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Sandia National Laboratories

SAND2017-10006C

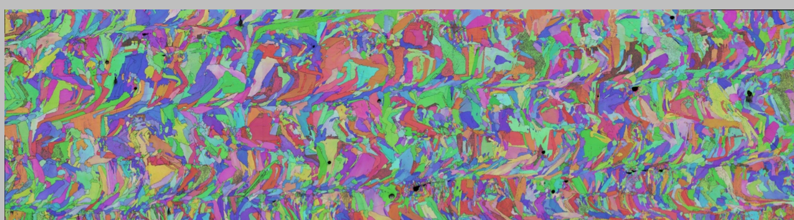
Recent Advances in Integrated Computational and Experimental Methods for Additive Manufacturing

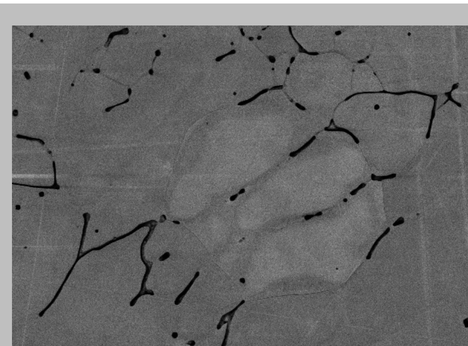
USACM

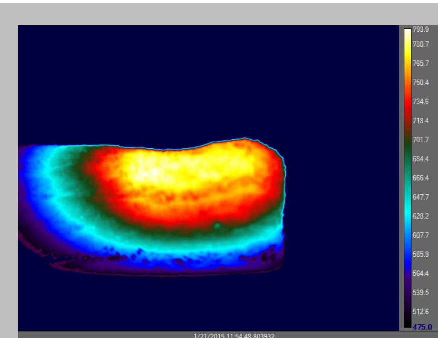
NSF

COLORADO SCHOOL OF MINES
EARTH • ENERGY • ENVIRONMENT

TMS
The Minerals, Metals & Materials Society







Microstructural Evolution, Mechanical Properties and Predictive Simulation of Additively Manufactured Austenitic Stainless Steels

J.D. Sugar, L. Beghini, M. Stender, M. Veilleux, S. Subia, D. Keicher, D. Dagel, M. Maguire, and C. San Marchi

Sep. 8, 2017

U.S. DEPARTMENT OF ENERGY

NNSA
National Nuclear Security Administration

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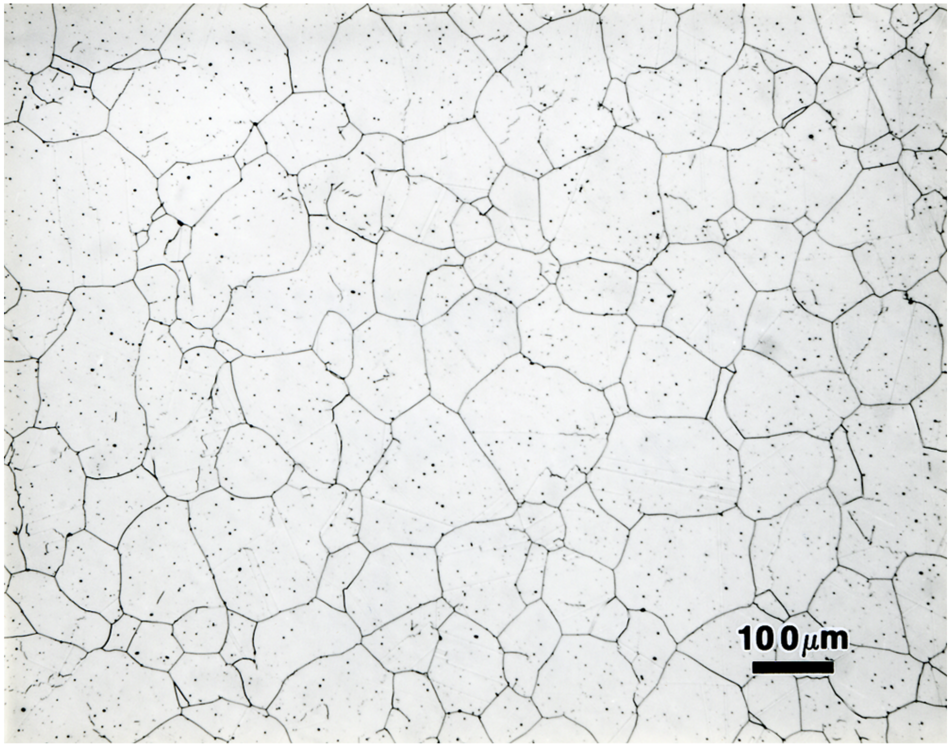
Acknowledgements

- Professor Todd Palmer (Penn State University) 2kW LENS material
- Thale Smith and Professor Julie Schoenung (UC Davis/Irvine): LENS material and Characterization
- LANL and NSC for PBF Materials

- Advertisement
  - Thale Smith's Poster "Microstructure and mechanical property heterogeneity in directed energy deposition (DED) austenitic stainless steel."

Centuries of Metallurgical Knowledge



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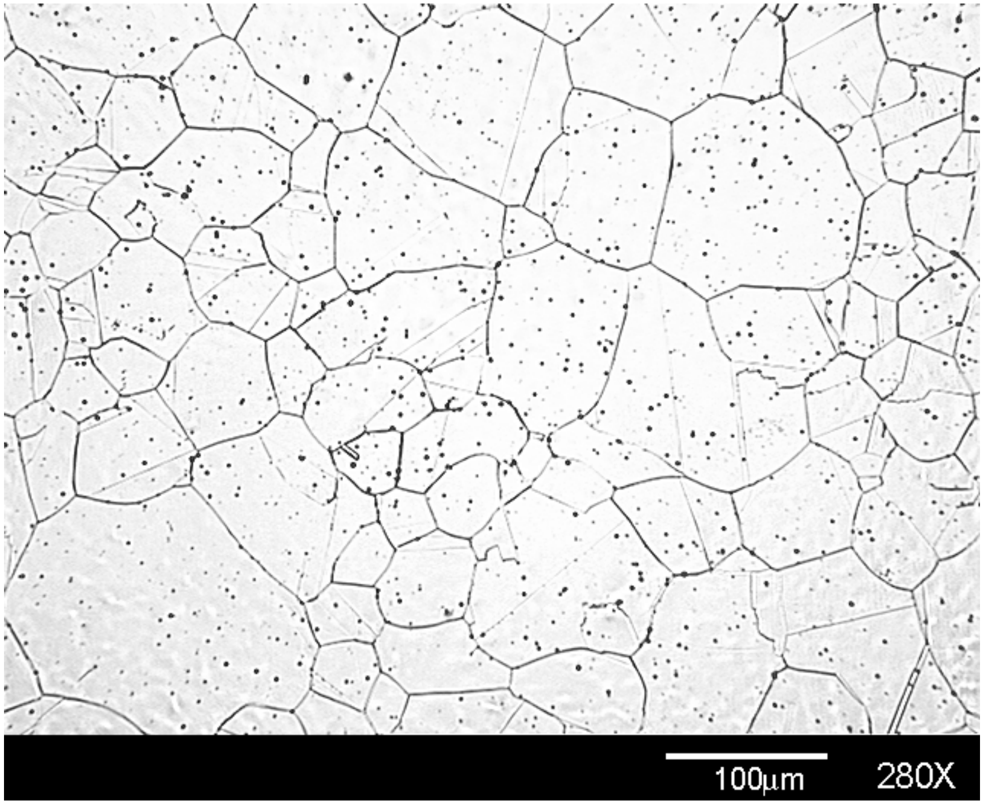

Annealed 316 Stainless Steel
ASM Micrograph Database

http://products.asminternational.org/mgd/index.aspx

Annealed 316 Stainless Steel
Courtesy of Chris San Marchi

- Annealing conditions that lead to this microstructure are well known, and the properties of this microstructure are well documented

Need To Fundamentally Understand the Processing-Microstructure-Property Relationships

- An alternative to an empirical database like ASM based on physics
- We must understand the mechanisms that contribute to the microstructural development during AM processes
- Properties and final form/function are coupled in AM through processing parameters (thermal history) and slice/build approach

- Goal is to answer:
- Can we relate the mechanical properties of a particular build to the details of the process?
- Develop a process model to predict lifetime performance that is validated by experiments (e.g. in situ thermal measurement, residual stress measurement)

Lifecycle Analysis of Additively Manufactured Components

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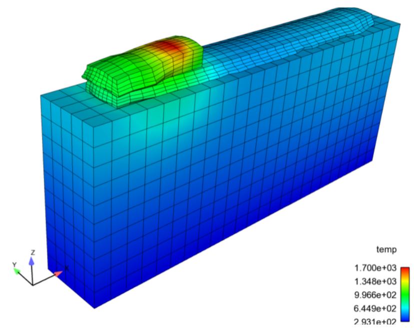
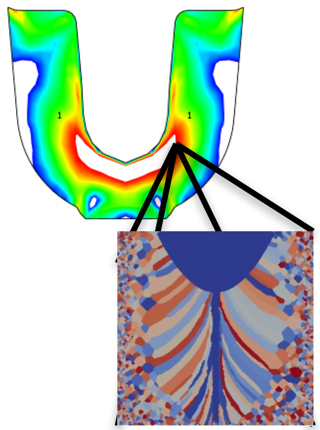
Process Design and Simulation

Advanced process controls and diagnostics enable simulation tools to "grow" near-net-shape structure

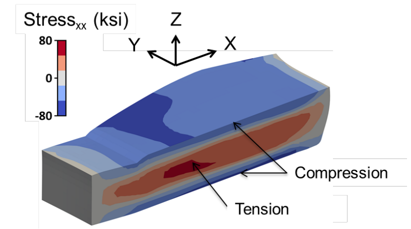


Microstructure and Properties



Internal state variable models account for microstructural evolution and distribution of properties (related to spatial variations of thermal history)

Residual Stresses

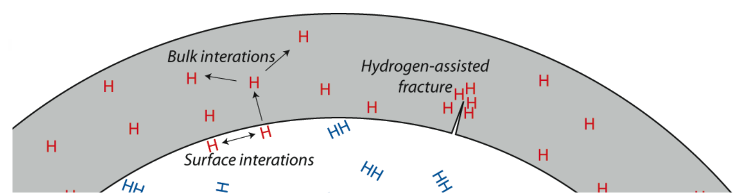


Solidification and thermal history result in strong residual stresses, which can impact performance

- Predictive uncertainties result in large safety factors, reduced lifetimes, and increased costs.
- Our approach develops tools to reduce uncertainty, increase understanding, and enhance predictive capability.

Assembly and Service

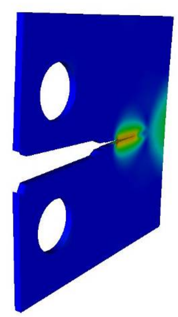
Multiphysics approaches for fully coupled simulation of chemical/thermal transport, mechanical loading, etc. to predict performance



(includes unique service environments, such as hydrogen embrittlement, corrosion, microstructural aging, etc)

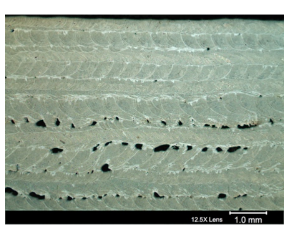
Crack Initiation, Growth and Failure

Transition from crack initiation to failure is not well characterized and depends on microstructure and defects



Margin/Uncertainty → Design Life

Service requirements may dictate design iteration to assure sufficient margin based on predictive uncertainties.
The lifecycle analysis provides a tool to enable design optimization to meet the requirements.



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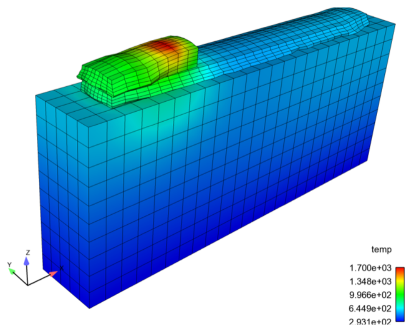

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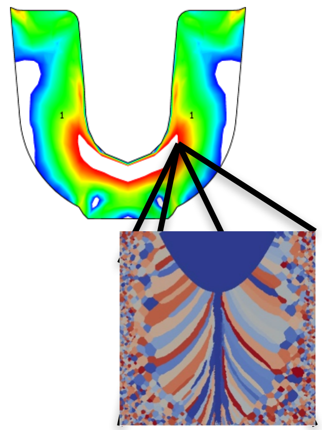

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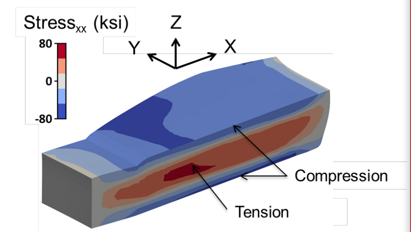

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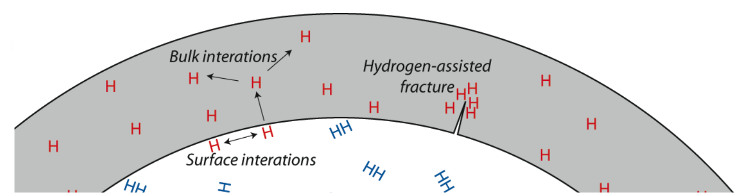

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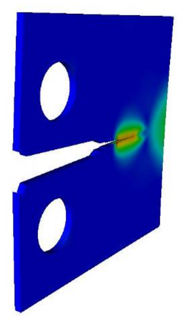

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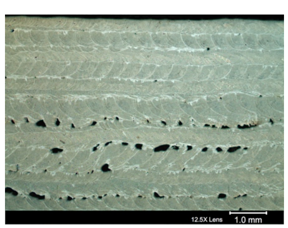
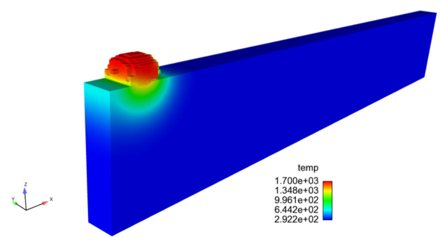
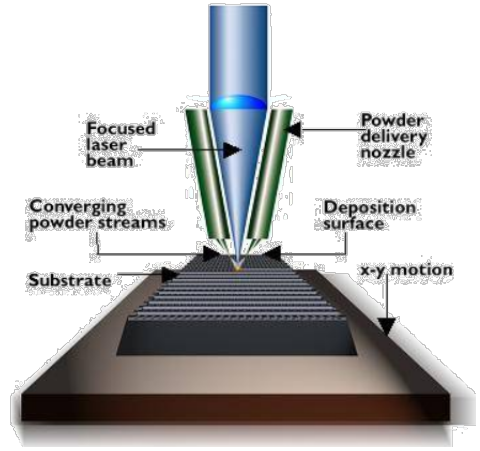


Spherical Moving Heat Source

- Material is activated via a spherical, volumetric heat source
  - Inputs: raster path, melt temperature, diameter, efficiency, radius and spatial influence factor
  - Activation user variable – toggles conductivity on/off within the sphere





LENS Process

  - Activation and melt pool size based on variable input power

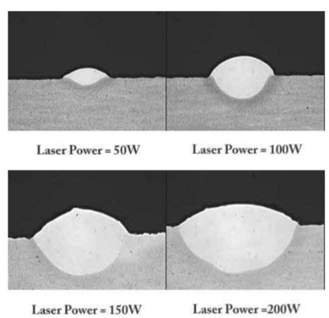
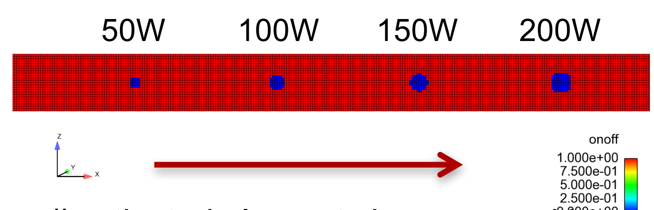
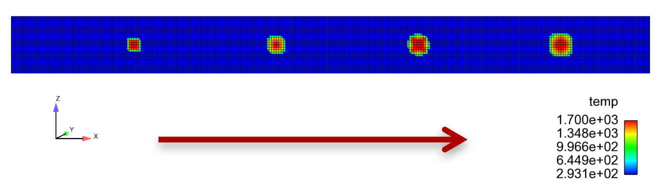


Figure 2: Cross-sectional photographs showing semi-circular type melt pool geometry over a range of laser powers. Travel speed = 5 mm/s, powder mass flow rate = 0.08 g/s.

