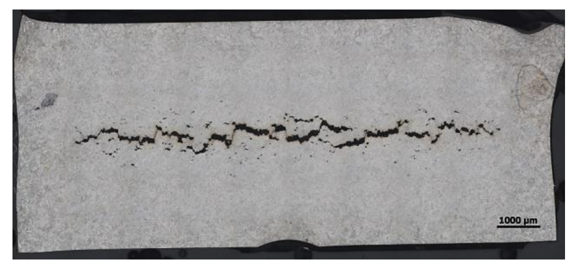
- Difference in processing results in microstructural differences







- Difference in microstructure results in performance differences



257m/s Flyer Impact Triple Shot

Ref: Gray, LANL MST-8

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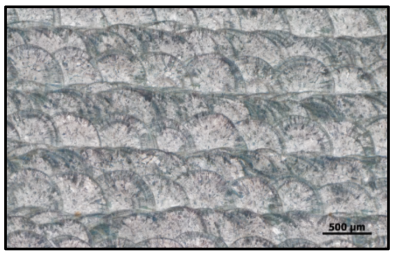
Theoretical and Computational Approach Needs

- Integration of processing and performance through microstructure prediction

316L SS AM



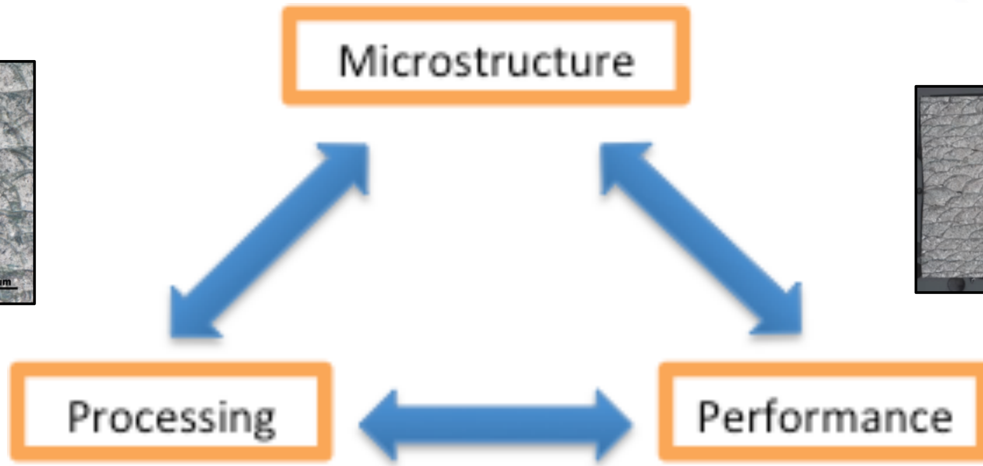


Plate impact response

- Need to develop **advanced modeling and simulation capabilities** for AM processes along with **experimental testing** as part of our methodology **towards prediction and control**

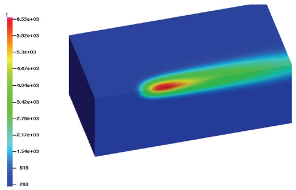
Long term vision: microstructure-aware modeling from materials processing to mechanical performance

Process Modeling ⟷ Microstructure Modeling ⟷ Properties Modeling ⟷ Performance Modeling

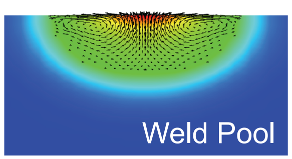
Liquid/solid phase change

Solid/solid phase transformation

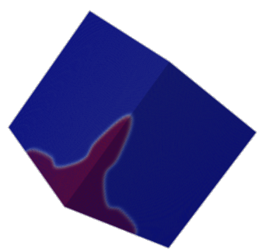
3D multi-physics microstructure-aware solidification capability



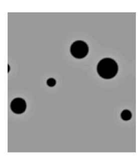
Moving heat source



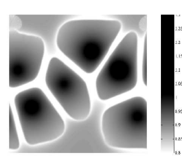
Direct numerical simulation of grain growth



3D single grain growth

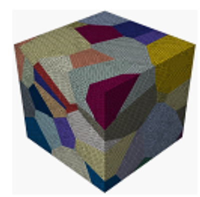


Initial grain distribution (nucleation site)

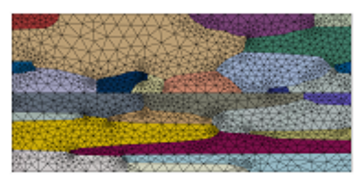


Final grain shape and composition

Polycrystal models to determine elastic, plastic, and damage properties

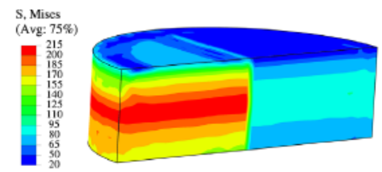


Polycrystal and grain boundary properties



AM specific interface properties

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



Mesoscale to macroscale prediction of performance

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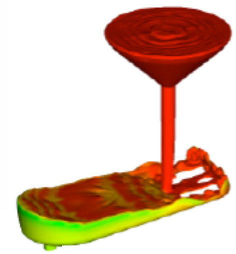
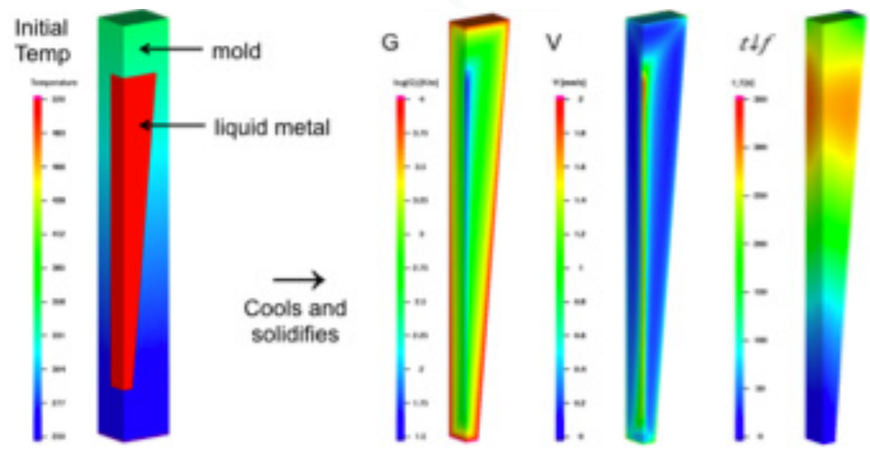
TRUCHAS a computational tool for modeling material processing

