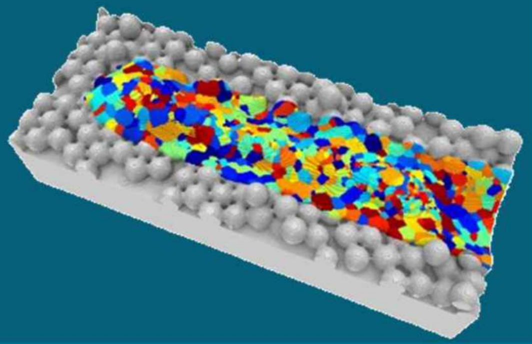
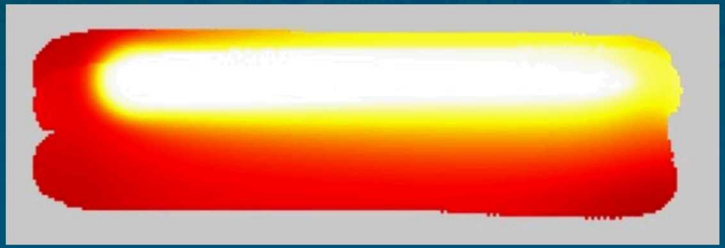
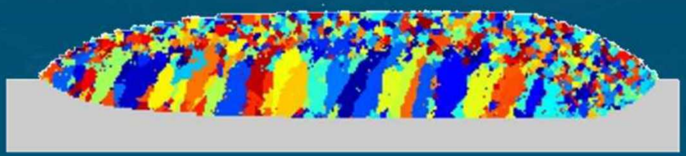
SAND2019-4403PE

Computational Materials for Qualification of Advanced Manufacturing Metals







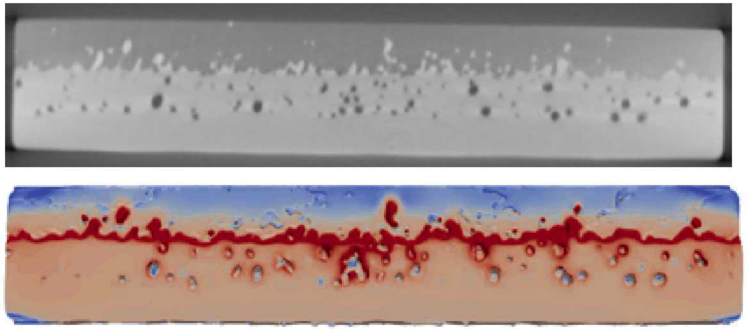
PRESENTED BY

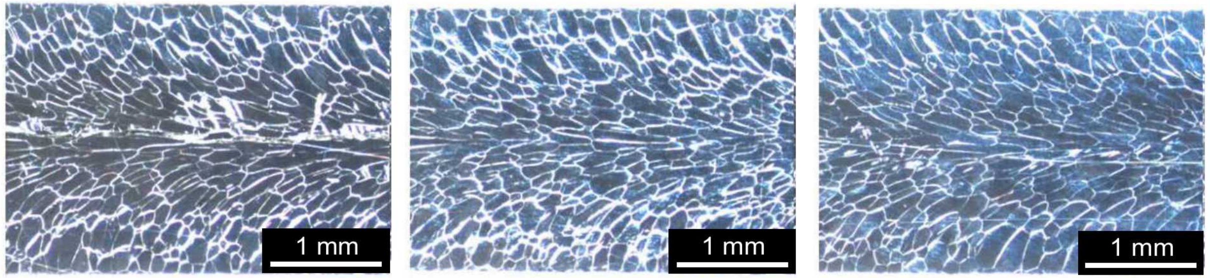
Theron Rodgers

Simulation Needs for Advanced Manufacturing

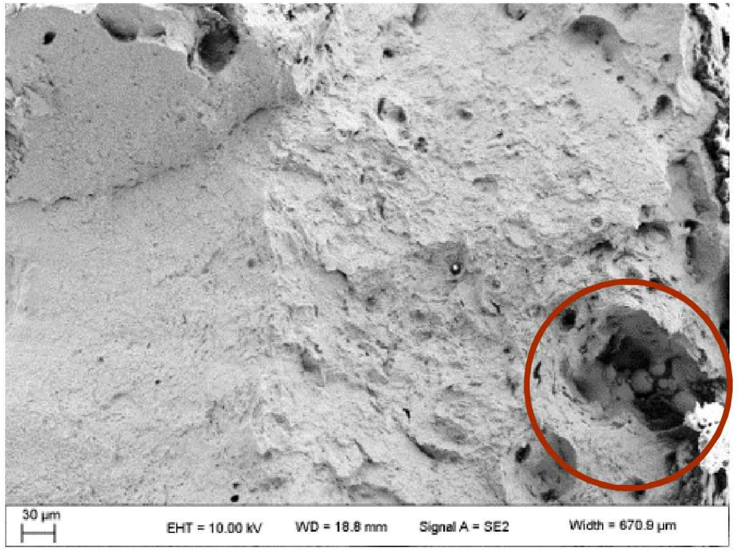
Many processing methods result in materials with non-traditional microstructures, significant defect populations, and residual stresses.

