

# Predicting Residual Stress and Microstructural Equiaxed-to-Columnar Grain Transition in 304L Stainless Steel LENS Parts

Kyle Johnson, Theron Rodgers, Olivia Underwood, Jonathan Madison, Kurtis Ford, and Joe Bishop

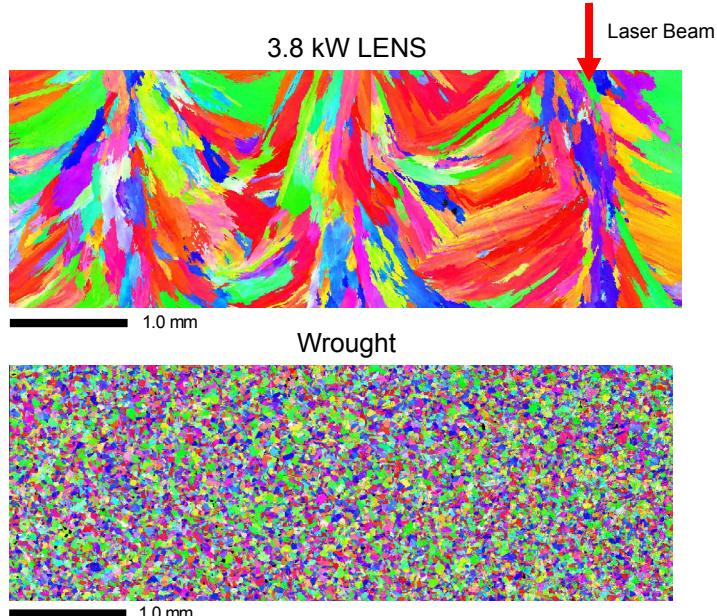
# Acknowledgements

- Collaborators
  - Joe Bishop
  - Kurtis Ford
  - Theron Rodgers
  - Sam Subia
  - Daryl Dagel
  - Dave Keicher
  - Shaun Whetten
  - Bradley Jared
  - Jon Madison
  - Olivia Underwood
  - Sierra Code Team

# Outline

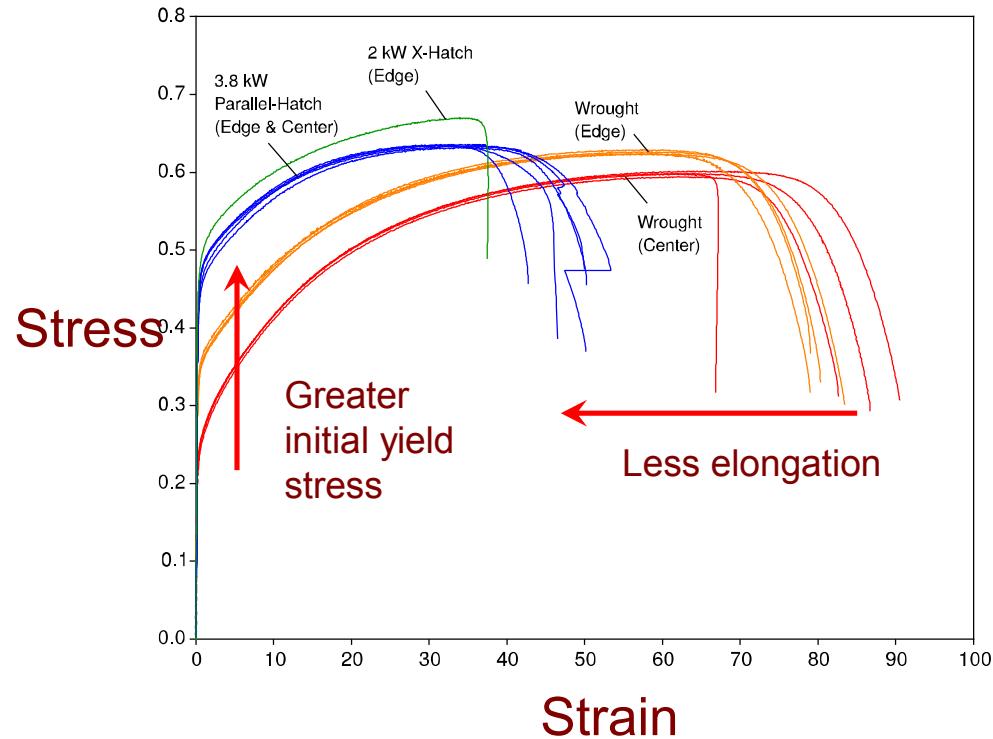
- Background and Motivation
- Thermal, Solid Mechanics and Microstructure Modeling Methodology
- Single Build Results
- Comparison of Different Inter-layer Delay Time Predictions
- Conclusions and Future Work

# AM Can Produce Extreme Properties



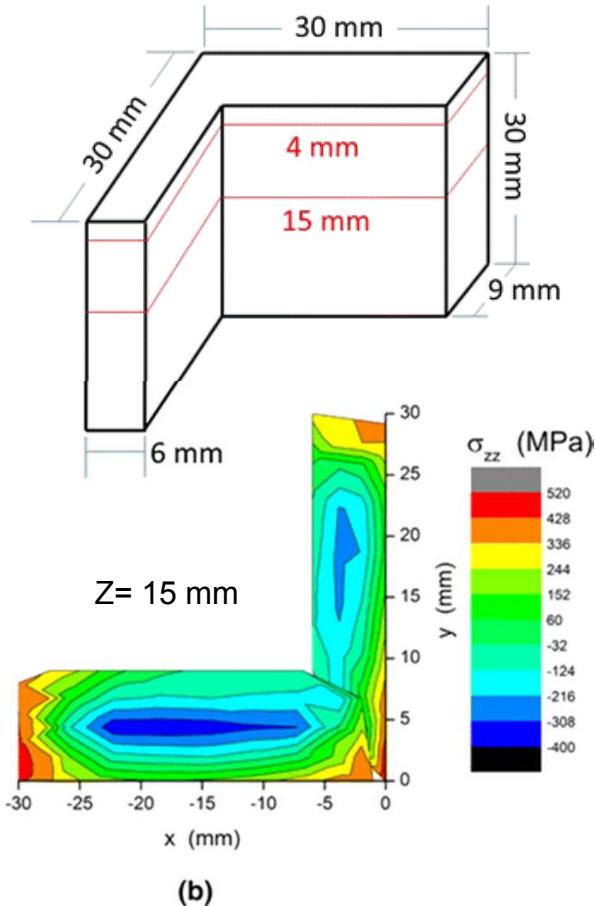
(J. Michael, SNL)

- 304L Stainless Steel



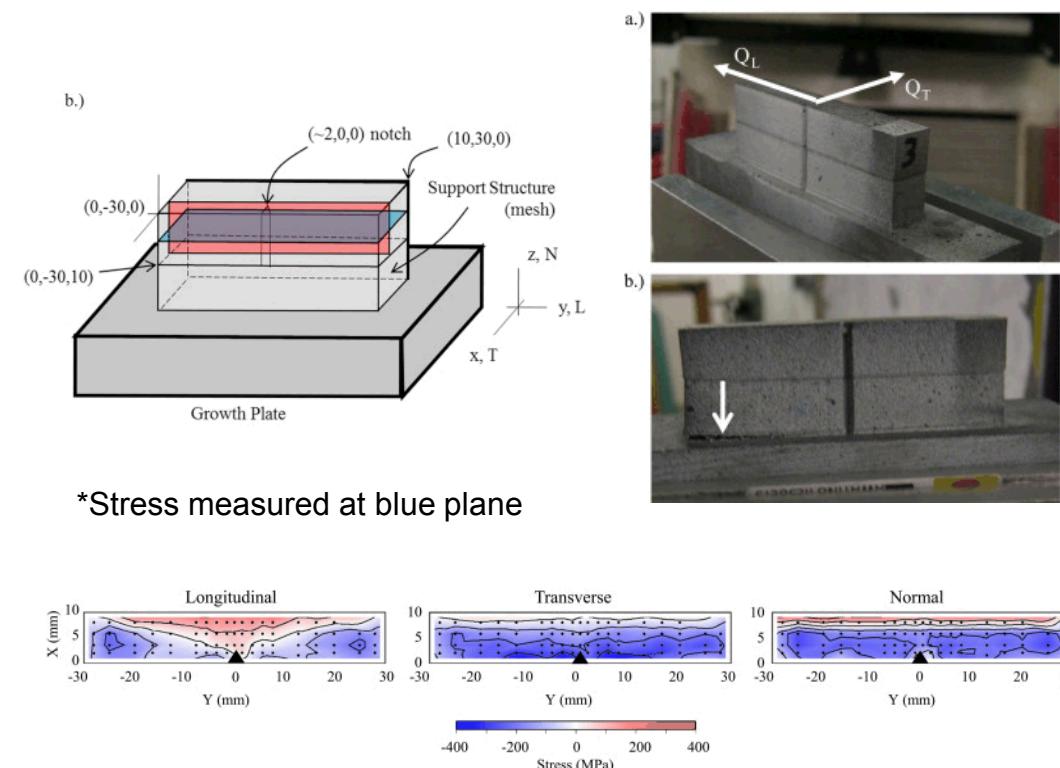
(J. Carroll, SNL)

# High Thermal Gradients Produce High Residual Stresses



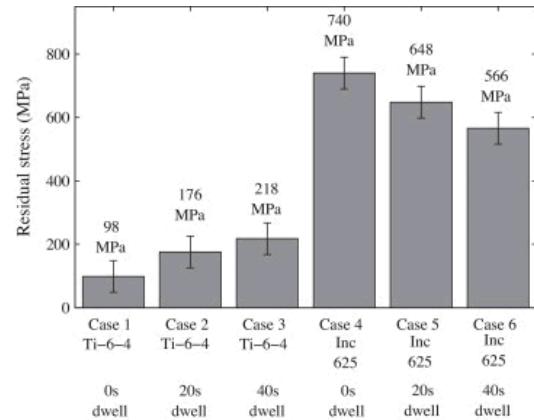
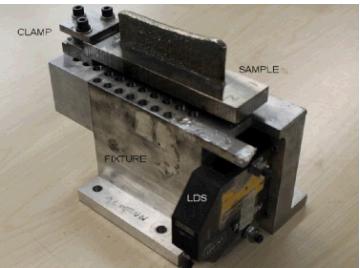
(b)

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

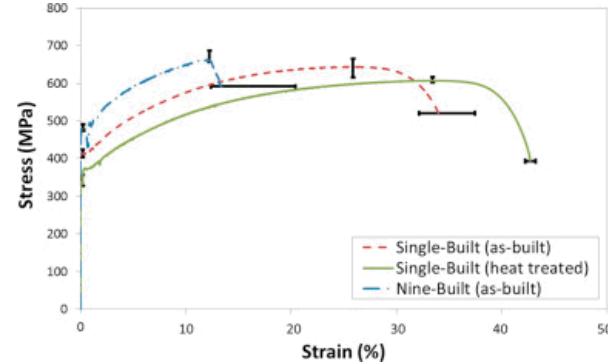


17-4 Stainless Steel Powder Bed  
Brown *et al.* 2016 (LANL)

# Inter-layer Time Affects Residual Stress and Mechanical Properties



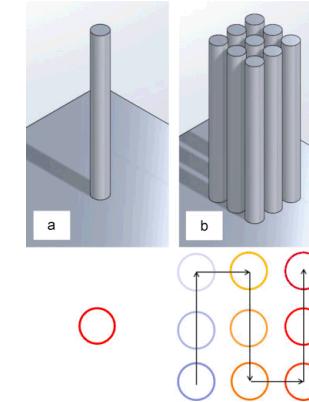
Denlinger et al., J. Mater Process Technol 2015



Yadollahi et al., Mat Sci Eng A 2015

Inter-layer dwell times can change residual stresses

Building multiple parts can change mechanical properties based on different process time intervals

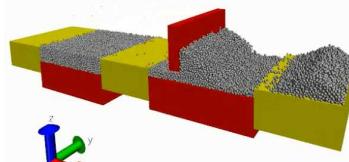


# SNL Modeling Work

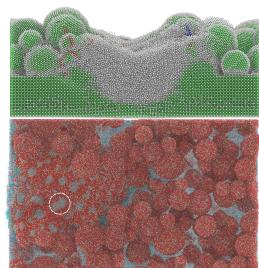
## Codes

LAMMPS, SPPARKS,  
Sierra/Aria,  
Sierra/Adagio

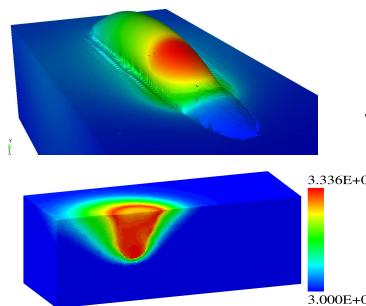
Powder Spreading  
Dan Bolintineanu



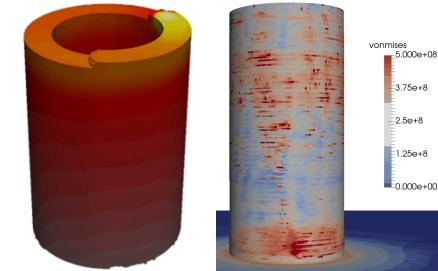
Powder Behavior  
Mark Wilson



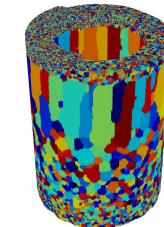
Mesoscale Thermal Behavior  
Mario Martinez & Brad Trembacki



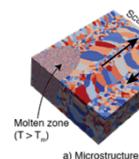
Part Scale Thermal & Solid Mechanics  
Kyle Johnson, Kurtis Ford & Joe Bishop



Part Scale Microstructure  
Theron Rodgers



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



$10^{-6}$

$10^{-3}$

Length Scale (m)

1

7

# 304L Tube Example

## Case 1

No inter-layer delay  
(continuous build)

## Case 2

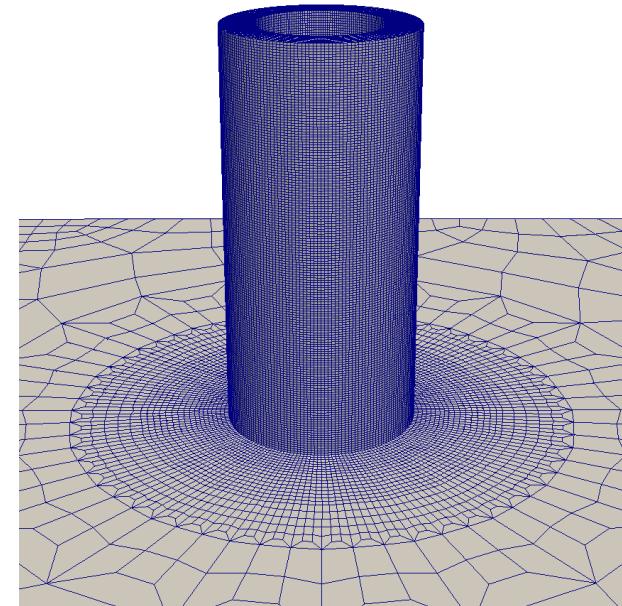
8 second delay added  
between layers  
(double build)



Can we capture the difference in  
microstructure and residual  
stress due to changing thermal  
gradients?