http://www.lehigh.edu/~inemg/Framset/Research_Activities/JLP/LENS/LENS_4.htm



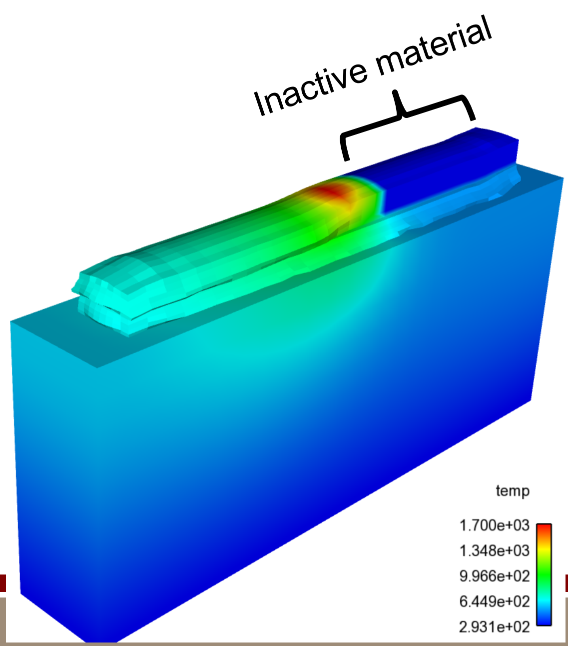
activated elements increases with power

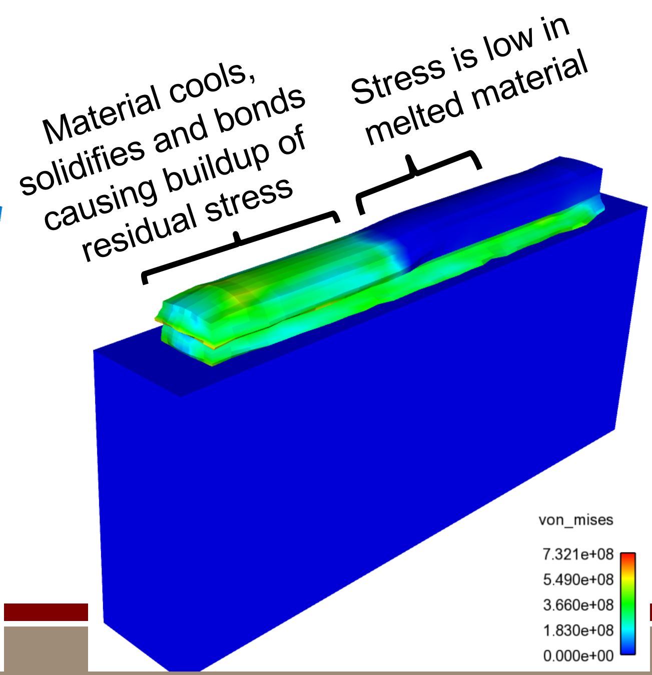


Melt pool size increases with power

Building Models to Birth AM Material: LENS

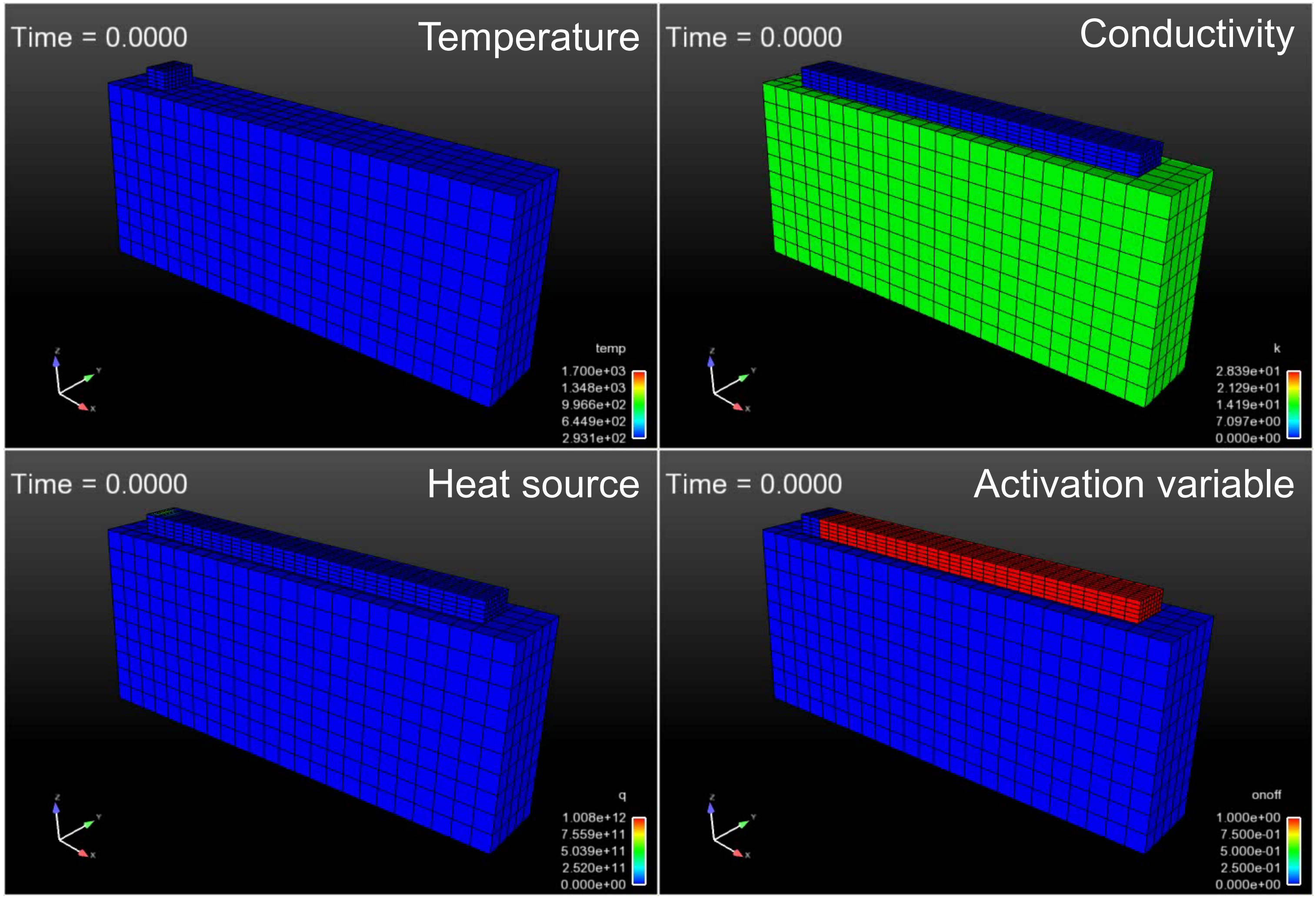
- Sandia Solid Mechanics based code
  - Traveling volumetric heat source based on path (x,y,z), power, efficiency, diameter
  - Element birth from inactive elements: physical properties turn on when interact with traveling heat source
  - Phase transformation ~ 1700k
  - Deformation from gravity
  - Contact transitions from Coulomb to glued (sliding to tied friction model)





Modeling of Material Birthing

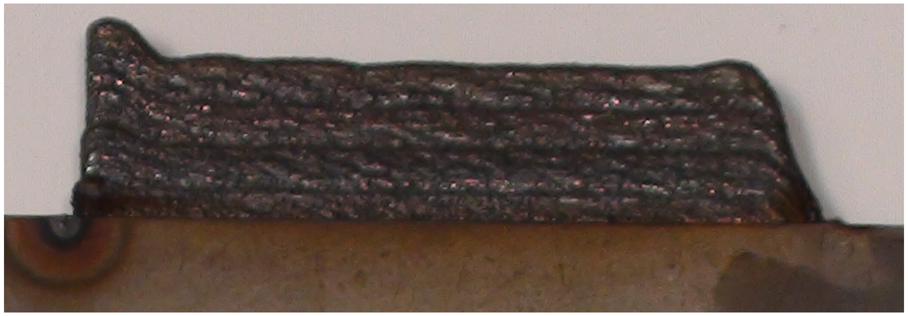
- Thermal solution



Thermal profiles demonstrate effect of laser power

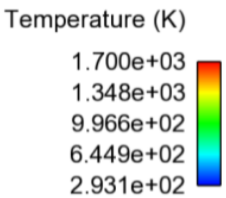
Thin walled LENS part build

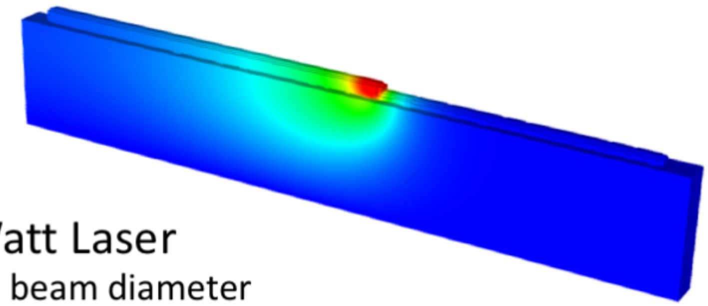
- ~1.8 inches long
- Efficiency = 36%
- Print Speed 20 inches/min
- Material melt temperature = 1700 K



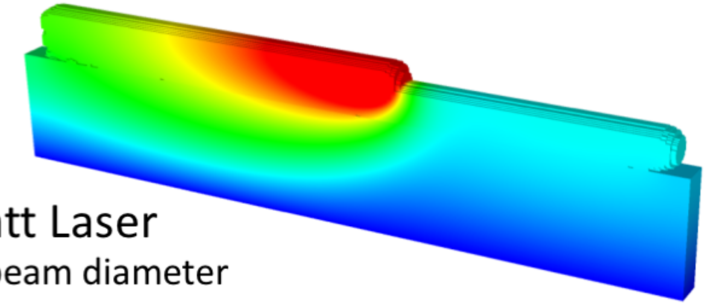
500 W Laser

2 kW Laser





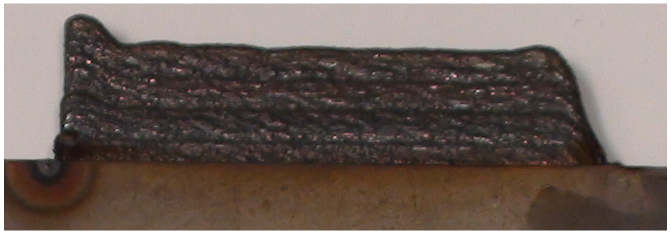
500 Watt Laser
0.001 m beam diameter

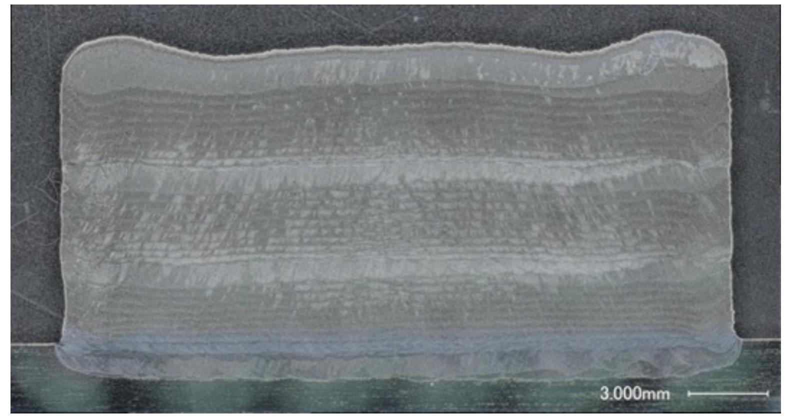


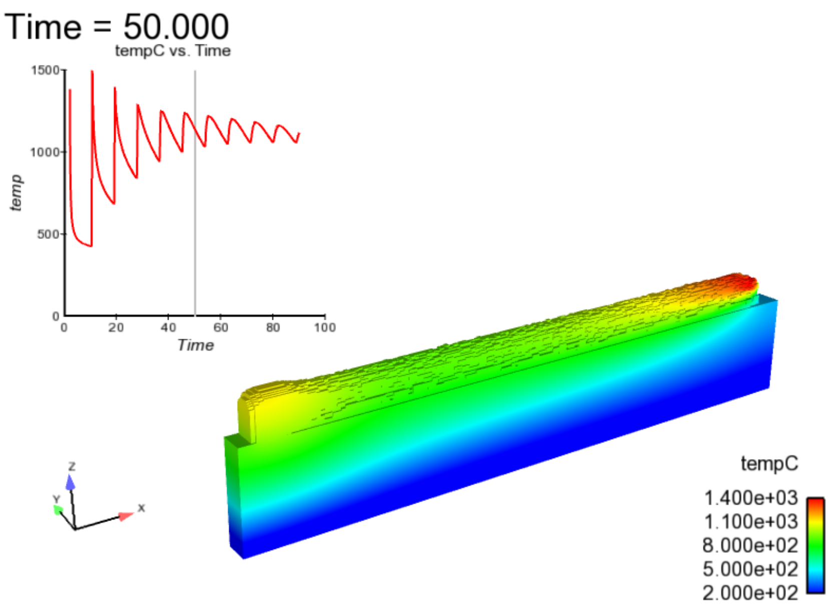
2000 Watt Laser
0.0025 m beam diameter

Models can predict general shape

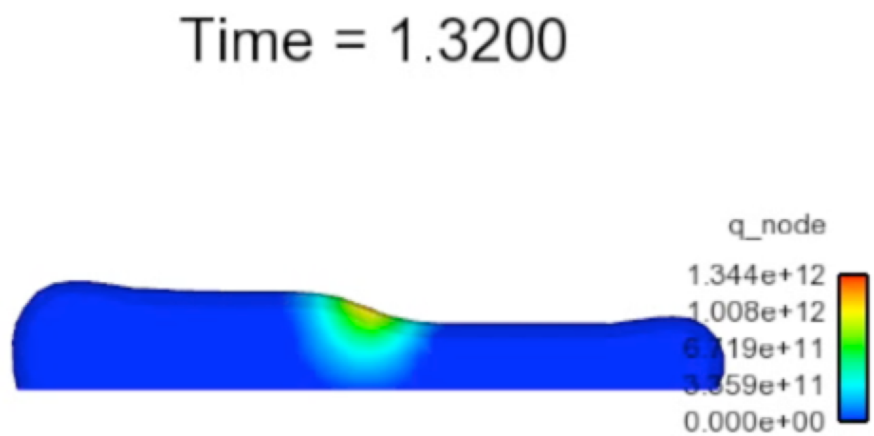
- Validation activities







Modeling the thermal history of thin wall build



Process modeling of LENS manufacturing

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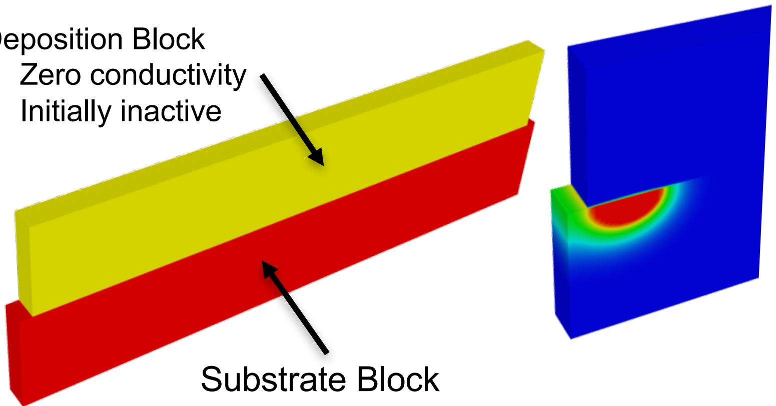
Step 1 Thermal Activation

Initial mesh:

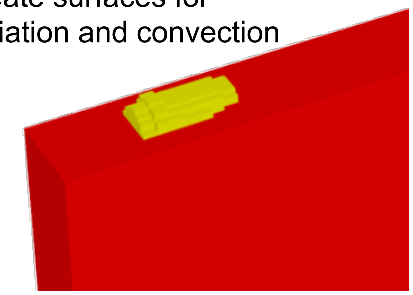
Deposition Block
- Zero conductivity
- Initially inactive



Substrate Block

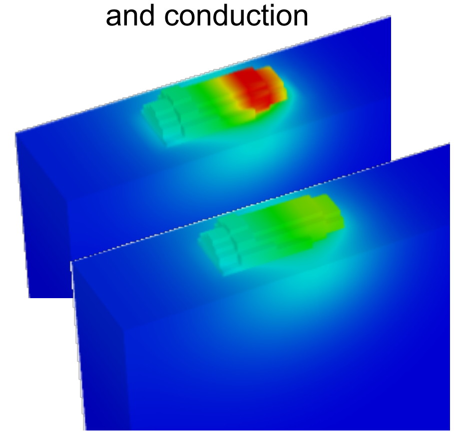
Step 2 Remove Inactive Elements

- Remove elements that are below melt temperature
- Create surfaces for radiation and convection



Step 3 Thermal Analysis

- Radiation, convection, and conduction

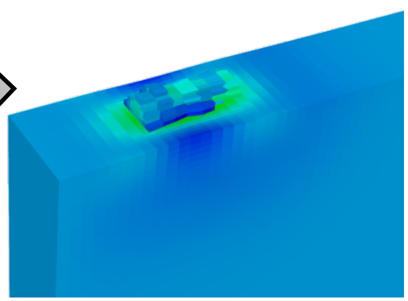


Step 4 Map and/or Initialize Mechanical Variables

- Map material state variables and displacements from previous solid mechanics solution
- Newly activated elements are given initial material parameters

Step 5 Structural Analysis

- Calculate residual stresses as a result of thermal gradients
- Solid elements (below melt temperature)
  - Solid material properties
  - Tied contact
- Fluid elements
  - Newtonian fluid material model
  - Sliding frictional contact

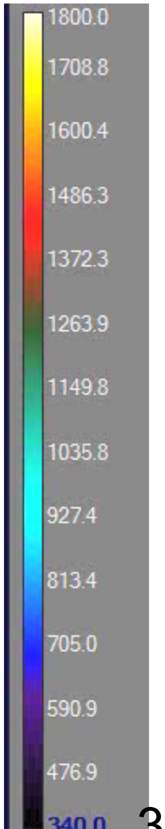


* Displacements shown 15x

Step 6 Map Back to Reference Configuration

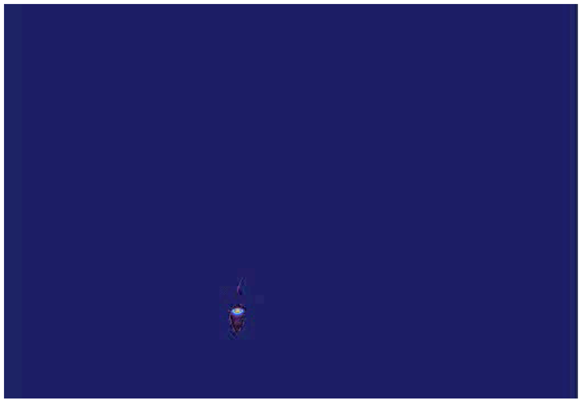
- Map material state variables, displacements, and temperatures back to original mesh

