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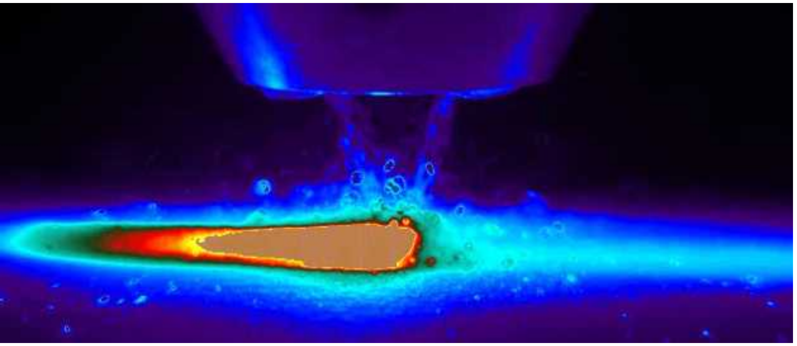

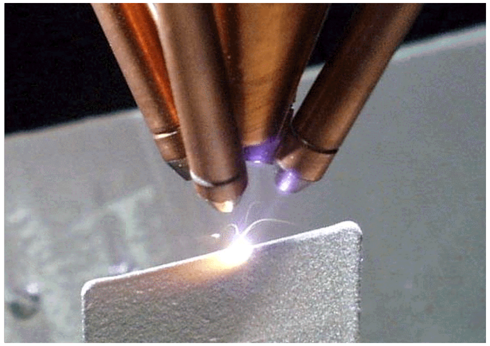

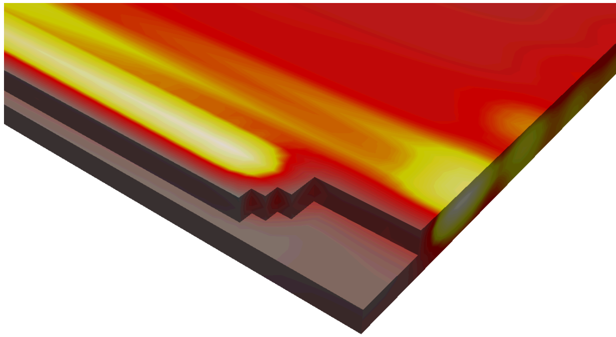

Modeling the Life Cycle of High Throughput Tensile Specimens Produced by Laser Powder Bed Fusion: From Fabrication to Performance

Kyle Johnson, Kurtis Ford, Joe Bishop, John Emery, Bradley Jared, Jon Madison, Carl Jacques, and Burke Kernen

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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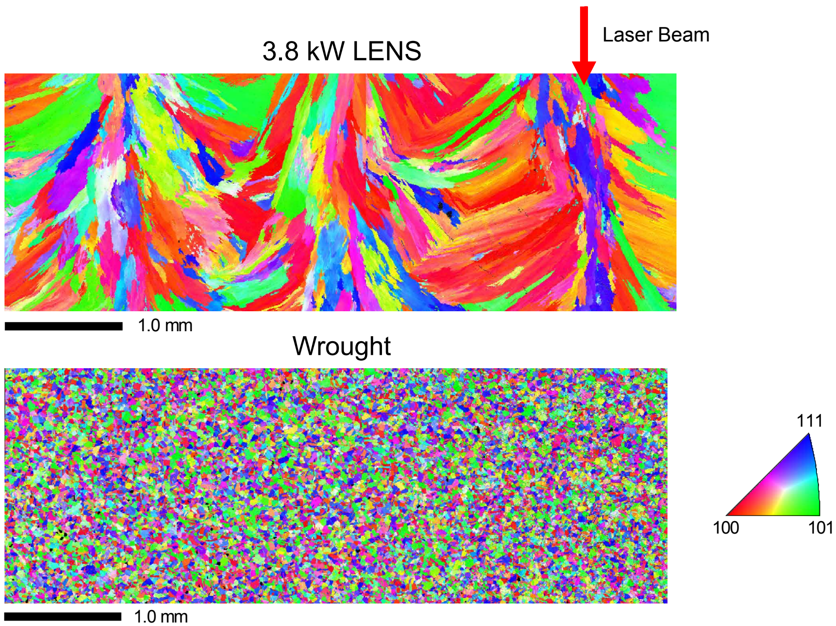
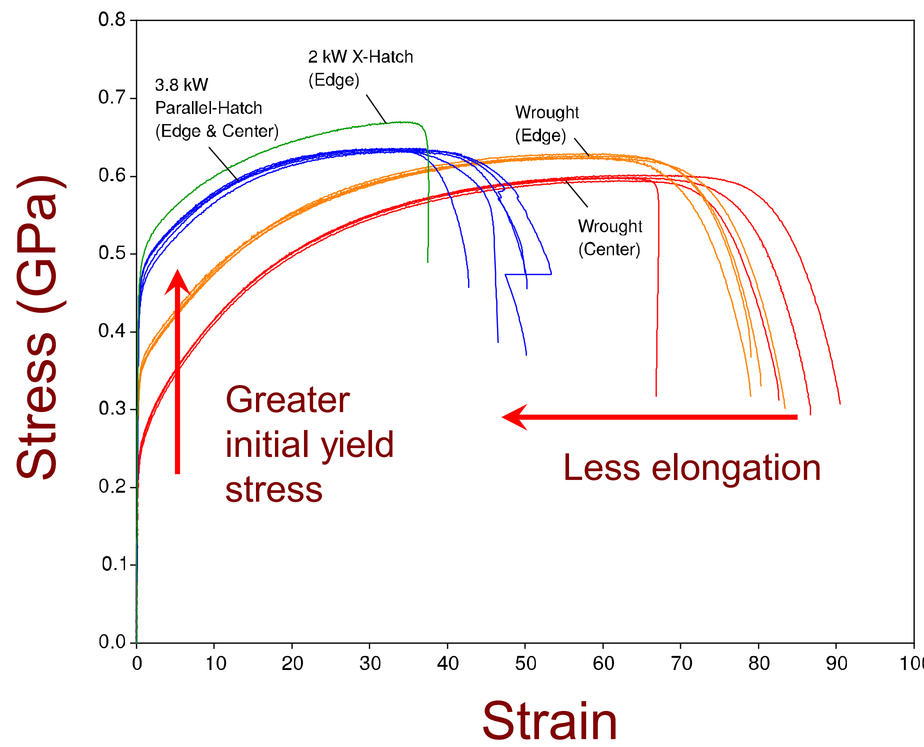
Outline

- Background
- Thermal Modeling and Solid Mechanics Modeling in Sierra
- Dogbone Gage Section Models
- Mechanical Property Predictions
- Future Work

AM Can Produce Extreme Properties



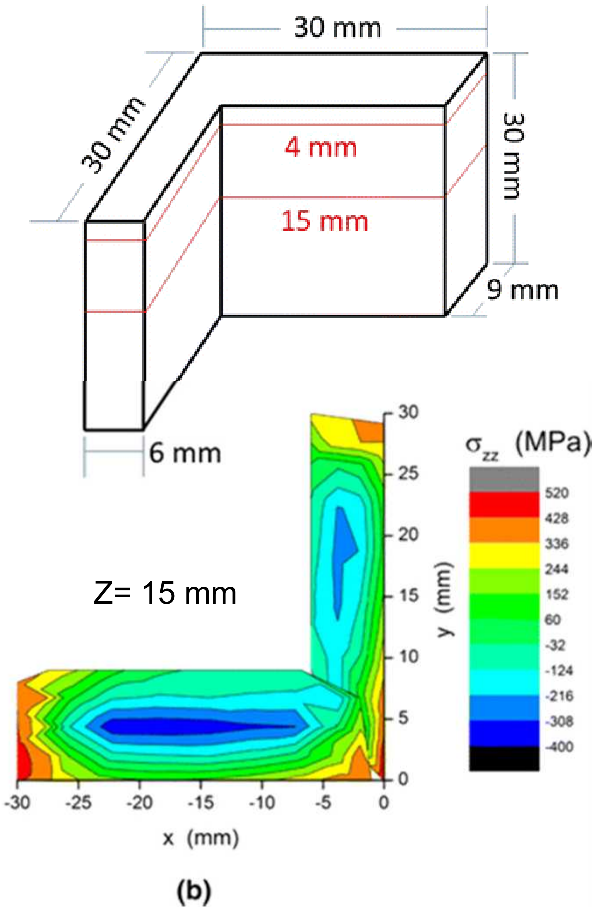
(J. Michael, SNL)