- Dimensions: 2" H x 1" W
- LENS process
- Laser diameter = 4 mm
- Laser Speed = 8.46 mm/s
- Layer Thickness = 0.9 mm
- Laser Power = 2000 > 1750 > 1500 > 1250 W

Submitted to: *Computational Mechanics*



# Outline

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- Thermal, Solid Mechanics and Microstructure Modeling Methodology
- Single Build Results
- Comparison of Different Inter-layer Delay Time Predictions
- Conclusions and Future Work

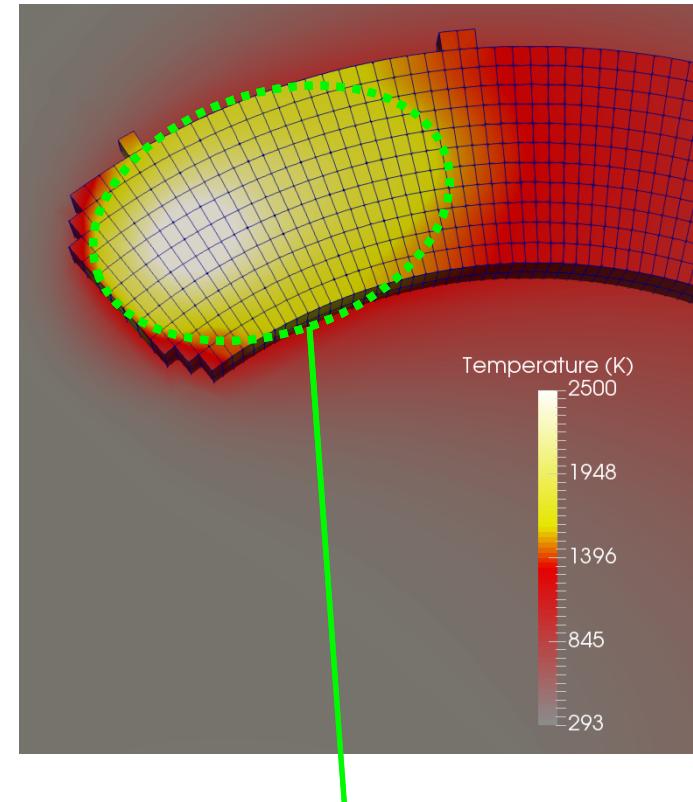
# Thermal Approach

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

Laser heat source is scanned according to input path.

Elements are activated once they reach melt temperature.

Conduction, convection, and radiation are considered.



Approximate Melt Pool

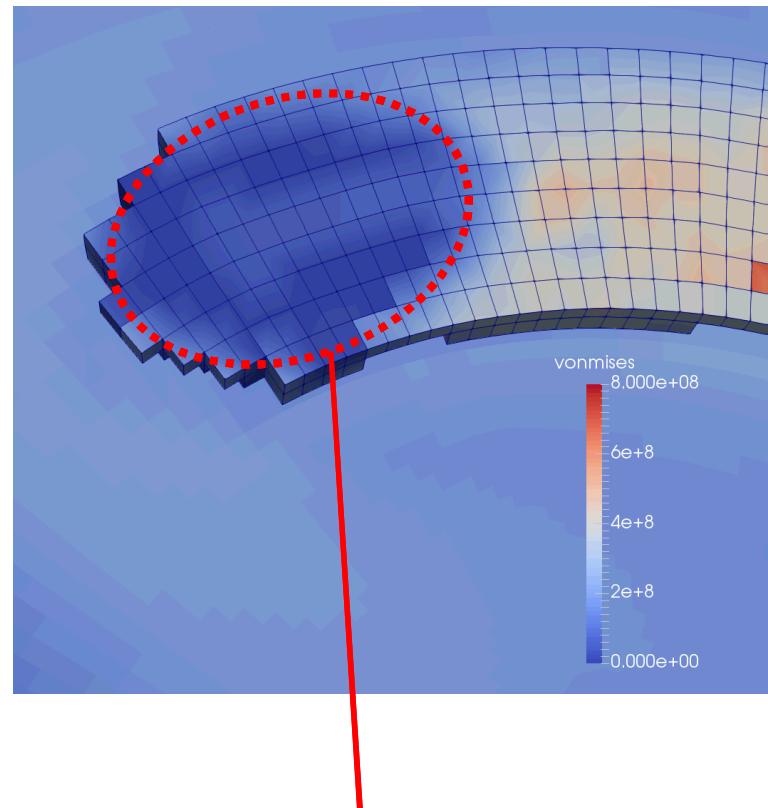
# Solid Mechanics Approach

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

Aria output file is read at every time step to provide temperature fields.

Elements are activated 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
- Flow rule includes yield stress and hardening internal state variable

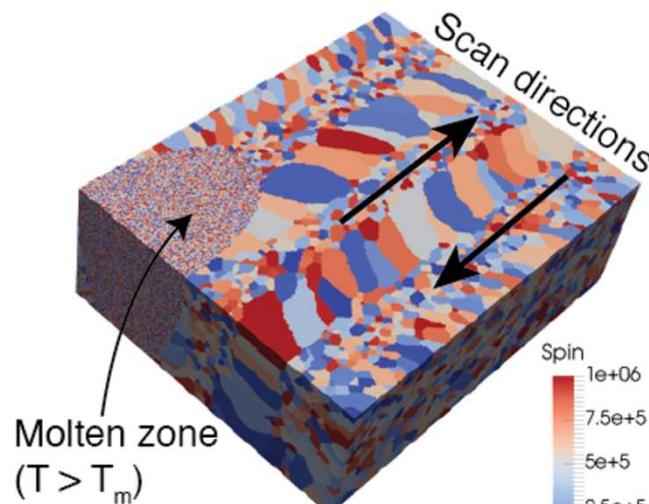
$$\dot{\varepsilon}_p = f \sinh^n \left( \frac{\frac{\sigma_e}{1-\phi} - \kappa}{Y} - 1 \right)$$

- The isotropic hardening variable  $\kappa$  evolves in a hardening minus recovery form.

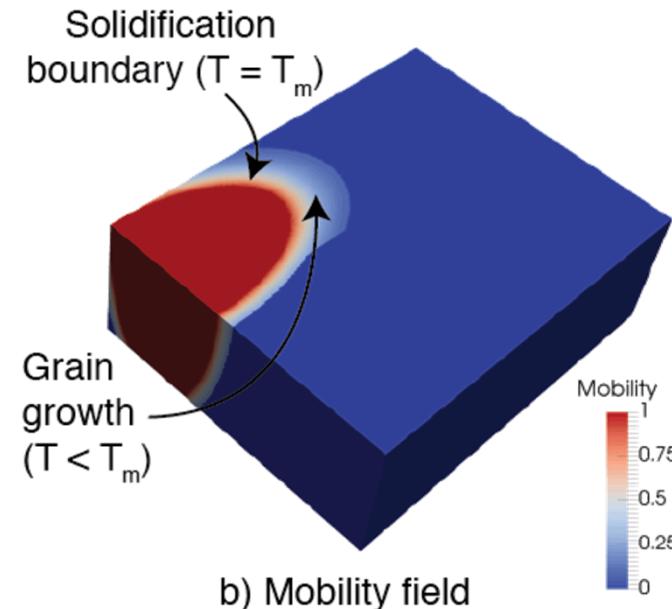
$$\dot{\kappa} = \kappa \frac{\dot{\mu}}{\mu} + (H(\theta) - R_d(\theta)\kappa) \dot{\varepsilon}_p$$

- Model is calibrated to experimental data over a range of temperatures

# Microstructure Prediction in Stochastic Parallel PARticle Kinetic Simulator (SPPARKS)



a) Microstructure



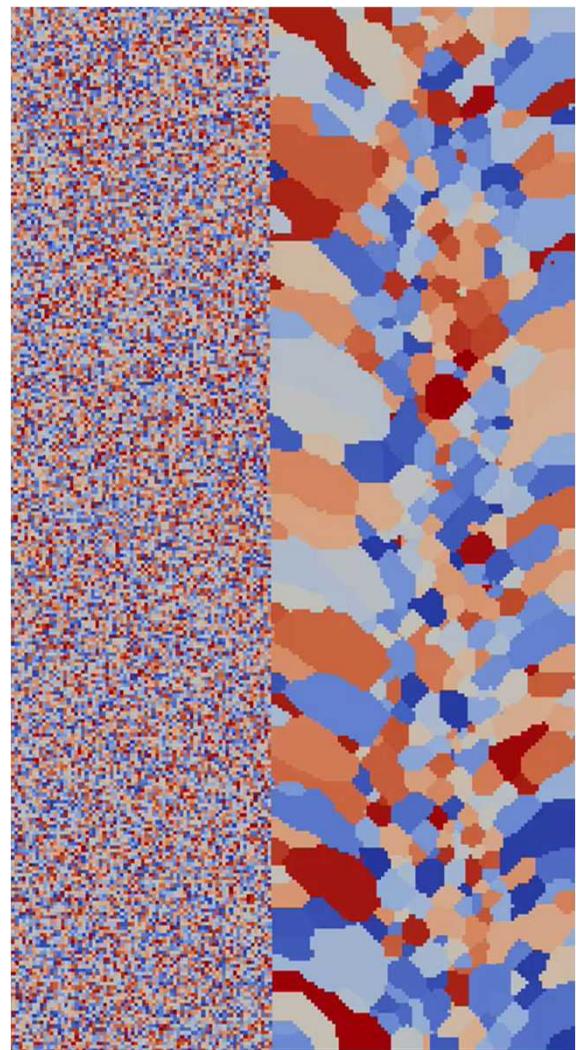
b) Mobility field

$$M(T) = M_0 \exp\left(\frac{-Q}{RT}\right)$$

$$P = \begin{cases} M(T) \exp\left(\frac{-\Delta E}{k_B T_s}\right), & \text{if } \Delta E > 0 \\ M(T), & \text{if } \Delta E \leq 0 \end{cases}$$

- Aria temperature history is used as material state in SPPARKS
- Captures bulk heating effects on microstructure
- See Rodgers *et al.*, “Simulation of metal additive manufacturing microstructures using kinetic Monte Carlo,” *Computational Materials Science*, 2017

# 3D Microstructure Prediction in SPPARKS



a) Experimental

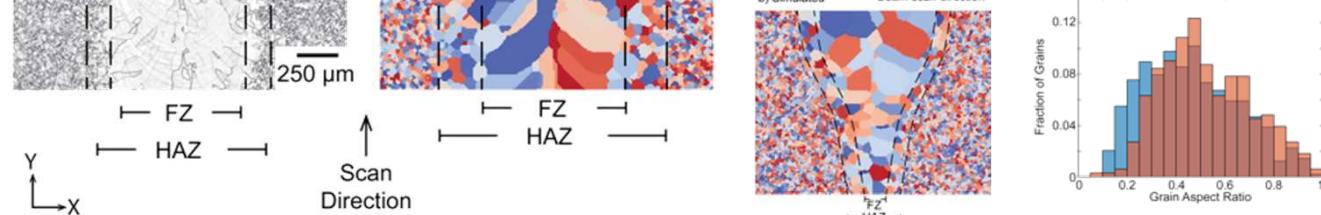
b) Simulated

a) Experimental

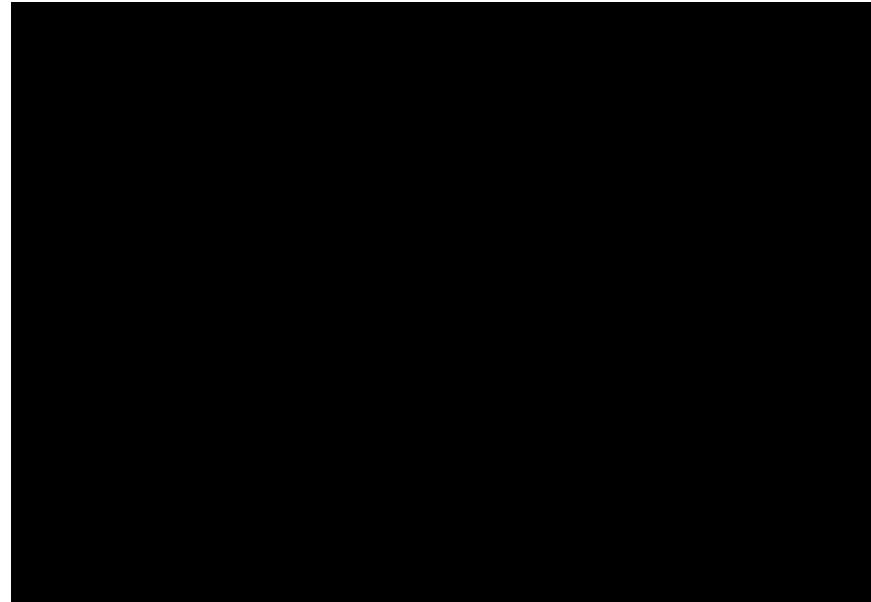
b) Simulated

a) Equivalent circular diameter distribution

b) Grain aspect ratio distribution



Rodgers et al., JOM 2016, Comp Mat Sci 2017



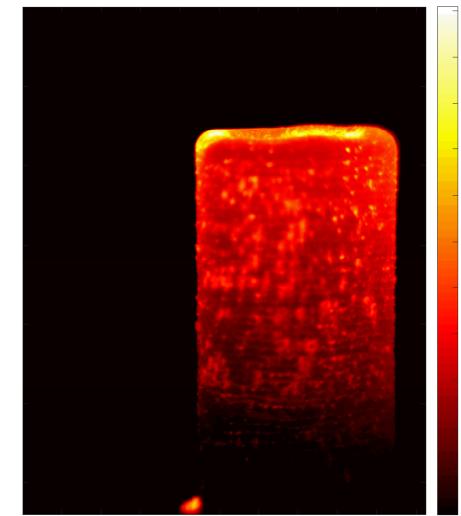
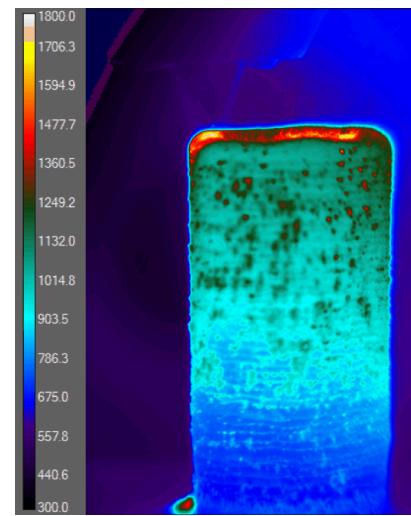
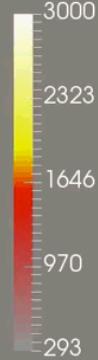
# Outline

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# Experimental Comparison - Thermal