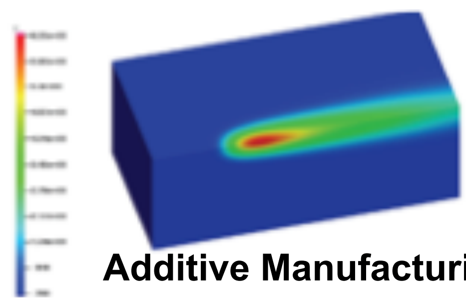


Mold Filling

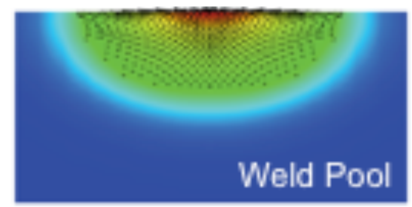
- A 3D multiphysics package: fluid flow with interface tracking and surface tension, heat transfer with phase change, species diffusion, chemical reaction and solid mechanics
- Complex geometries
- Initially developed to model casting processes, extended to model welding in 2006
- Currently being extending to model direct energy deposition AM processes



Nuclear Fuel Rod Casting



Additive Manufacturing



Welding

3D Simulations of Laser Spot Welding of 304 Stainless Steel – a Validation Study

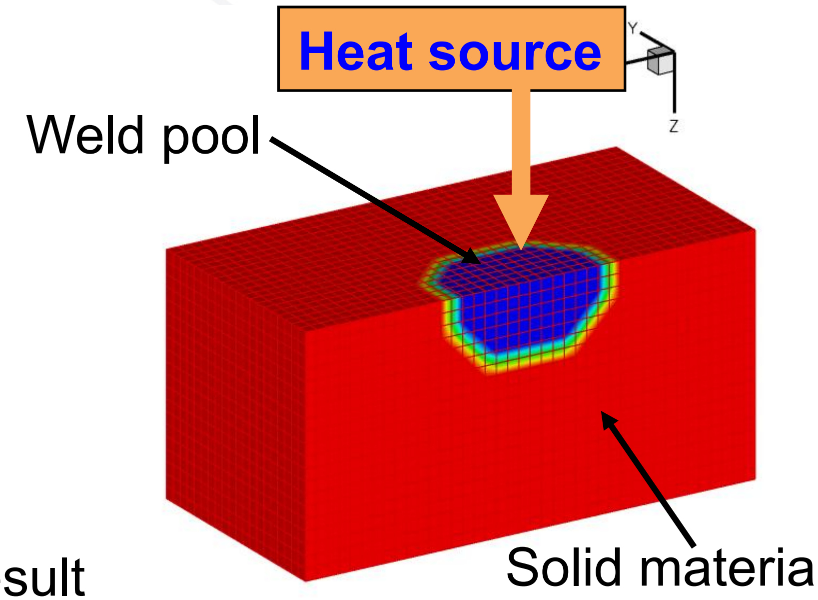
Ref: Parietti, Lam, LA-UR-06-7622

- Domain [-0.5,0.5]x[0,0.5]x[0,0.5] mm
- Laser power Q = 530 W
- Properties as in He et al. (2003)

  Solidus temperature 1697 K

  Liquidus temperature 1727 K

  $d\sigma/dT = -4 \times 10^{-4}$ N/m
- Heat Transfer + Phase change + Flow
- Heat source applied from t=0 to 4 ms result in melting of the solid material
- At t=4ms, solidification starts
- Convection in melt driven mainly by thermocapillary force



Surface Heat Flux with Gaussian distribution

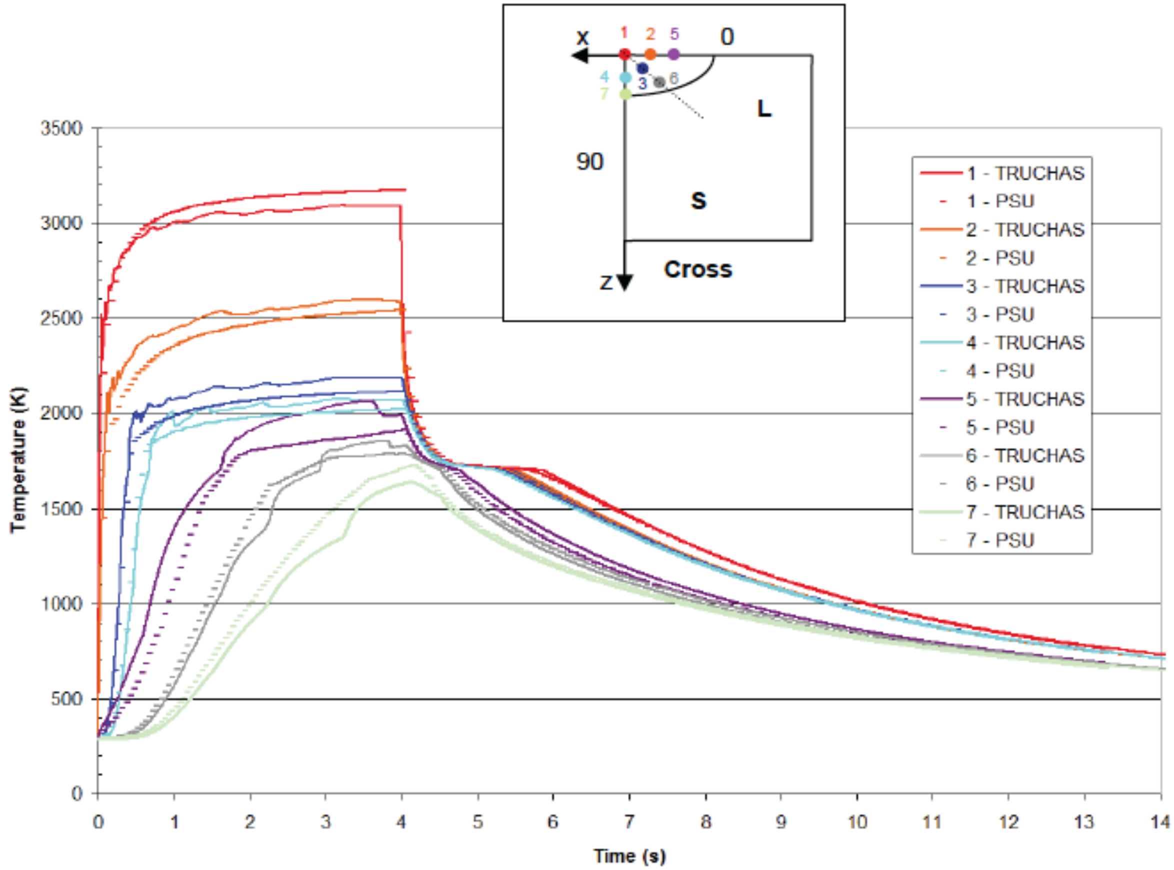
$$\Phi(x,y) = \frac{3Q\eta}{\pi r_b^2} e^{\frac{3(x^2-y^2)}{r_b^2}}$$