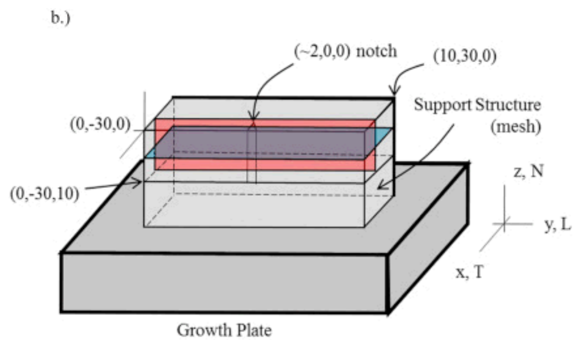
(J. Carroll, SNL)

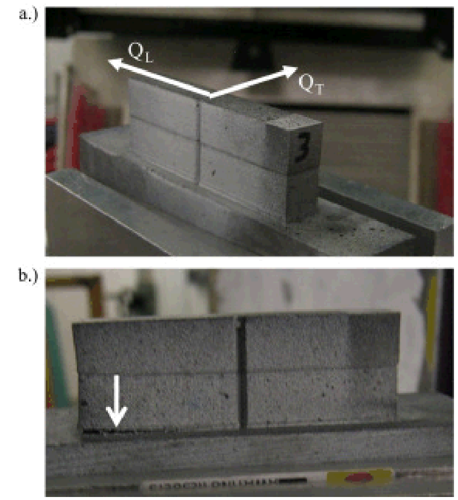
- 304L Stainless Steel

High Thermal Gradients Produce High Residual Stresses

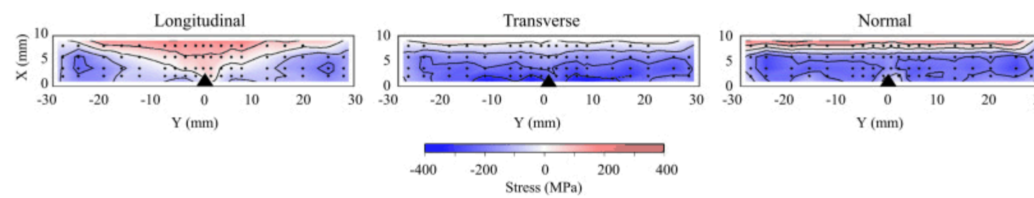


316L Stainless Steel Powder Bed
Wu *et al.* 2014 (LLNL, LANL)





*Stress measured at blue plane



17-4 Stainless Steel Powder Bed
Brown *et al.* 2016 (LANL)

AM Materials Exhibit Higher Dislocation Density

Brown *et al. 2017, Met Trans A*

Table III. Microstructural Parameters Determined from DLPA

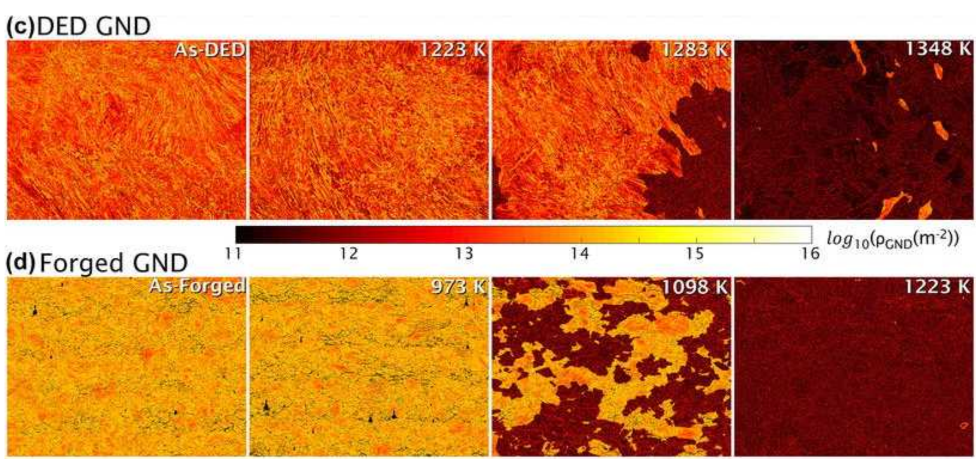
Sample	T/C geometry	Applied Strain	X_A (nm)	$\rho \times 10^{14}$ (1/m^2)	M
W–U	C	0		0.13 (3)	
W–U	T	0		0.30 (3)	
P–U	C	0		2.4 (2)	2.25
P–U	T	0		2.4 (2)	2.14
X–U	C	0		1.2 (1)	3.50
X–U	T	0		1.5 (1)	3.73
W–C					3.03
P–C					1.86
X–C					2.29
W–T					1.49
P–T					1.32
X–T					1.61
W					

Wrought 304L

LENS 304L

Can we predict the higher yield caused by increased dislocation density?

Smith *et al. 2018, JOM*



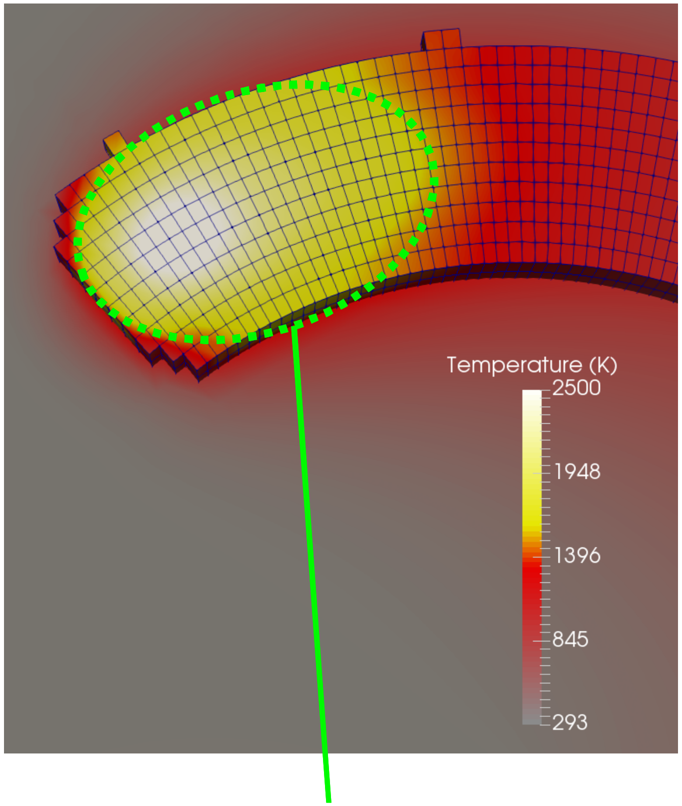
Thermal Approach

Pre-meshed part is initialized with "inactive" elements. Baseplate elements are active.

Laser heat source is scanned according to input path

Elements are activated by a thermal conductivity increase once they reach melt temperature

Conduction, convection, and radiation are considered.