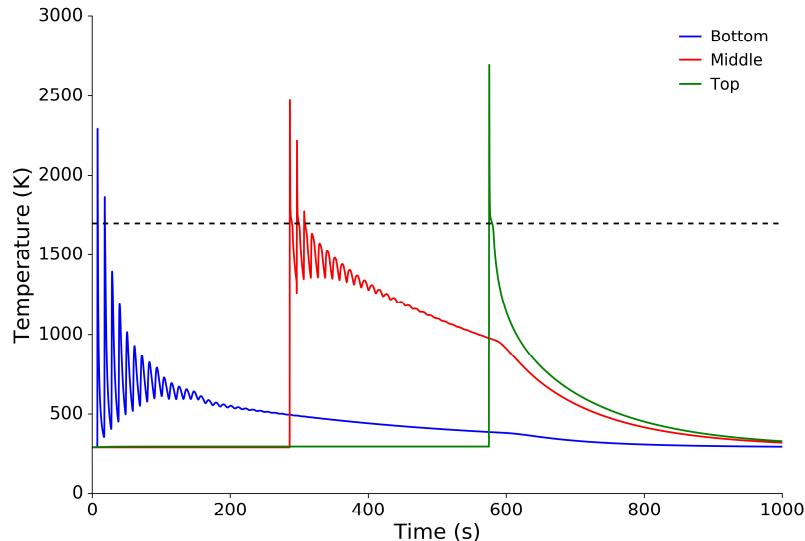
Time: 0.00 s

Temperature (K)

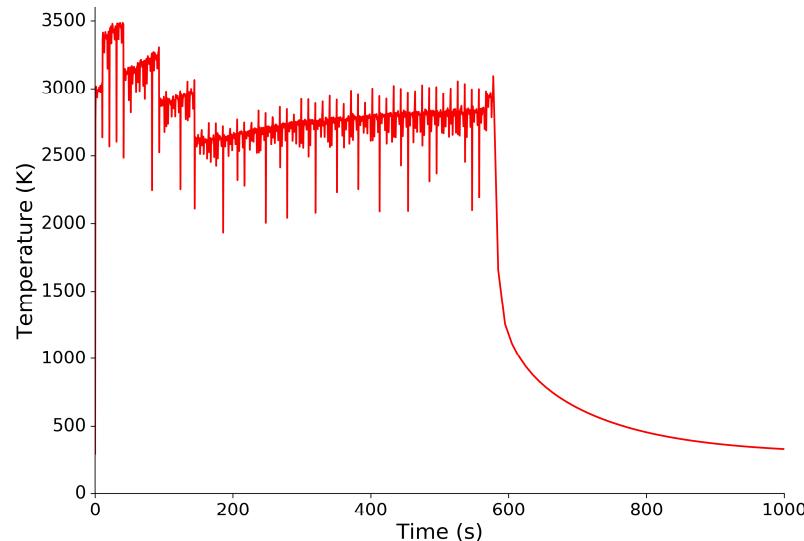


# Thermal Histories

Temperature Histories at 3 Different Tube Heights

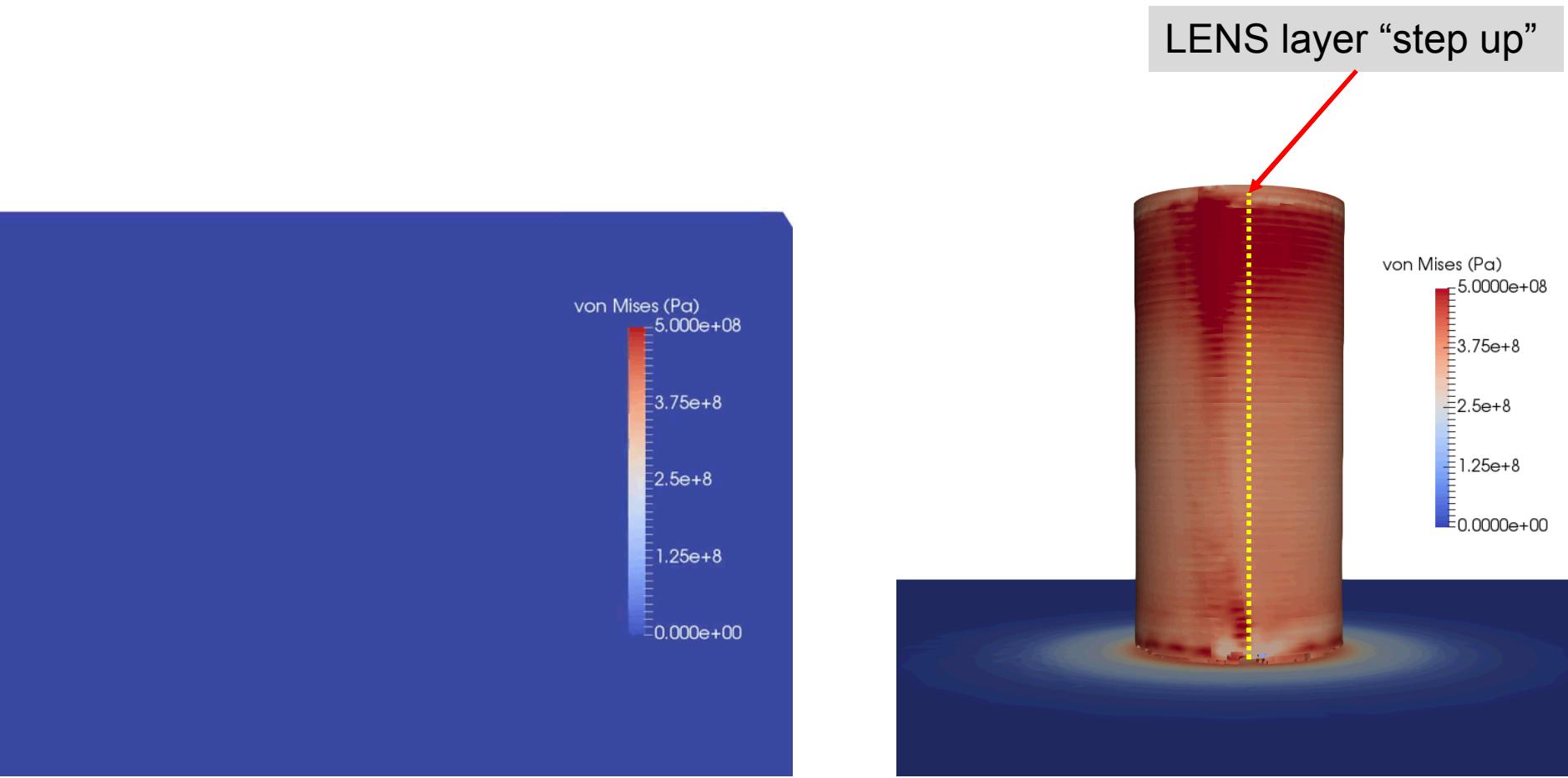


Maximum Temperature Across Entire Part

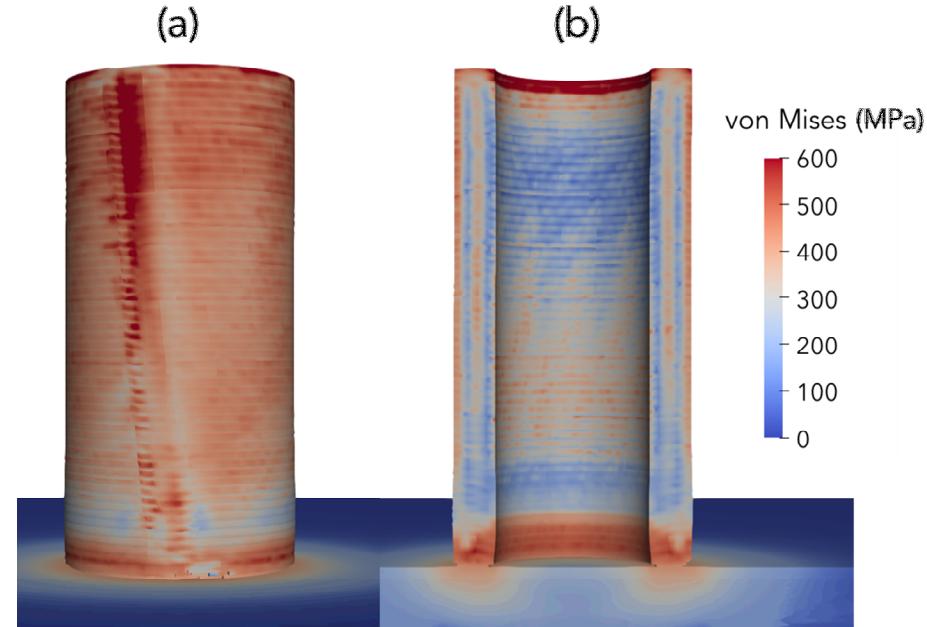
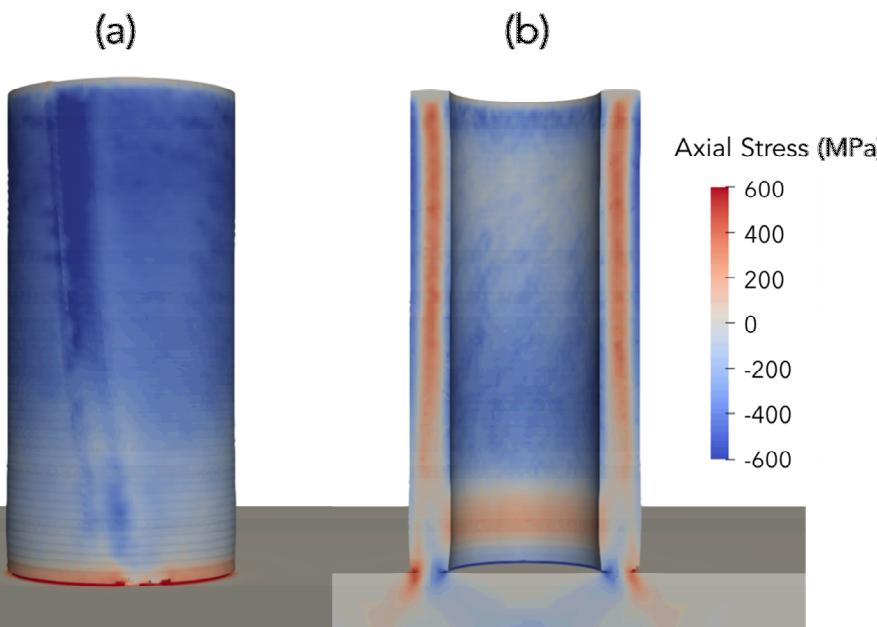


- Different part locations show very different thermal histories
- Middle location goes through 3 melting cycles
- Different thermal gradients throughout cool down
- Drops in maximum temperature demonstrate laser power drops

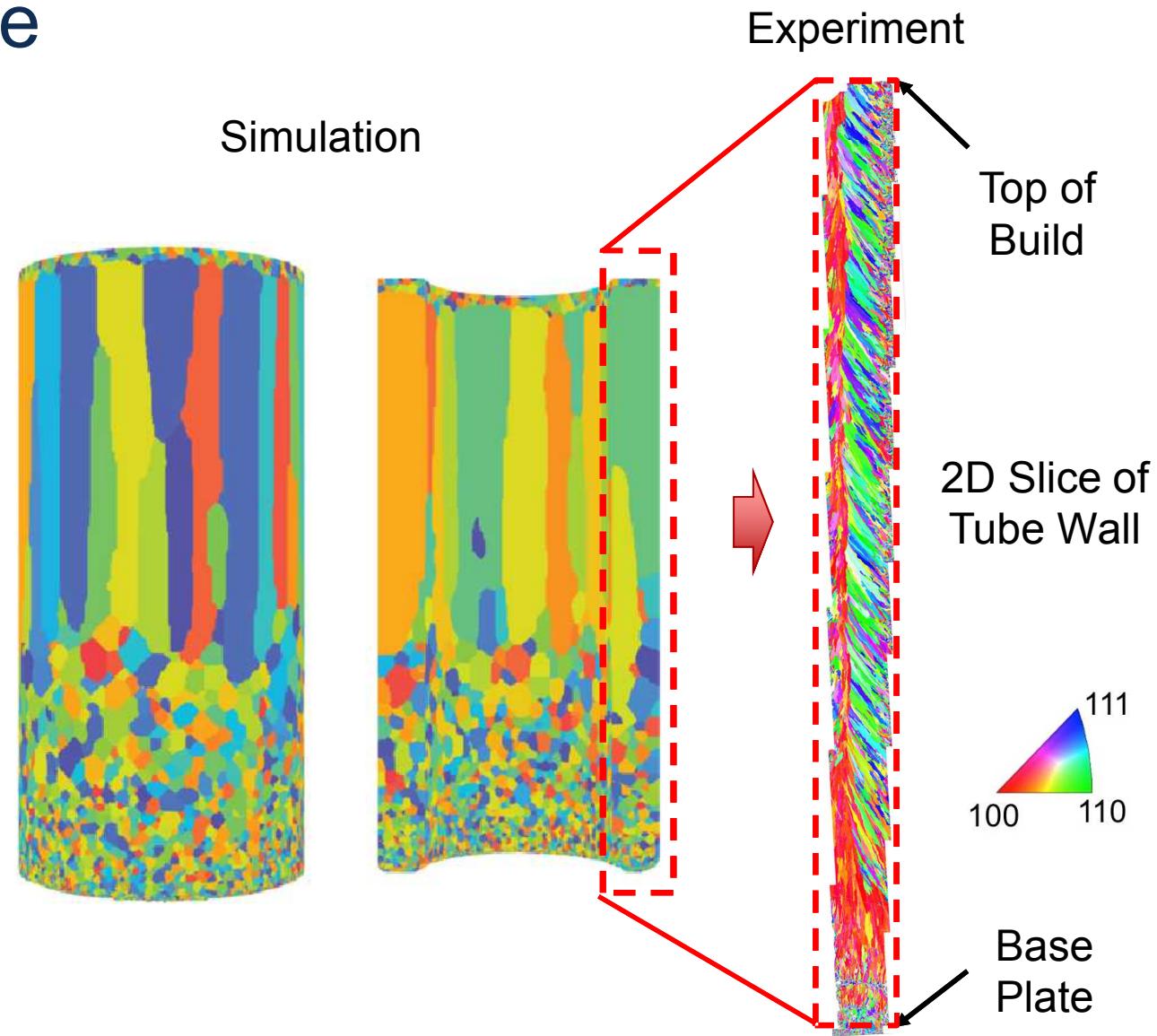
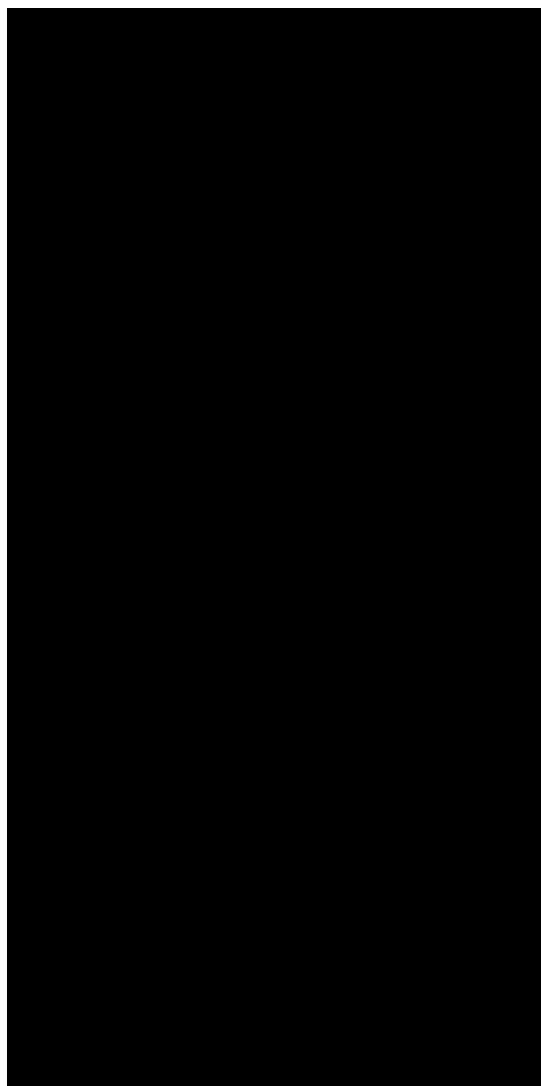
# Residual Stress Prediction