η absorption coefficient

r_b beam radius

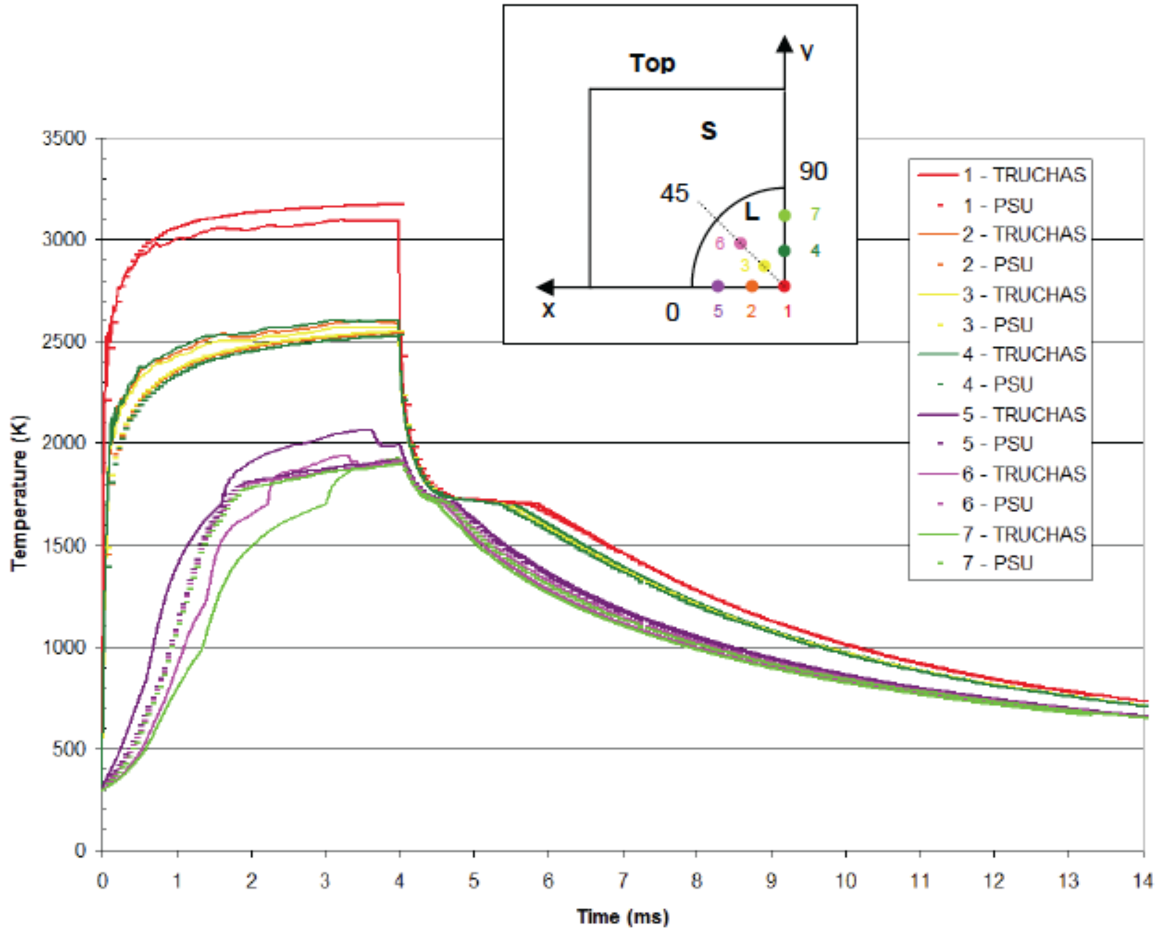
Laser Spot Welding of 304 Stainless Steel - Validation Temperature Histories Cross-section

Ref: Parietti, Lam, LA-UR-06-7622



Laser Spot Welding of 304 Stainless Steel - Validation Temperature Histories Top Surface