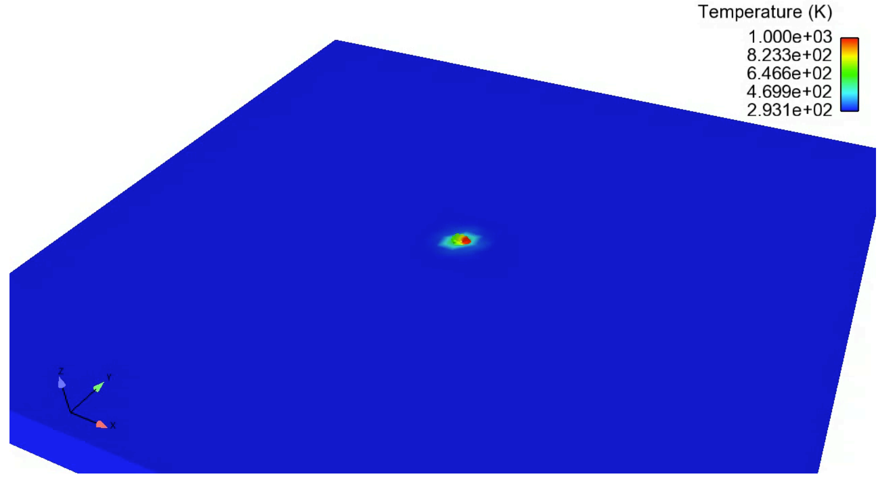
Coupled Thermal and Mechanical Modeling

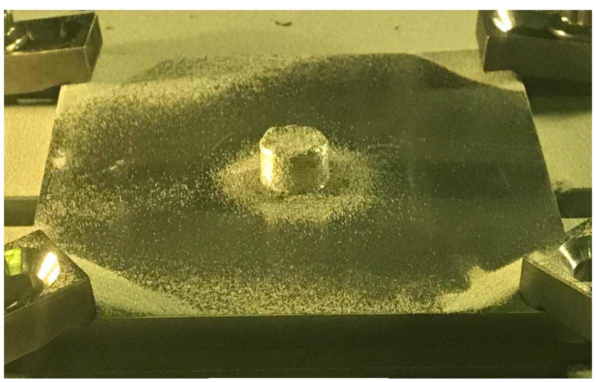


1800°C

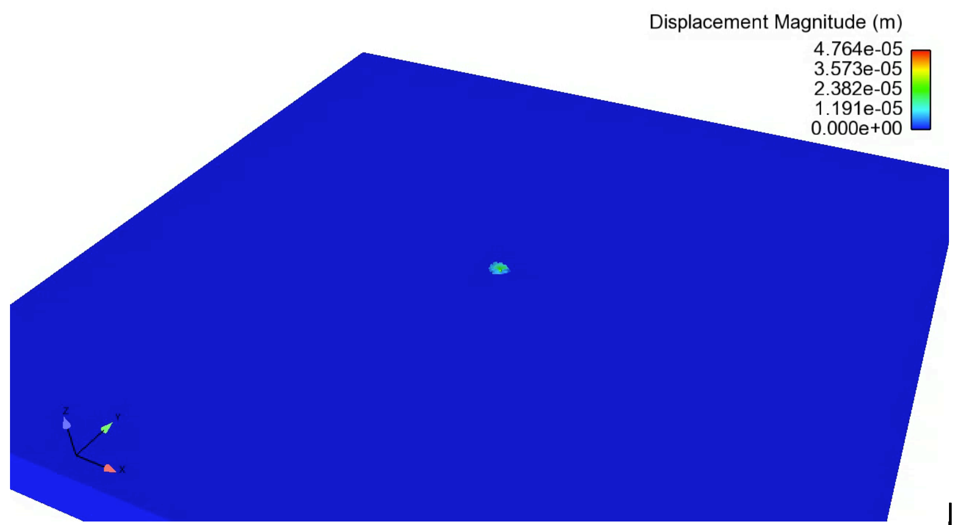
340°C







4 inch



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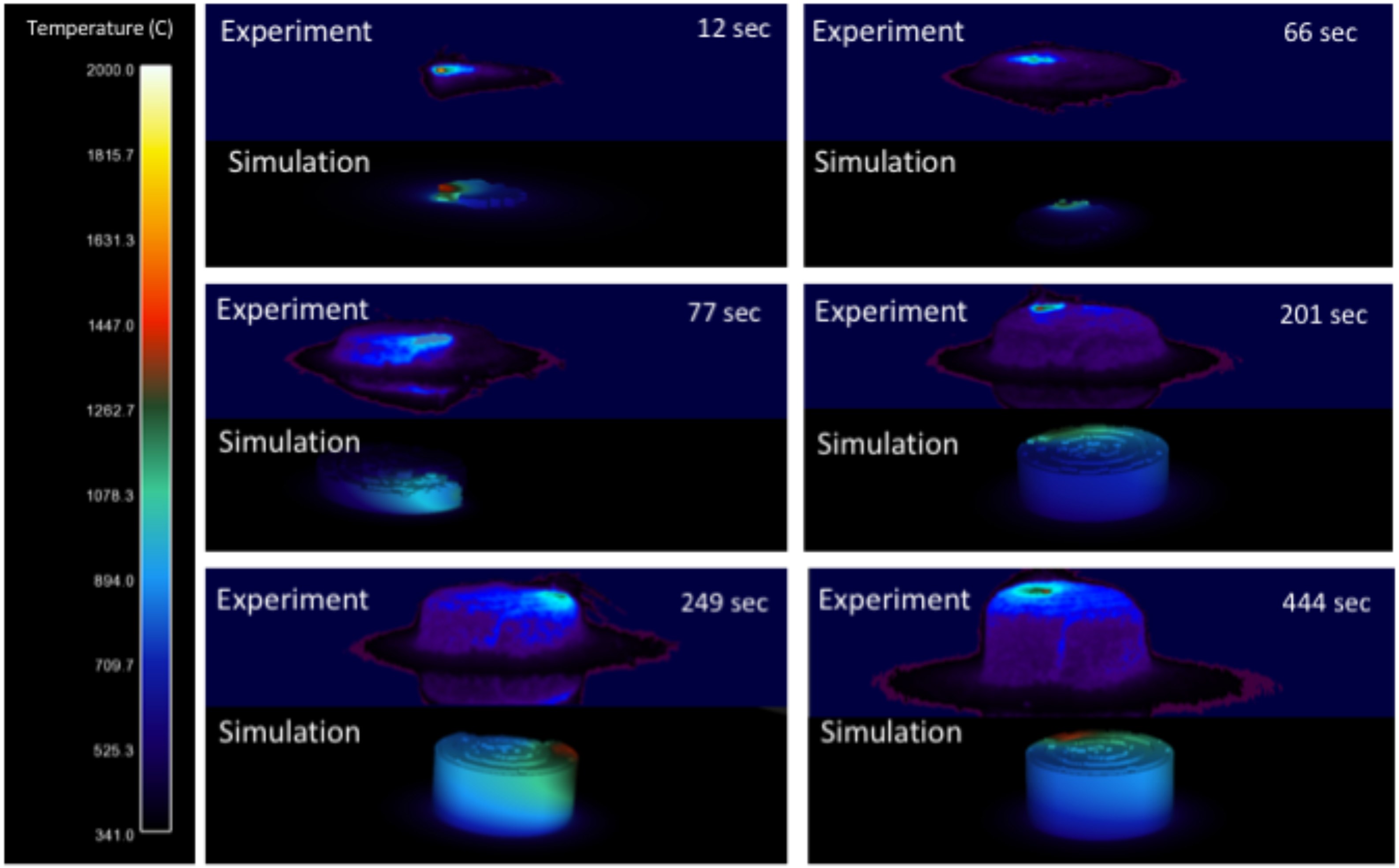
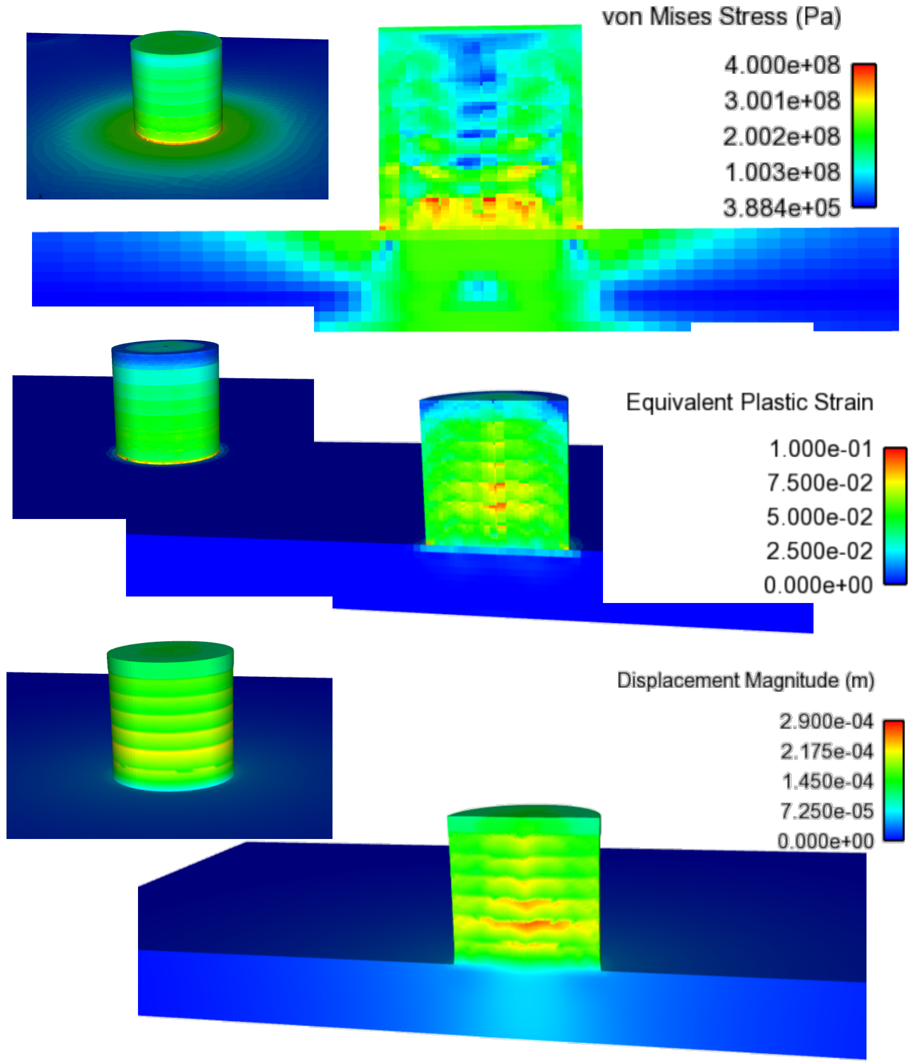
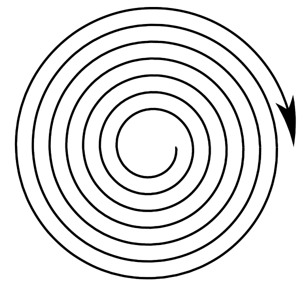


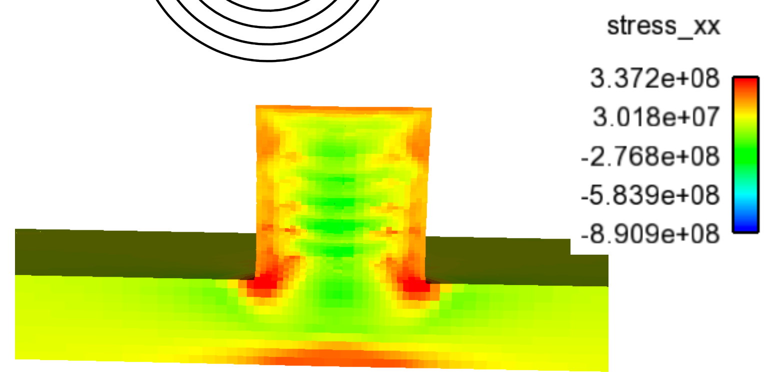
The temperatures are not all equivalent, but the general shape and motion of the melt pool is similar to the experiment. Frame time in experiment and simulation doesn't line up perfectly.

Coupling of Mechanical and Thermal Modeling

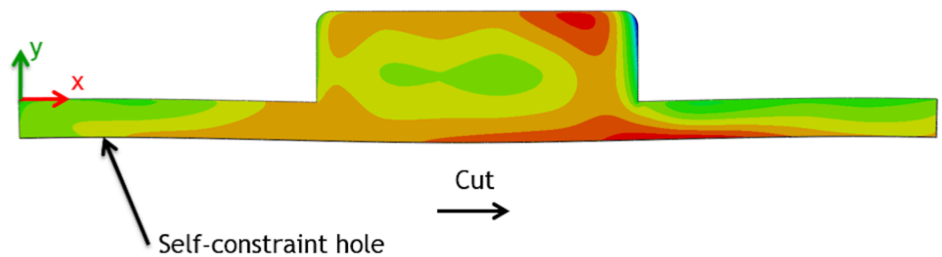




Build Pattern



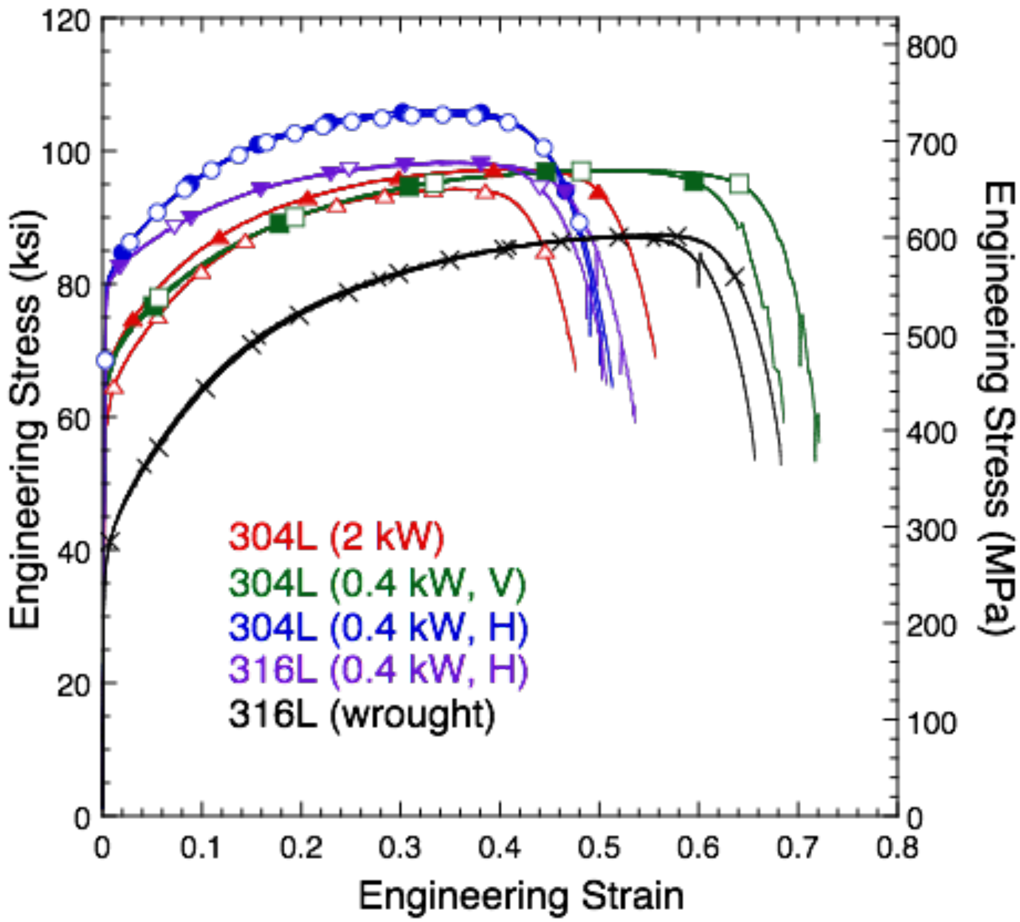
Simulation Residual Stress Results (Pa)

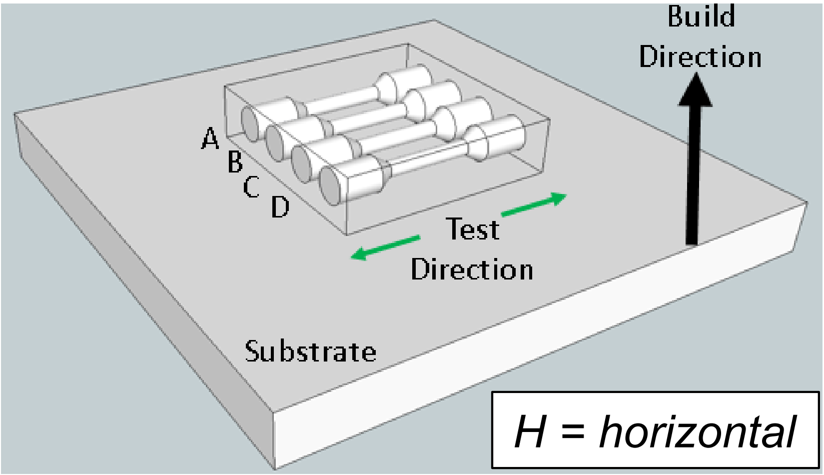


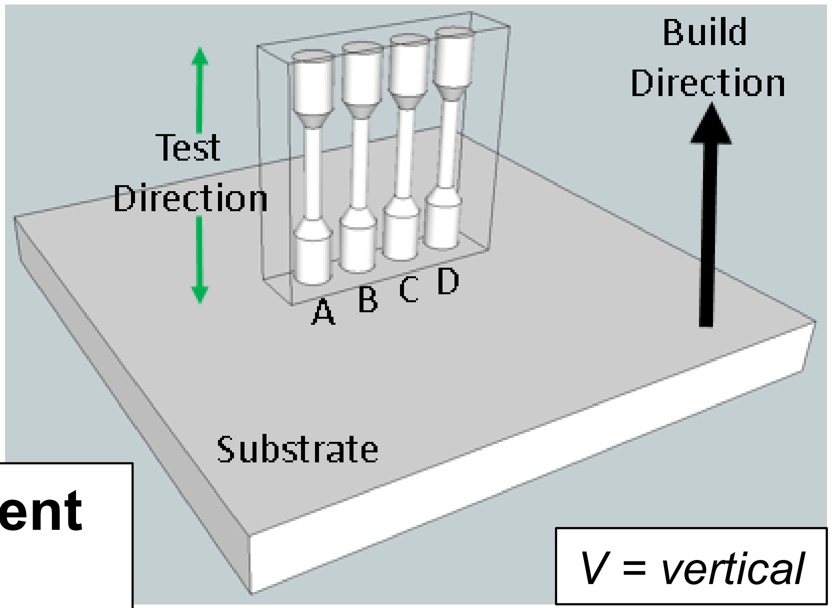
Example LENS Build Residual Stresses (Pa)

Modeling shows higher stress, strain, and displacement near the base plate?
Do we see any effects of this in the microstructure and properties?