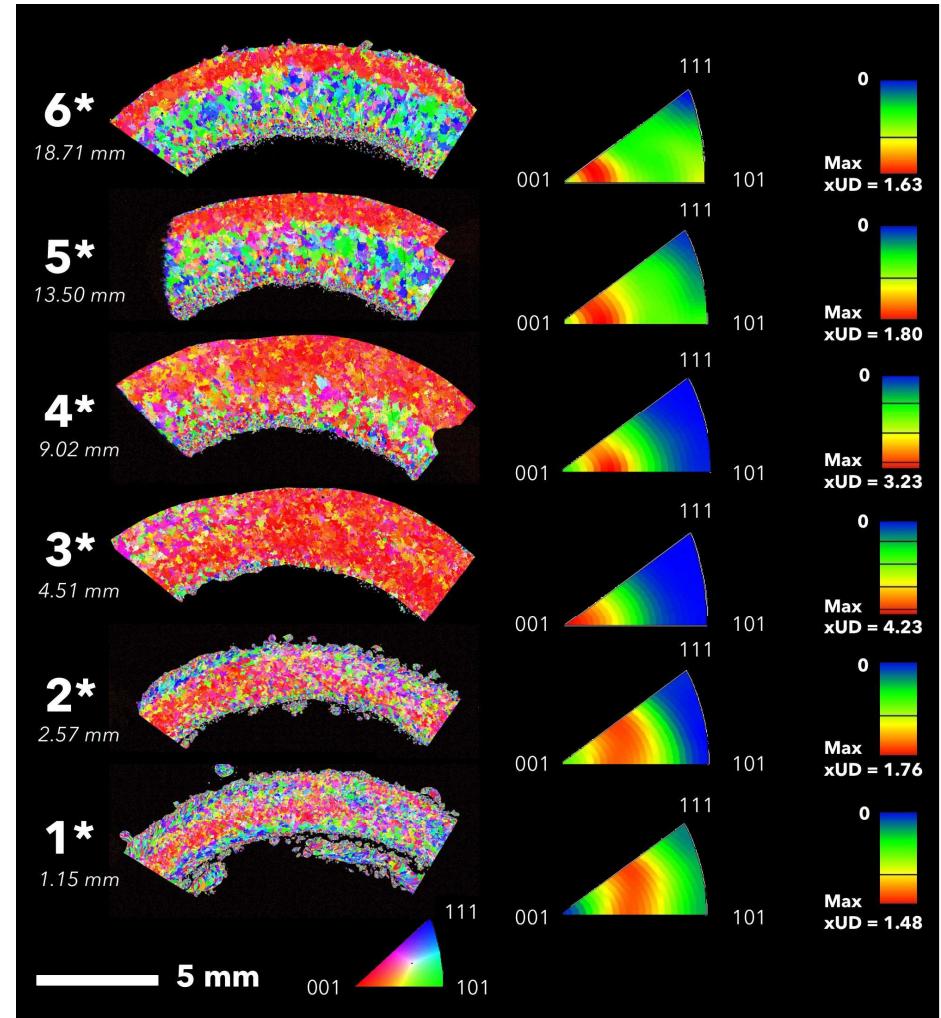
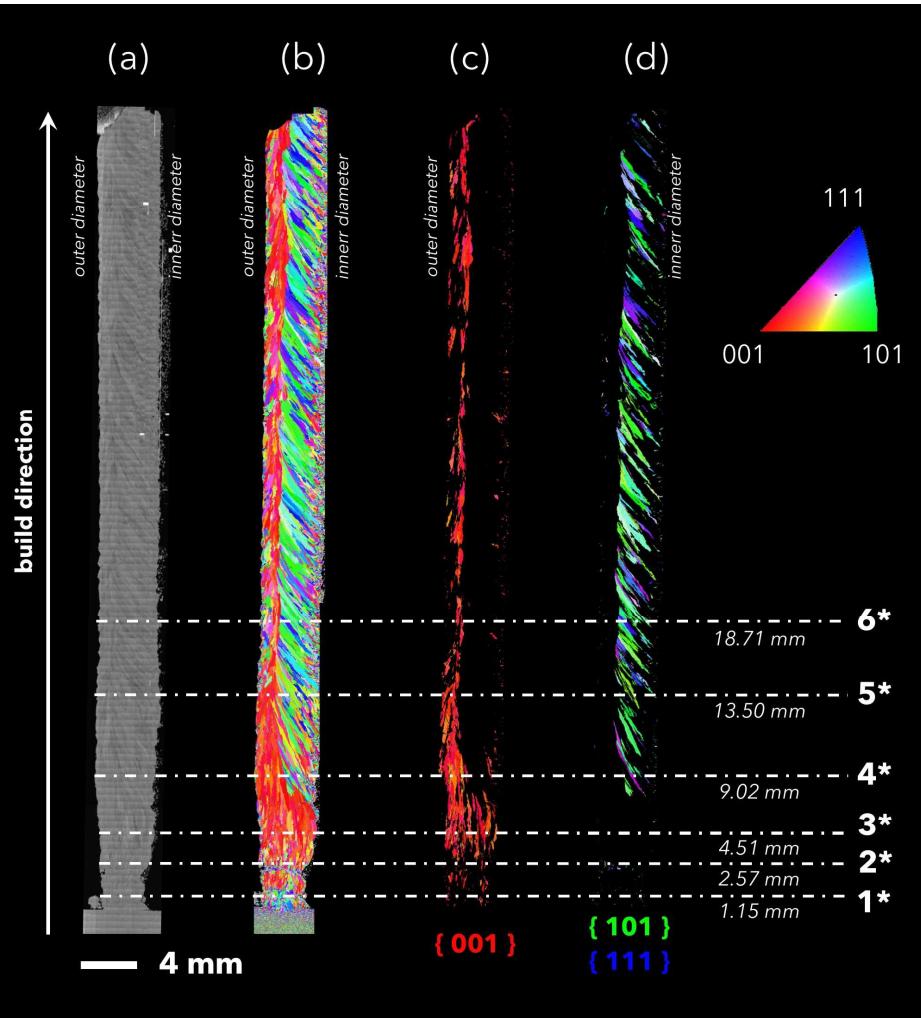
# Residual Stress Predictions Show Gradient Through Wall Thickness



# Experimental Comparison - Microstructure



# EBSD Shows a Transition Region of (001) Grains With Centerline Offset to O.D. Side



# Outline

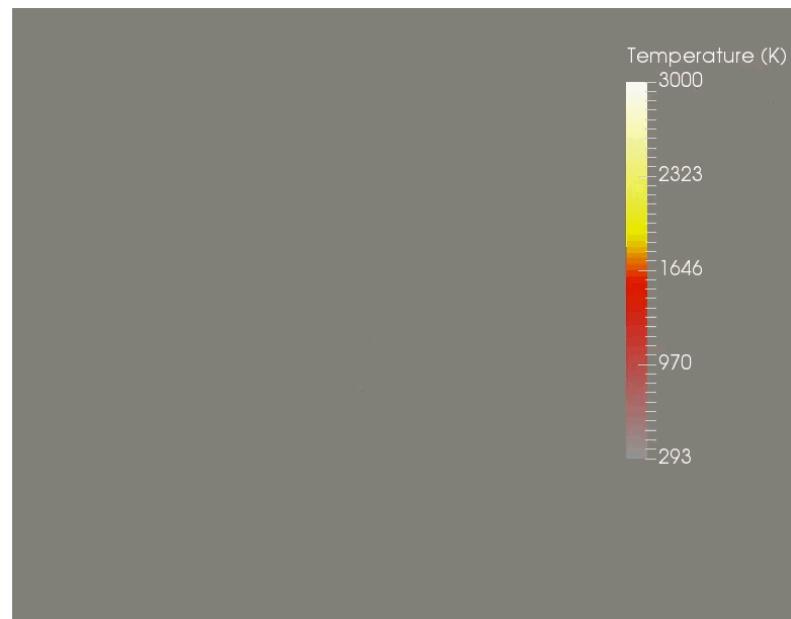
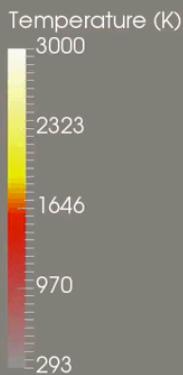
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# Thermal Comparison

Single Build

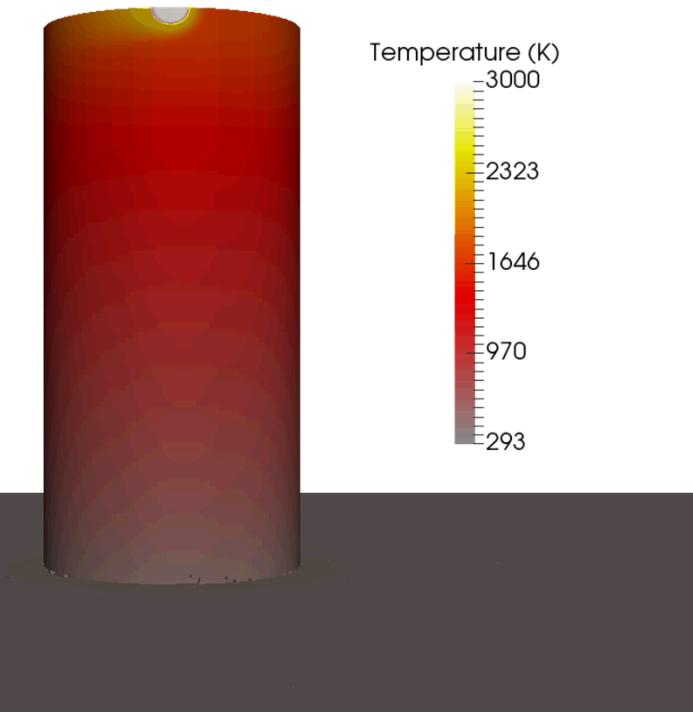
Double Build – 8 Second  
Inter-layer Delay