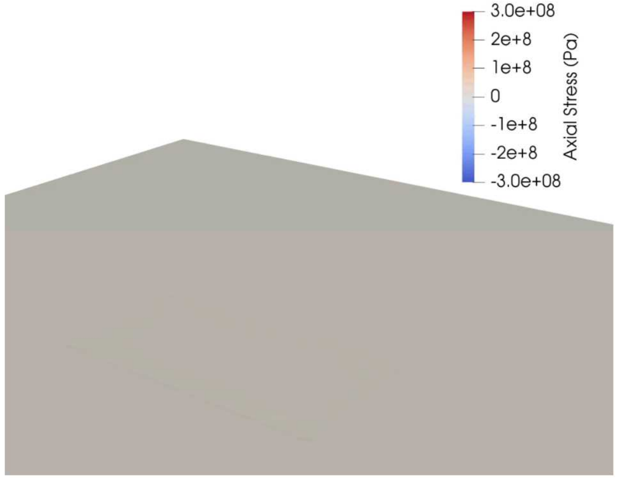
Laser welding

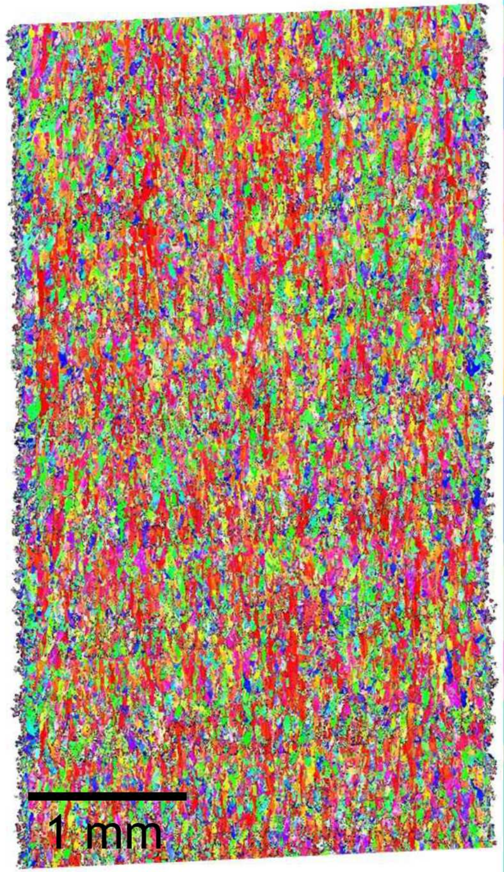




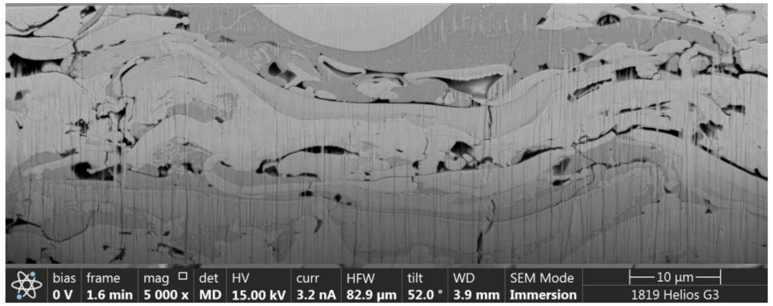
Additive manufacturing

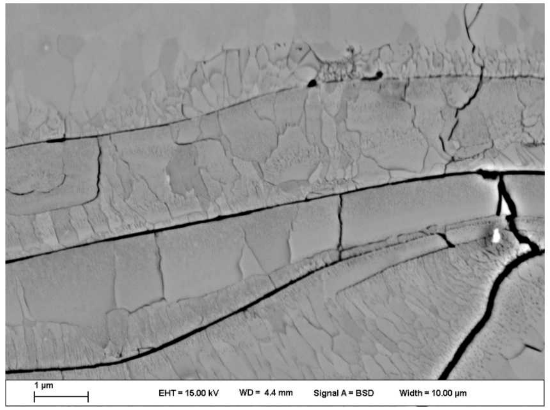




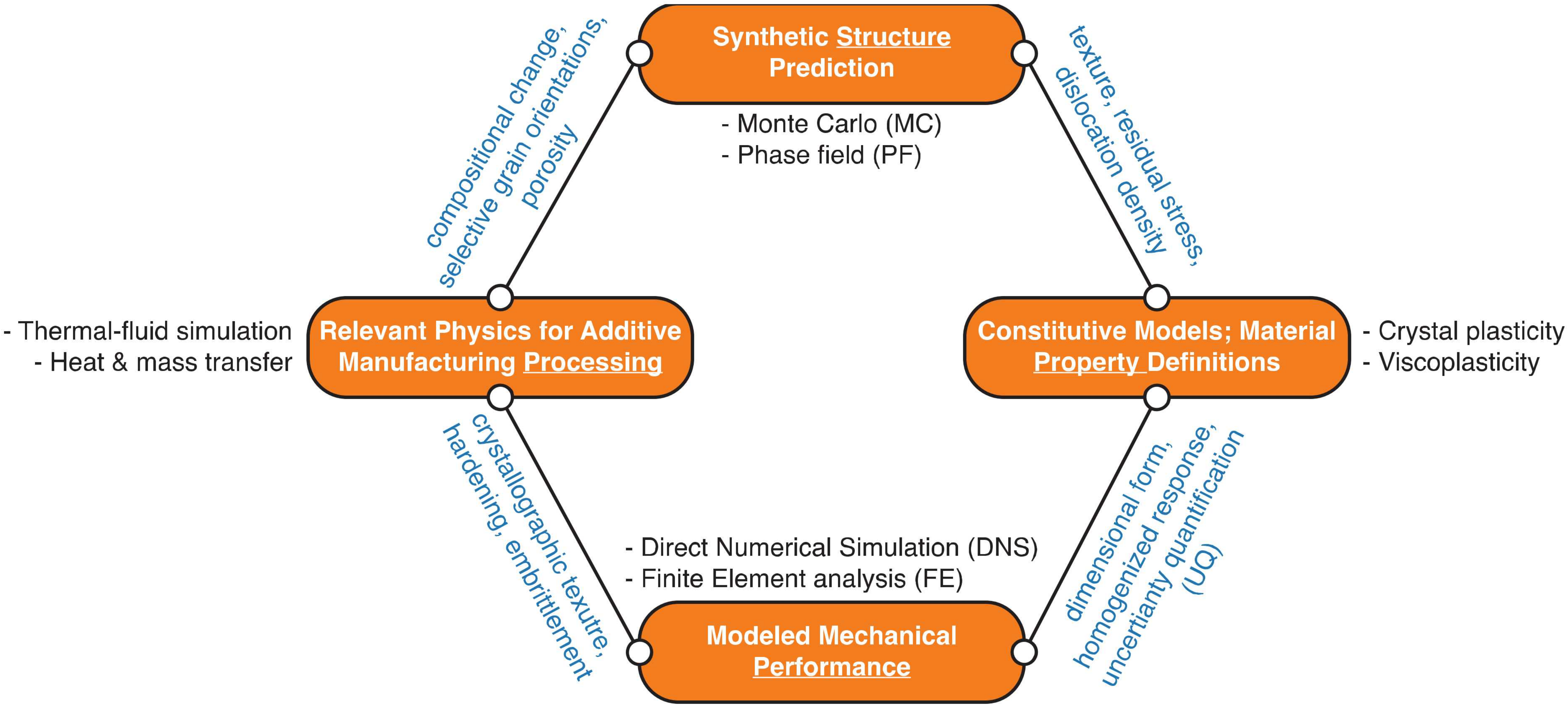


Thermal Spray





Making PSPP linkages at microscale and above

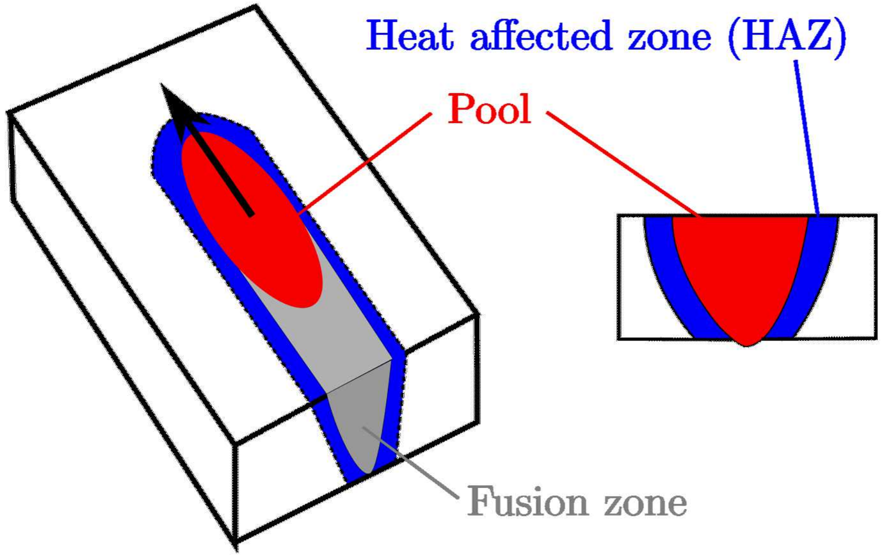


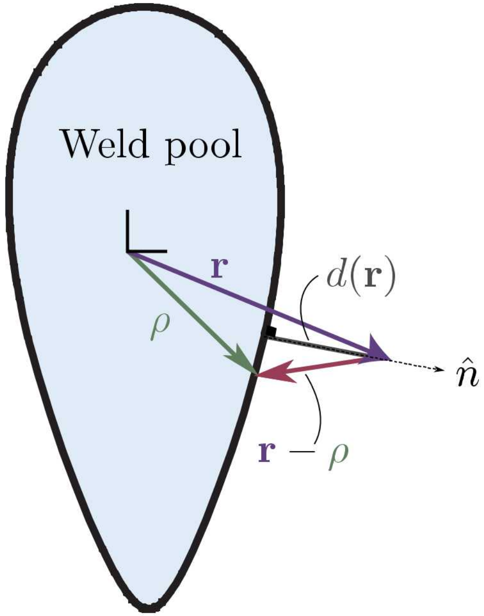
Outline

- Laser welding
- Additive manufacturing
- Thermal Spray
- Enabling technologies & methods

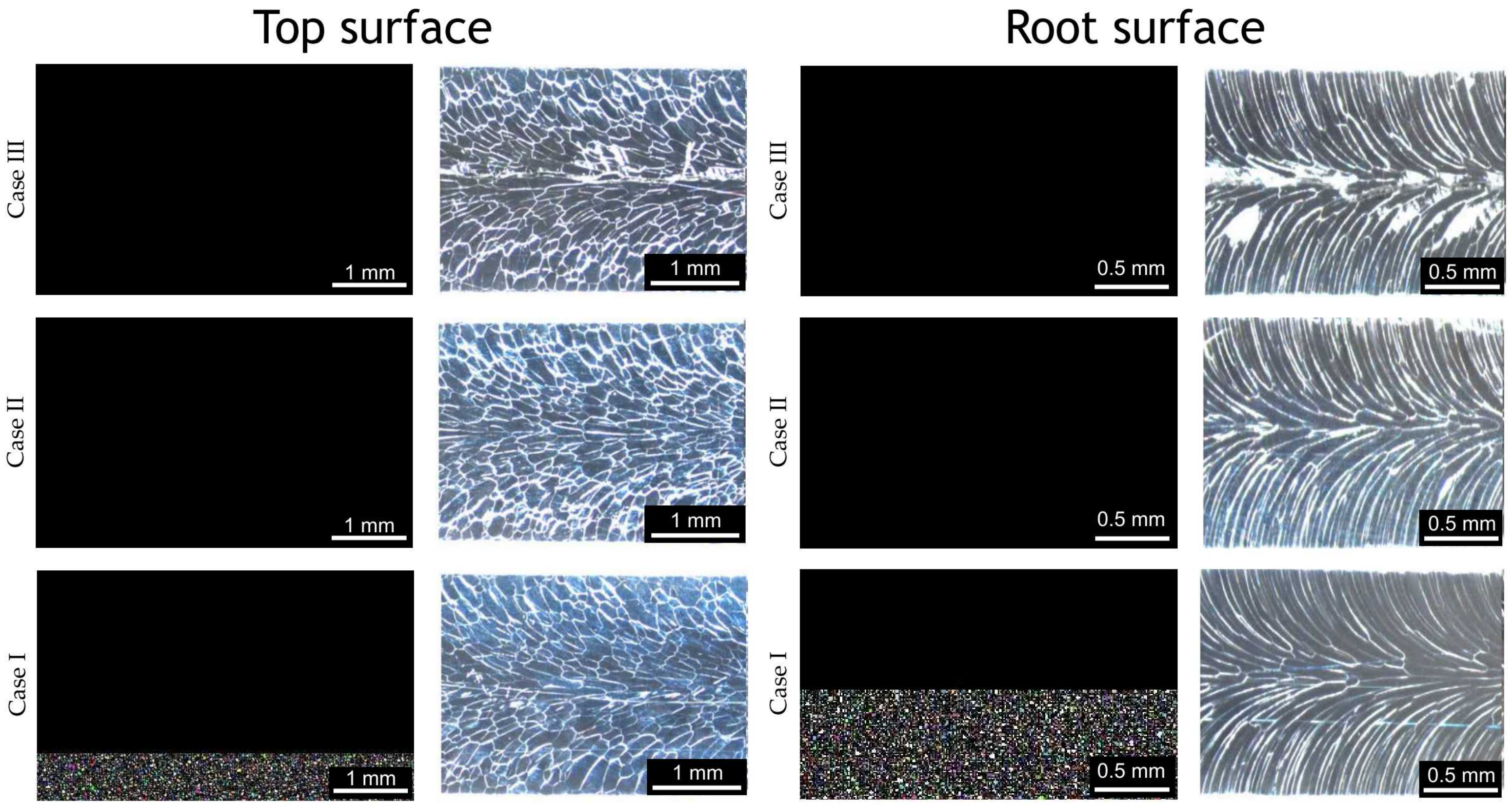
Microstructure prediction for laser welding

John Mitchell



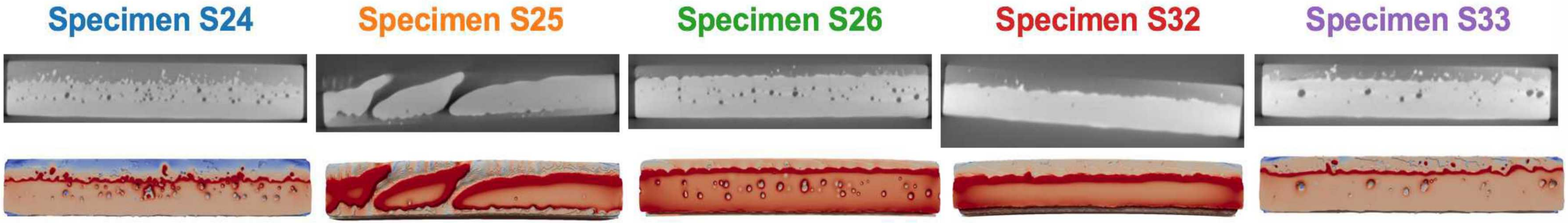


- Spline-based weld pool shapes allow rapid simulation of 3D weld microstructures.
- Solid-state grain coarsening in heat-affected zone is also simulated.
- Pulsed welding can be simulated.