Approximate Melt Pool

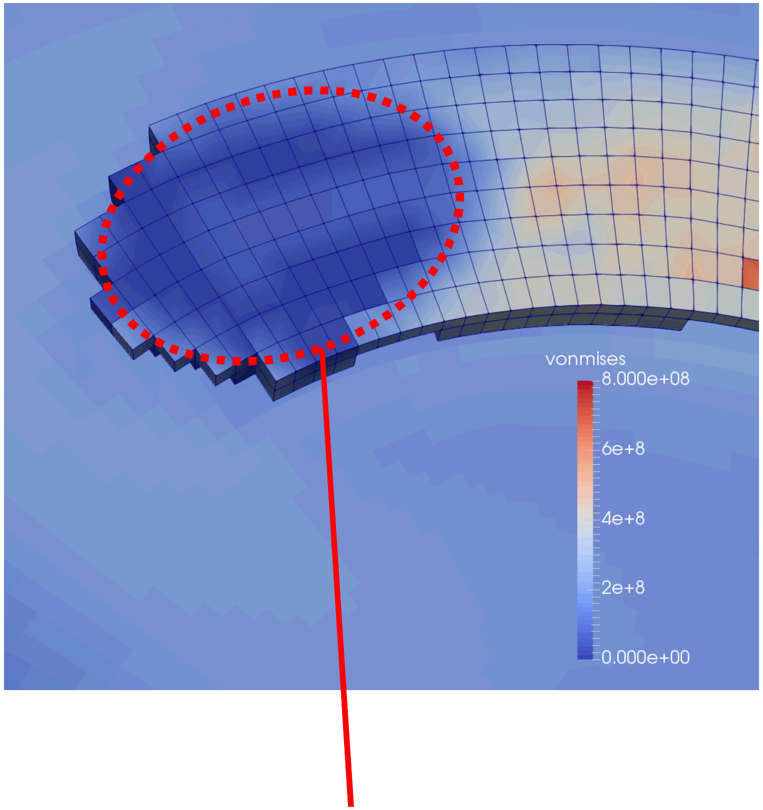
Solid Mechanics Approach

Pre-meshed part is initialized with "inactive" elements. Baseplate elements are active.

Thermal output file is read at every time step to provide temperatures

Elements are activated using once they reach melt temperature

Residual stress builds as elements contract upon cooling and build thermal strain



Approximate Melt Pool (~zero stress)

BCJ Material Model

- Temperature and history-dependent viscoplastic internal state variable model
- Stress is dependent on damage ϕ and evolves according to

$$\dot{\sigma} = \left(\frac{\dot{E}}{E} - \frac{\dot{\phi}}{1-\phi}\right)\sigma + E(1-\phi)(\dot{\epsilon} - \dot{\epsilon_p})$$

- Flow rule includes yield stress and internal state variables for hardening and damage

$$\dot{\varepsilon}_p = f sinh^n\left(\frac{\frac{\sigma_e}{1-\phi} - \kappa}{Y} - 1\right)$$

- Statistically stored dislocations are represented by isotropic hardening variable κ

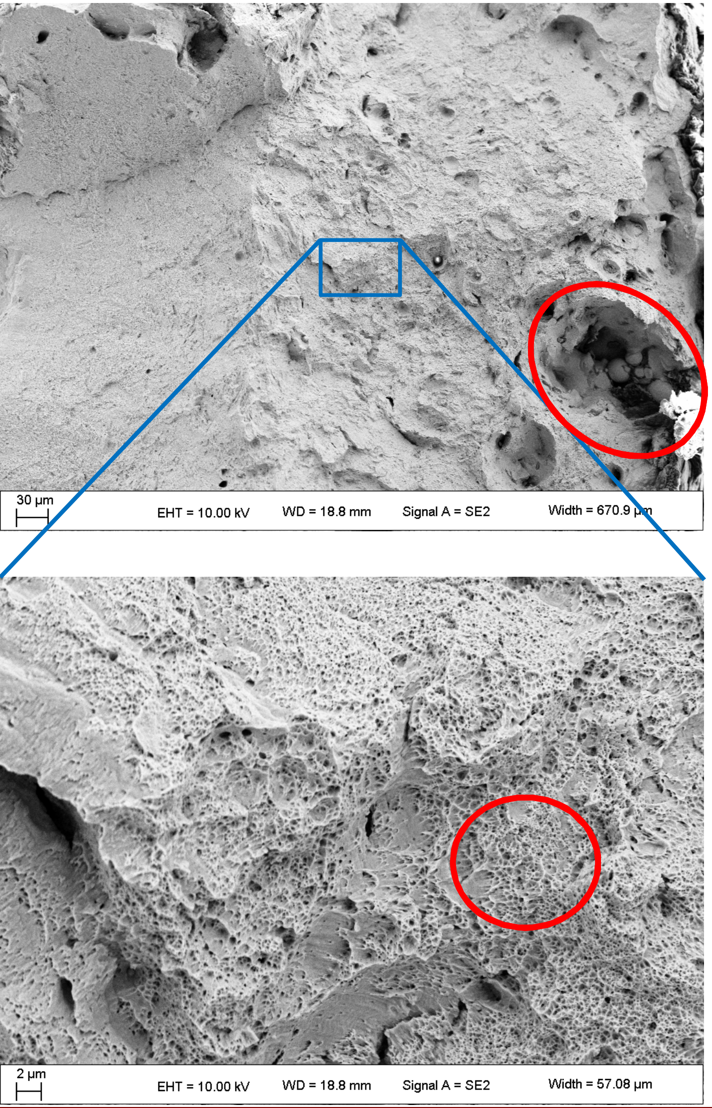
$$\bar{\kappa} = c_{\bar{\varepsilon}_{ssds}} b\mu(\theta)\sqrt{\bar{\rho}_{ssds}} \qquad \dot{\bar{\rho}}_{ssds} = \left[\frac{k_1}{L_s} + \frac{k_2}{L_g} - R_d(\theta)\bar{\rho}_{ssds}\right]\dot{\varepsilon}_p$$

- The isotropic hardening variable κ evolves in a hardening minus recovery form.

$$\dot{\kappa} = \kappa\frac{\dot{\mu}}{\mu} + (H(\theta) - R_d(\theta)\kappa)\dot{\epsilon}_p$$

(Bammann *et al.* 1993, Brown and Bammann 2012)

Incorporating porosity as initial damage



Void Growth

Pre-existing voids captured by void growth

$$\dot{\phi} = \sqrt{\frac{2}{3}}\dot{\epsilon}_p \frac{1-(1-\phi)^{m+1}}{(1-\phi)^m} \sinh\left[\frac{2\,(2m-1)}{2m+1}\frac{\langle p\rangle}{\sigma_e}\right]$$

Void Nucleation

Fine scale voids ($< 1\mu$m) indicate nucleation

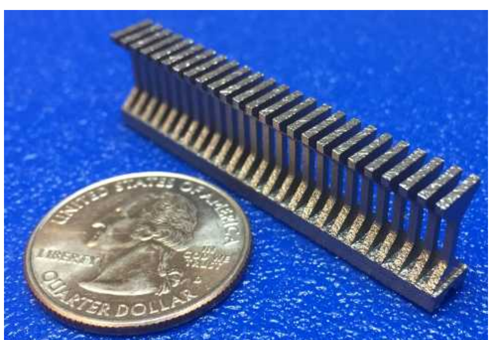
$$\dot{\eta} = \eta\dot{\epsilon}_p \left(N_1 \left[\frac{4}{27} - \frac{J_3^2}{J_2^3}\right] + N_2 \frac{J_3}{J_2^{\frac{3}{2}}} + N_3 \frac{\langle p\rangle}{\sigma_e} \right)$$

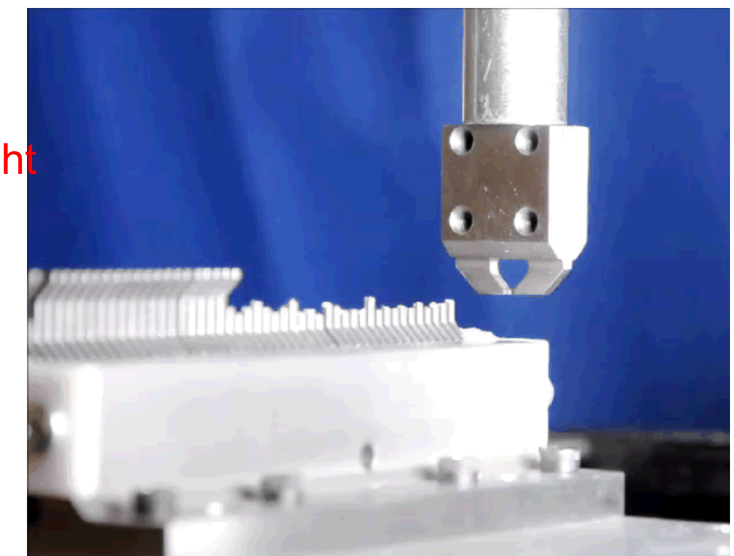
*Fractography taken from 3rd Sandia Fracture Challenge