Time: 0.00 s

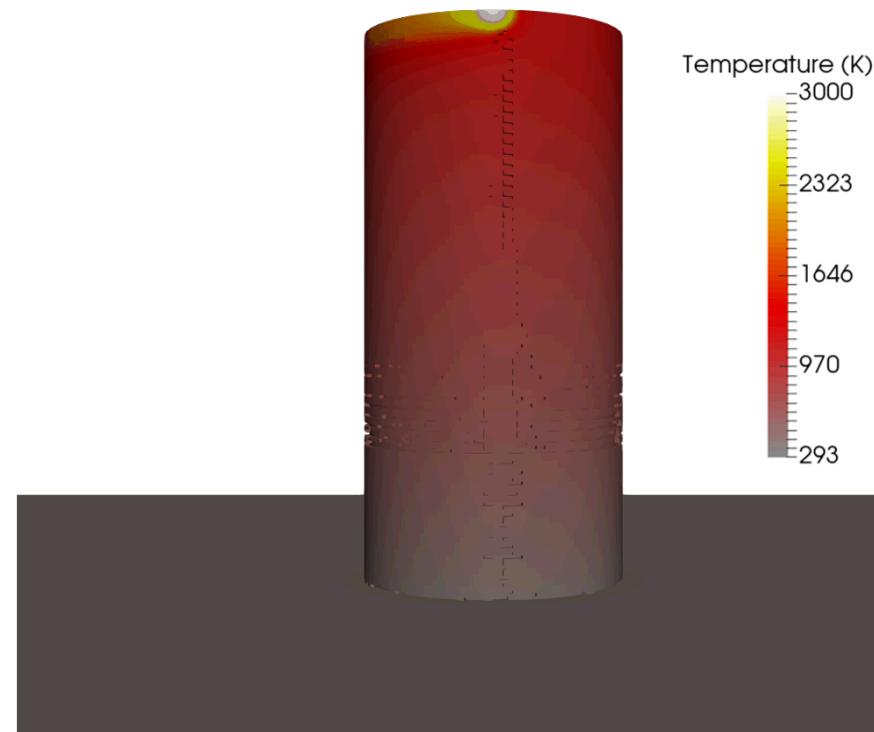


# Delay Time Lowers Global Part Temperature

Single Build

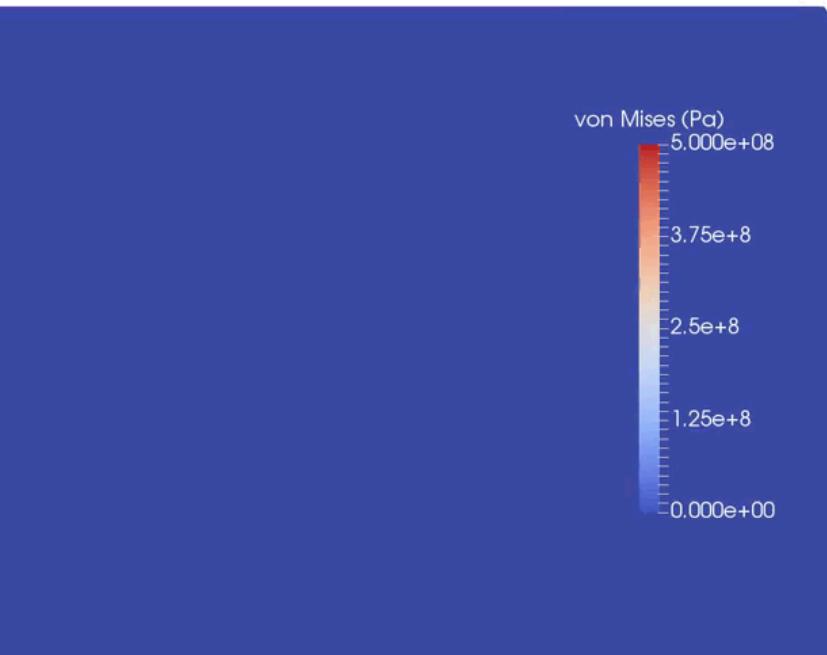


Double Build – 8 Second  
Inter-layer Delay

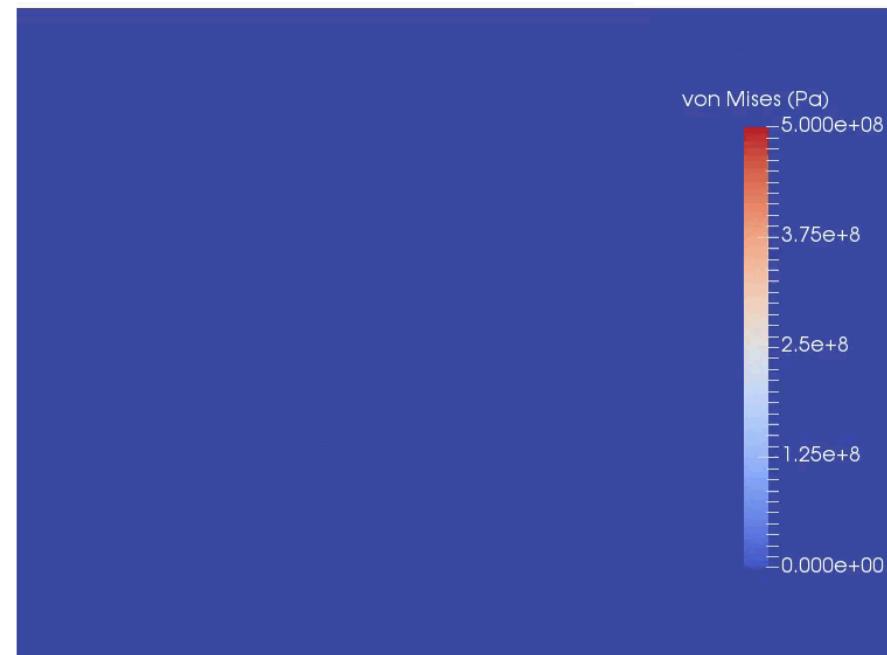


# Residual Stress Comparison

Single Build

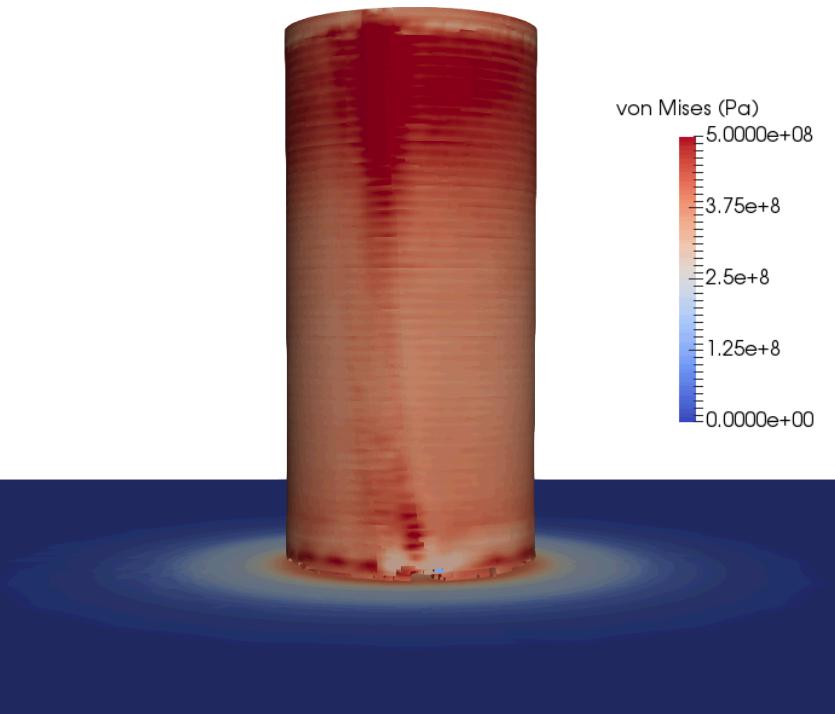


Double Build – 8 Second  
Inter-layer Delay

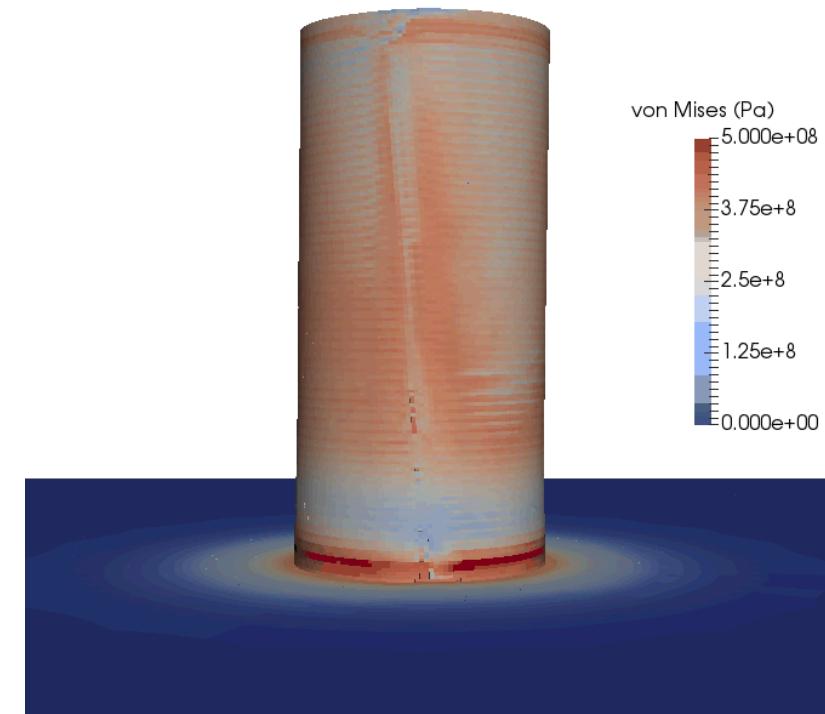


# Delay Time Causes Lower Overall von Mises Stress

Single Build

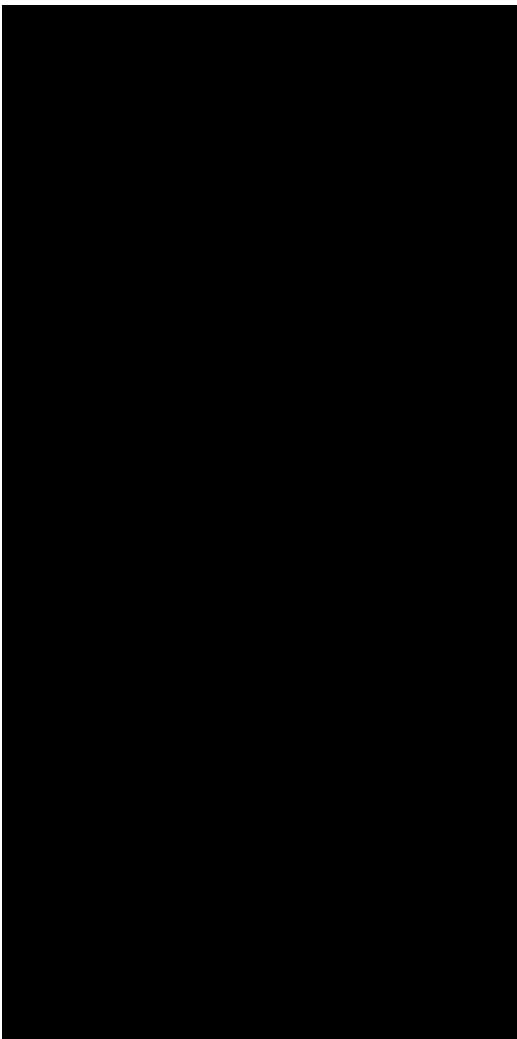


Double Build – 8 Second Inter-layer Delay

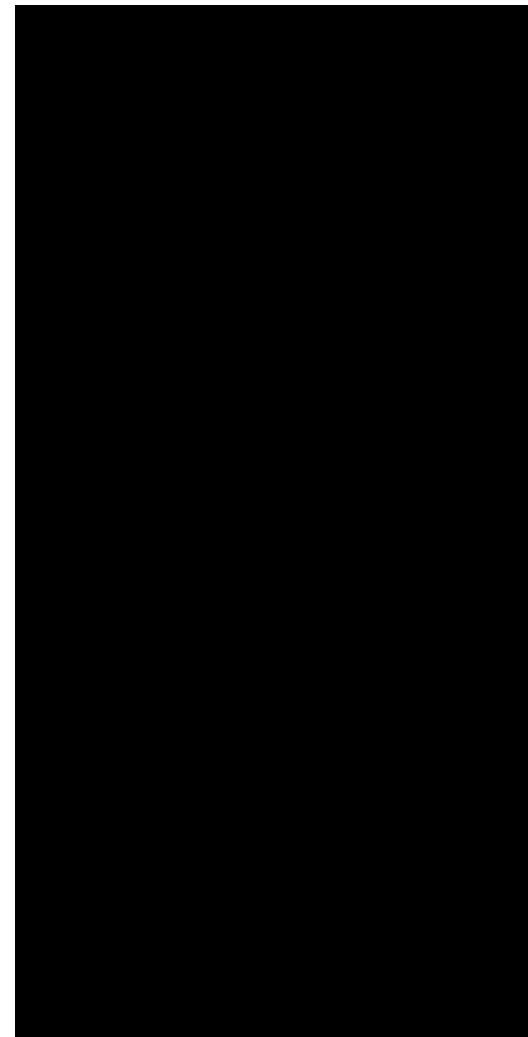


# Microstructure Comparison

Single Build

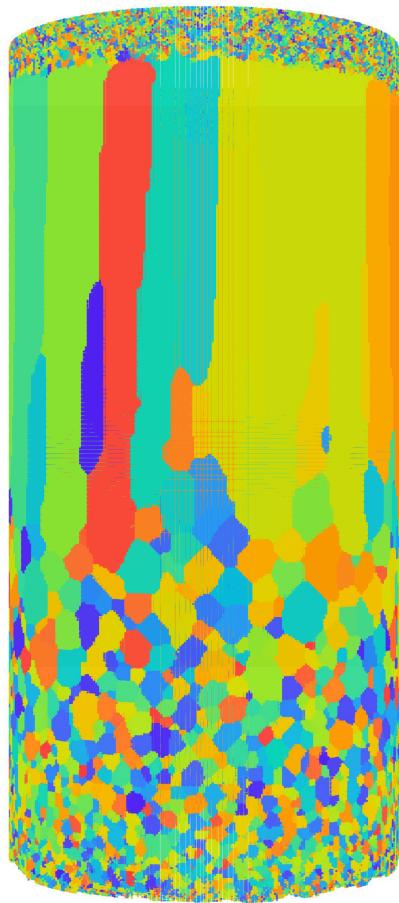


Double Build – 8 Second  
Inter-layer Delay

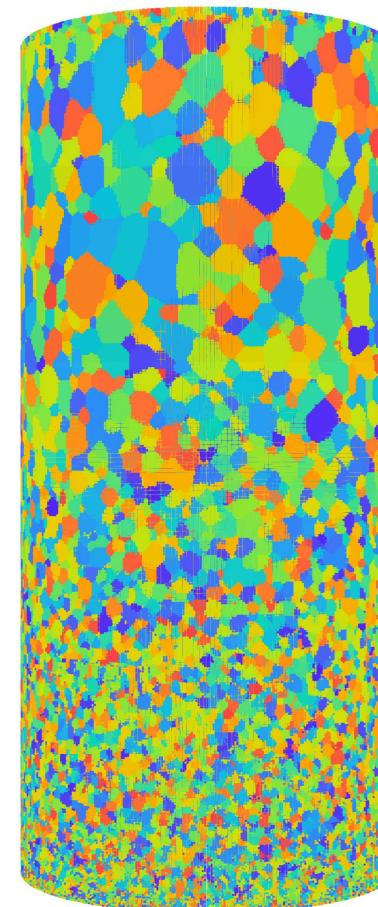


# Delay Time Inhibits Equiaxed-to-Columnar Transition

Single Build



Double Build – 8 Second  
Inter-layer Delay



# Outline

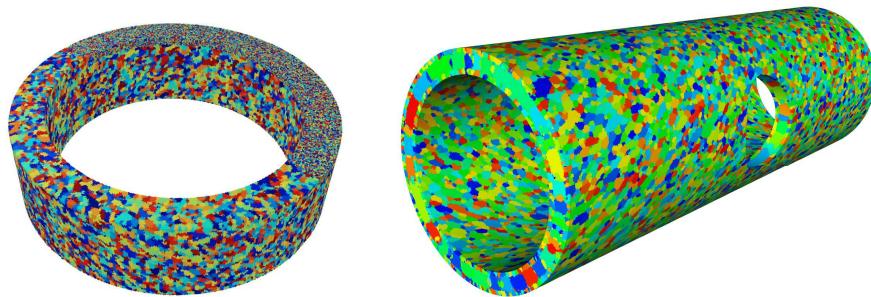
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# Conclusions and Future Work

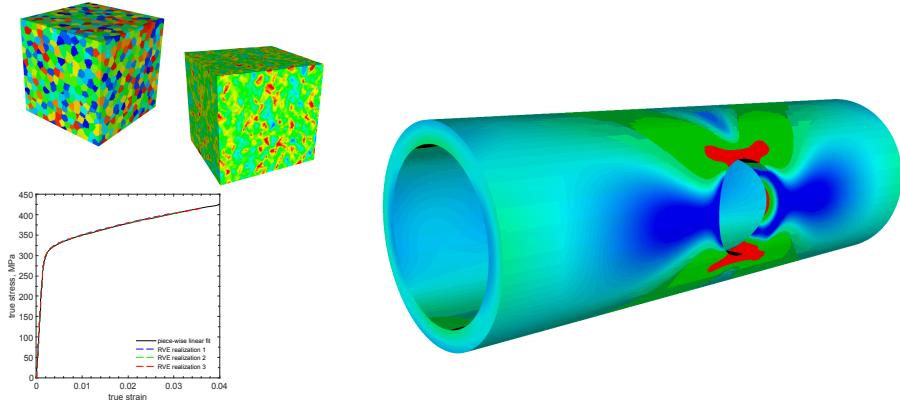
- Thermal, residual stress, and microstructures have been predicted and compared to experiments
- Residual stress decreases with short inter-layer dwell time relative to continuous build
  - Likely specific to this build and process settings
- Inter-layer delay time inhibits equiaxed to columnar transition for selected process settings
- Work ongoing to predict grain orientation
- Currently comparing effects of part-scale thermal model to combined thermal fluid model on residual stress

# Quantifying material variability using multiscale *a posteriori* error-estimation techniques

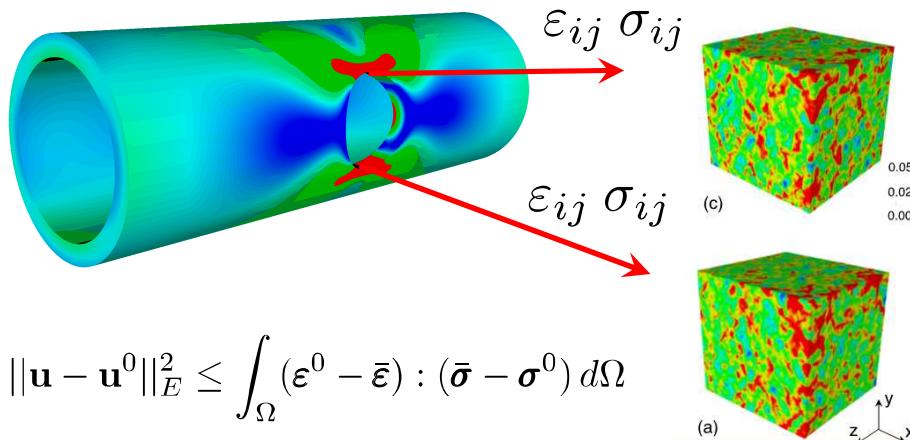
## 1. Generate Microstructures Using Kinetic Monte Carlo (KMC)