Ref: Parietti, Lam, LA-UR-06-7622



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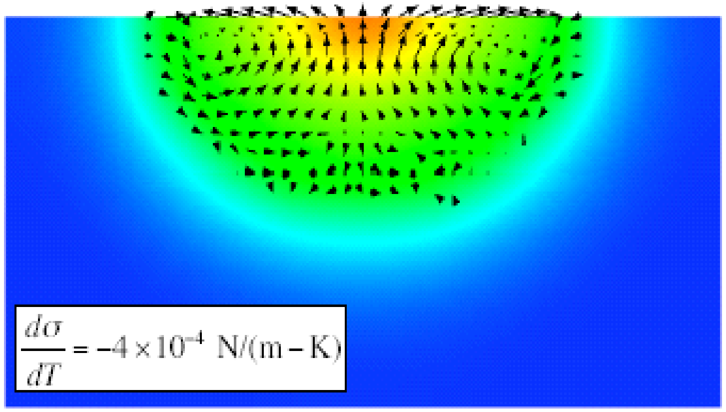
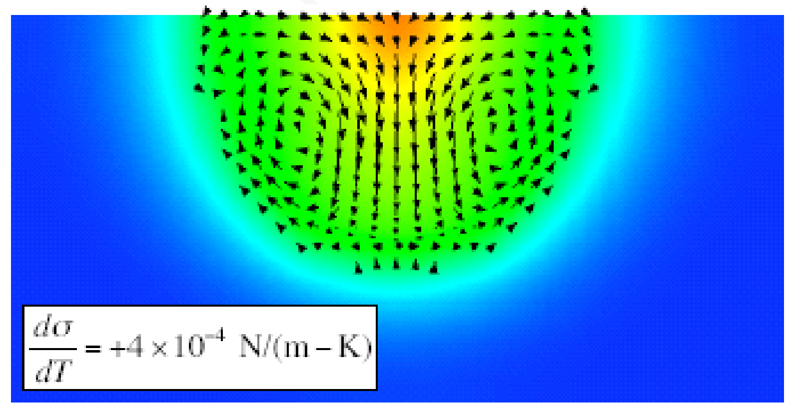
Marangoni convection determines weld pool shape

Laser Spot Welding of 304 Stainless Steel
Temperature contours and velocity vectors



Negative gradient
→ outward flow
→ shallower weld pool



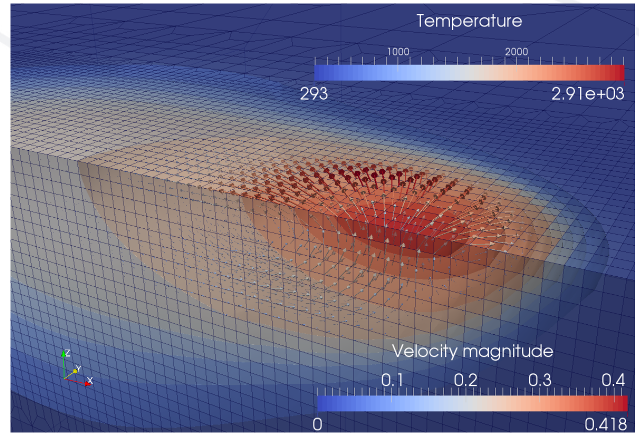
Positive gradient
→ inward flow
→ deeper weld pool

- Surface tension properties vary with composition and temperature
- Any impurity will change melt pool shape and size
- In AM: powder particles effects (fully or partially melted), melting and re-solidification cycle (scanning pattern effect), chemical composition, surface instabilities, …

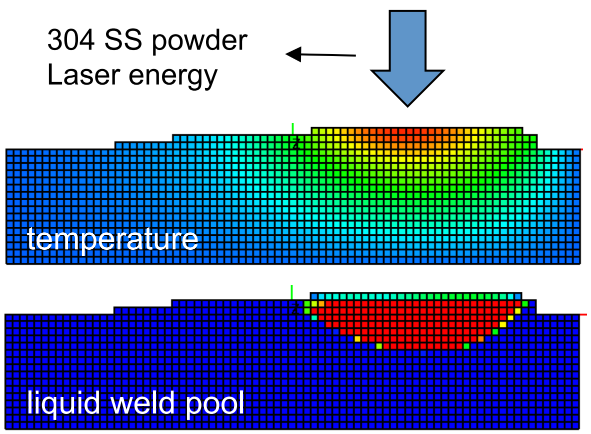
ASC Truchas code extended to model AM

- Open source Truchas metal casting code is being extended to AM process modeling, esp. directed energy processes (e.g. LENS)

- Capabilities assessed via testing on AM process problems involving heat transfer/phase change, weld pool fluid flow (Marangoni effect), and residual stress/distortion.



Marangoni flow in weld pool during single weld bead pass in 304 SS.



- Short-term: Implemented preliminary heat/mass deposition models:
  - moving heat flux boundary conditions for simpler models;
  - fully moving powder/laser energy deposition at evolving material surface embedded within the computational domain (volume-of-fluid).
- Next: more physics models and V&V
- Microstructure-aware solidification models

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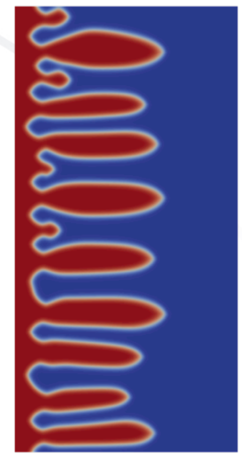
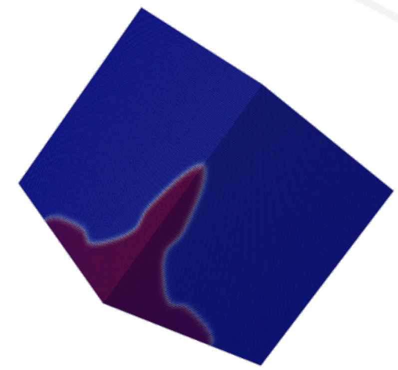
Microstructure capability development

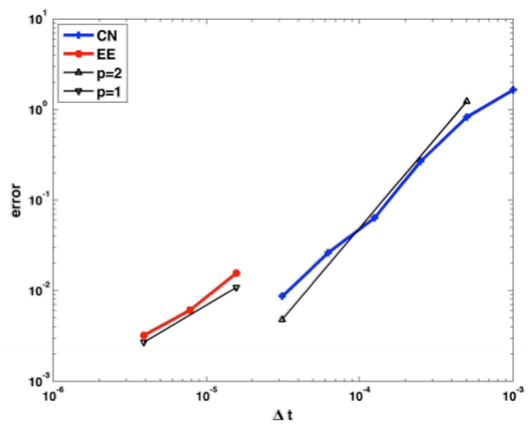
- Phase field approach to microstructure solidification simulation utilizing modern algorithms and software.
- *Finite element* allows for high-order spatial discretization on unstructured 2D/3D meshes.
- *Implicit time integration* allows for stable, second order with large time steps.
- Second-order implicit shows better efficiency over first-order explicit.
- Unstructured mesh allows for irregular (curved) geometries.