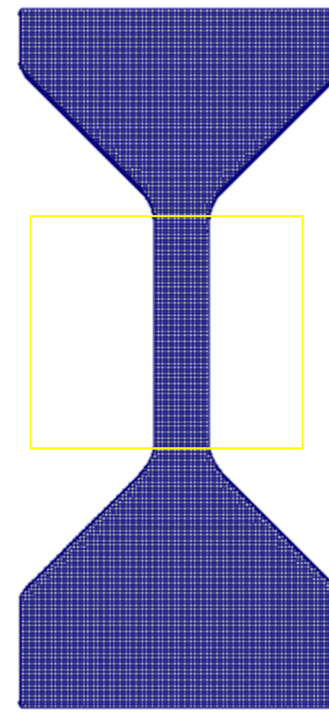
LPBF High Throughput Dogbone Example

Process	Structure	Property	Performance
Thermal and Structural Model (Scan path, laser power, laser speed)	Initial dislocation density, defects	Residual Stress, Higher yield, UTS	Component behavior using as-built properties, residual stress, and porosity

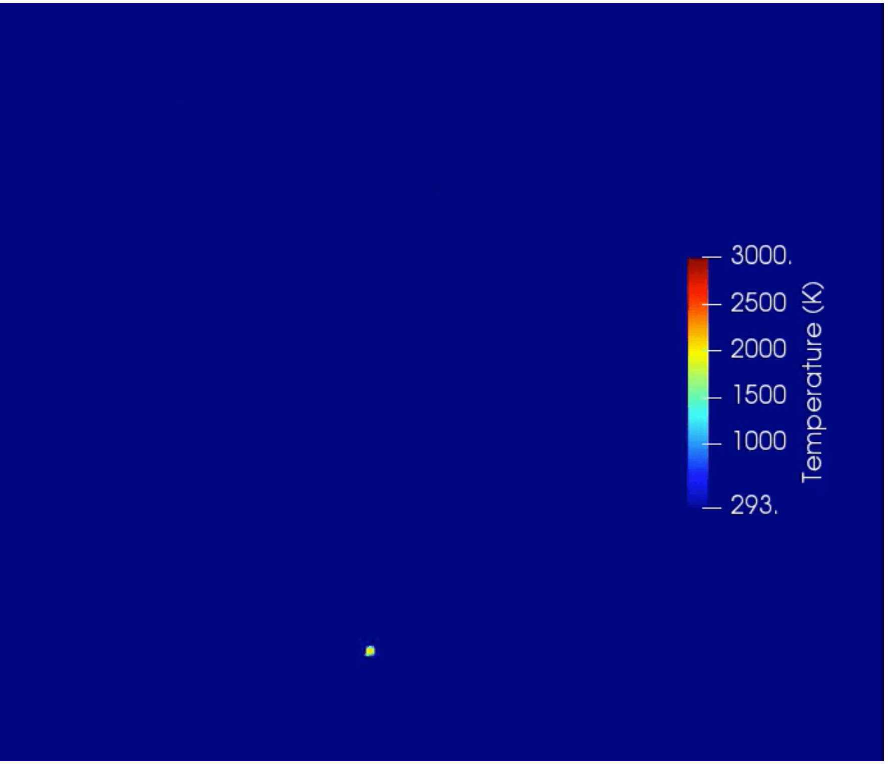
- Laser diameter = 120 μm
- Laser Speed = 1400 mm/s
- Layer Thickness = 0.03 mm
- Laser Power = 120 W
- Hatch Spacing = 60 μm
- Material model calibrated to wrought data