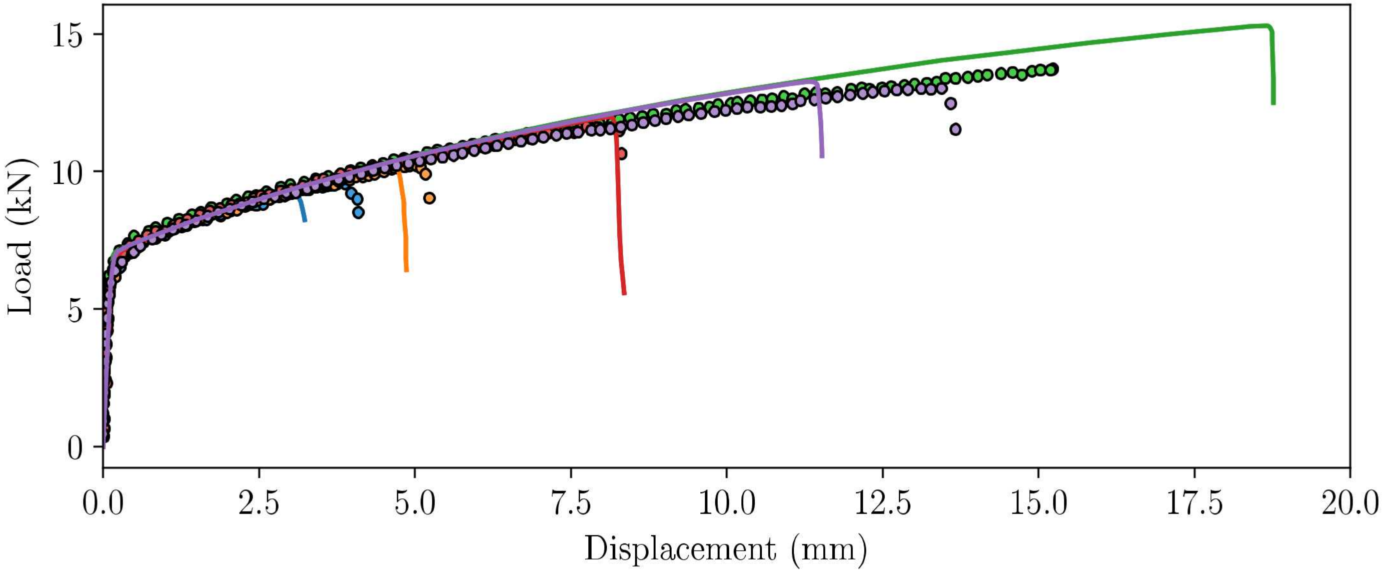
Micro-CT based models of laser welds for determination of failure

Kyle Karlson, Alyssa Skulborstad, Maher Salloum



Nonlinear solid mechanics models generated from micro-computed tomography (mCT) scans were used to evaluate primary drivers for observed laser weld structural variability.

A new laser weld material model parameter set was developed to evaluate laser failure using novel full field calibration techniques. Results show geometric variability (e.g. porosity, weld root geometry) is the primary driver for global structural variability observed among laser welds in tension.



The upper images show simulation results calculated using models generated from CT scans of actual laser welds and the lower plot shows the strong agreement between simulation result predictions (lines) and the experimental load displacement curves (dots)

Outline

- Laser welding
- **Additive manufacturing**
- Thermal Spray
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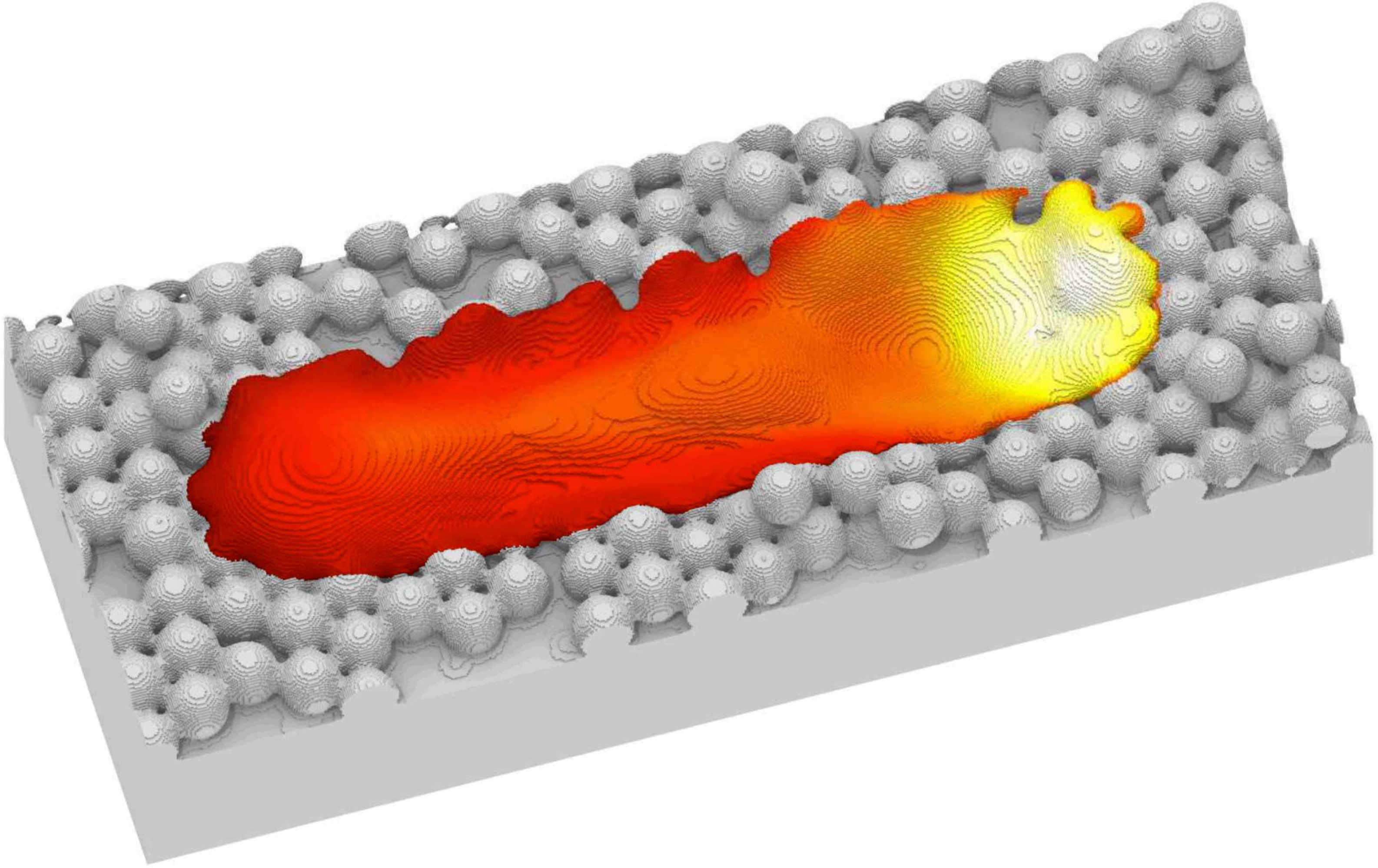
Thermofluid powder bed simulations