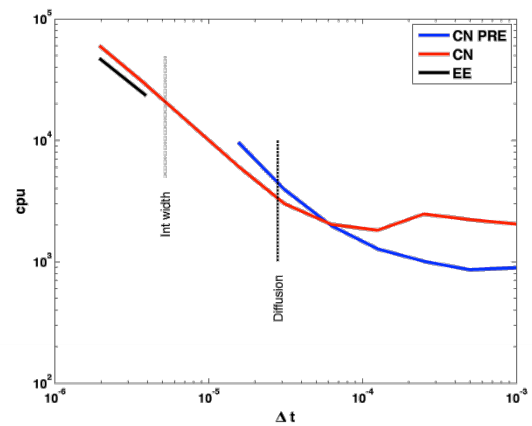
Multiple dendrite growth along flat boundary. (Preliminary result)



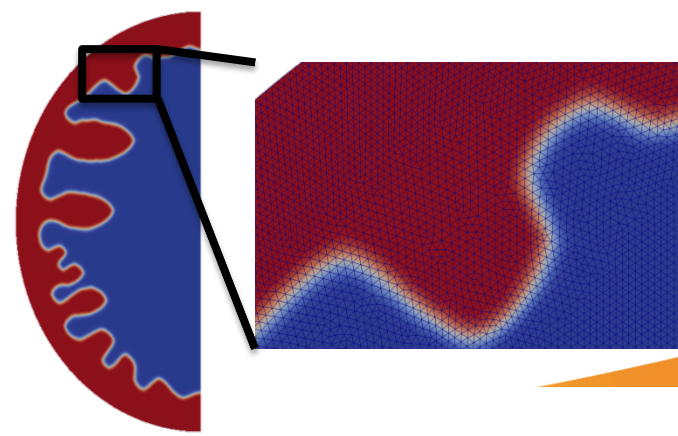
3D single dendrite growth.



Accuracy as a function of timestep size for implicit (--) vs explicit (--).



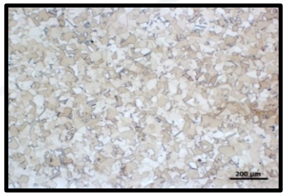
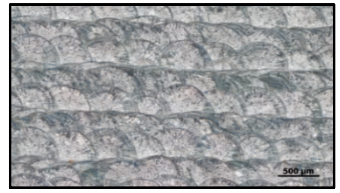
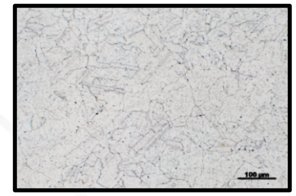
Efficiency as a function of timestep size for implicit (--,--) vs explicit (--).



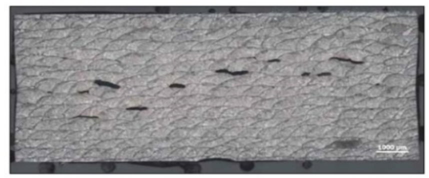
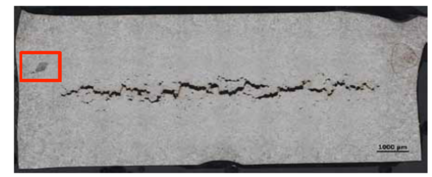
Multiple dendrite growth along curved boundary, unstructured mesh. (Preliminary result)

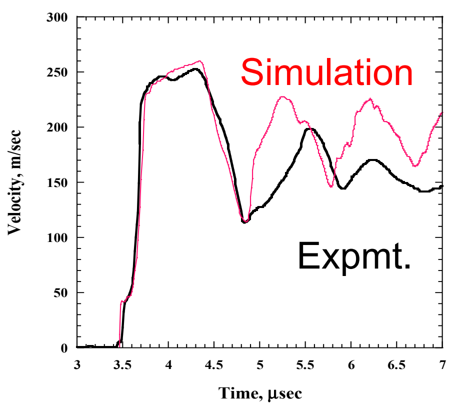
Additively Manufactured Material – 316L Performance Modeling of Plate Impact Response

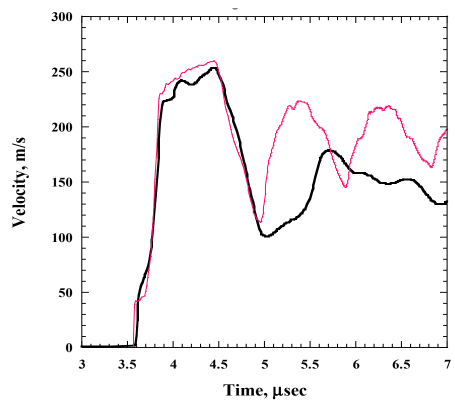
AMIT Materials & Expmts., G. Gray et al.