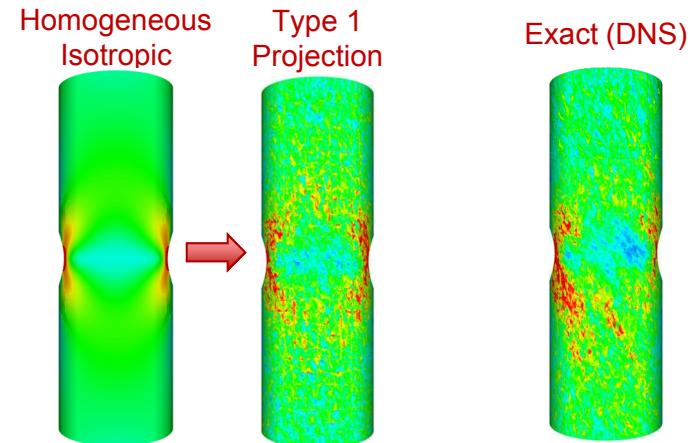
## 2. Run Homogenous Simulation With Isotropic Material Model



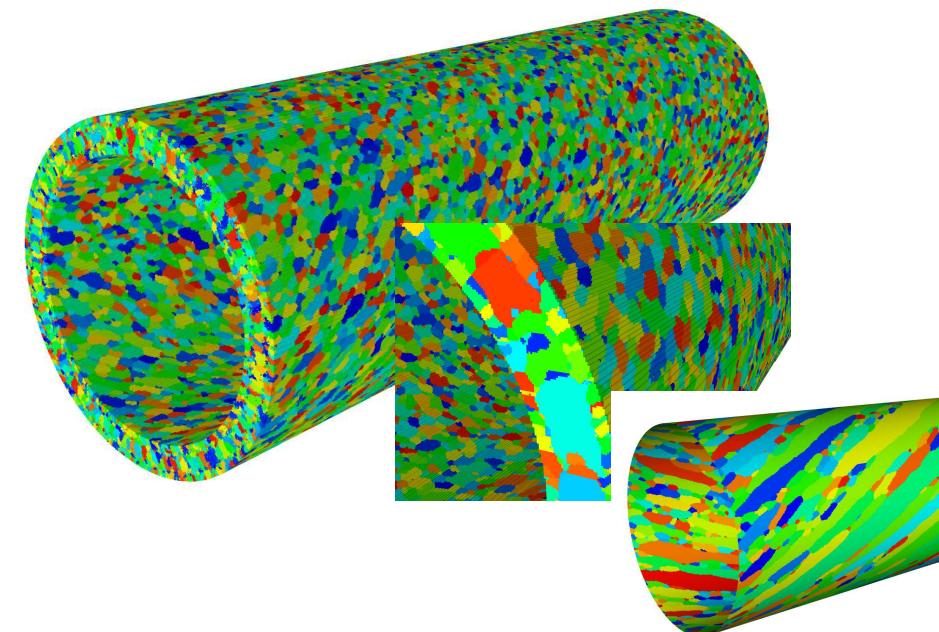
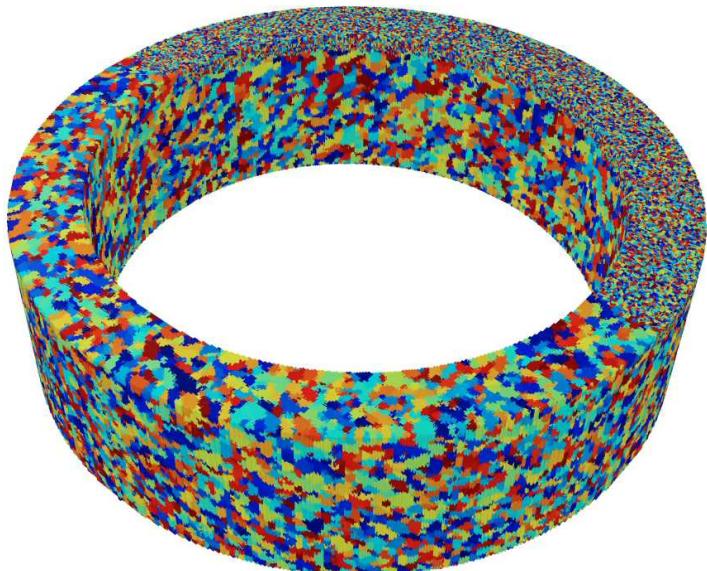
## 3. Recover Localized Stresses Using *a posteriori* Error Methods



## 4. Compare to Direct Numerical Simulations of Full KMC Microstructure



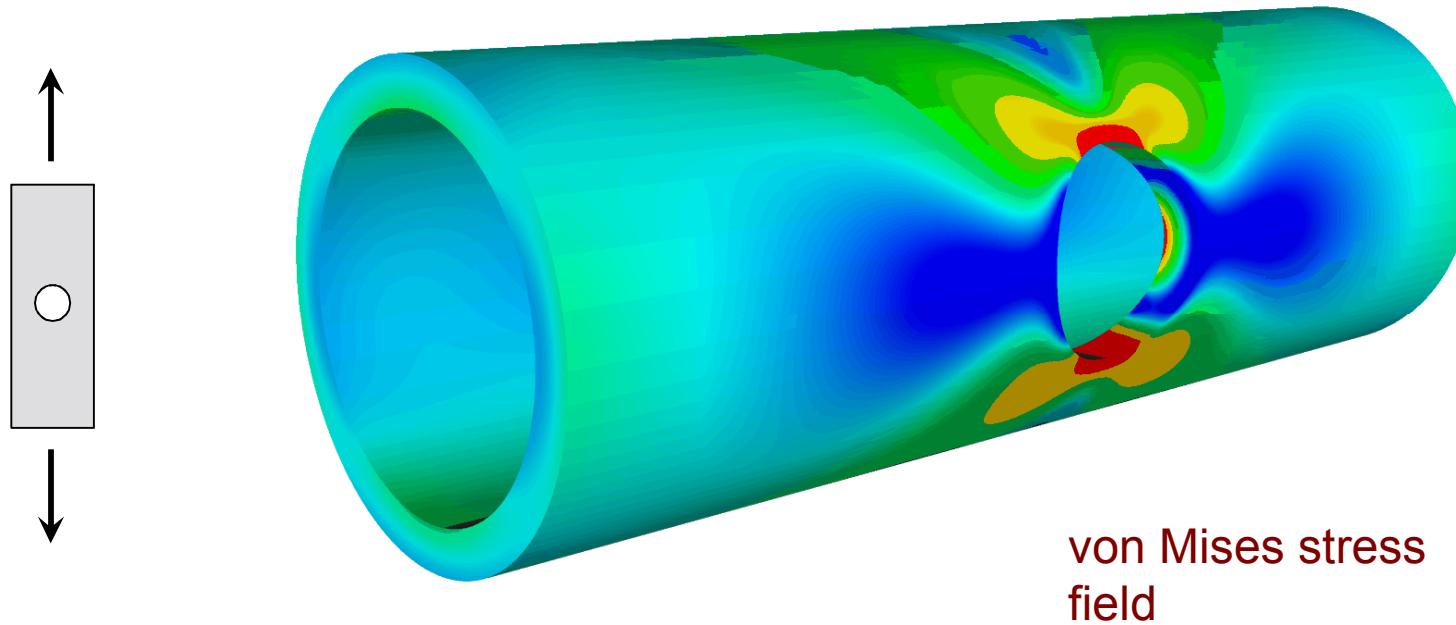
# Synthetic additive microstructure using KMC



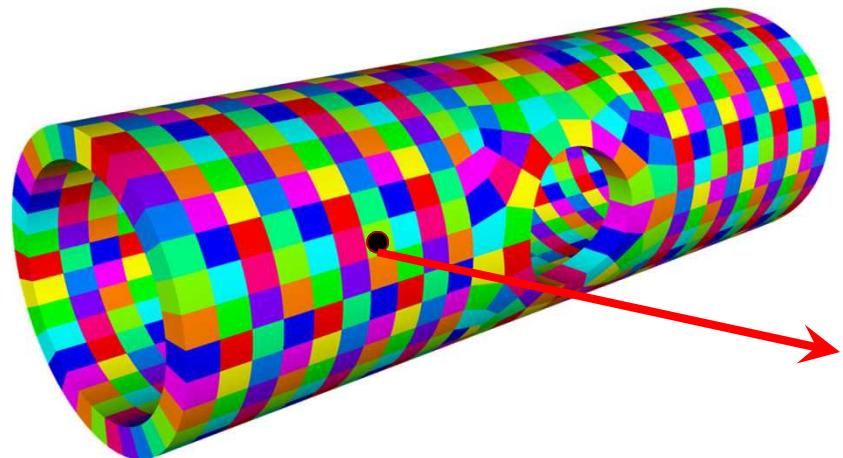
- KMC (SPPARKS) voxelated geometry
  - 55M voxels
- Two laser passes per layer (difference between surface and interior microstructure)
- Map to conformal finite-element mesh
  - 30M elements

# Homogeneous analysis results

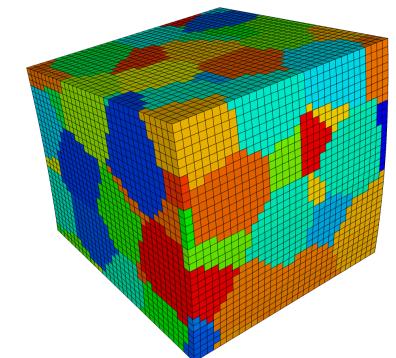
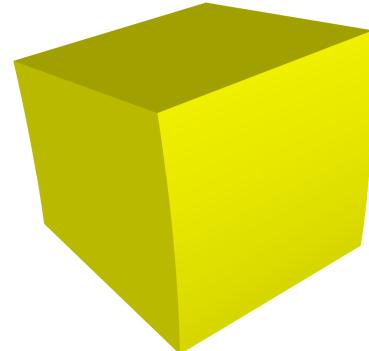
- Using homogenized material properties for wrought 304L
- Isotropic (no texture)