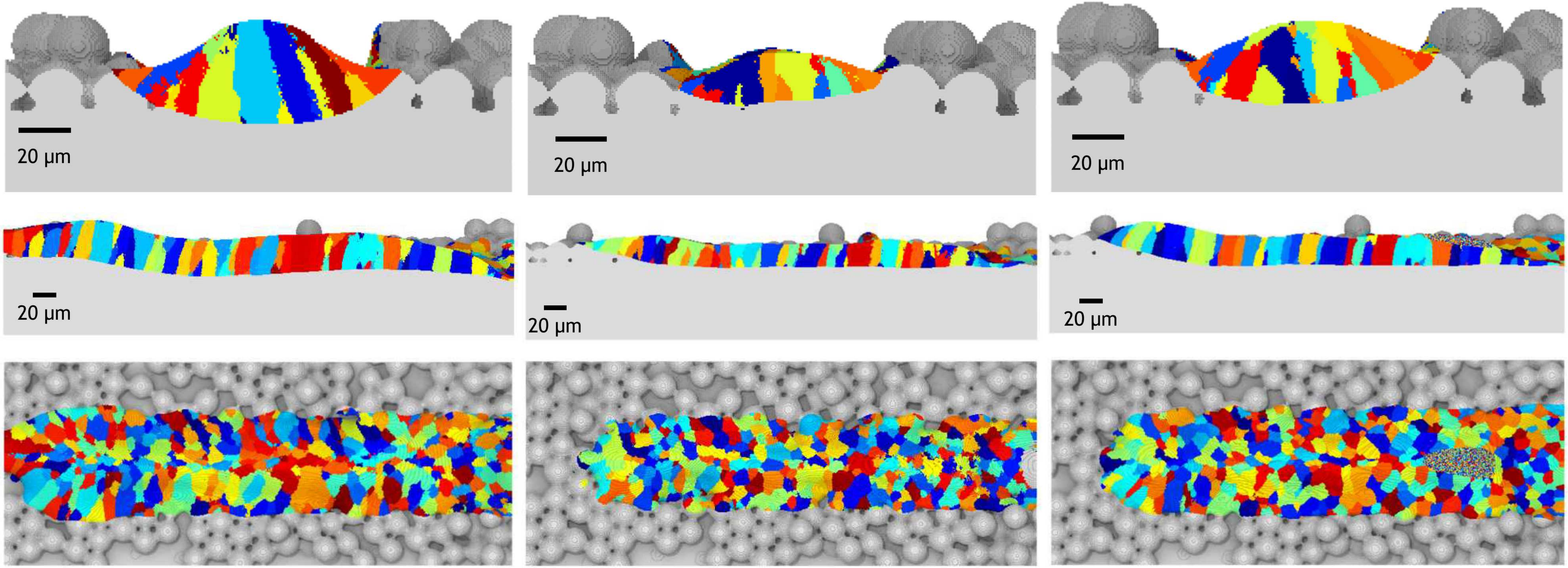
Mario Martinez & Daniel Moser

- Highly detailed level-set simulations with extensive physics.
  - Molten metal & gas flow
  - Vapor recoil pressure
- Very expensive to run
- CD-FEM mesh, mapped to a cubic mesh
  - 0.75 µm mesh size



Powder bed results

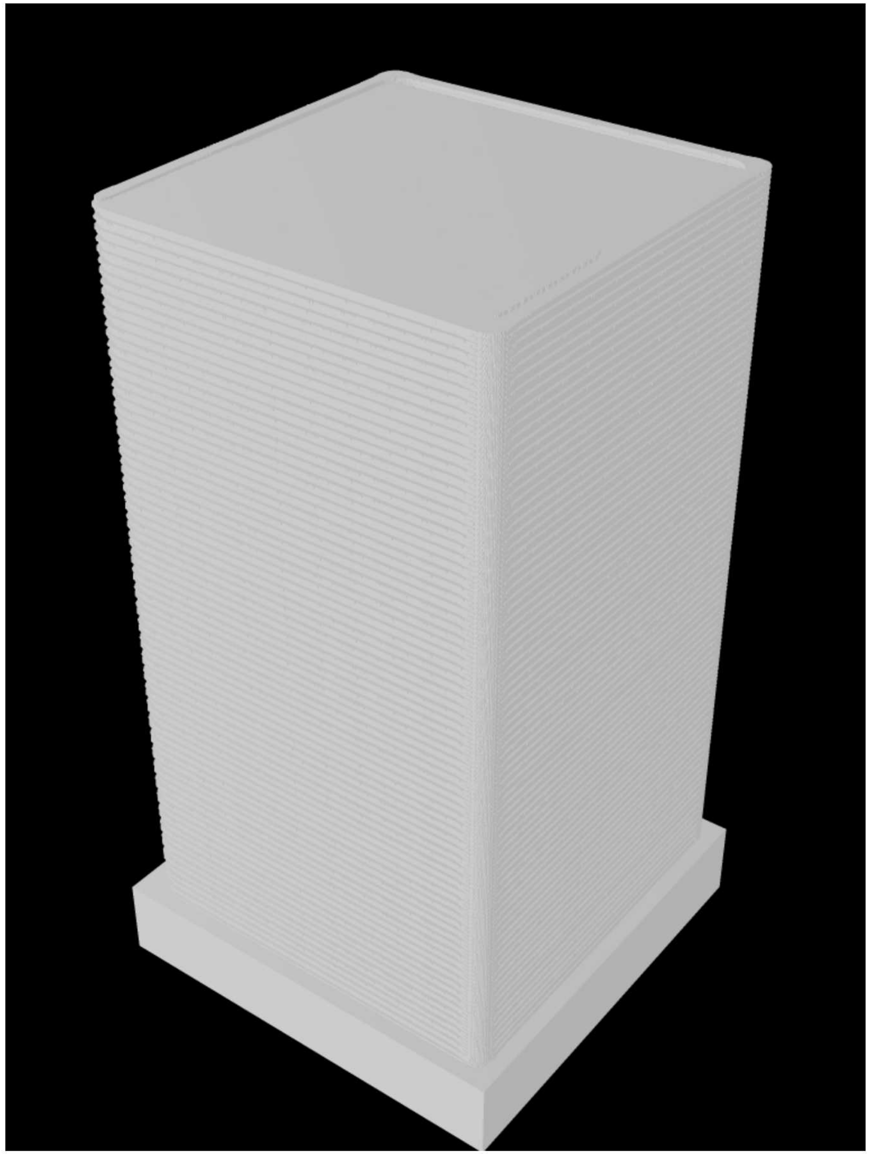
30W, 80 cm/s | 30W, 140 cm/s | 40W, 140 cm/s



Example Simulated Pillar

Daniel Moser & Fadi Abdeljawad

- 2.8 x 2.8 x 5.5 mm domain
- Process parameters calibrated for 3D Systems ProX DMP 200 machine
  - Layer thickness = 30 μm
  - Hatch spacing 50 μm
  - Scan rate = 1400 mm/s
  - Laser power = 129 W
  - Scan strategy = +/-90 alternating
- Includes powder phase with 0.01 of solid conductivity
- Simulation domain boundaries fixed at 300K
- 5 μm grid
- 21.8 m of scan path simulated
- 157 layers
- Critical undercooling 5K