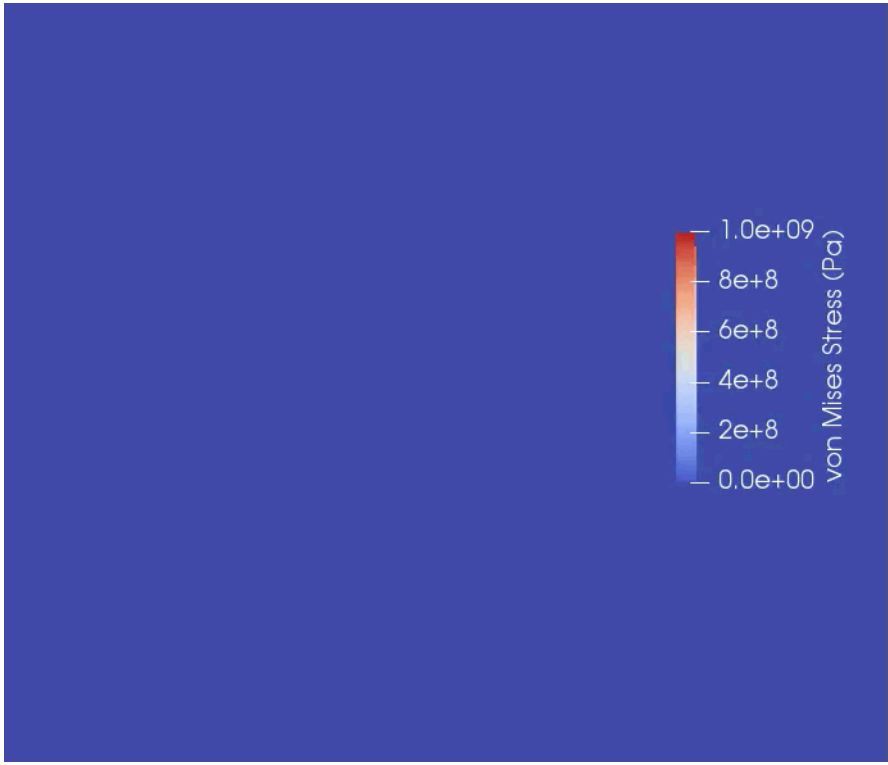




Thermal and Structural Results

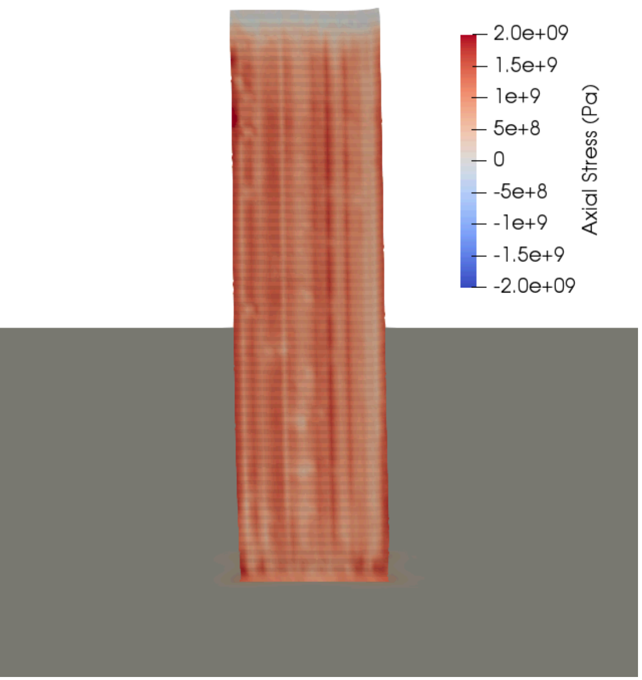


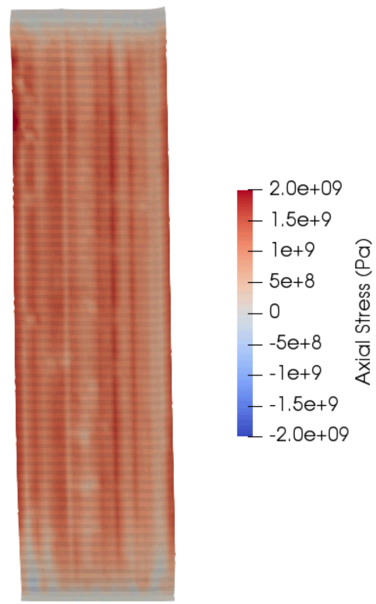
Thermal



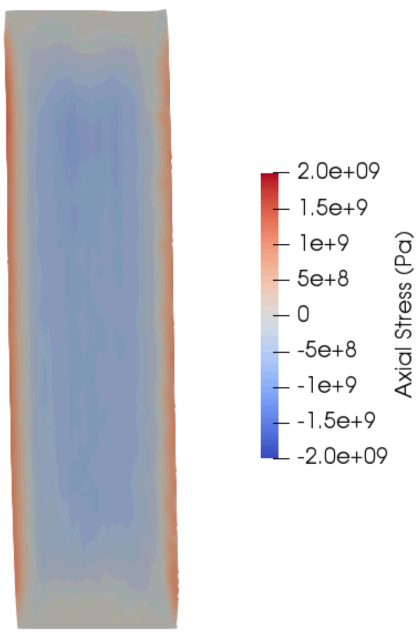
Structural

Significant Tensile and Compressive Residual Stresses Remain

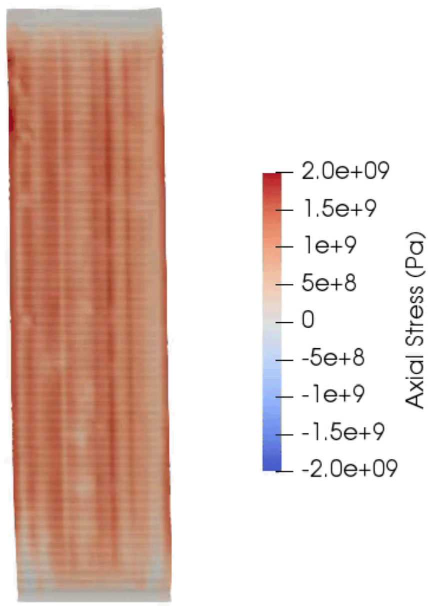


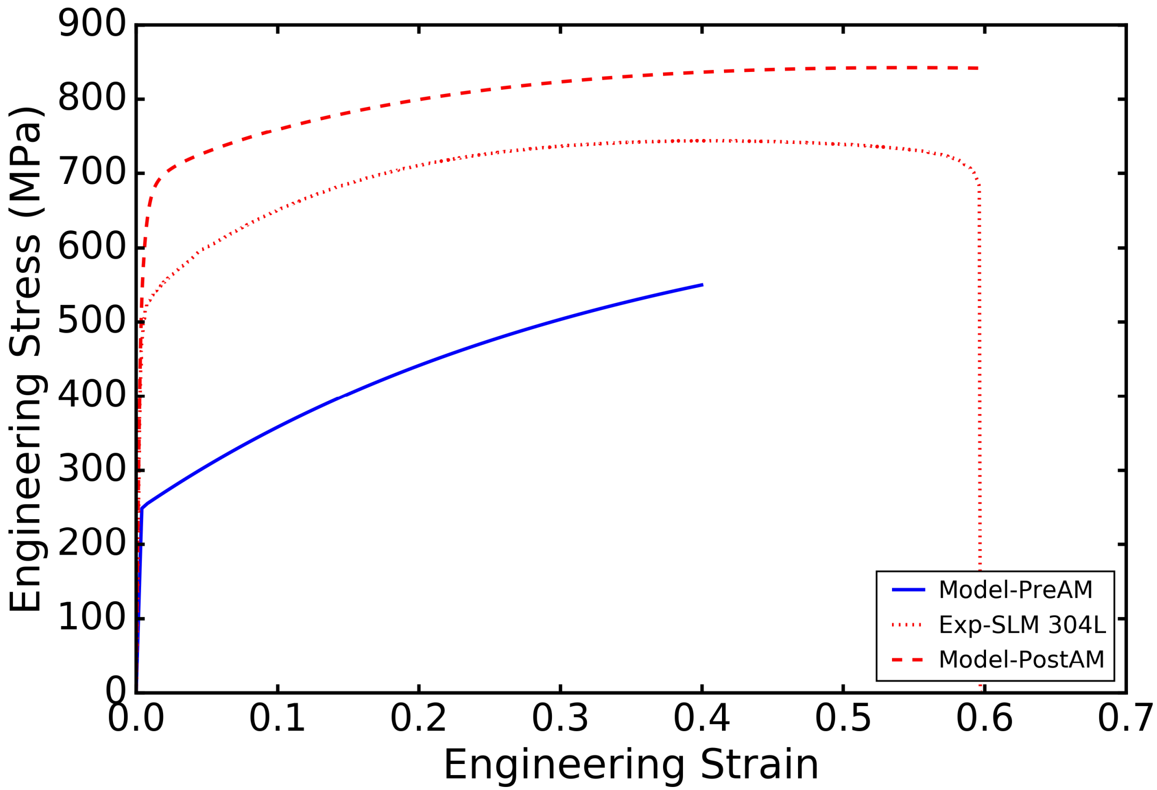


Mid-plane Cut View



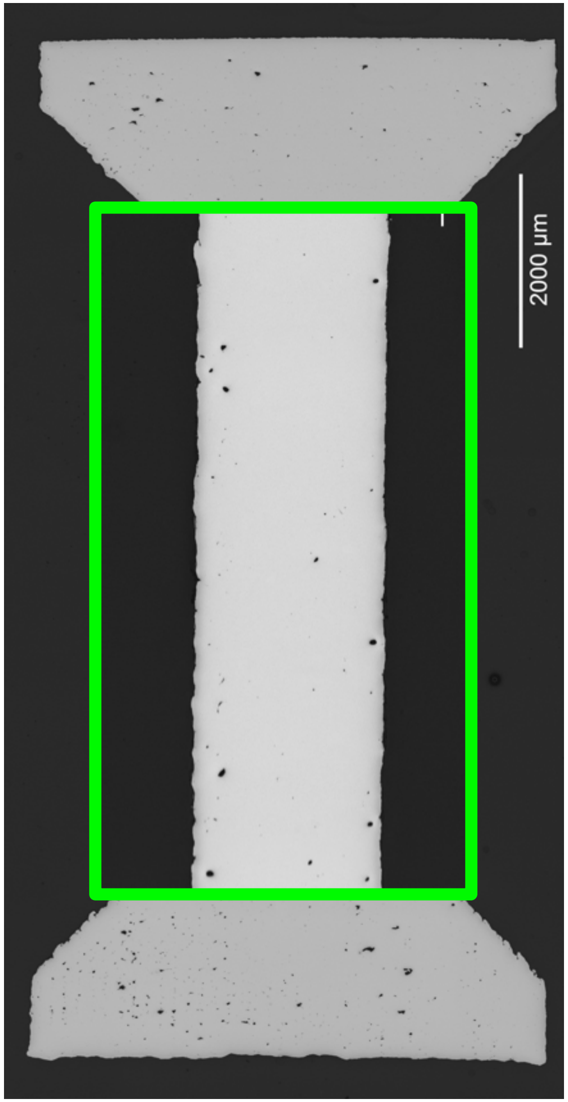
Model Captures Higher Yield but Over Predicts Stress