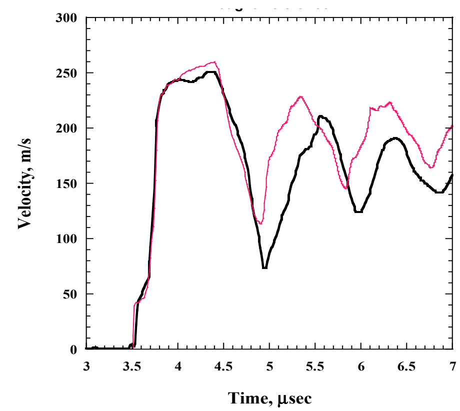




Wrought | LENS Additive | Heat Treated Additive





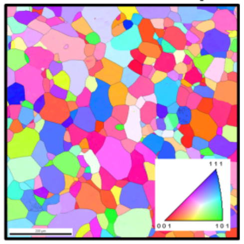


Parameterization | Prediction | Prediction

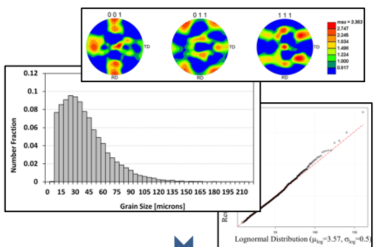
- Influence of microstructure on damage performance is significant.
- Not yet possible to represent the additive microstructure adequately to successfully predict dynamic damage with simple macro-scale models.

316L Metallographic Characterization

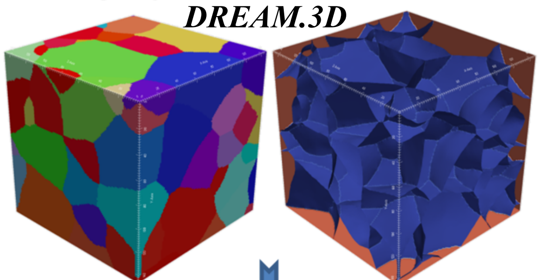
Real 2D/3D Data from Experiments



Microstructure Statistics



Digitally Generated Microstructure
DREAM.3D

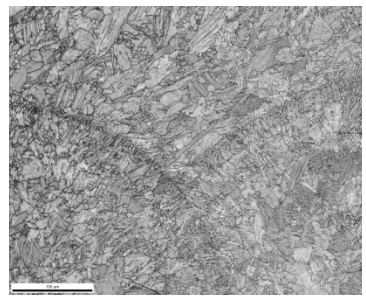


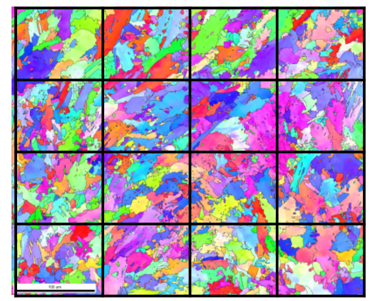
PATRAN FEM Software with Advanced Surface Meshers

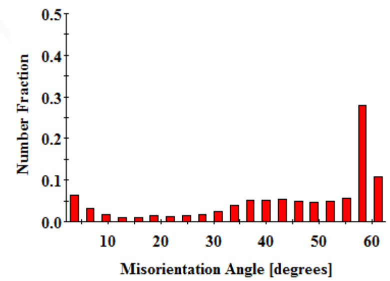
ABAQUS + Dynamic Damage Model

AM material

- EBSD data acquired
- Working on texture and Euler angles data export

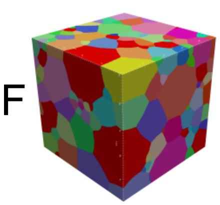




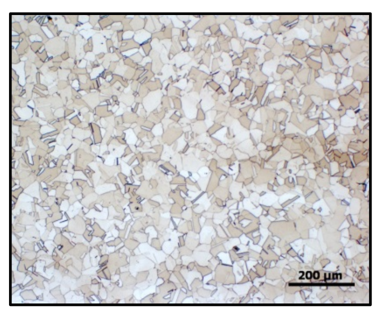


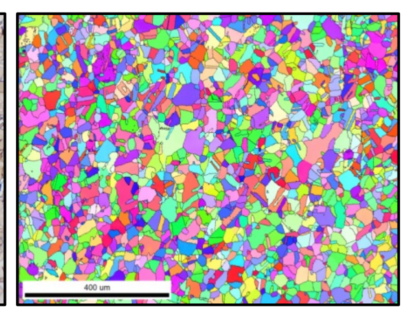
Wrought material

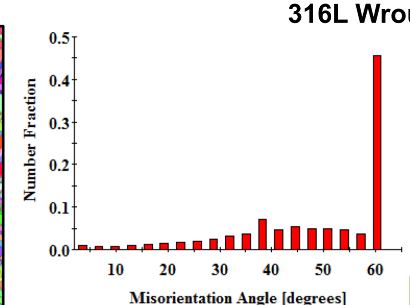
- EBSD data collected
- Found statistical distribution of grain sizes and ODF
- Working on twin insertion within Dream3D



316L Wrought







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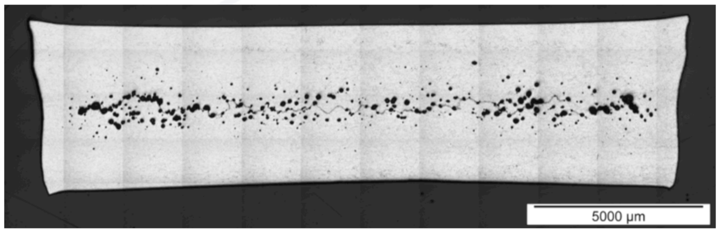
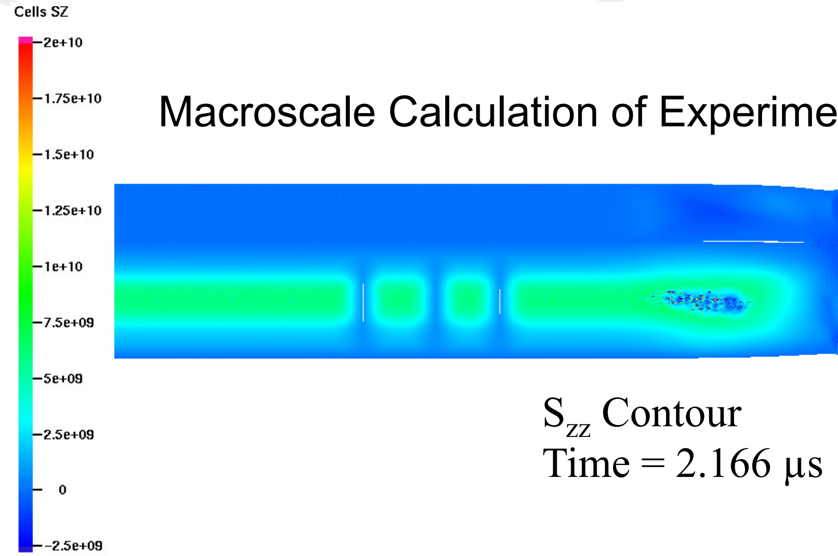
Macroscale Performance Linkages To Microstructural Modeling