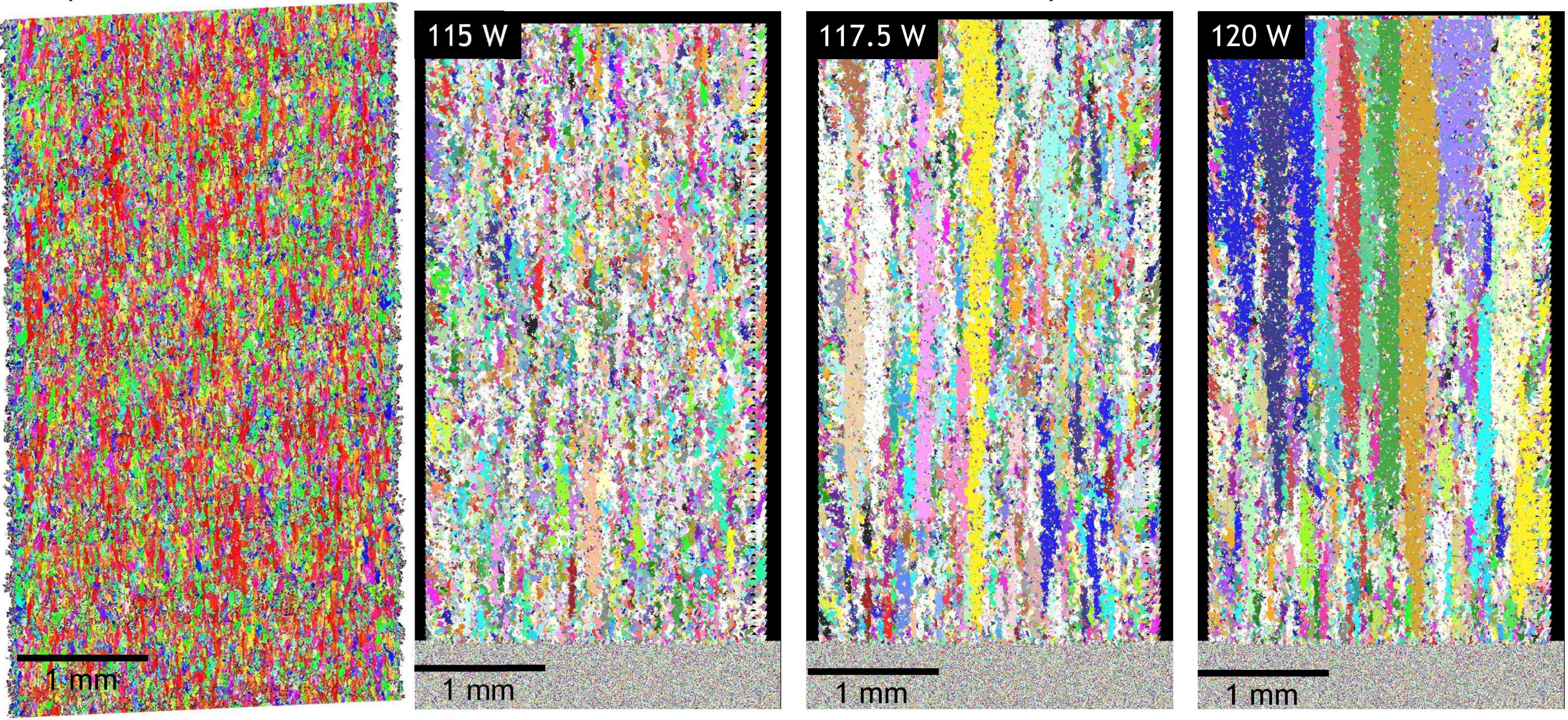


Microstructure evolution is quite sensitive to thermal parameters

Daniel Moser & Fadi Abdeljawad

Experiment

Absorbed laser power



All simulations performed with nucleation densities of 8e13

Using synthetic AM microstructures in SVE crystal plasticity simulations

Hojun Lim & Judy Brown

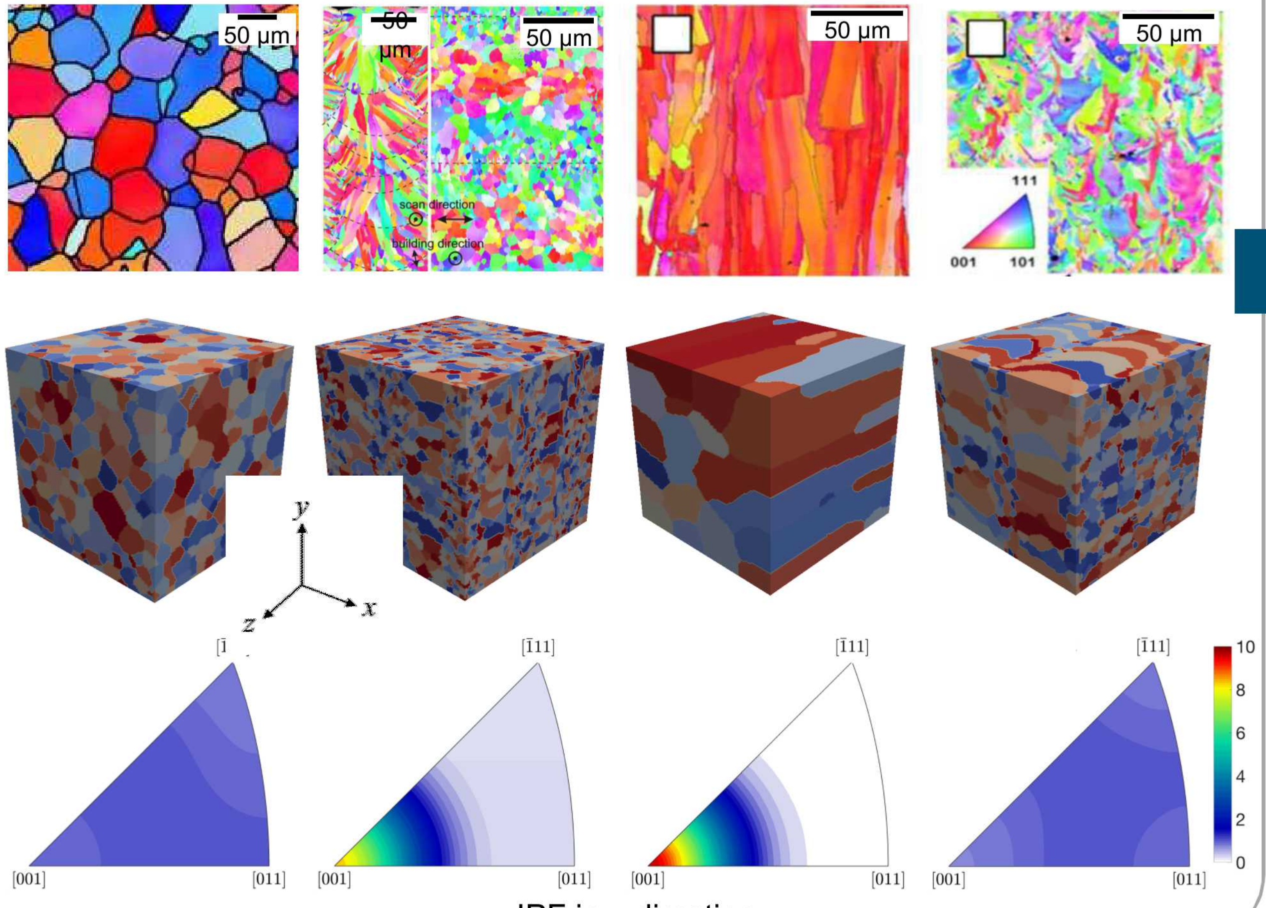
Microstructure generations (SPPARKS)

‘Equiaxed’

‘Bimodal’
Microtexture in alternating layers

‘Columnar’
Strong <100> fiber texture

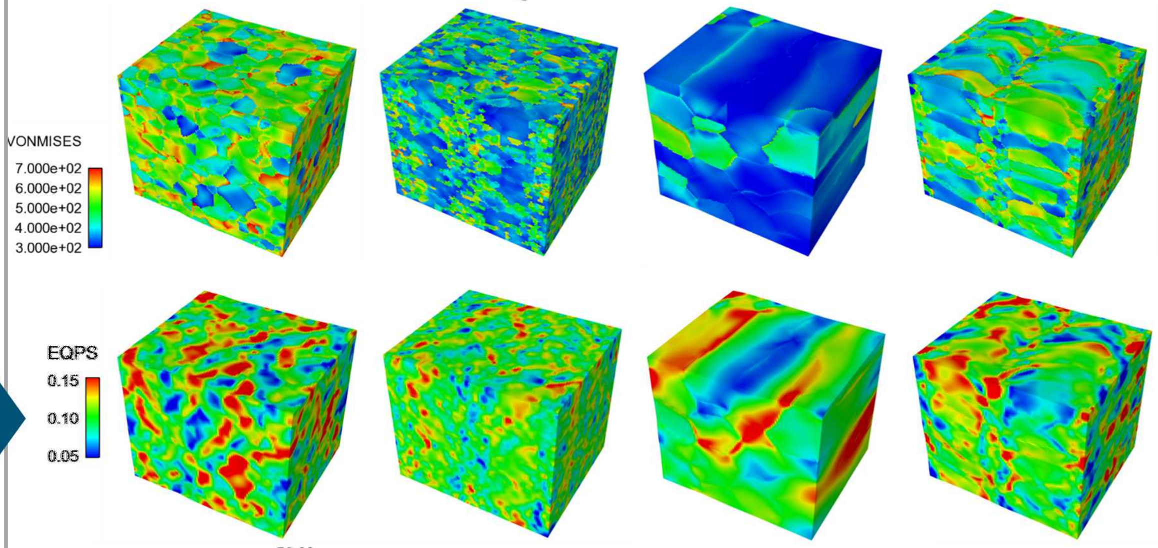
‘Uniform’
No macroscale texture

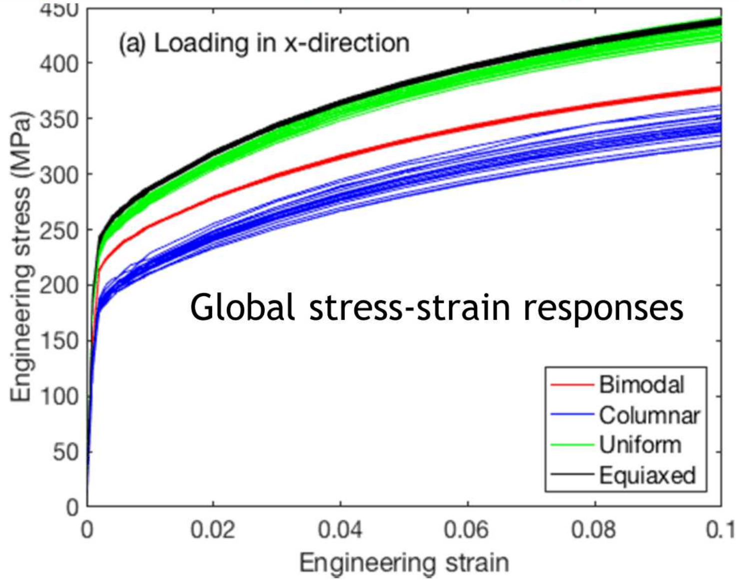


IPF in z direction

Mechanical simulations (CP-FEM)

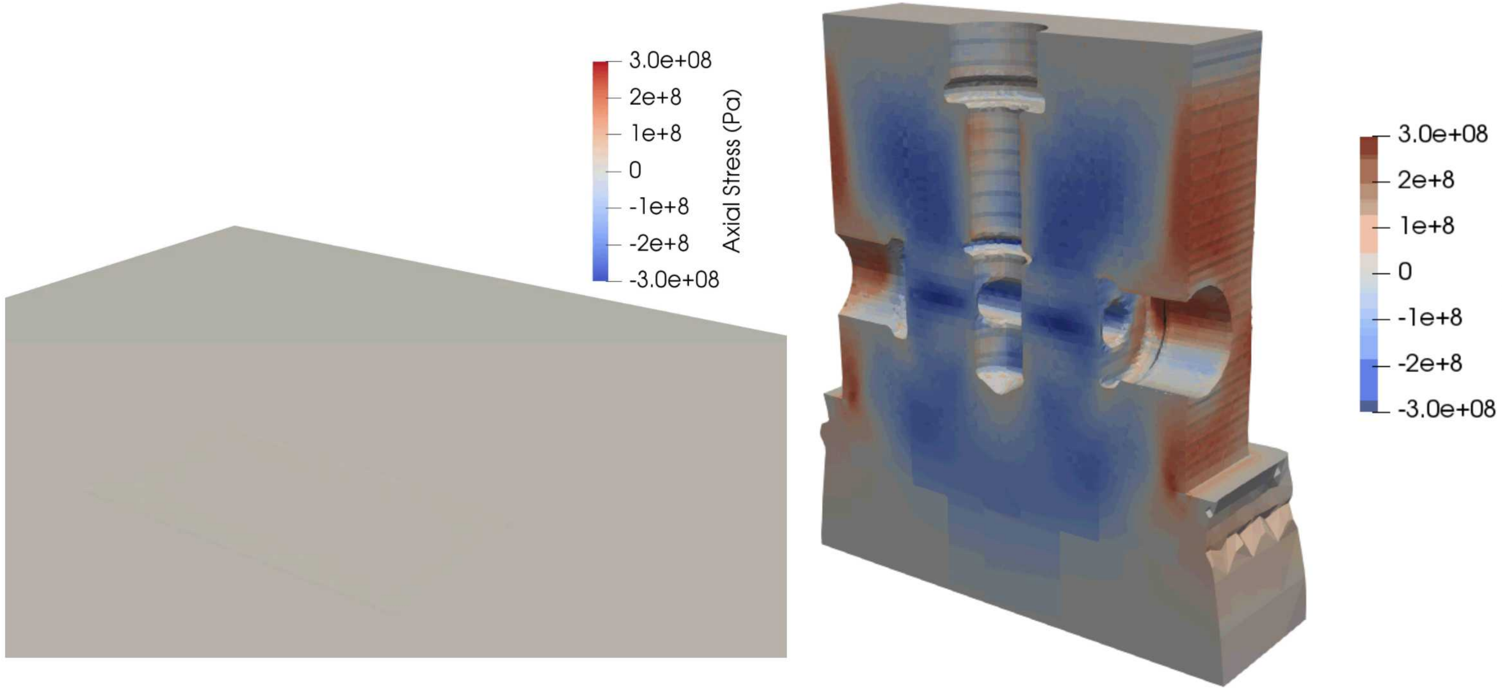
Local VM stress and EQPS values after 10% deformation