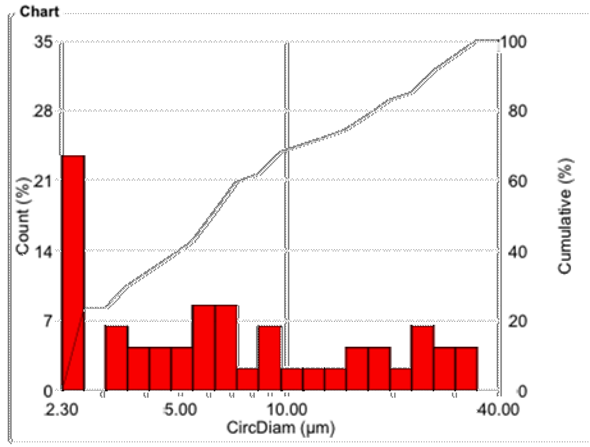




- Model with no residual stress was also simulated, but results were similar

Porosity Distribution is Directly Mapped to Mesh

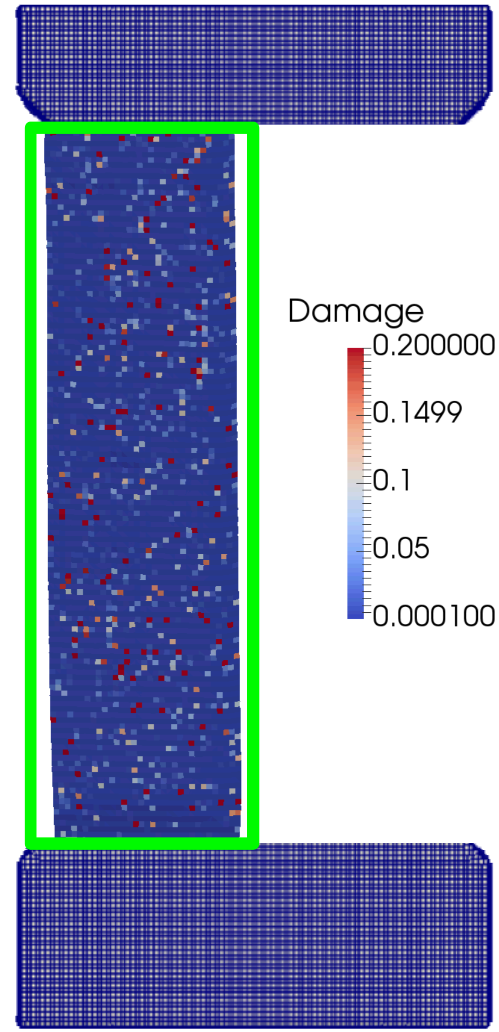




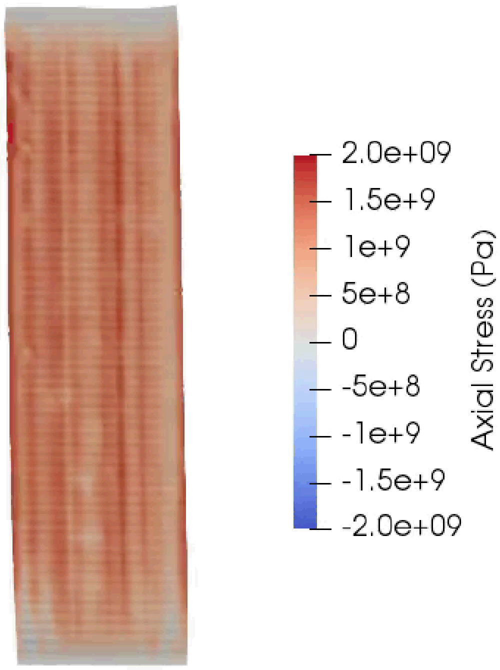
Porosity Mapping

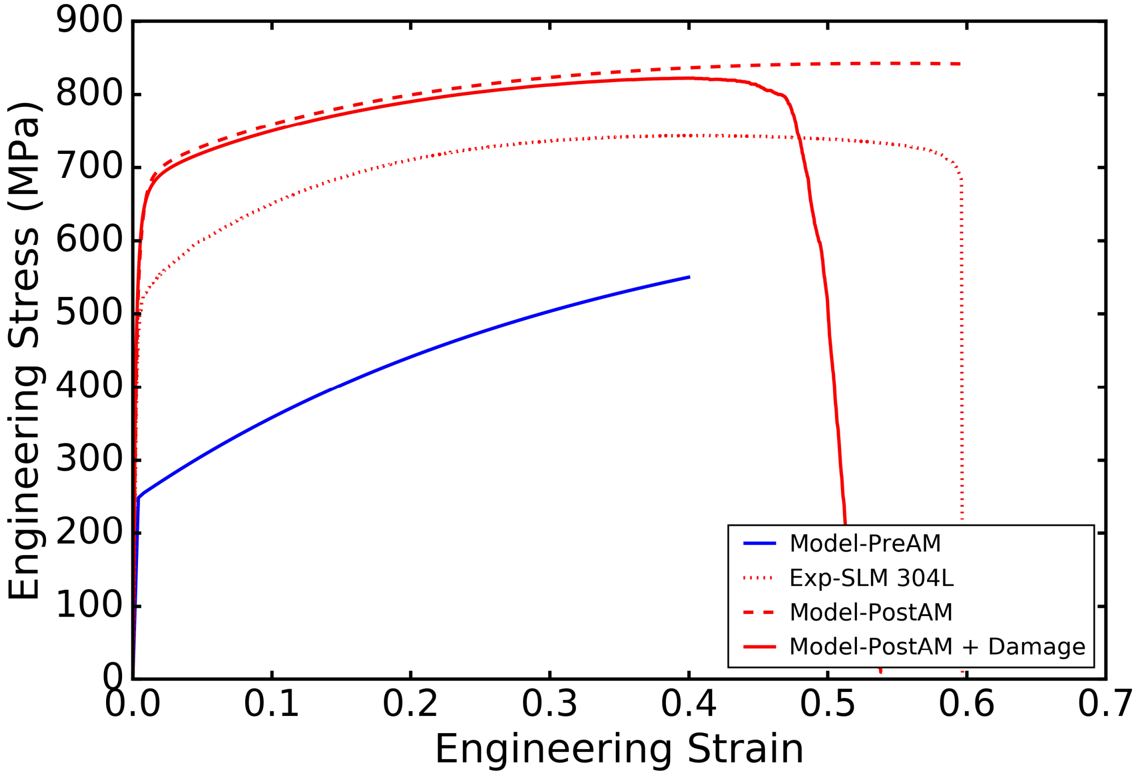
x,y,z,r_{pore}

- Total Porosity: 2%
  - Sample distribution taken from 3rd Sandia Fracture Challenge