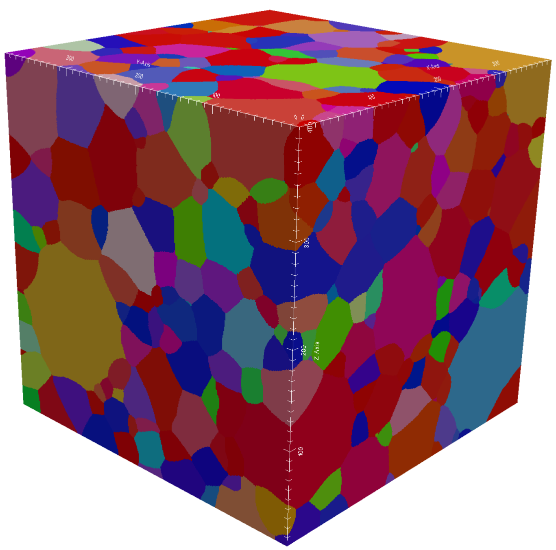


Tantalum on Tantalum Experiment

Macroscale Calculation of Experiment



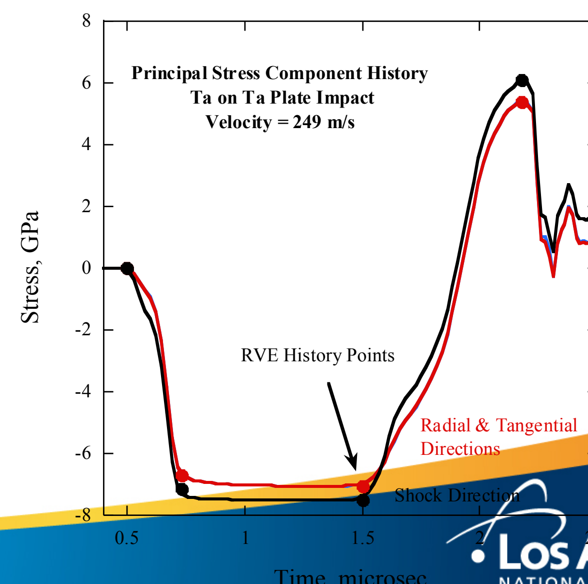
S_{zz} Contour
Time = 2.166 µs



Virtual Equivalent Microstructure

Prediction of macroscale performance will require microstructural representation

Calculated Principal Stress History



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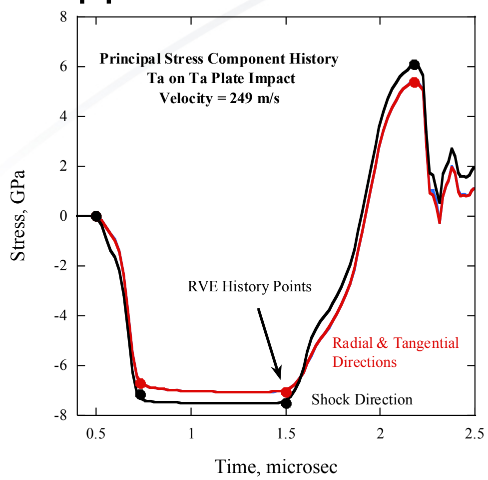
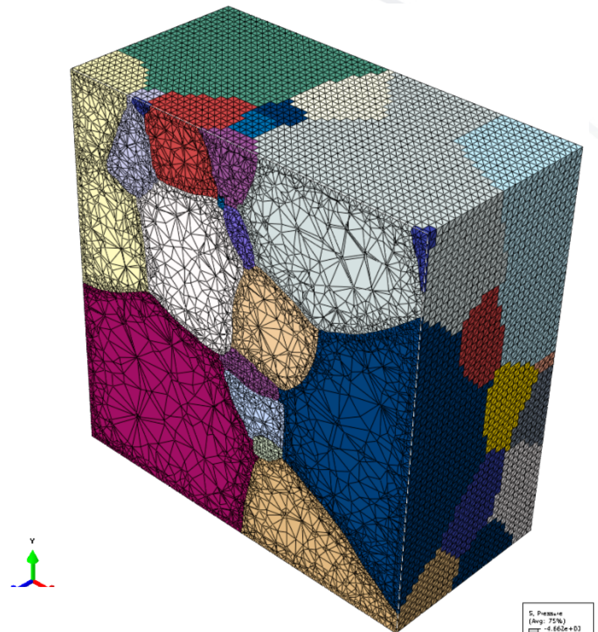
Dynamic Loading Conditions Applied to Statistically Equivalent Tantalum Numerical Microstructures