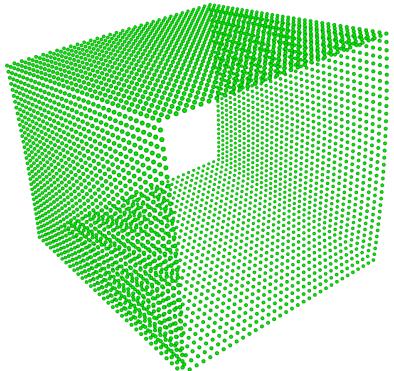
# Type 1 localization



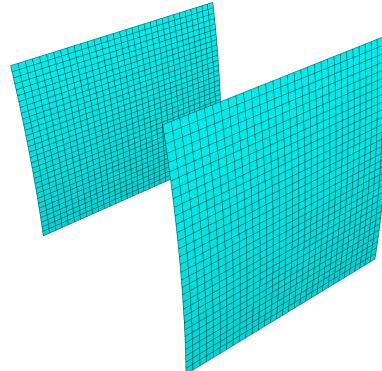
33K Hex Elements



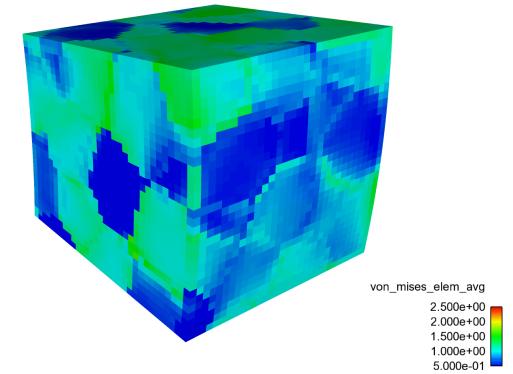
Displacement B.C.s



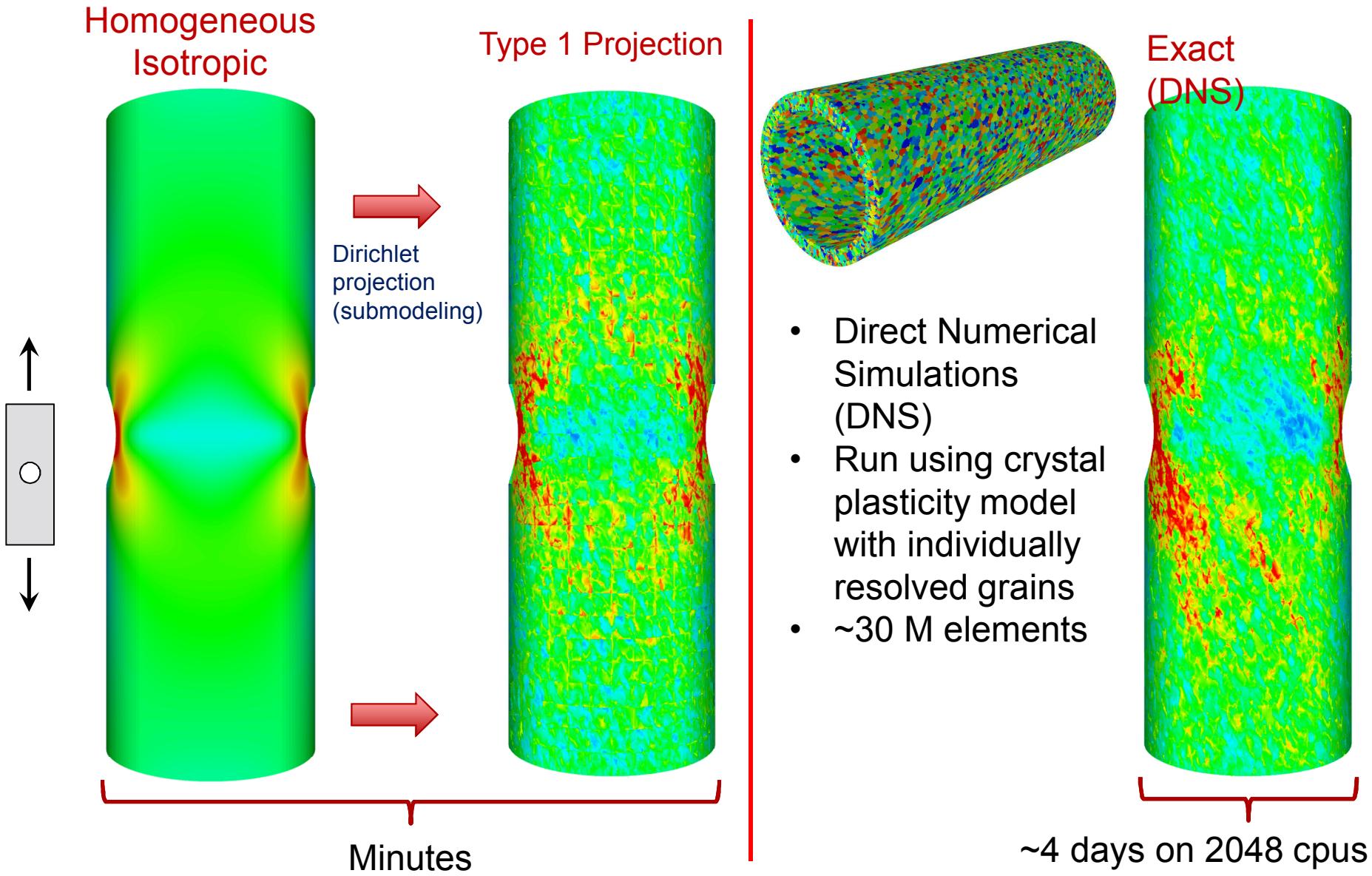
Traction B.C.s



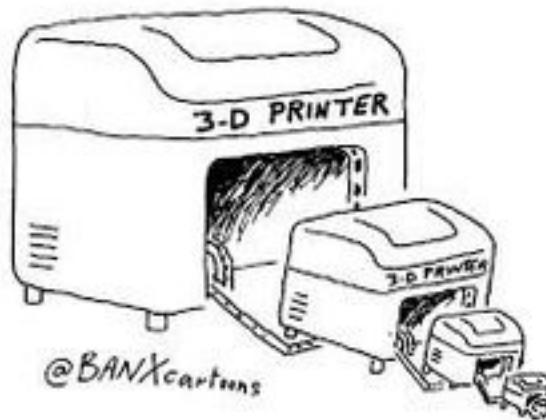
Local Stress Field



# Localization results (AM)

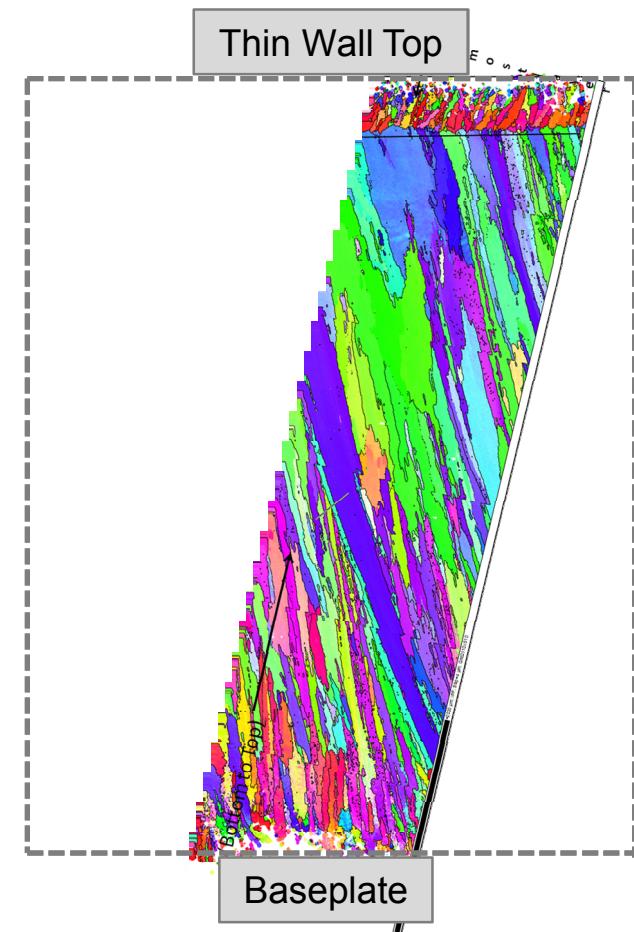
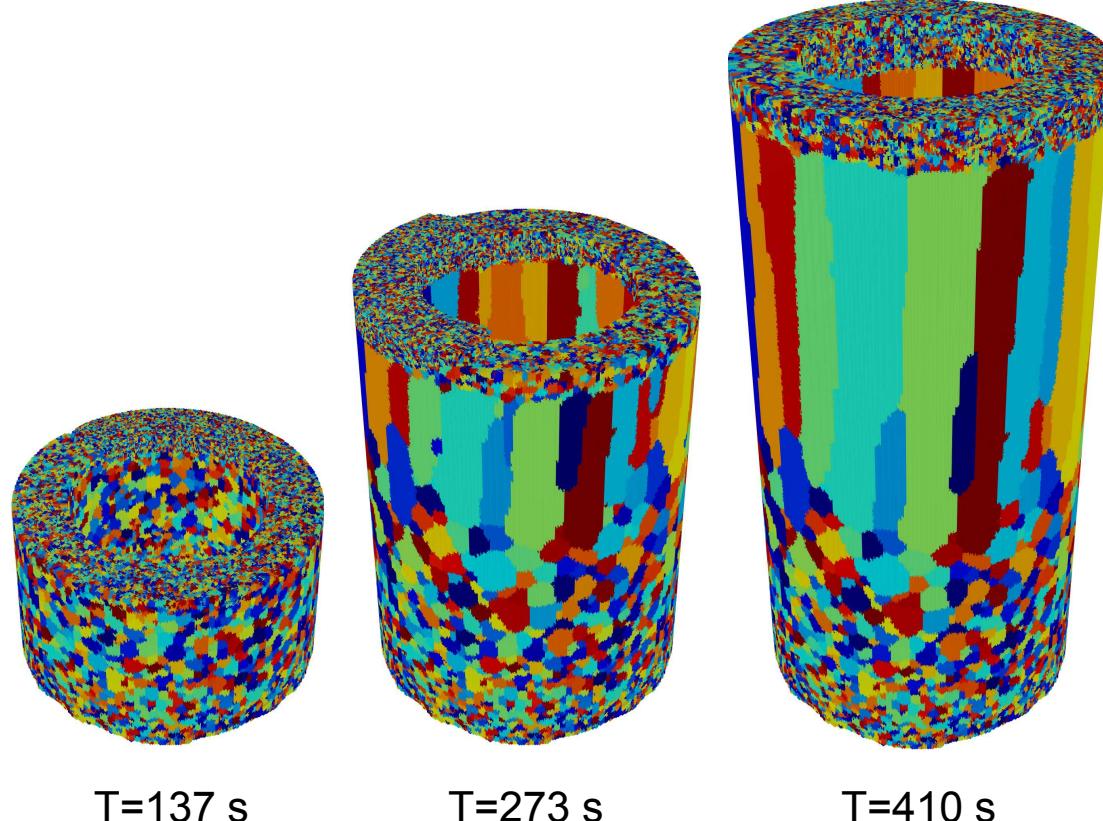


# Questions?



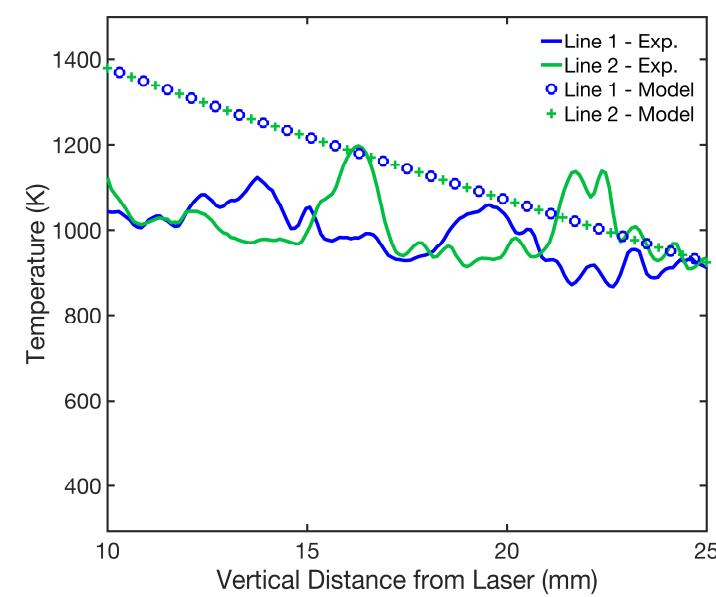
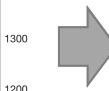
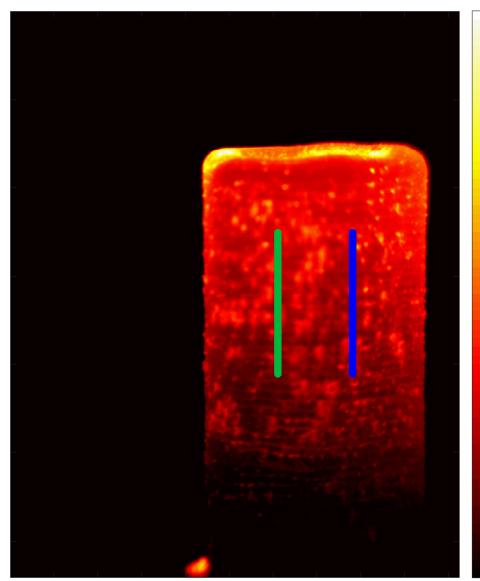
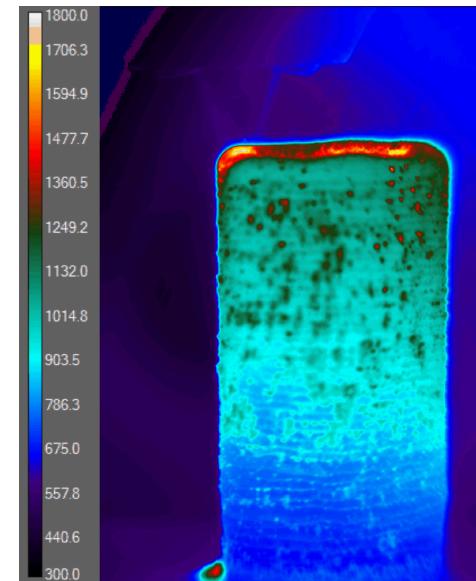
# Backup Slides

# Equiaxed to Columnar Transition Observed in Literature



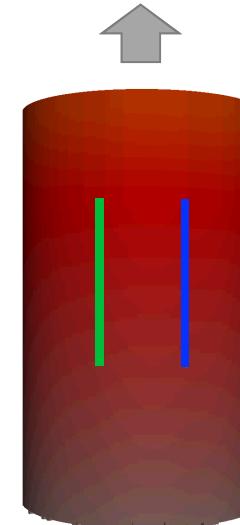
Thin wall IN718 LENS build at 900 W  
Parimi *et al.* 2013

# Comparison to IR Imaging

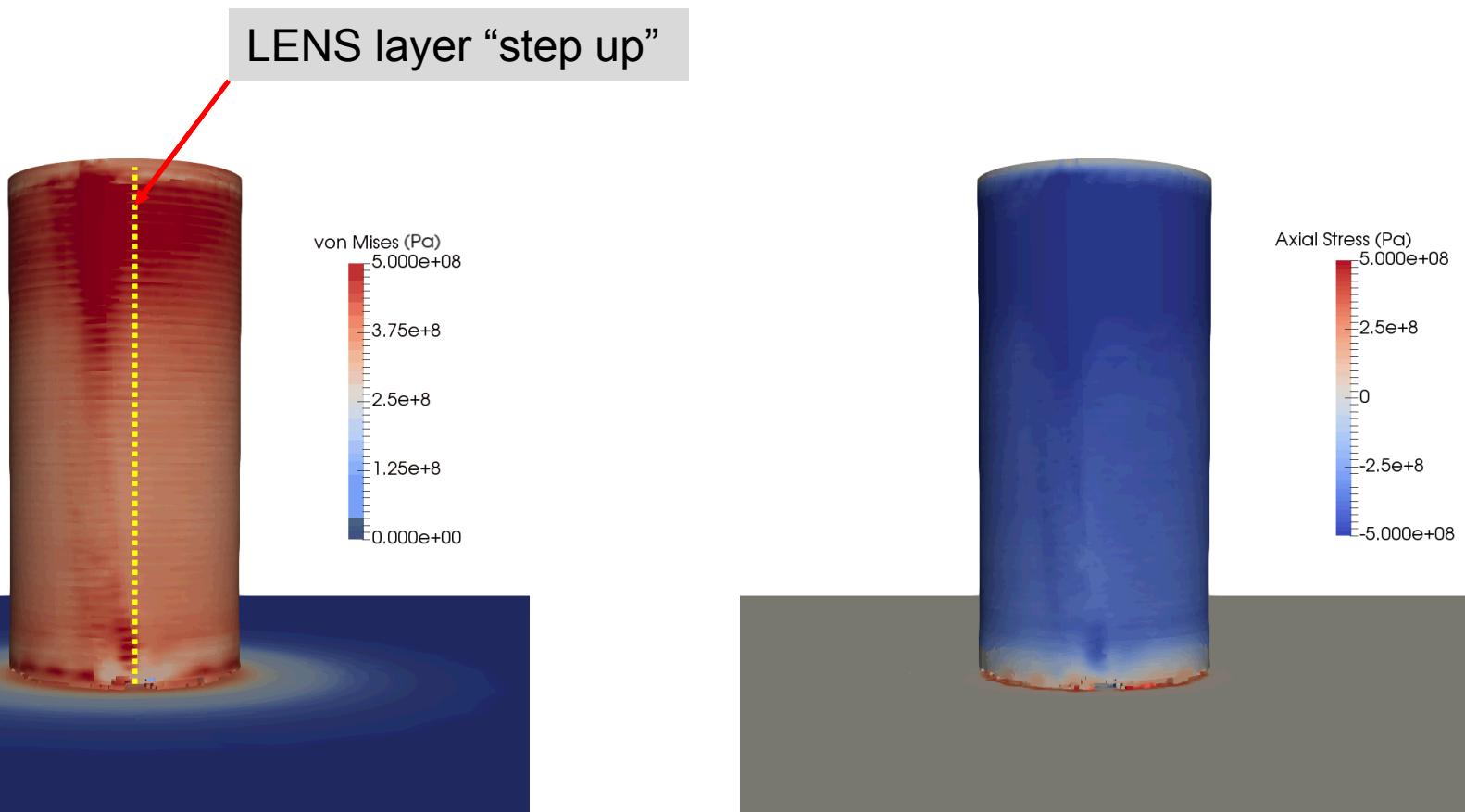


- IR camera mounted on LENS machine
- Assumes constant emissivity
- Compared to simulation