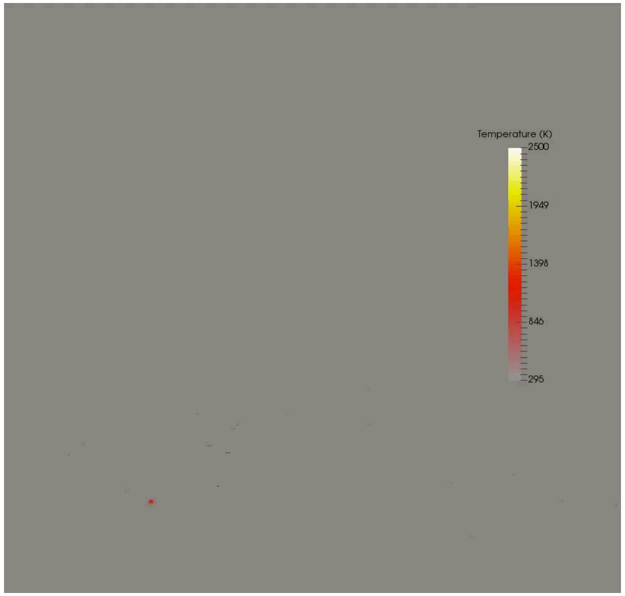
Tensile Results with Porosity





Future Work – Property Prediction

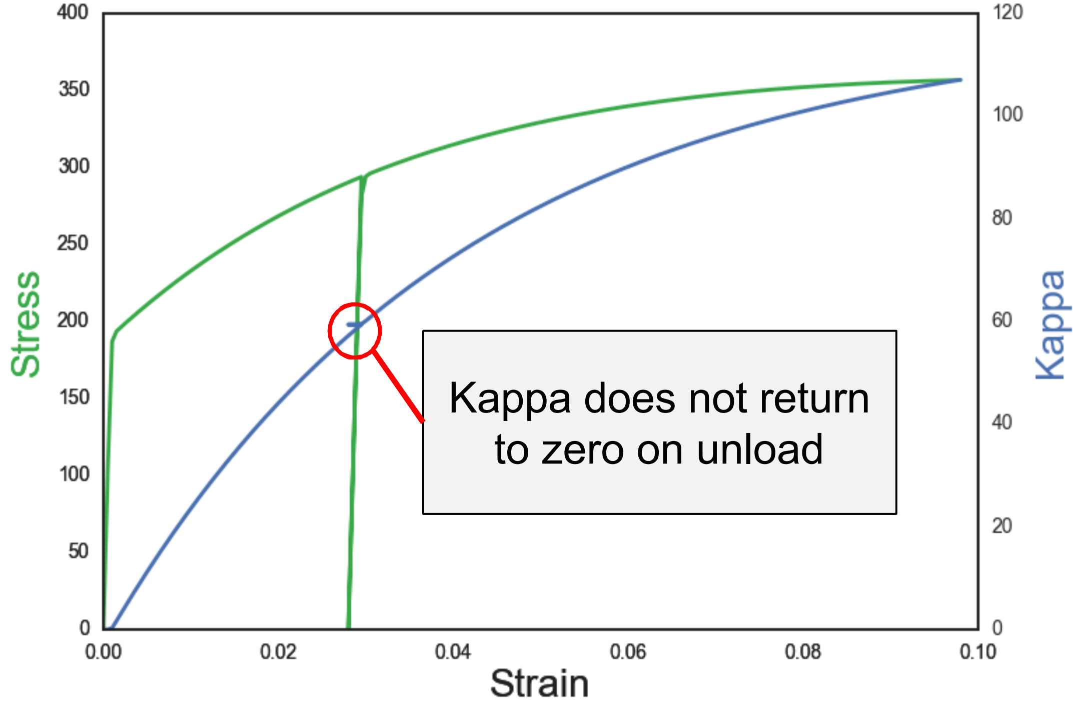
- Initial yield prediction is high
  - Refine material model at high temperatures with near melt Gleeble test data (Jeff Rodelas)
- Run more realizations of porosity for UQ (only 1 shown)
- Simulate full dogbone
- Simulate heat treatments
- Predict microstructure for crystal plasticity prediction



Johnson *et al. 2017, Computational Mechanics*

Questions?

Performance: Higher Yield Captured in 304L SS Upon Reloading



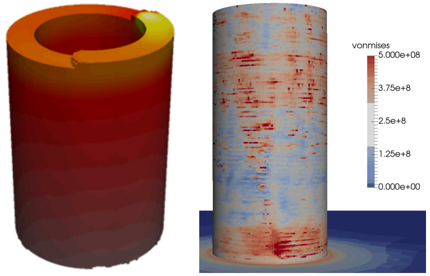
$$\dot{\kappa} = [H(\theta) - R_d(\theta)\kappa]\dot{\epsilon}_p$$

- Example: One element 304L SS loaded to 3 % strain, followed by unload and reload
- Model accurately captures loading history with kappa ISV

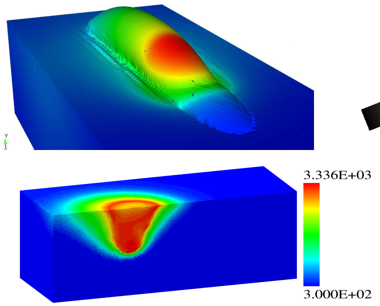
SNL Modeling Work

<u>Codes</u>
LAMMPS, SPPARKS,
Sierra/Aria,
Sierra/Adagio

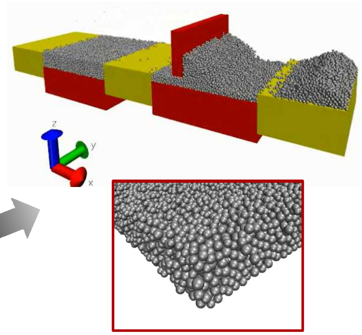
<u>Part Scale Thermal & Solid Mechanics</u>
Kyle Johnson, Kurtis Ford, Mike Stender,
Lauren Beghini & Joe Bishop



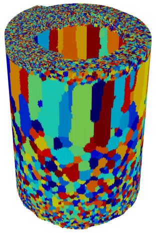
<u>Mesoscale Thermal Behavior</u>
Mario Martinez & Brad Trembacki



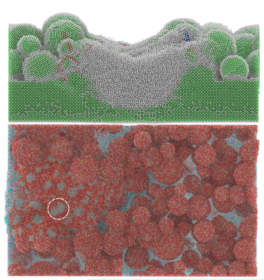
<u>Powder Spreading</u>
Dan Bolintineanu



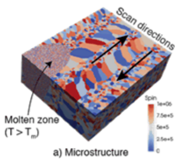
<u>Part Scale Microstructure</u>
Theron Rodgers



<u>Powder Behavior</u>
Mark Wilson



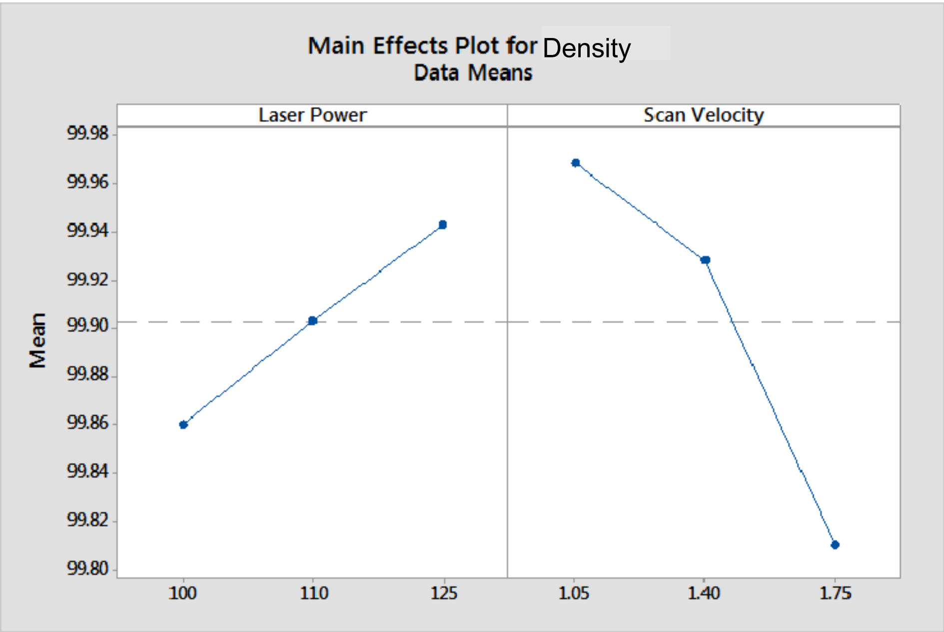
<u>Mesoscale Texture/Solid Mechanics/CX</u>
Judy Brown, Theron Rodgers and Kurtis Ford