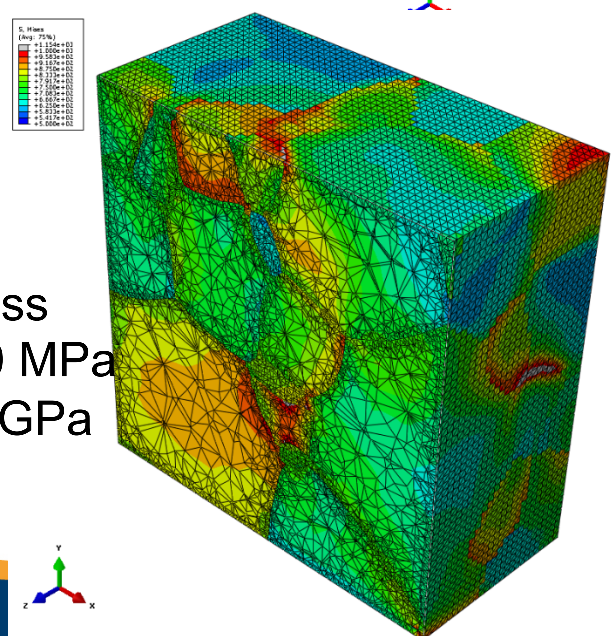
Applied Stress History



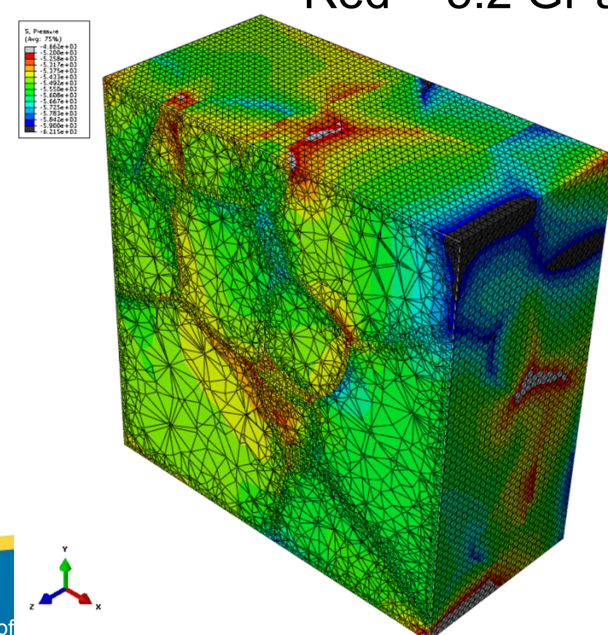


70 grain Realization

Pressure
Blue = 5.9 GPa
Red = 5.2 GPa

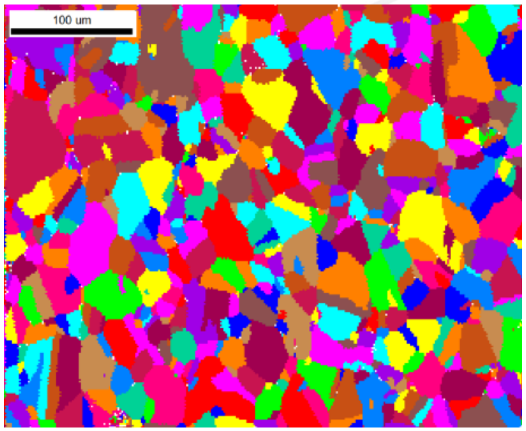


Mises Stress
Blue = 500 MPa
Red = 1.0 GPa



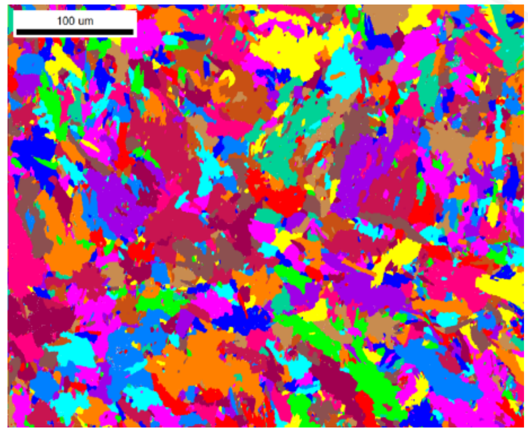
Additively Manufactured Material – 316L
Performance Modeling of Strength Difference

Different colors represent different crystallographic orientations



Wrought

Mean Grain Size = 15.9 μm

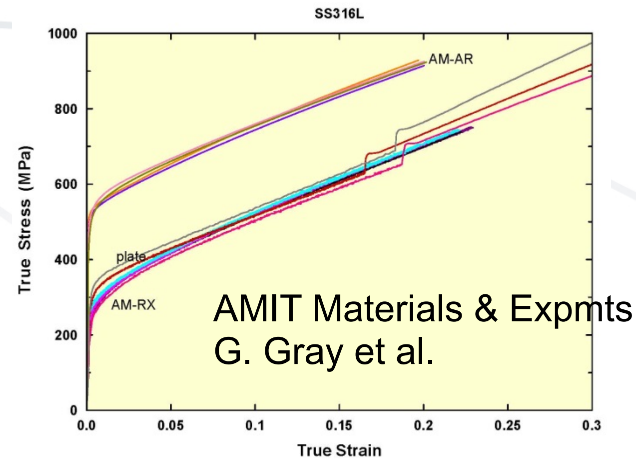


LENS Additive

Mean Grain Size = 4.4 μm

Numerical Polycrystal Models

Crystallographic orientation is translated to the numerical models but not color represented.



Greater strength in additive material

- Smaller grains generally increase strength in metals.
- Hypothesis: Grain size difference in part responsible for observed strength difference.

Hall-Petch relationship between grain size and plastic flow resistance being applied at grain level in polycrystal models.

Long-term Objectives for Predictive Methods in AM

- Integration of processing and performance modeling through microstructure prediction
- Validation with experimental testing (in-situ) as part of our methodology towards prediction and control
- Multiscale process modeling: microstructure-aware
- AM materials modeling and multiscale mechanical response (performance) modeling
  - Processing phase change and microstructural evolution
  - Cooling internal stress development linked to microstructure
  - Plasticity and structural feature damage prediction

Opportunities for Theoretical and Computational Predictive Methods in AM

- Material Processing
  - Melting/solidification and re-melting/solidification cycles, melt pools, microstructure morphology evolution, composition distribution (alloy), liquid-solid phase change models
  - Linkage of microstructure information to macroscale model (thermal gradient and cooling rate maps)
  - Residual stresses
- Mechanics of Materials
  - AM materials models (properties,…), solid/solid phase transformation
  - Plasticity/damage modeling
  - Linkage of microstructure information to macroscale model
- Faster computational methods
  - Reduced order models, fast emulators for process control
  - Robust, efficient and accurate numerical methods (implicit methods) for high-fidelity physics-based simulation