Strength of laser-deposited material is significantly greater than annealed materials



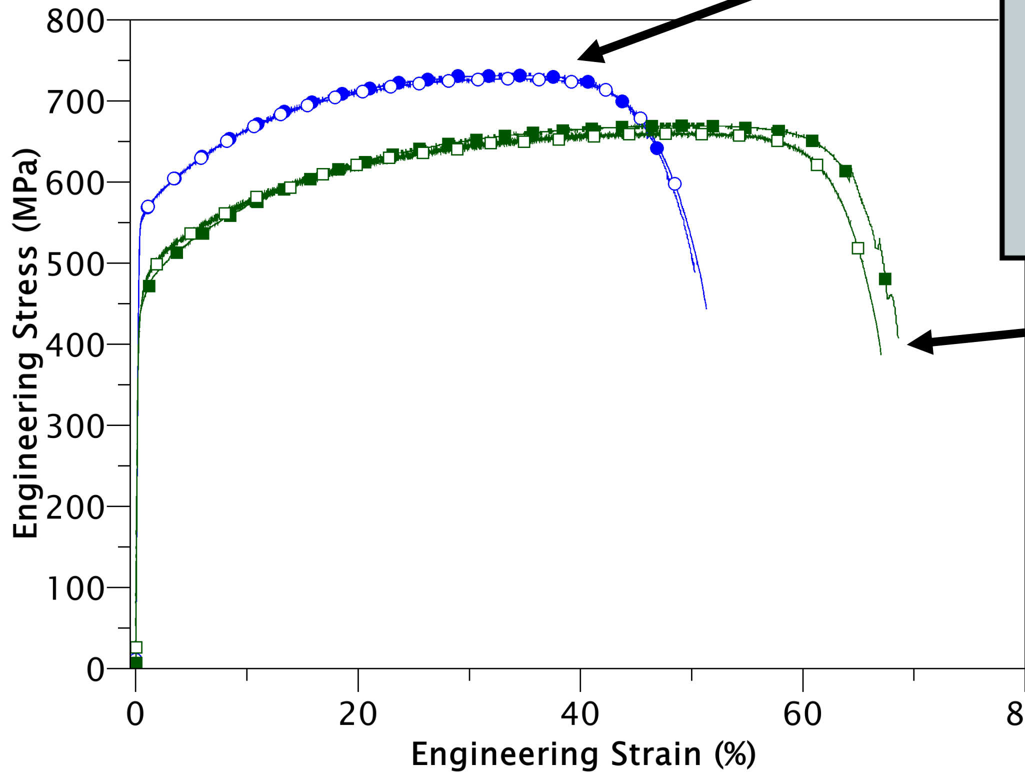


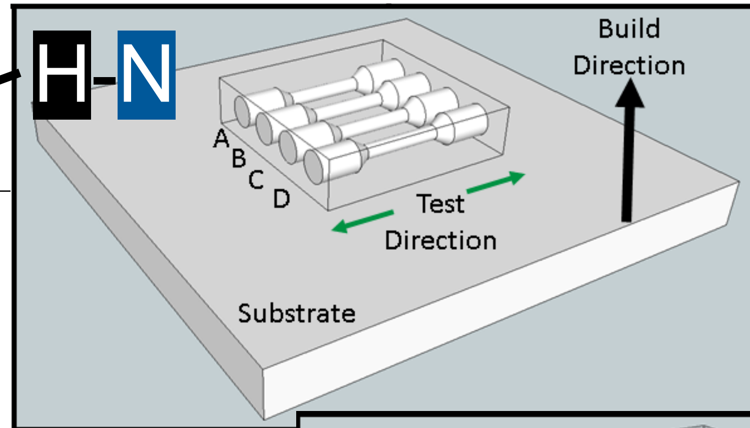


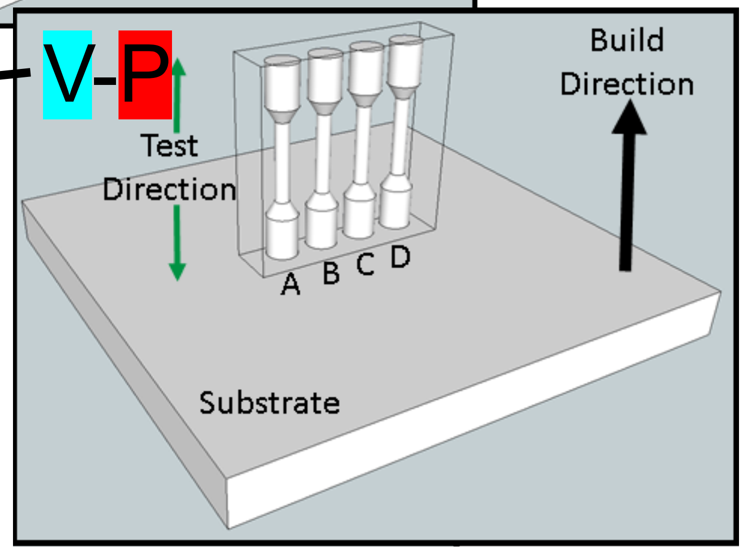
Laser-deposited material displays excellent combination of strength and ductility

Yield Strengths Are Higher Near Base Plate

Builds experience different thermo-mechanical histories





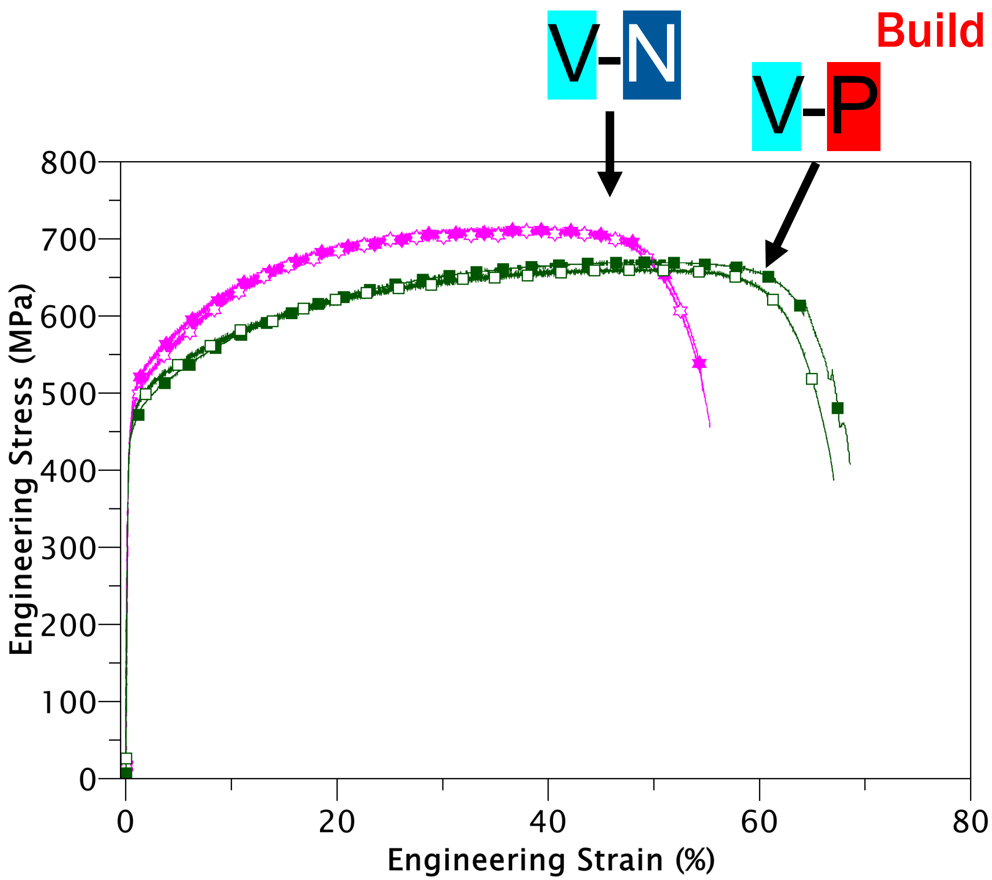


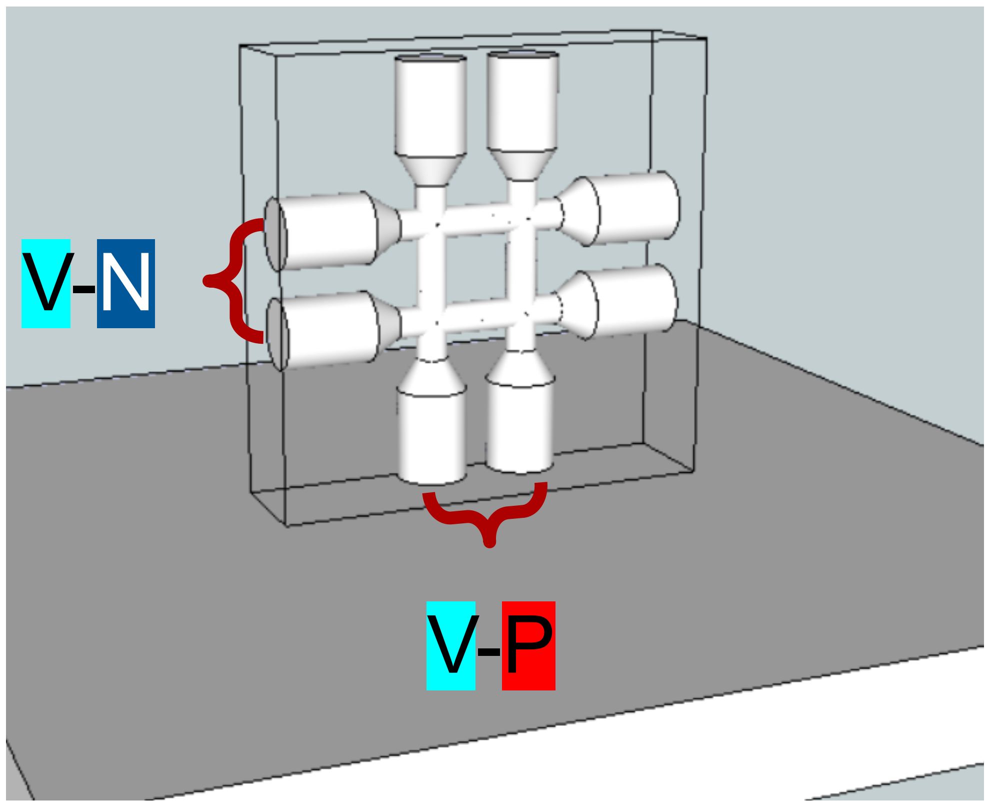
Grade	Yield Strength Horizontal-Normal (MPa)	Yield Strength Vertical-Parallel (MPa)	Percent Difference (%)
304L	552	445	22

T.R. Smith, J.D. Sugar, C. San Marchi, J.M. Schoenung. "Orientation effects on fatigue behavior of additively manufactured stainless steel." Pressure Vessel and Piping Conference (PVP 2017), ASME, 2017.

Specimen Orientation has Little Effect

Build volume has similar thermo-mechanical history

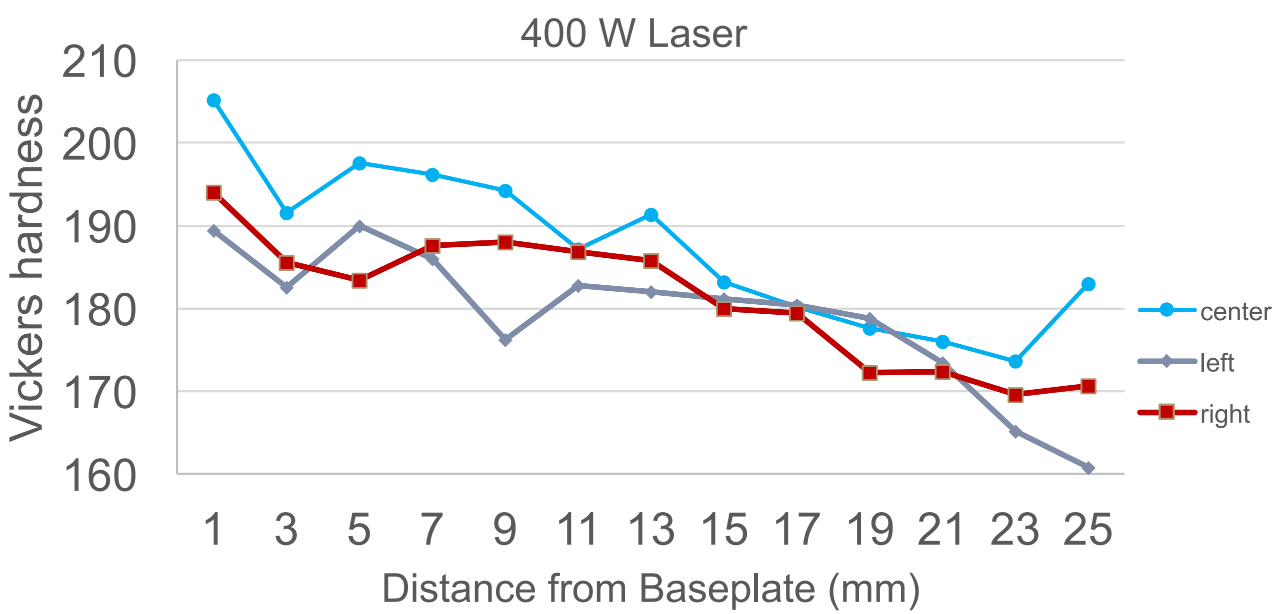


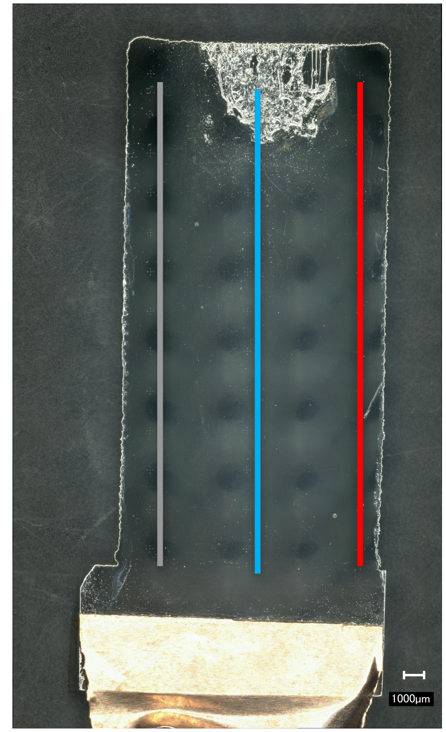


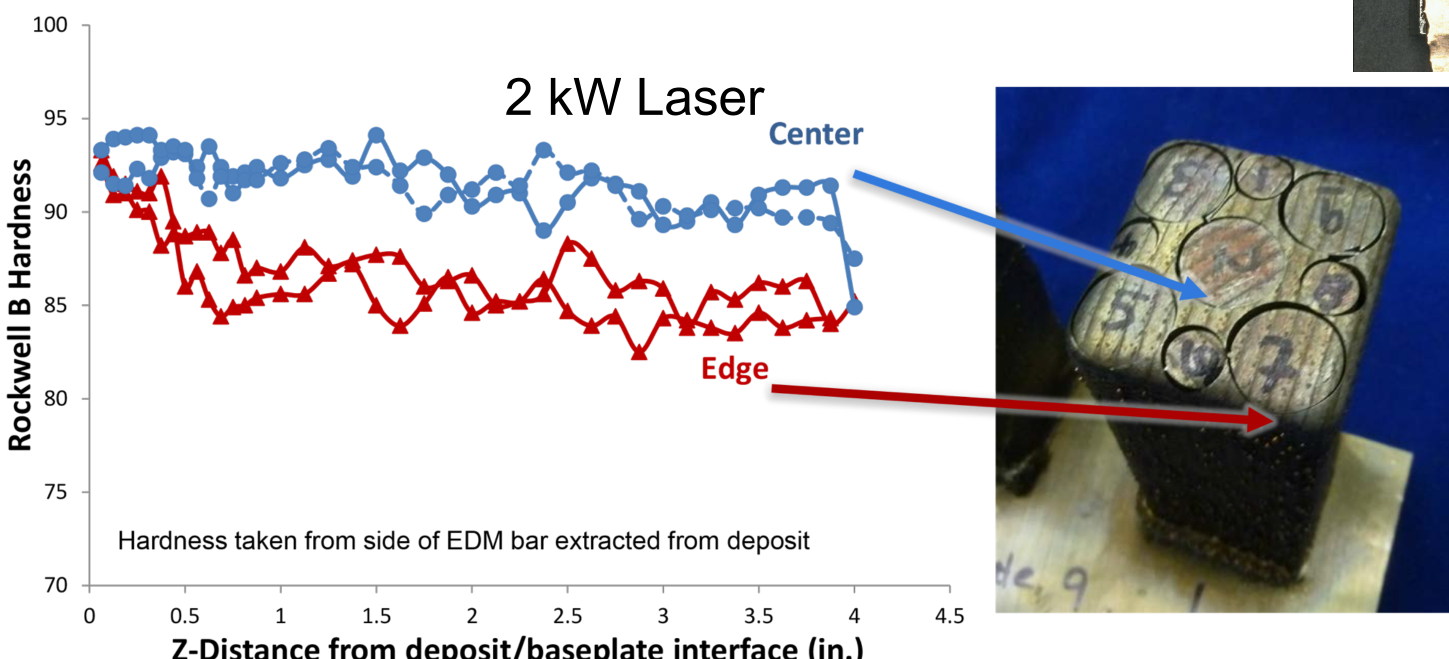
Grade	Yield Strength Vertical-Normal (MPa)	Yield Strength Vertical-Parallel (MPa)	Percent Difference (%)
304L	456	445	2

T.R. Smith, J.D. Sugar, C. San Marchi, J.M. Schoenung. "Orientation effects on fatigue behavior of additively manufactured stainless steel." Pressure Vessel and Piping Conference (PVP 2017), ASME, 2017.