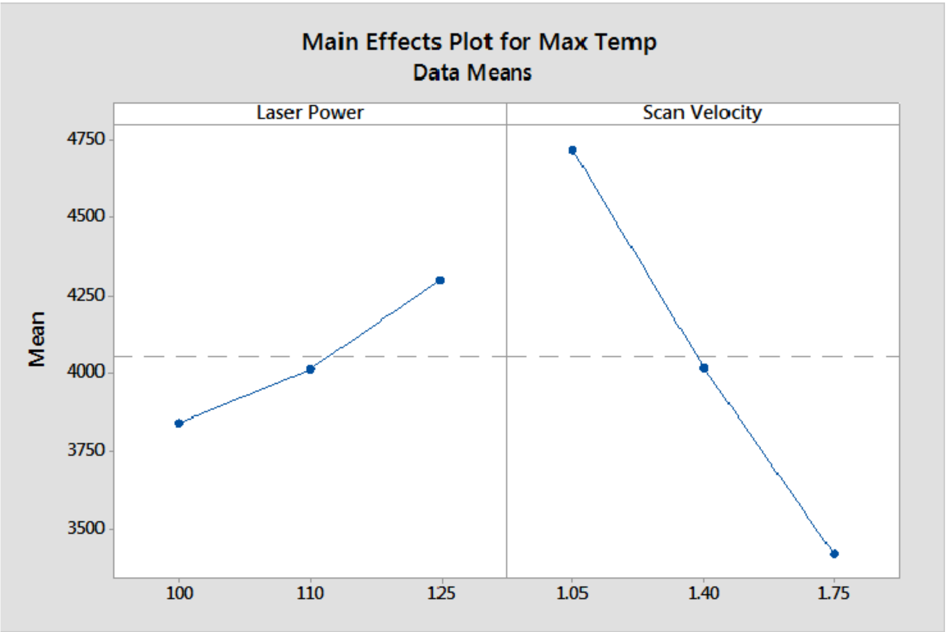


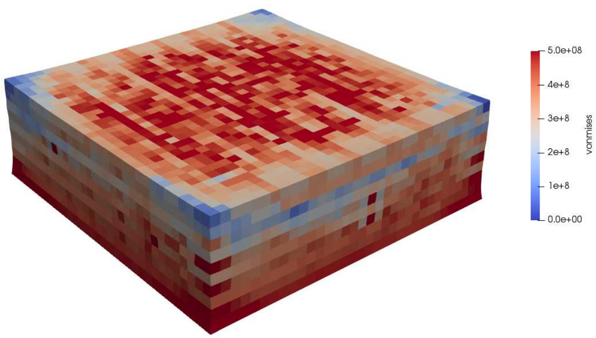
10^{-6} 10^{-3} 1

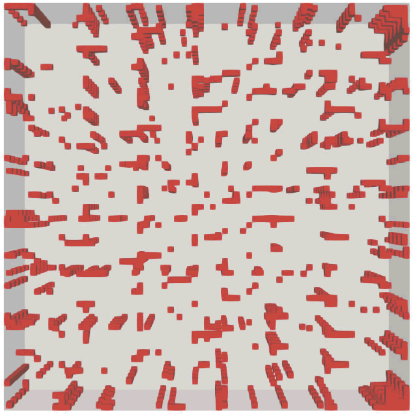
Length Scale (m)

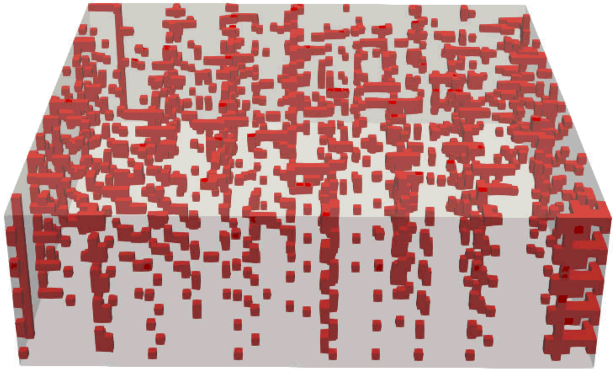
Process Setting Effects on Properties (Laura Swiler)











Thermal Modeling in Aria

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \boldsymbol{v} \cdot \boldsymbol{\nabla} T = -\boldsymbol{\nabla} \cdot \mathbf{q} + H_V$$

Volumetric Gaussian Laser Heat Source

```
begin laser heating
  Activation Temperature = 1698
  power = 2000
  beam diameter = 4.2
  efficiency = 0.4
  path function = path
  depth direction = -z
  distribution = gaussian
  source type = activation_hemisphere
  spatial influence factor = 1.2
  add volume block_40
end
```

Radiation and Convection

$$\mathbf{q} = \varepsilon\sigma(T^4 - T_r^4)$$

$$\mathbf{q} = h(T - T_\infty)$$

Conduction

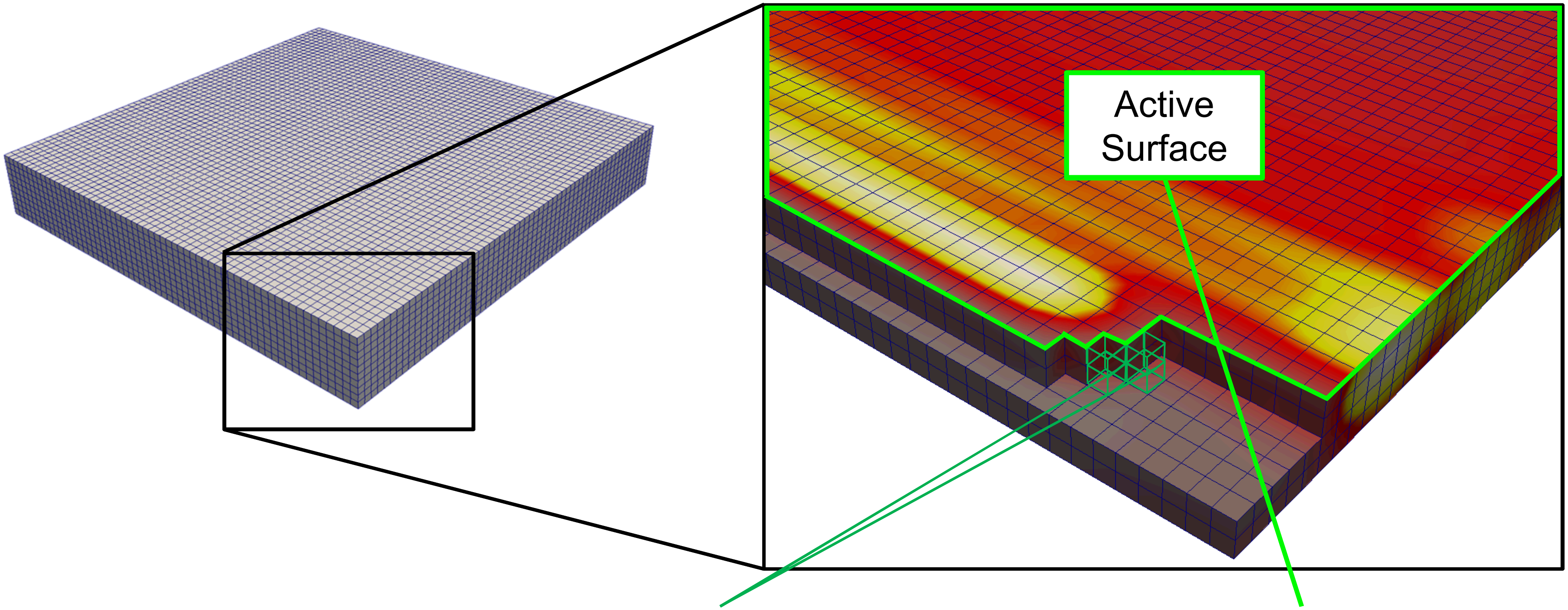
$$\mathbf{q} = -k\nabla T$$

Element Status	K Value $(W/(m * K))$
Inactive LENS	0
Inactive Powder Bed	Powder Property (< 1)
Active	Bulk Property

Material Addition in Aria

Pre-meshed Part

Part During Process



Elements ahead of laser are inactive

Convection and radiation are applied to active surface as it evolves

BCJ - Elasticity and Flow Rule

- Linear elasticity assumption

$$\overset{o}{\sigma} = \lambda tr(D^e)1 + 2\mu D^e$$

- The Cauchy stress is convected with the elastic spin as

$$\overset{o}{\sigma} = \dot{\sigma} - W^e\sigma + \sigma W^e$$

- The elastic stretching and spin tensors are written as:

$$D^e = D - D^p - D^{th}$$

$$W^e = W - W^p$$

- The plastic flow rule needed in the above equation is written as

$$D^p = f(\theta)\sinh[\frac{|\xi| - \kappa - Y(\theta)}{V(\theta)}]\frac{\xi'}{|\xi'|}$$

- Where θ is the temperature, κ is the isotropic hardening variable, ξ is the difference between the deviatoric Cauchy stress σ' and the tensor variable α'

$$\xi' = \sigma' - \alpha'$$

- The temperature dependence of the shear modulus is written as:

$$\mu(\theta) = \mu_0[1 - (\frac{\theta}{\theta_m})\exp[\theta_c(1 - \frac{\theta}{\theta_m})]]$$

- The temperature change due to plastic dissipation is:

$$\dot{\theta} = \frac{0.9}{\rho C_v}(\sigma \cdot D^P)$$