Simulation  
Results

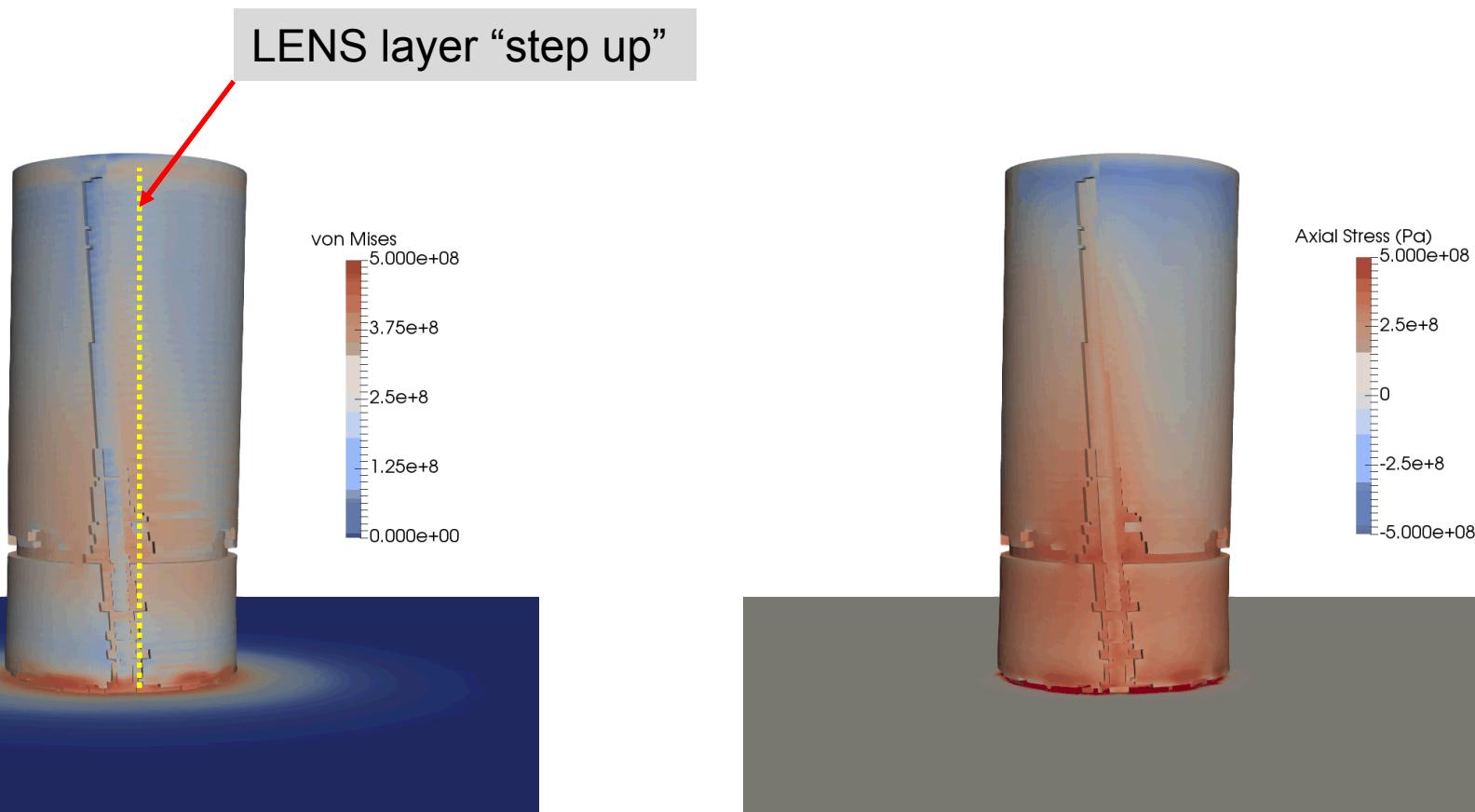


# Final Von Mises and Axial Stress



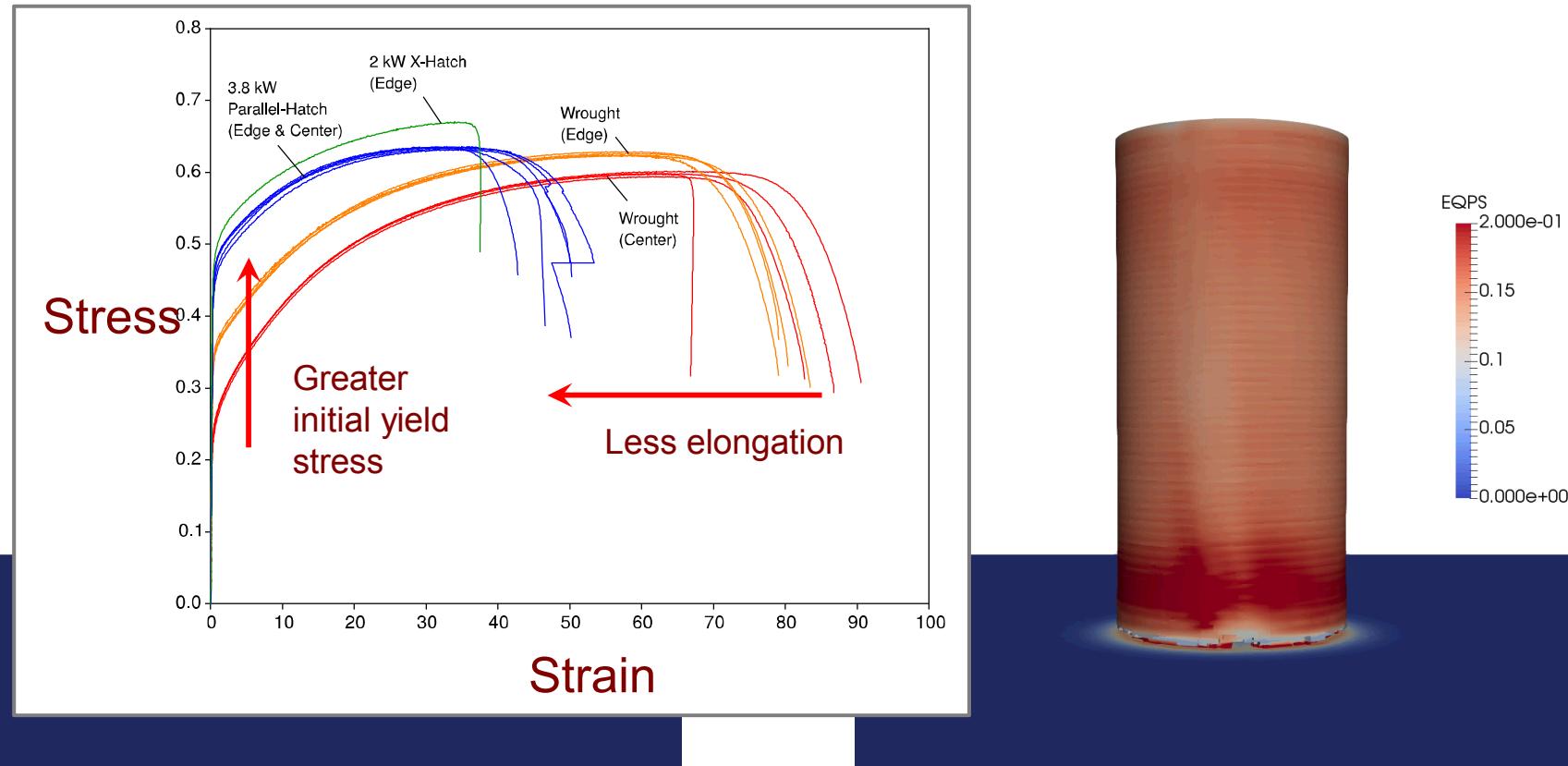
- Images taken after cool-down

# Final Von Mises and Axial Stress



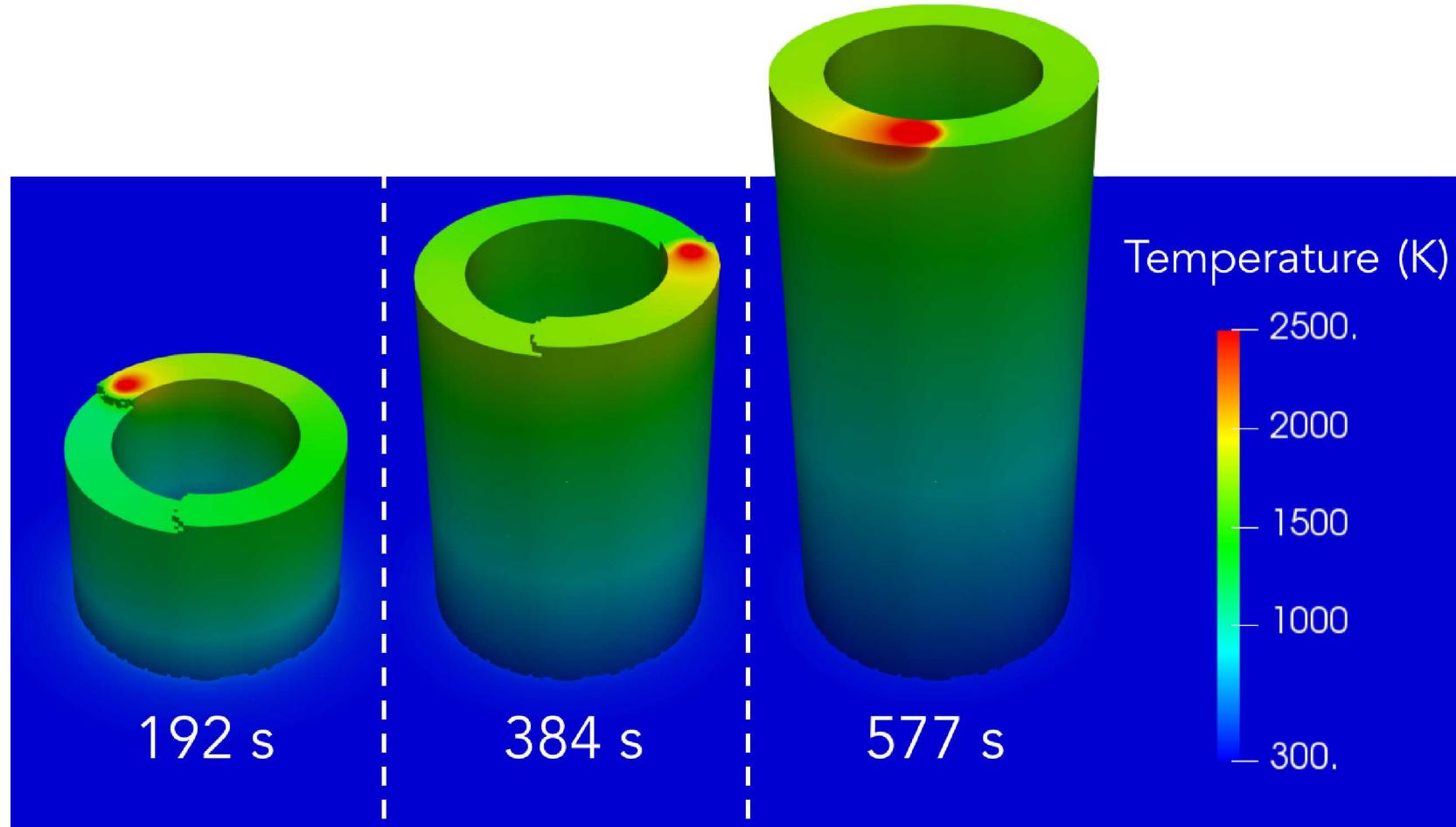
- Delay time causes lower overall von Mises stress and altered axial stress state

# Final Displacement and EQPS

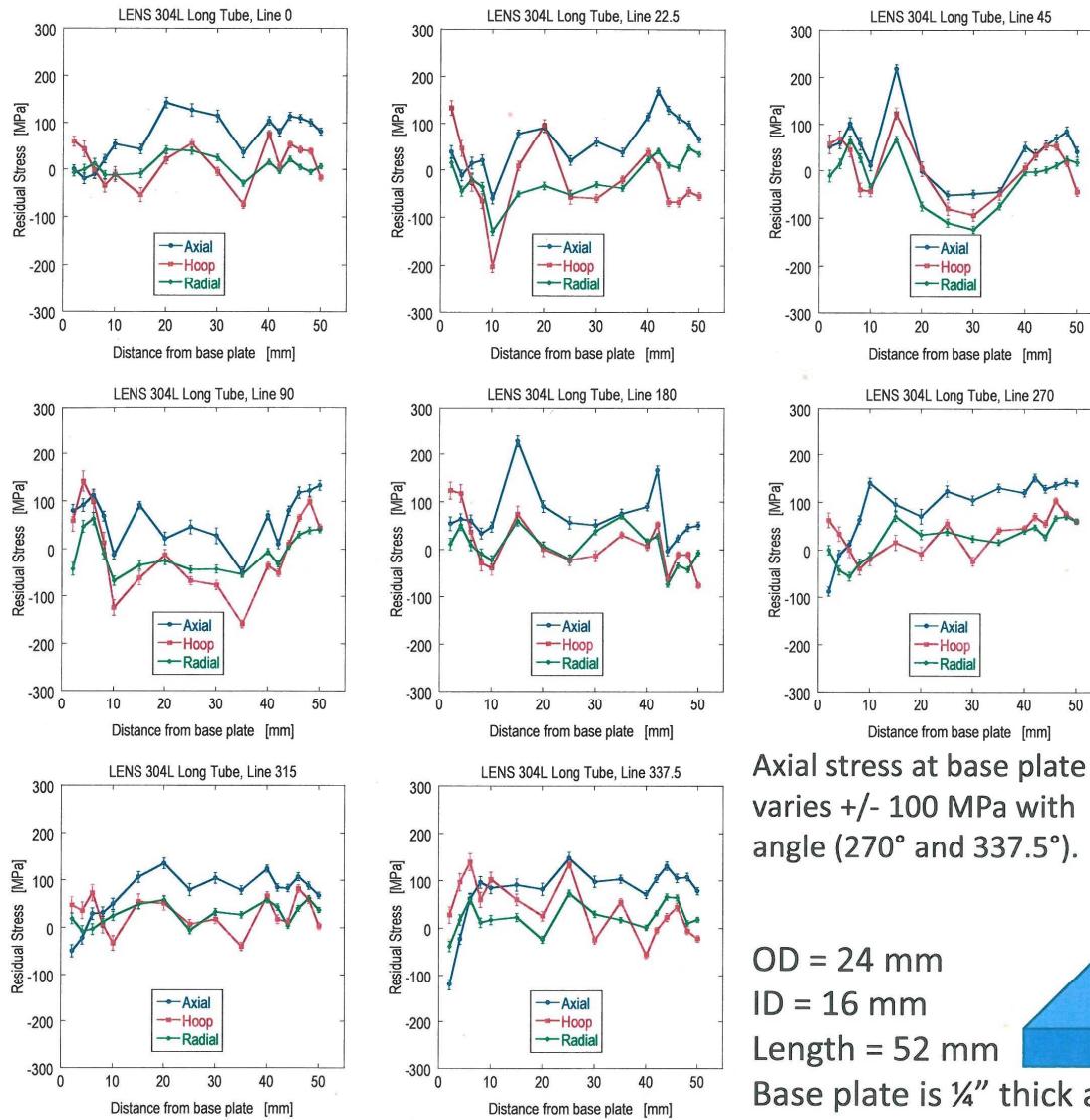


- High EQPS at baseplate indicative of plate warpage observed experimentally

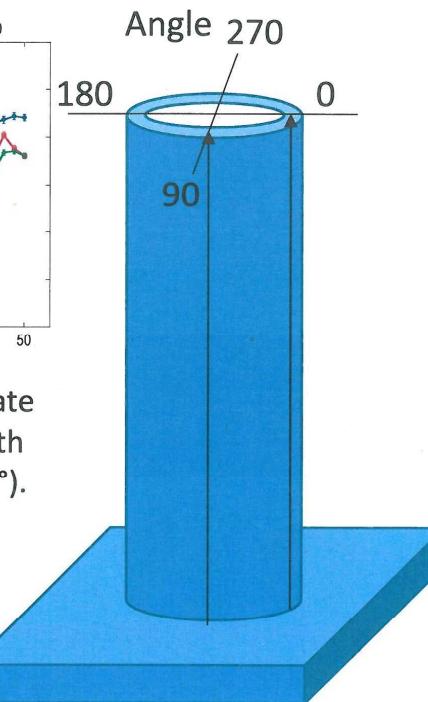
# Thermal Profile at 3 Different Times



# Experimental Comparison - Residual Stress



8 lines along axial direction.  
Transverse hole will be cut at mid length at 0 degrees.



Axial stress at base plate varies +/- 100 MPa with angle ( $270^\circ$  and  $337.5^\circ$ ).