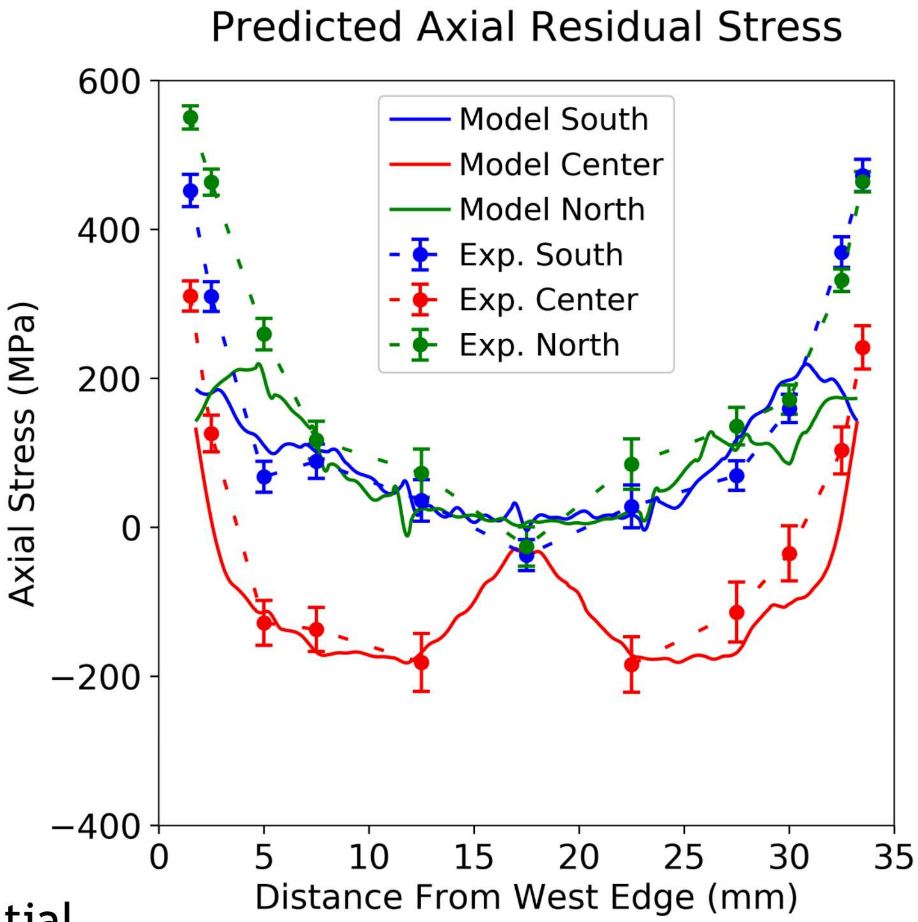




Predicting macroscopic residual stress with ”lumped laser” model

Kyle Johnson

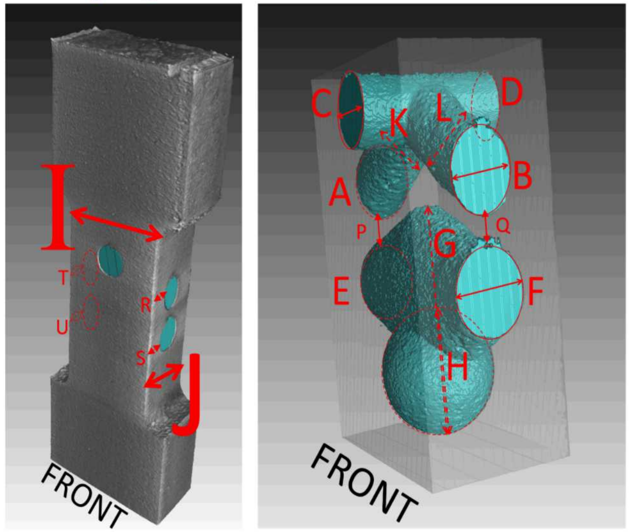


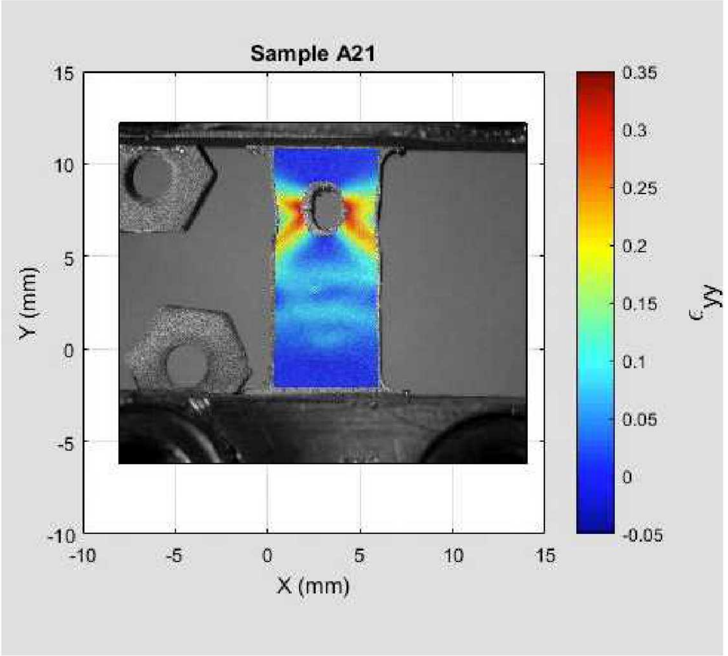


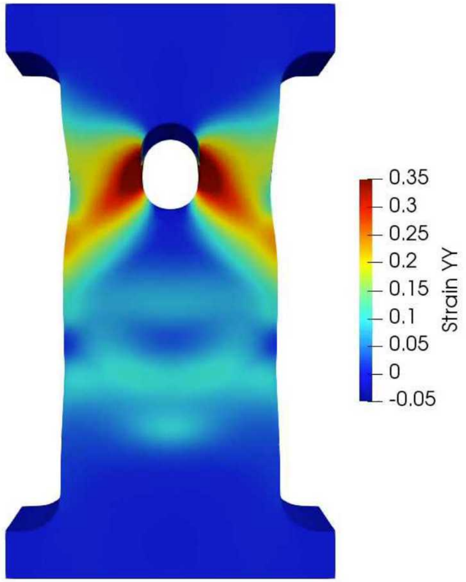
- Uses larger laser spot to reduce simulation time but still capture spatial dependence of thermal gradients.
- Laser radius to layer height ratio and total inter-layer cooling time held constant from actual conditions (~3mm laser diameter, 0.84 mm layer height).
- Bammann-Chiesa-Johnson (BCJ) material model used for response.

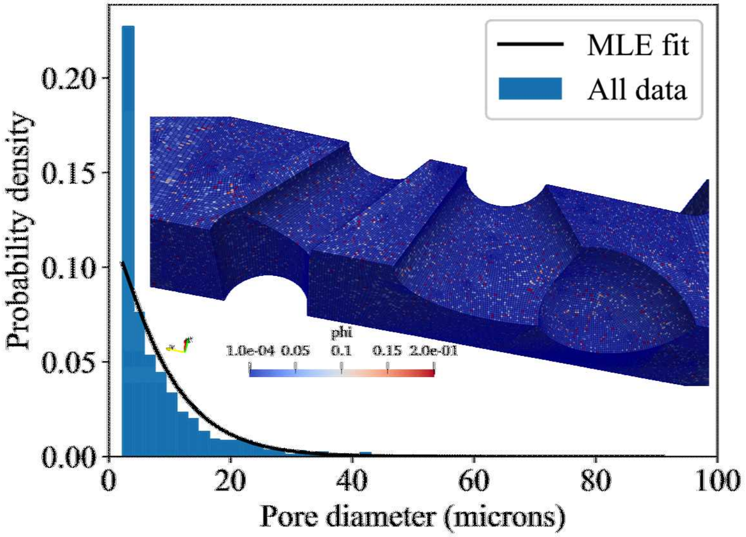
Mechanical simulations with porosity -3rd Sandia Fracture Challenge