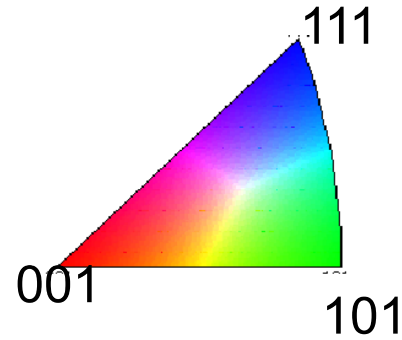
Hardness Values are Higher Near Baseplate

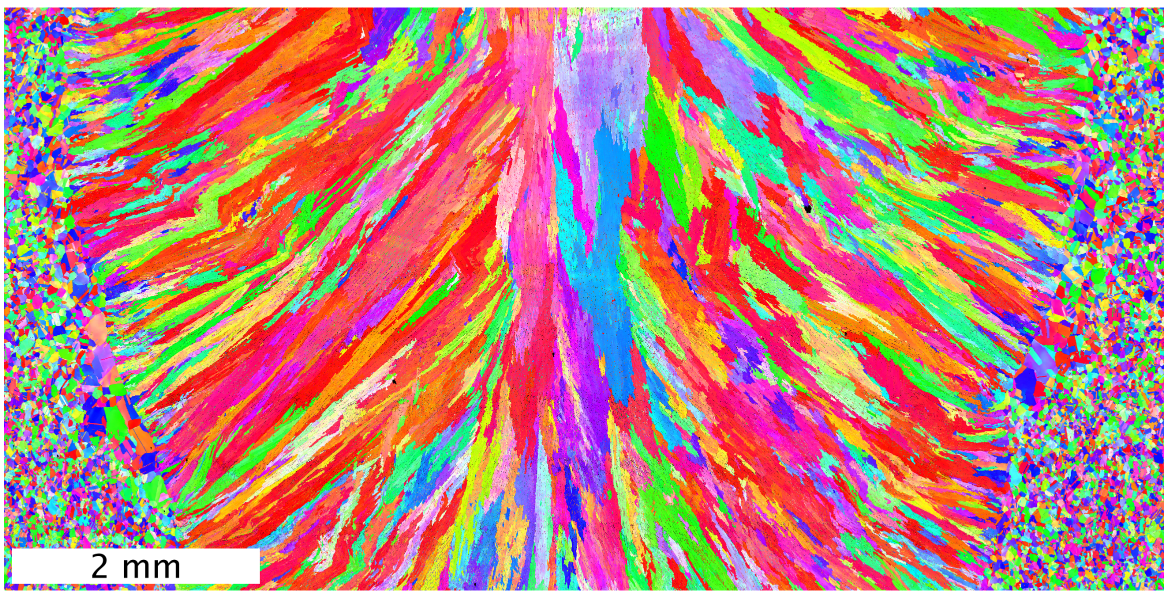


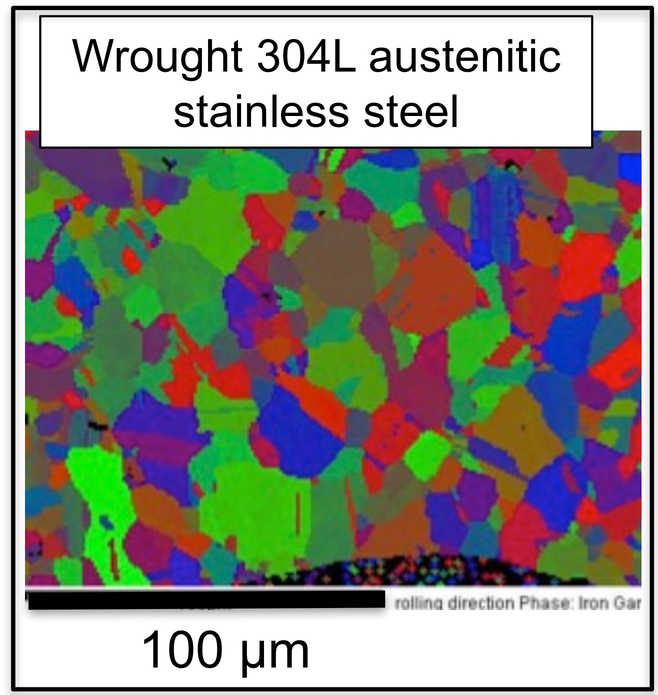




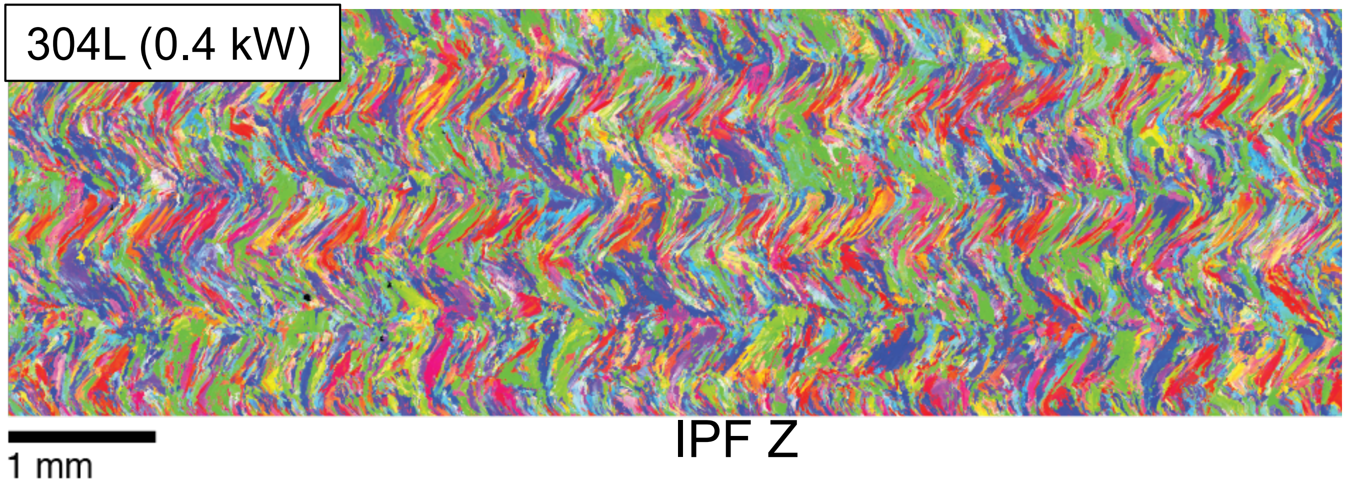
Grain structure is more characteristic of weld microstructure than wrought microstructure

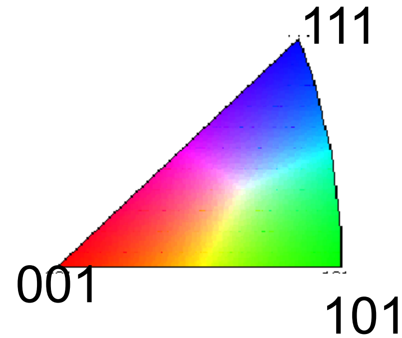




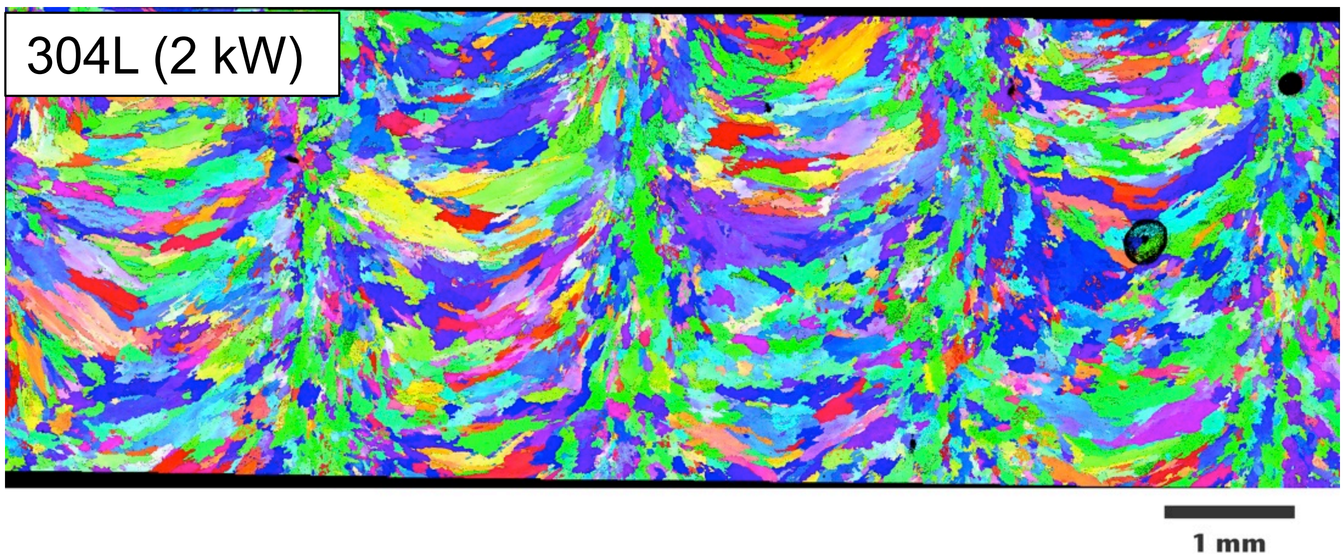


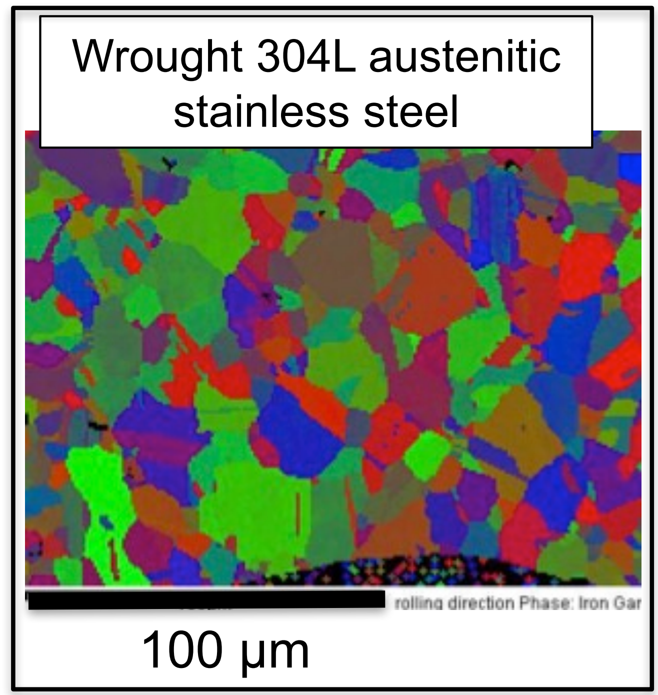
Grain structure is more characteristic of weld microstructure than wrought microstructure





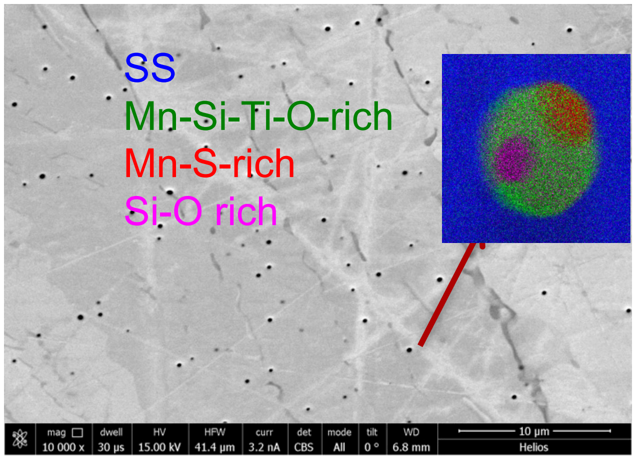
IPF Z





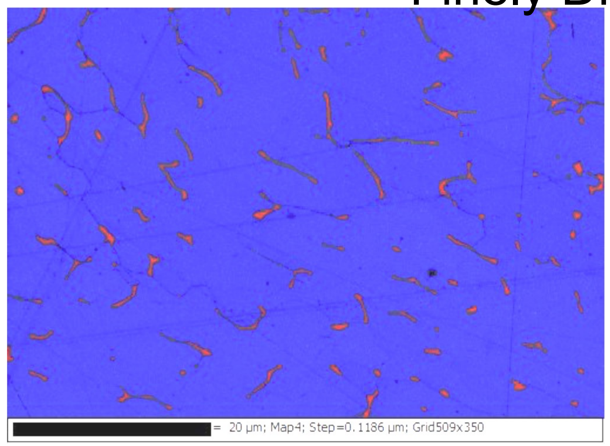
- AM and wrought microstructure differ
- ***What is the effect on structural properties?***