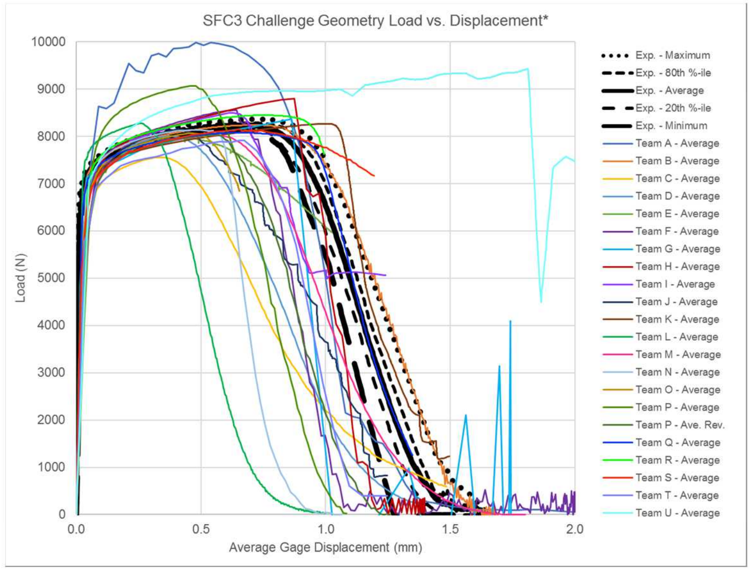
Kyle Johnson



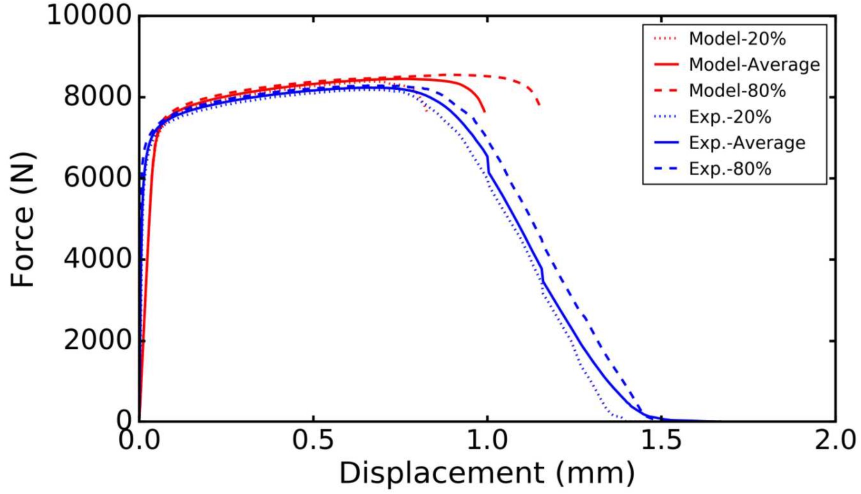








All Participant Predictions with Experimental in Black



SNL/NM Prediction

Kramer, *Boyce* et al., *IJF (In preparation)*, *Johnson* et al. *IJF (In preparation)*

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- Laser welding
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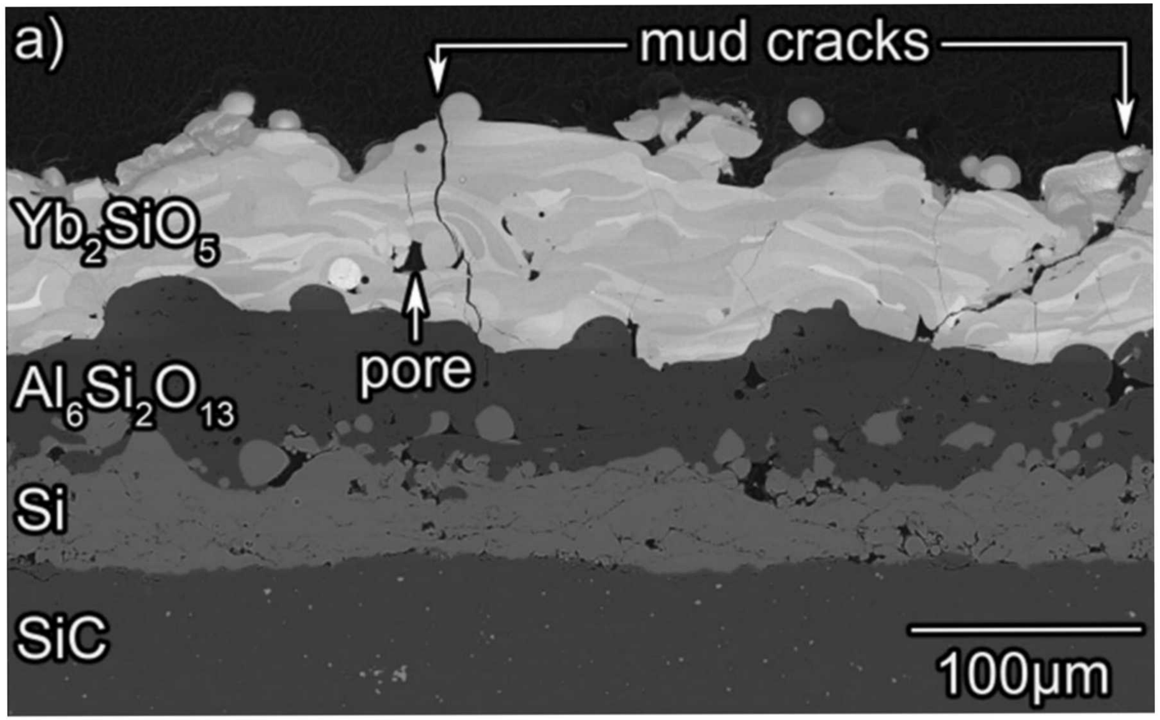
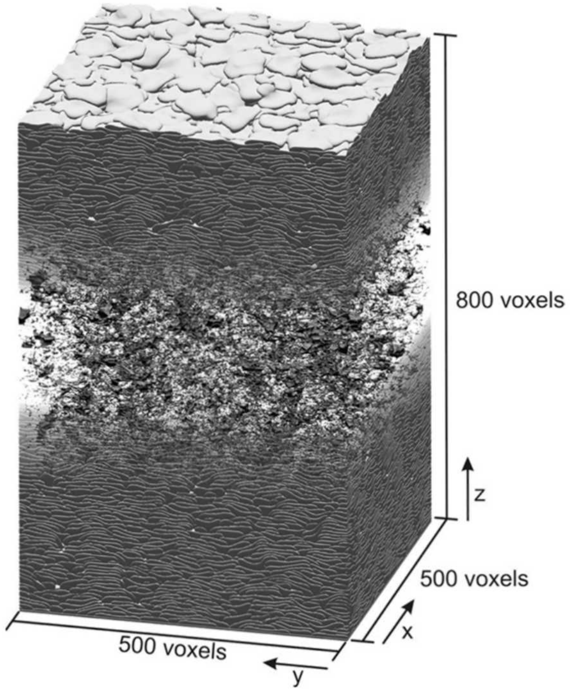
- Enabling technologies & methods

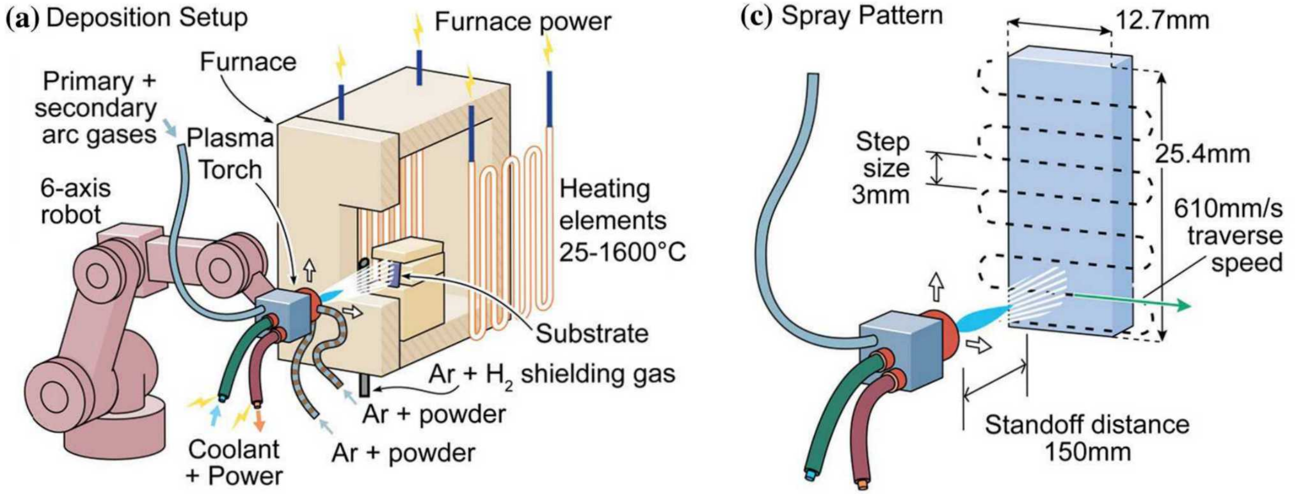
Thermal spray process and example microstructures

- Coatings are formed by the successive impact of molten particles.
- Resulting microstructures are stochastic and include pores, unmelted particles, cracks and anisotropic structures.
- Grain sizes often less than 1 µm.