Several Fine-Scale Features to Consider in the Overall Microstructural Picture



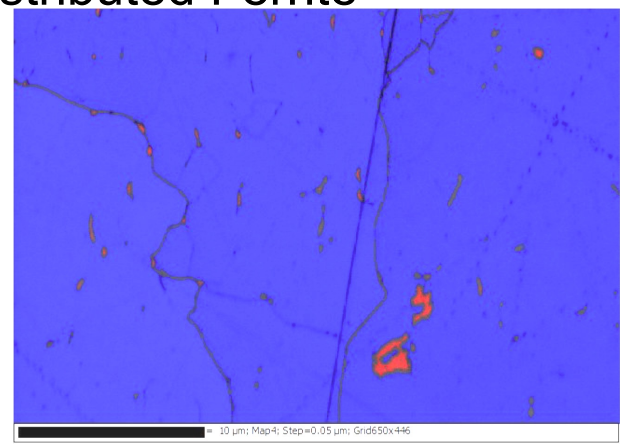
2 kW PSU 304

Finely Distributed Ferrite



20 μm

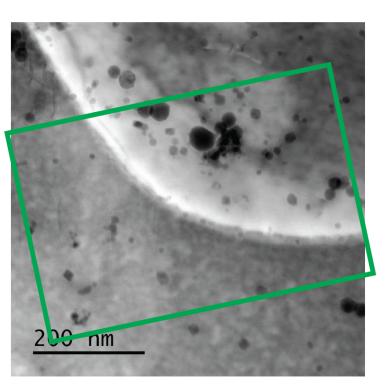
2 kW PSU 304L

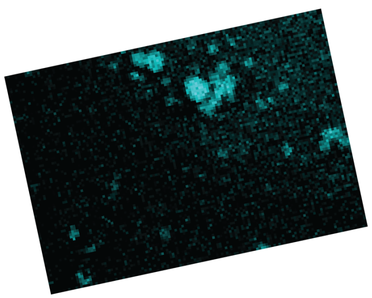


10 μm

400 W UCD 316

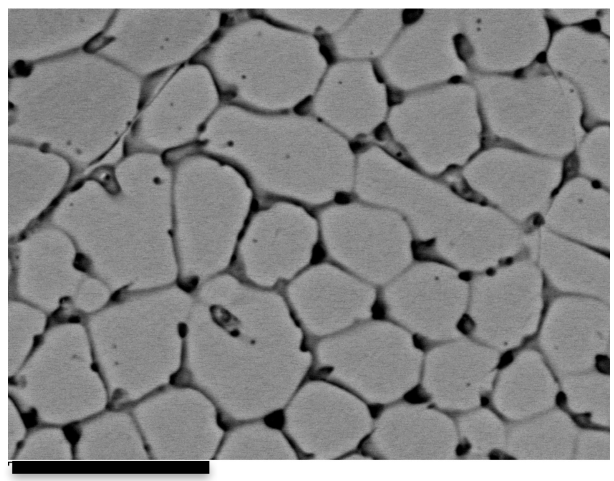
Oxide Particles



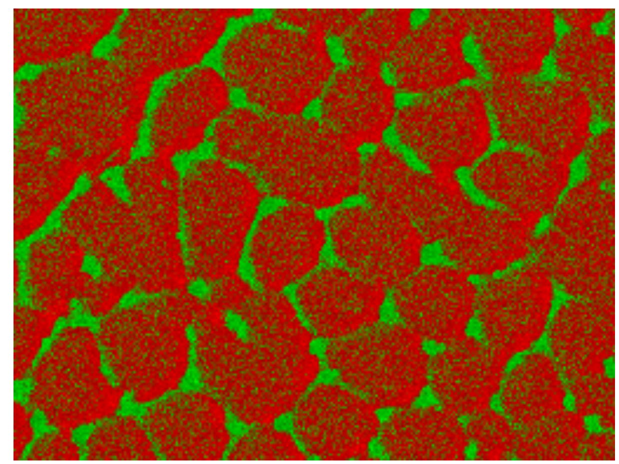


Cr-O rich

400 W UCD 316



10 μm



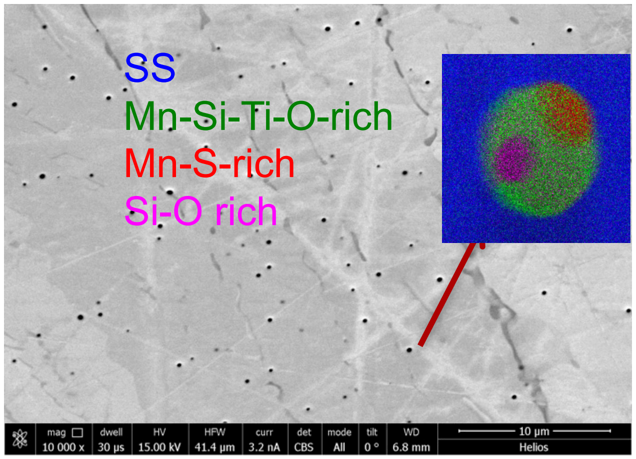
Cellular Solidification Structure

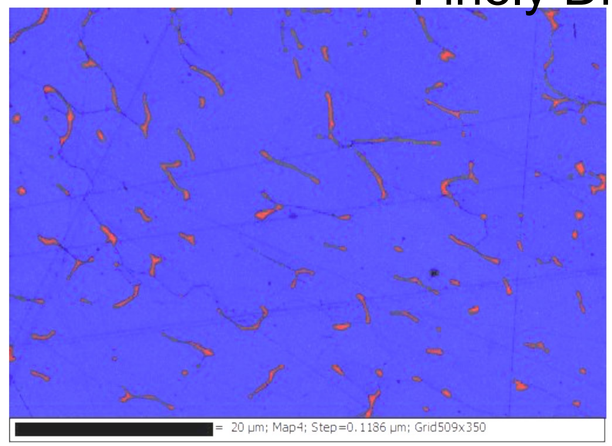
Cr-rich

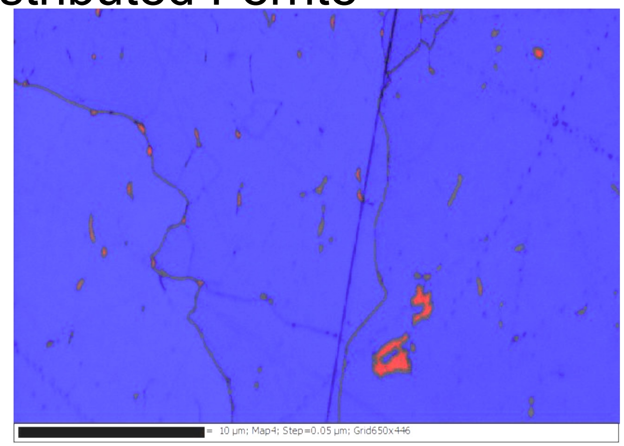
Ni-rich

Several Fine-Scale Features to Consider in the Overall Microstructural Picture

Finely Distributed Ferrite







20 µm

10 µm

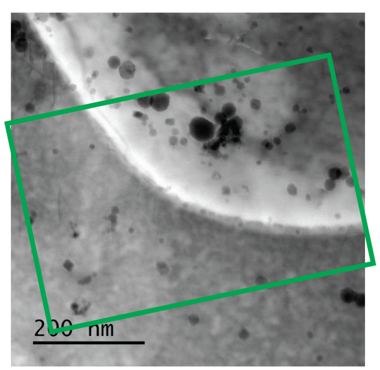
2 kW P

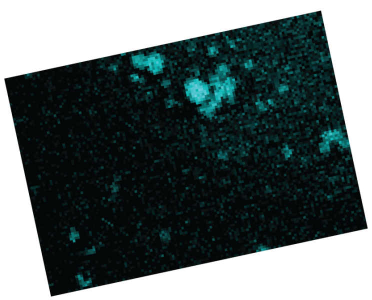
400 W

CD 316

None show an obvious significant variation with distance from baseplate

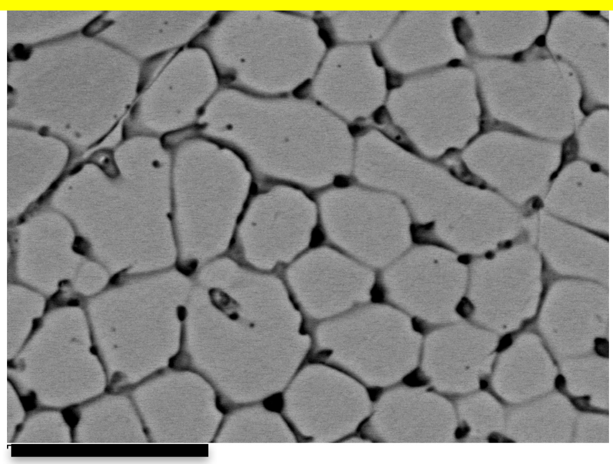
Oxide Par



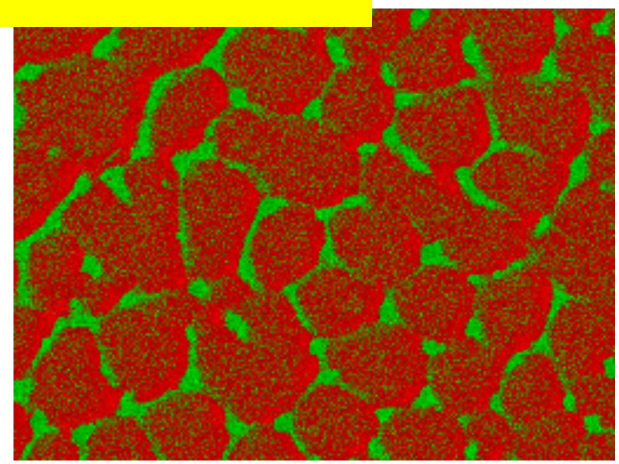


Cr-O rich

400 W UCD 316



10 µm

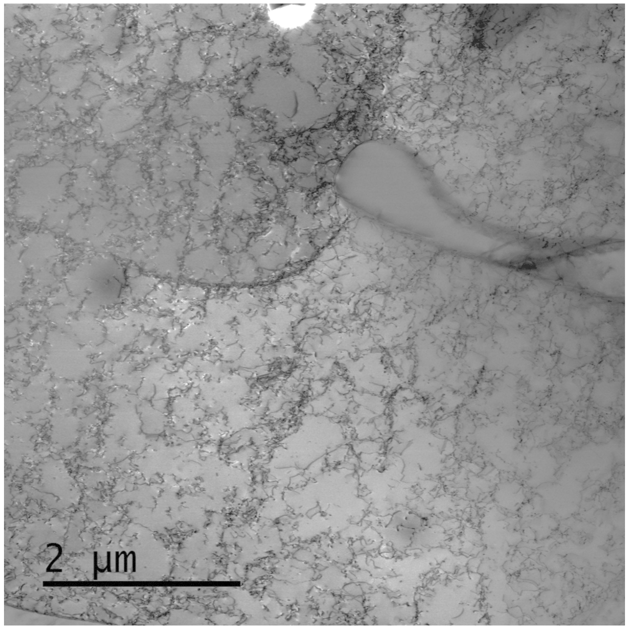


Cellular Solidification Structure

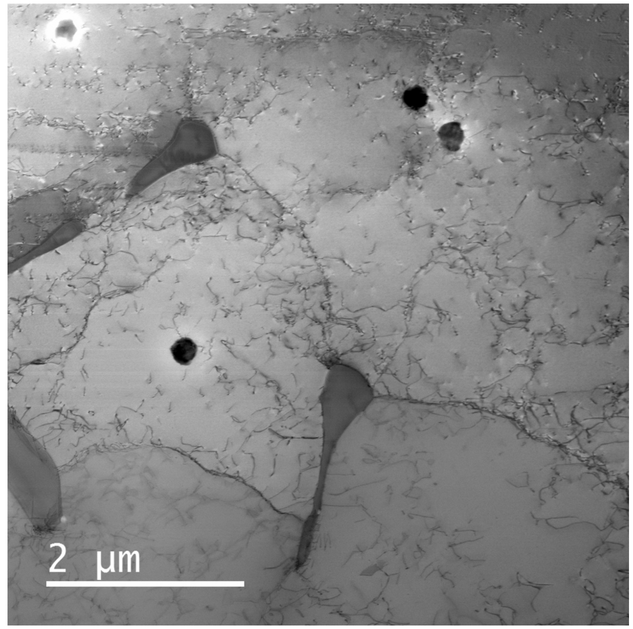
Cr-rich

Ni-rich

Dislocation Structure Dependent on Location in Build

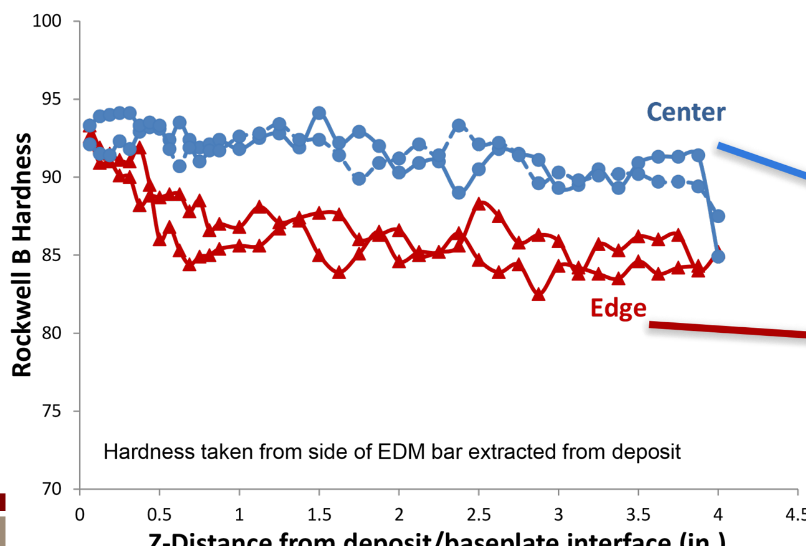


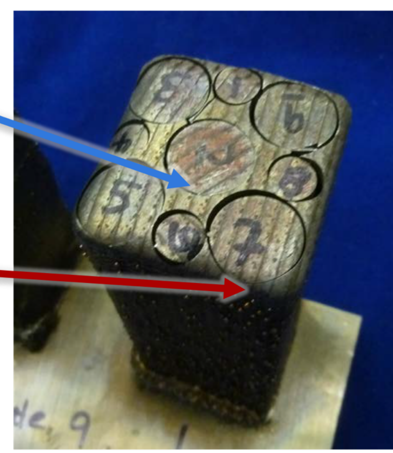
2 mm from Base BF STEM



2 mm from Top BF STEM

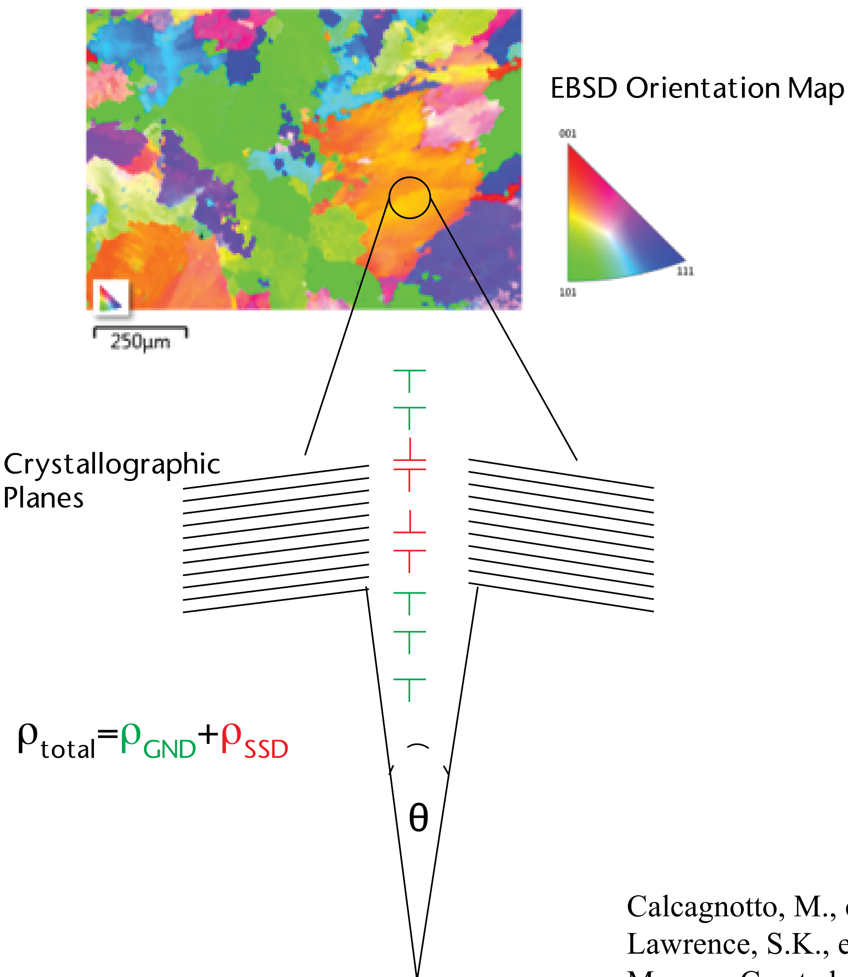
- Qualitatively, there appear to be less dislocations near the top of the build
- This correlates with lower hardness numbers near the top of the build

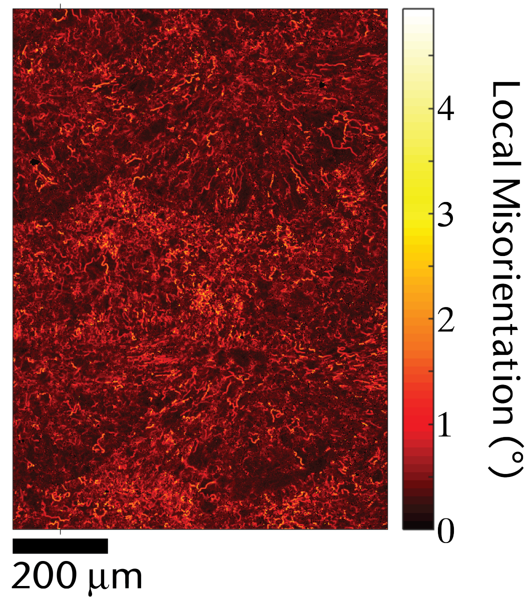


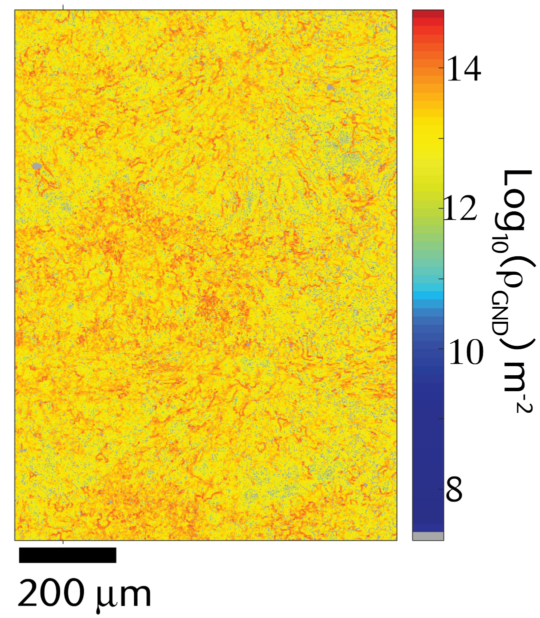


Can we quantify the dislocation structure at a scale larger than what TEM allows?

Measurement of Geometrically Necessary Dislocations with EBSD







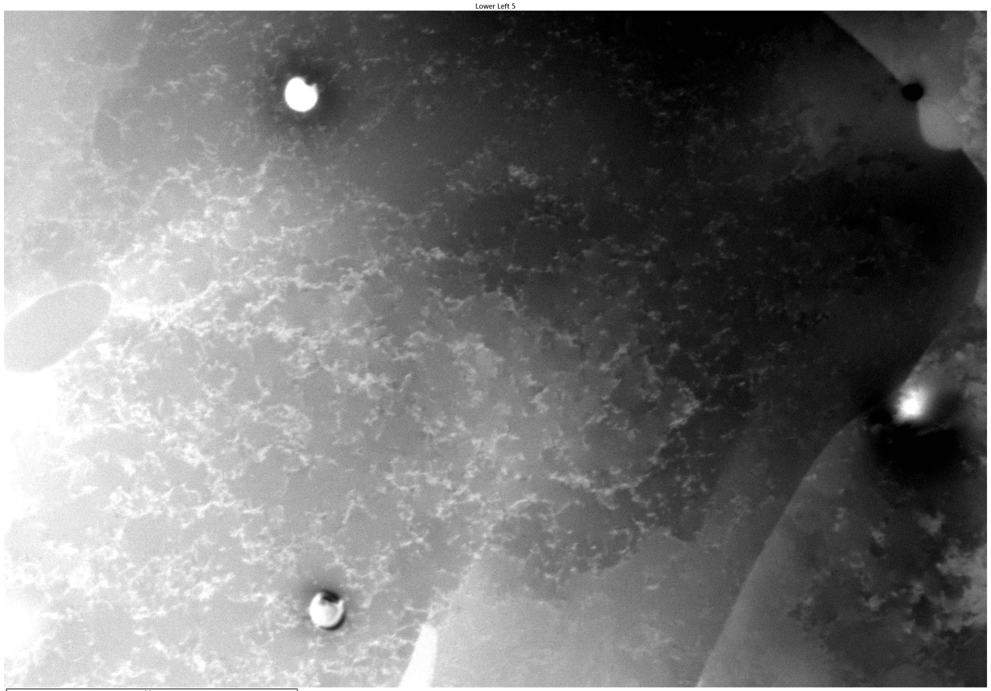
$$\rho_{GND} = \frac{2\theta}{ub} = \frac{2(KAM)}{ub}$$

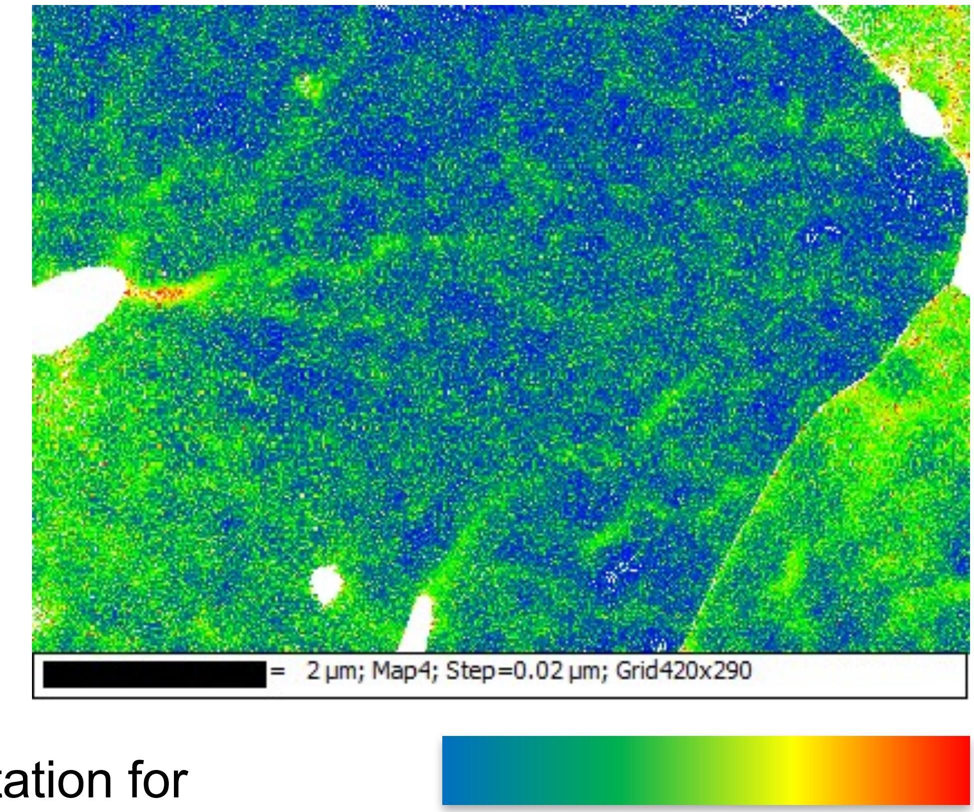
ρ_{GND} = GND density
b = burgers vector
u = unit length

Calcagnotto, M., et al., Materials Science and Engineering: A, 2010. **527**(10–11): p. 2738-2746.
Lawrence, S.K., et al., Metallurgical and Materials Transactions A, 2014. **45**(10): p. 4307-4315.
Moussa, C., et al., IOP Conference Series: Materials Science and Engineering, 2015. **89**(1): p. 012038.
Kubin, L.P. and A. Mortensen, Scripta Materialia, 2003. **48**(2): p. 119-125.
Gao, H., et al., Journal of the Mechanics and Physics of Solids, 1999. **47**(6): p. 1239-1263.
Kamaya, M., Ultramicroscopy, 2011. **111**(8): p. 1189-1199.

GND Measurements Correlate With STEM Images of Dislocation Structure

$$\rho_T = \rho_{GND} + \rho_{SSD}$$





0° 1°

Local Averaged Misorientation

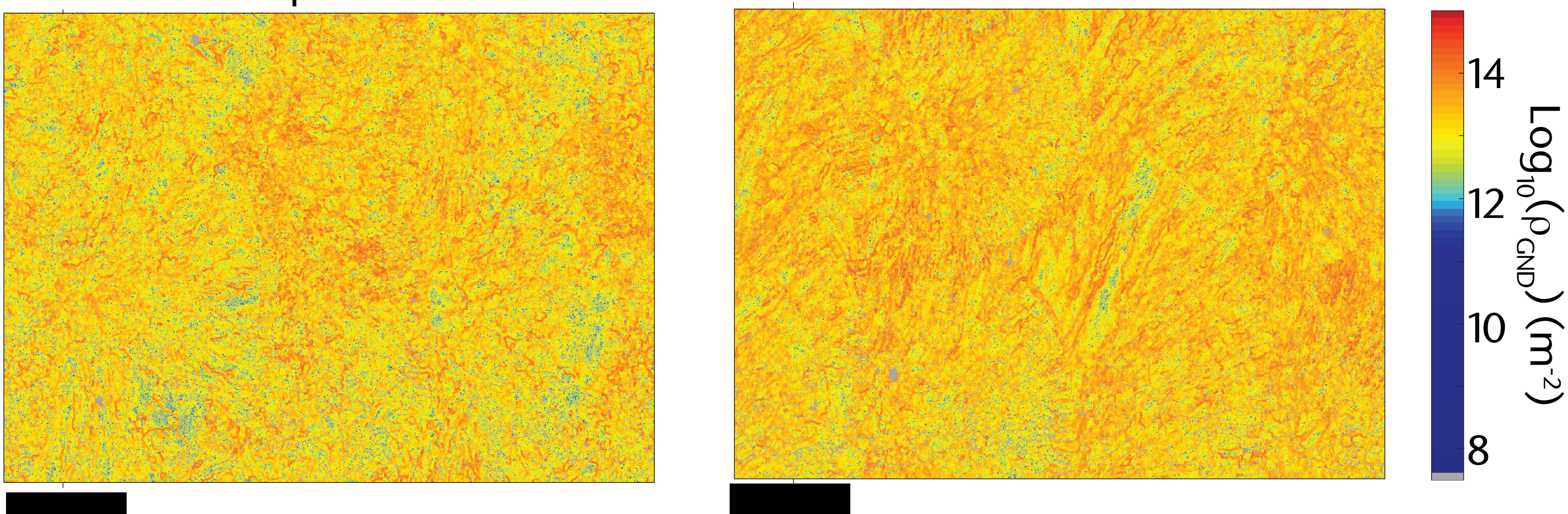
Measurements of local averaged misorientation for GNDs are consistent with images of the more general dislocation structure. Higher misorientations occur where the images show higher dislocations densities.

GND Distribution Varies with Build Location

400 W 304L LENS

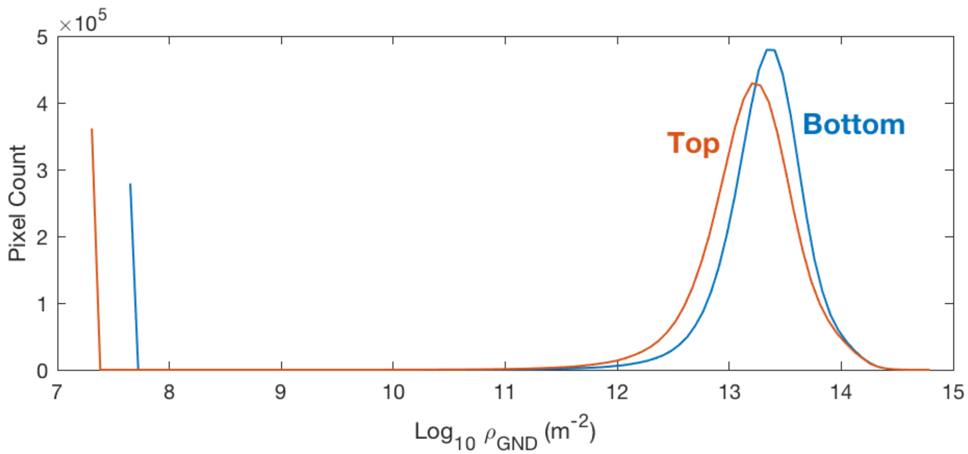
Top

Bottom



200 μm $\bar{\rho}_{GND} = 2.3\times10^{13}\ m^{-2}$

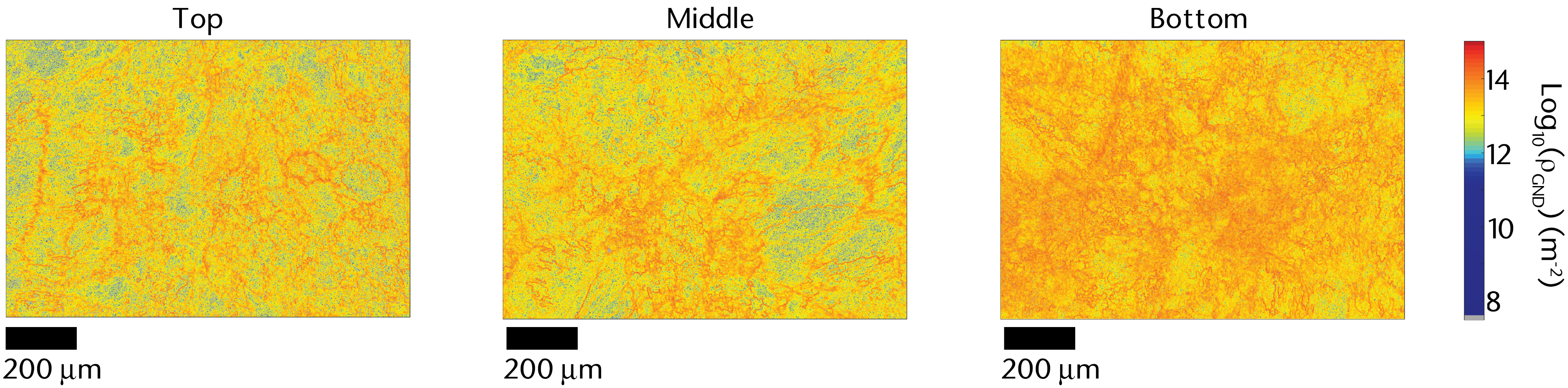
200 μm $\bar{\rho}_{GND} = 2.8\times10^{13}\ m^{-2}$



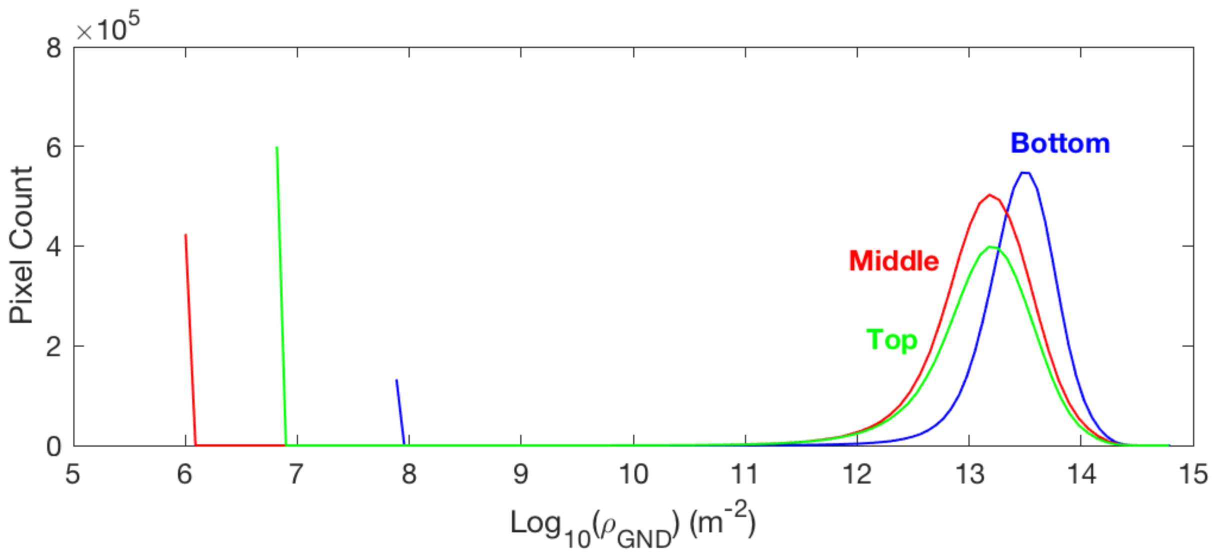
Average GND density and GND distribution show higher densities closer to baseplate

GND Distribution Varies with Build Location

2kW 304L LENS

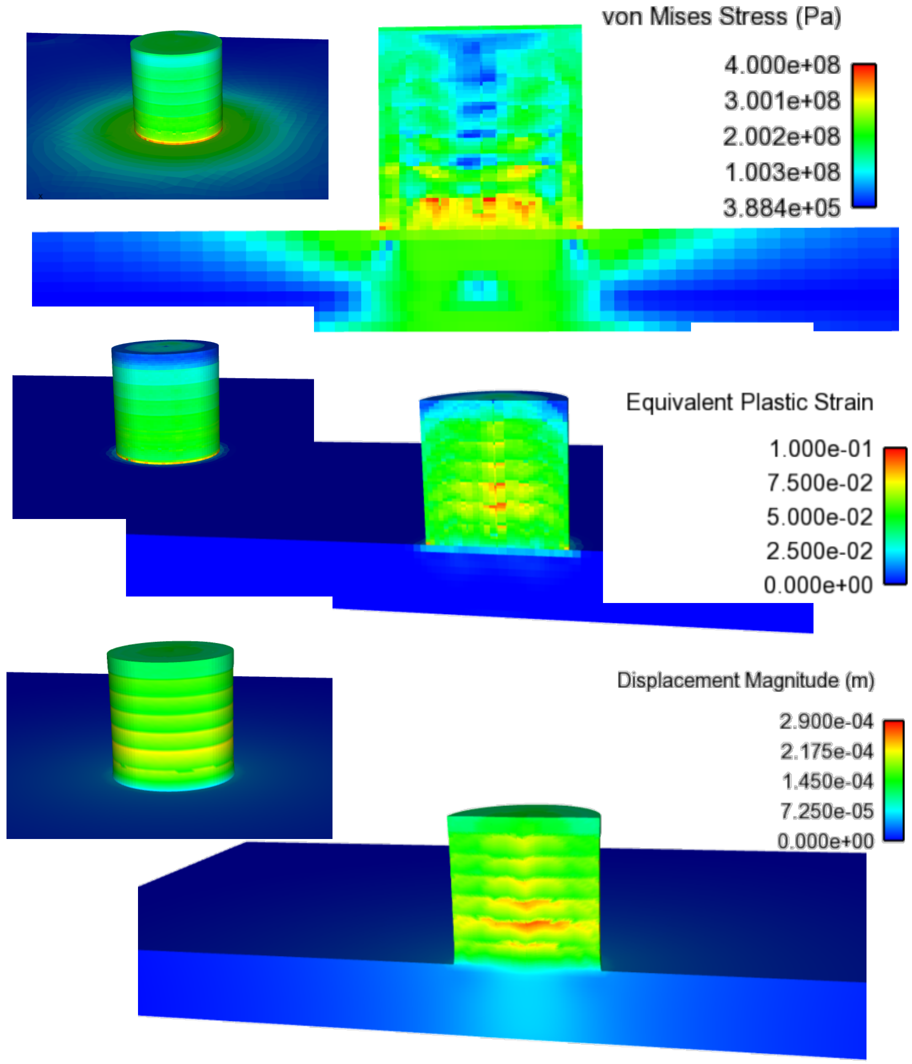


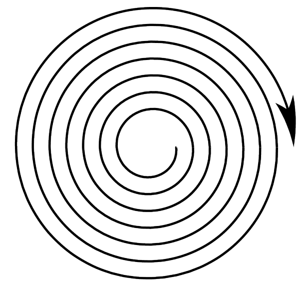
$\bar{\rho}_{GND} = 2.07{\times}10^{13}\ m^{-2}$ $\bar{\rho}_{GND} = 2.09{\times}10^{13}\ m^{-2}$ $\bar{\rho}_{GND} = 3.62{\times}10^{13}\ m^{-2}$



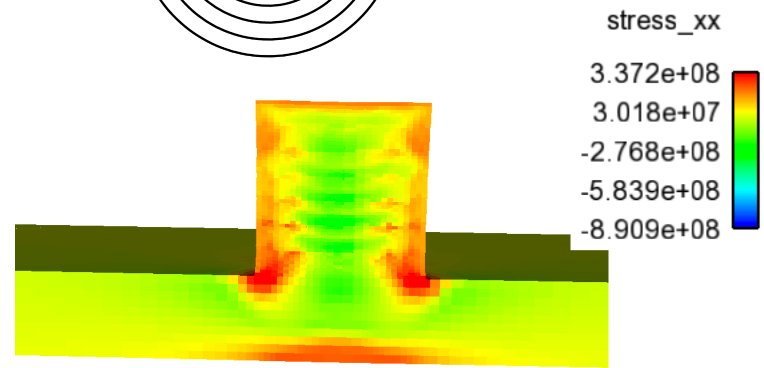
Higher energy builds shows same trend of higher dislocation density closer to the base plate

Coupling of Mechanical and Thermal Modeling

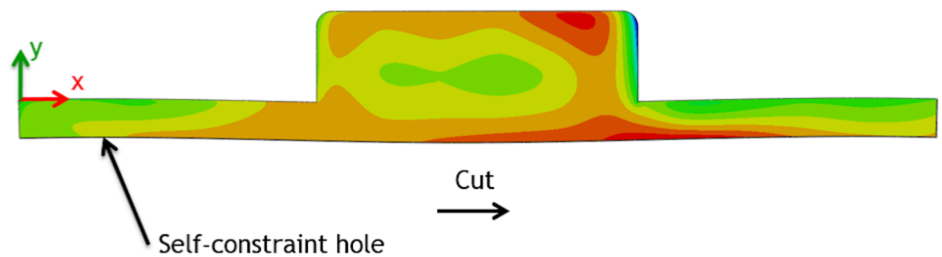




Build Pattern



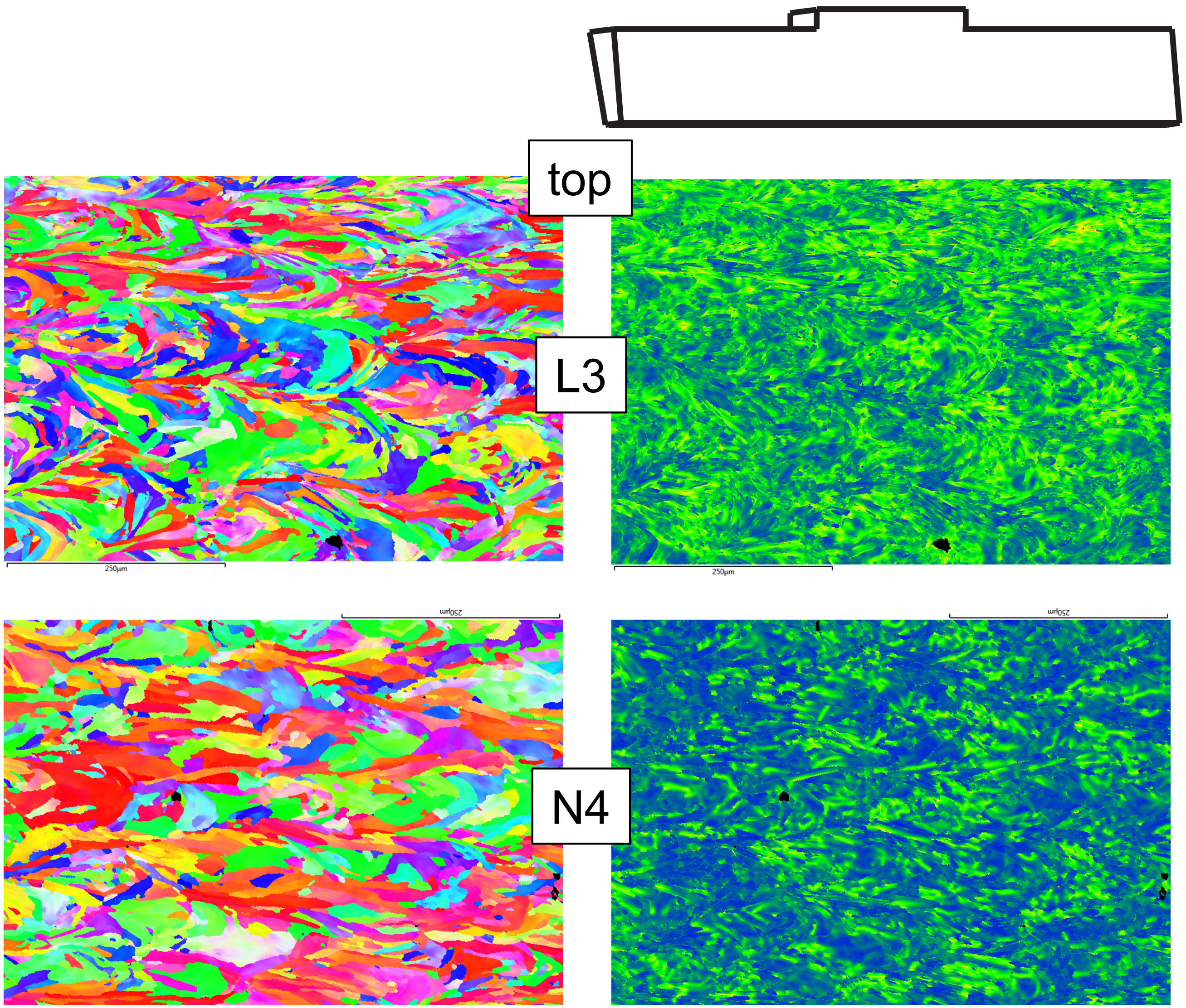
Simulation Residual Stress Results (Pa)



Example LENS Build Residual Stresses (Pa)

Modeling shows higher stress, strain, and displacement near the base plate?
Do we see any effects of this in the microstructure and properties?

Dislocation Mapping in PBF



Orientation maps

Misorientation maps

- Preliminary survey suggests about the same microstructure bottom to top
- Grain size appears slightly larger for Rennishaw ring (N4)
- Misorientation is greater for EOS ring (L3)
- No observable ferrite

Dislocation Mapping in PBF

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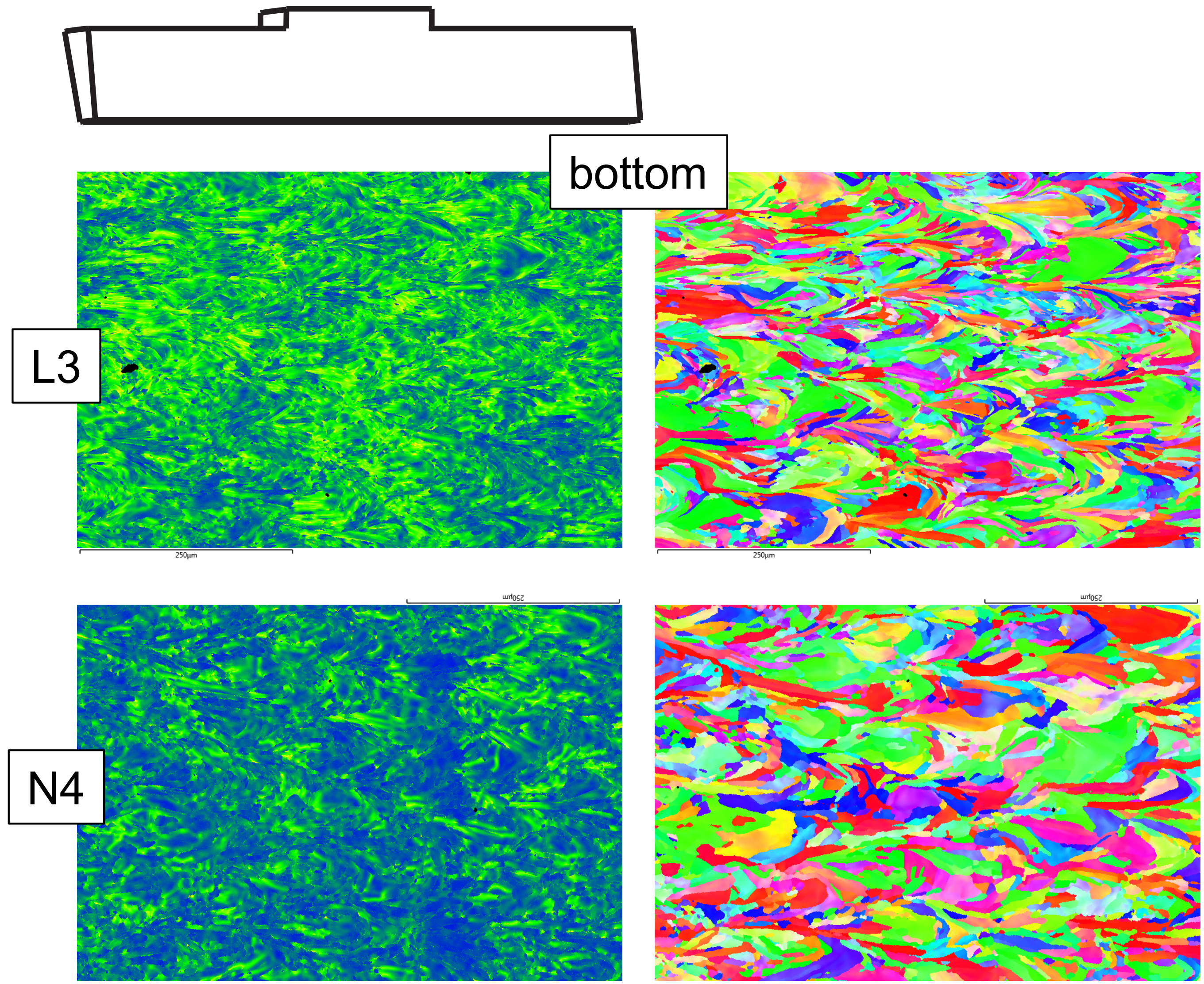
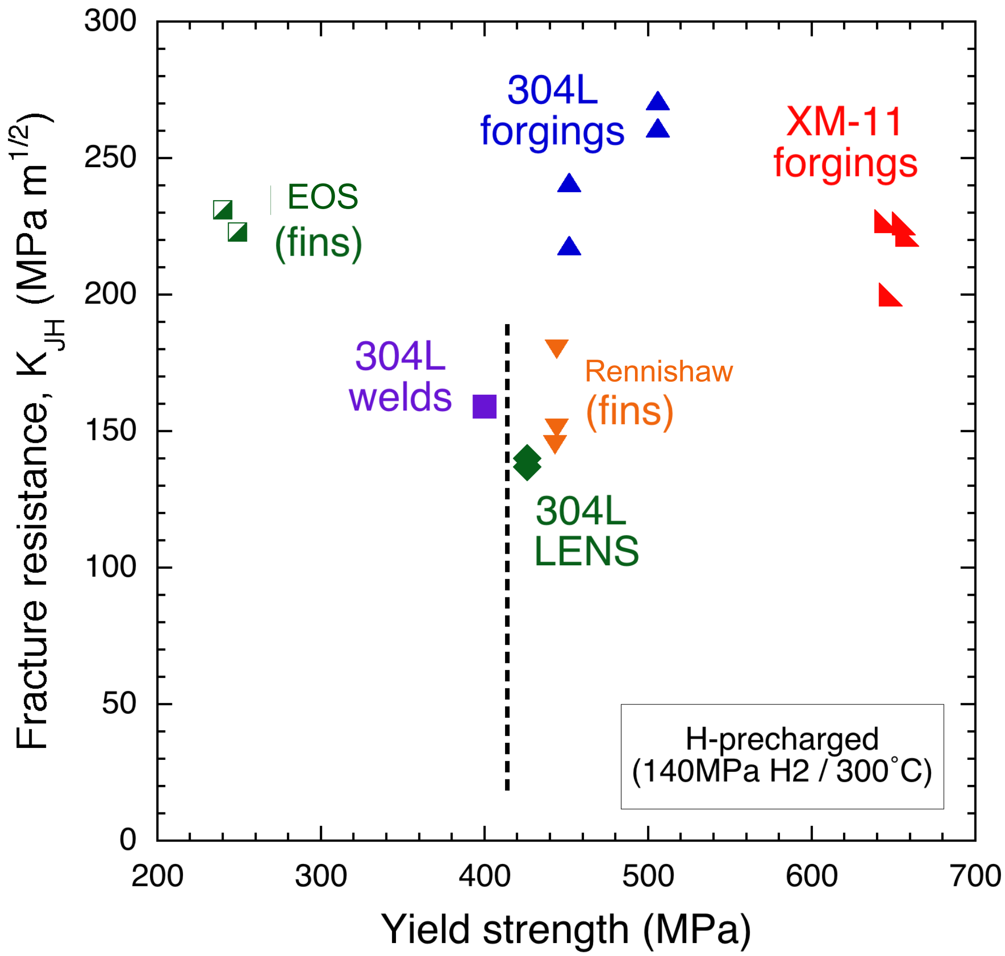


Misorientation maps

Orientation maps

Fracture measurements

Sandia National Laboratories

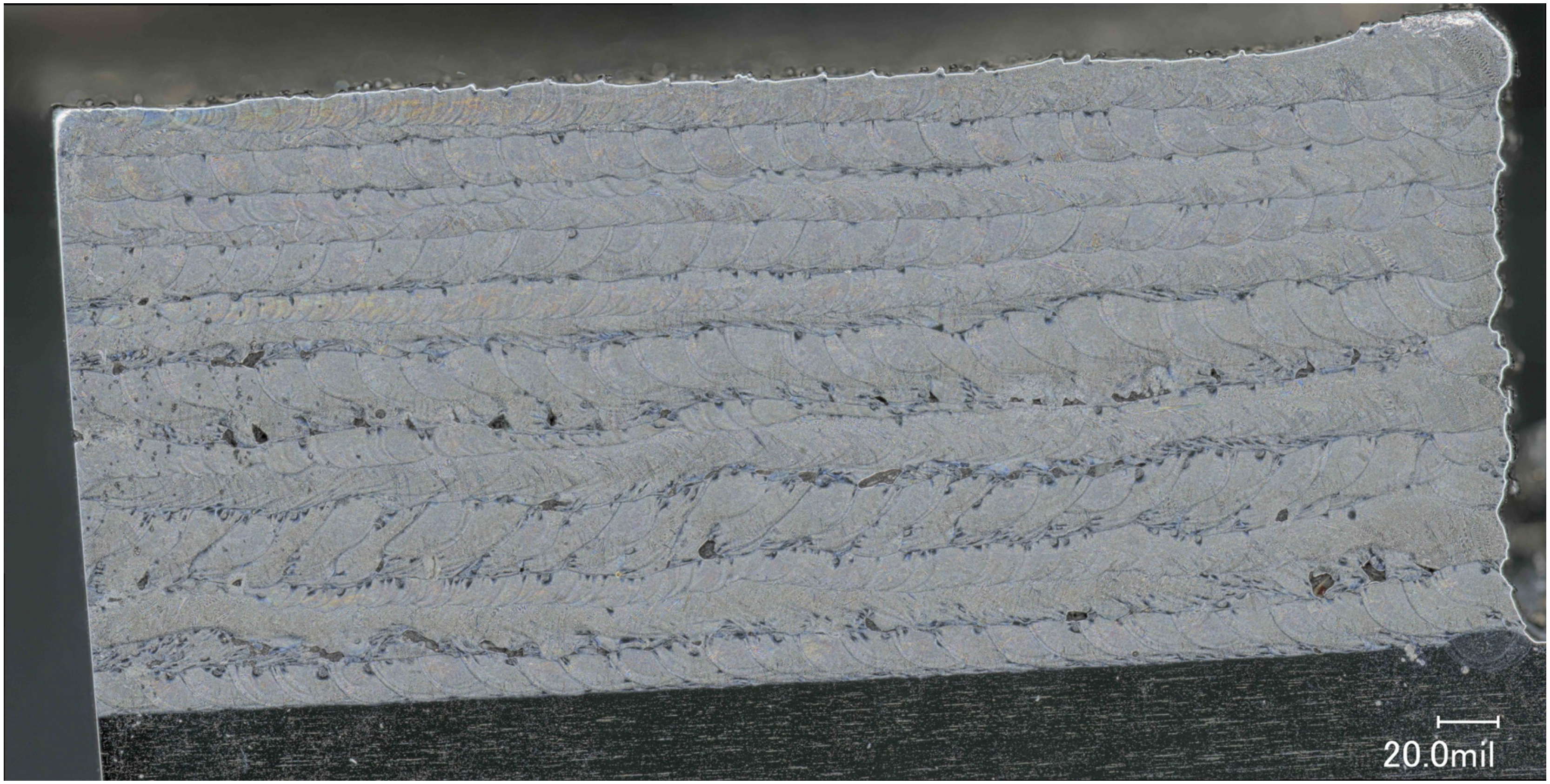


304L forgings: Jackson, Metall Mater Trans 47A
XM-11 forgings: Nibur, Acta Mater 57
Welds: Jackson, Corros Sci 60

Fracture resistance of H-precharged AM 304L

- Lower than wrought (forged) 304L with same strength
- Similar to welded 304L
- Higher fracture resistance of EOS fins consistent with lower strength (*as expected*)

Thermally Induced Plasticity During Processing is Critial

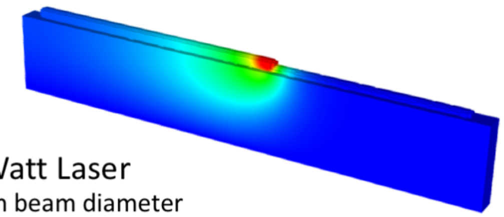


Relatively simple builds and the constraint of the baseplate and thermally induced plasticity during processing make a difference in the dislocation structure and distribution of hardness in these materials

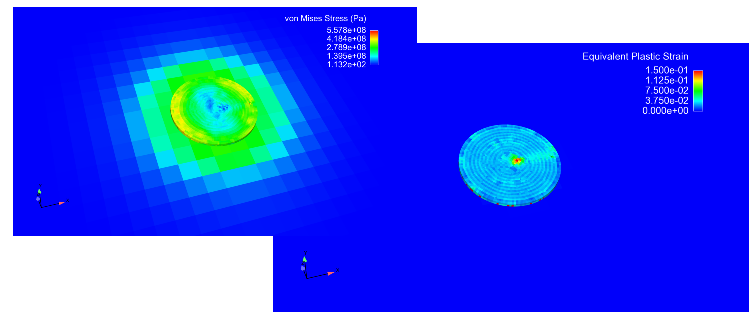
This plasticity and the resultant dislocation/hardness/yield distribution will be completely different in a more complex geometry build

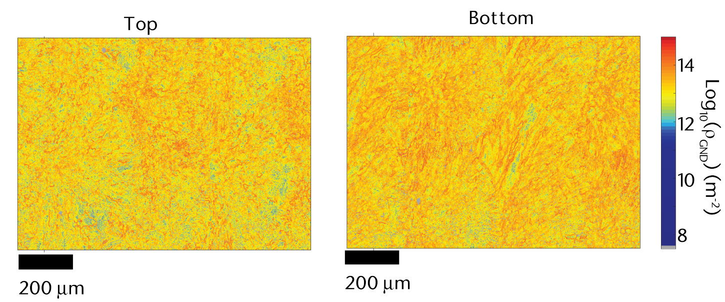
Summary

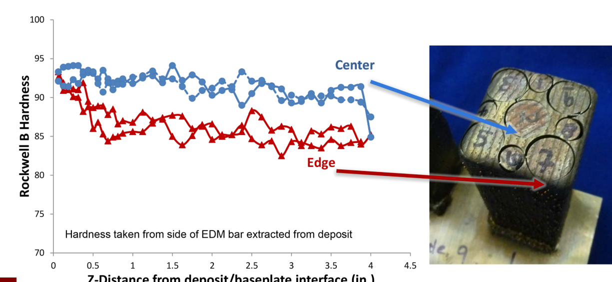
- Moving heat source has been developed that enable multiphysics thermal and mechanical modeling of the LENS process for part-scale builds
- We can perform coupled simulations that predict residual stresses at values near the yield strength 304L
- The prediction of yielding and plastic strain near the baseplate is consistent with microstructural measurements of dislocation density
- Measurements of higher GND density near the baseplate is consistent with our measurements of higher hardness values near the baseplate



500 Watt Laser
0.001 m beam diameter

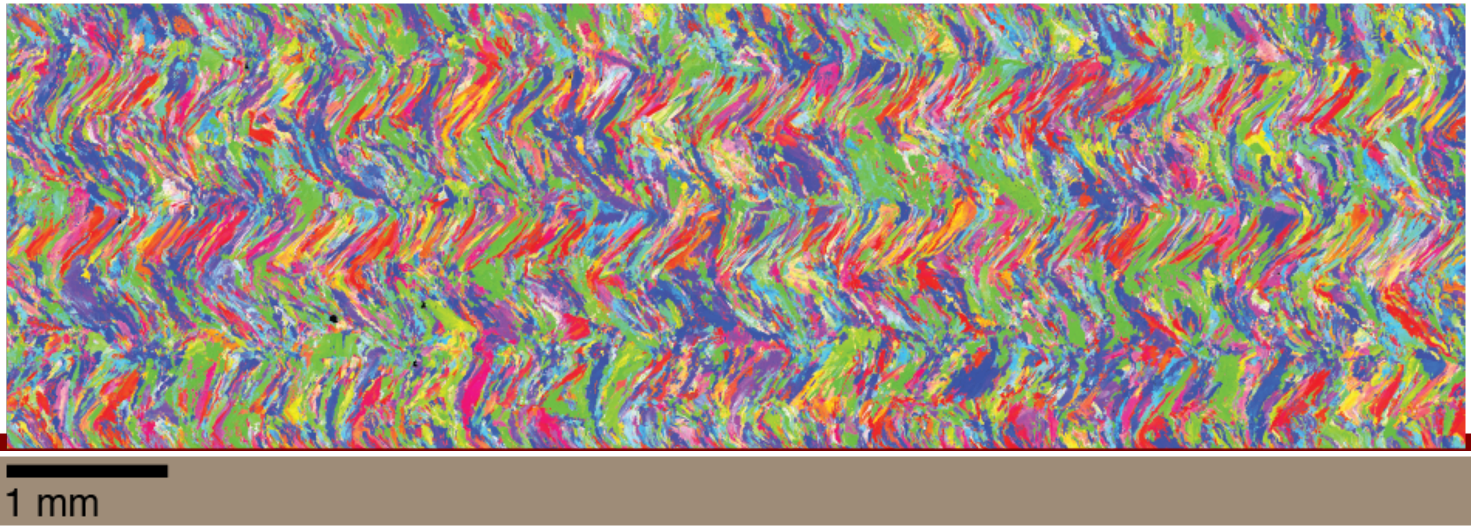






Conclusions

- The thermally-induced strain and resultant dislocation structure is an important factor to understanding the mechanical property variation in a build
  - The effect of the base plate as a heat sink and a constraint is significant in the development of microstructure and properties of a build
  - We have measured this in simple builds, but the effect could be more complicated in more complicated builds
- Eventually, these models can be used to optimize build parameters for each specific build geometry
  - Laser pattern can be optimized for residual stress before the build (e.g. spiral out, spiral in or cross hatch)



LENS 304L
400 W Laser