Wiederkehr and Müller, ***JTST 2015***

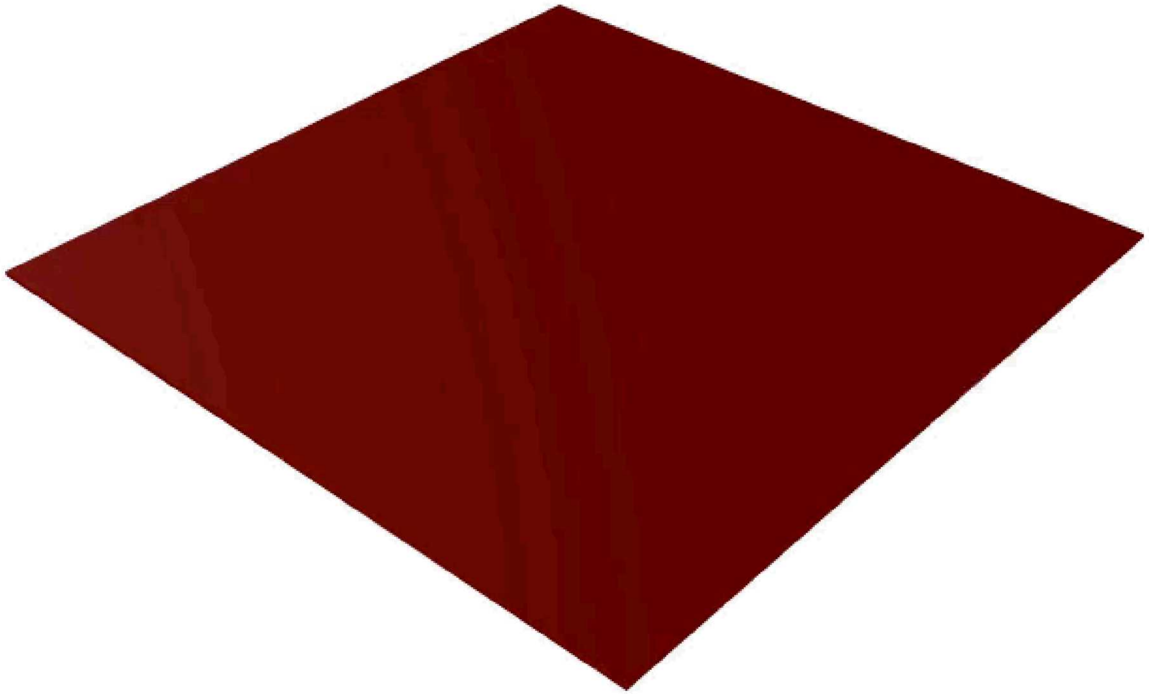


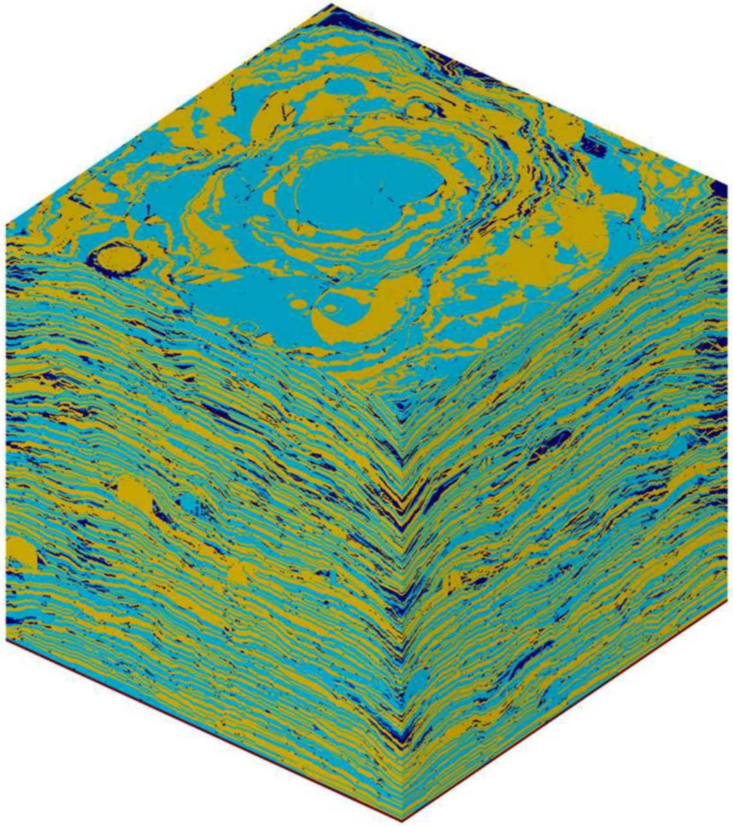
Richards et al., ***J. Mater Sci 2015***

Rules-based thermal spray microstructure model

Thermal Spray Microstructures
Preliminary Simulation Results

- 500x500x500 lattice
- Particle diameters varied from 10-50 voxels
- Unmelted particles are 2.5 % of incident
- Particles had a “flattening ratio” of 4 (melted particle diameters are 4x larger than incident particles)

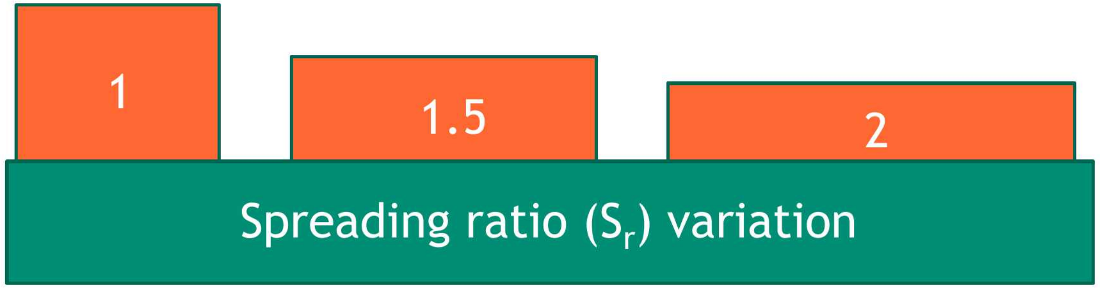


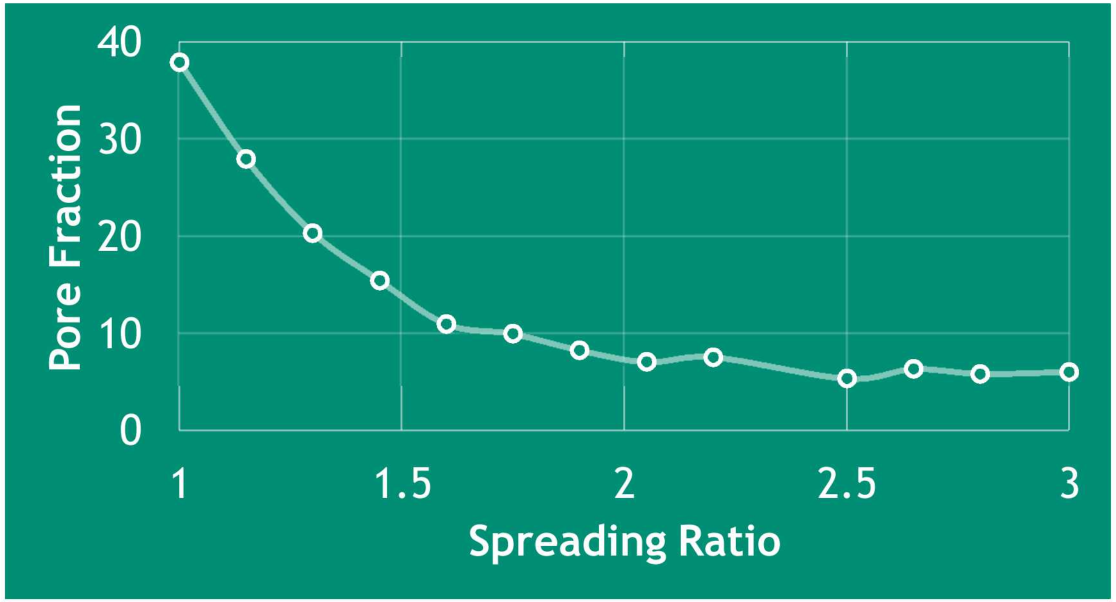


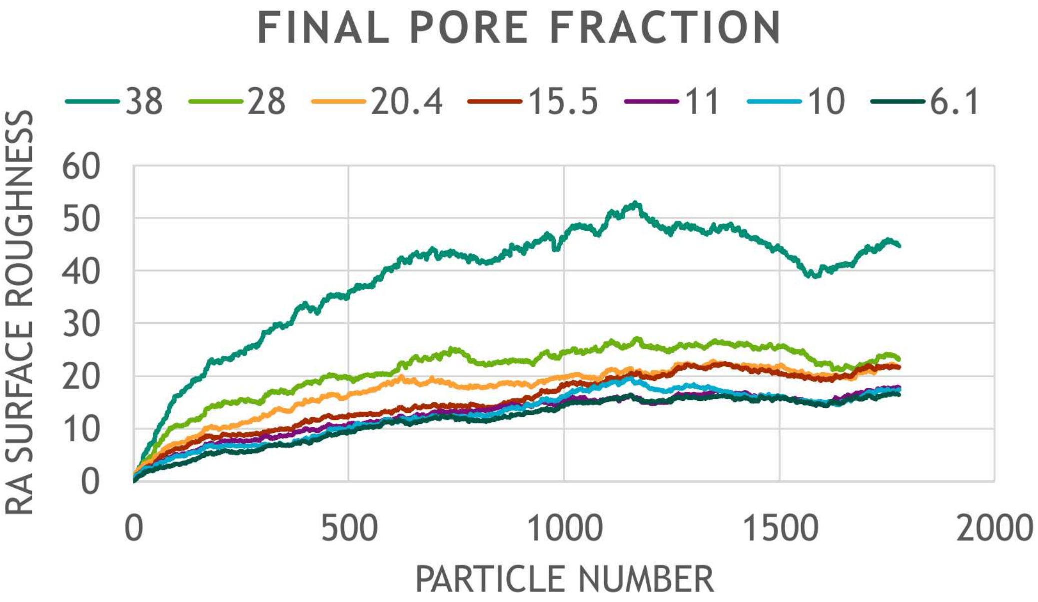
Thermal spray parameter study

Thermal spray model performance has been evaluated for variation in particle/splat spreading ratio, S_r.

Porosity decreases with increasing spreading ratio before leveling off around 5%. Increased spreading ratio also impacts in-process surface roughness. Larger S_r result in lower surface roughness and final total porosity.







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Predicting plastic anisotropy using microstructure measurements

Hojun Lim

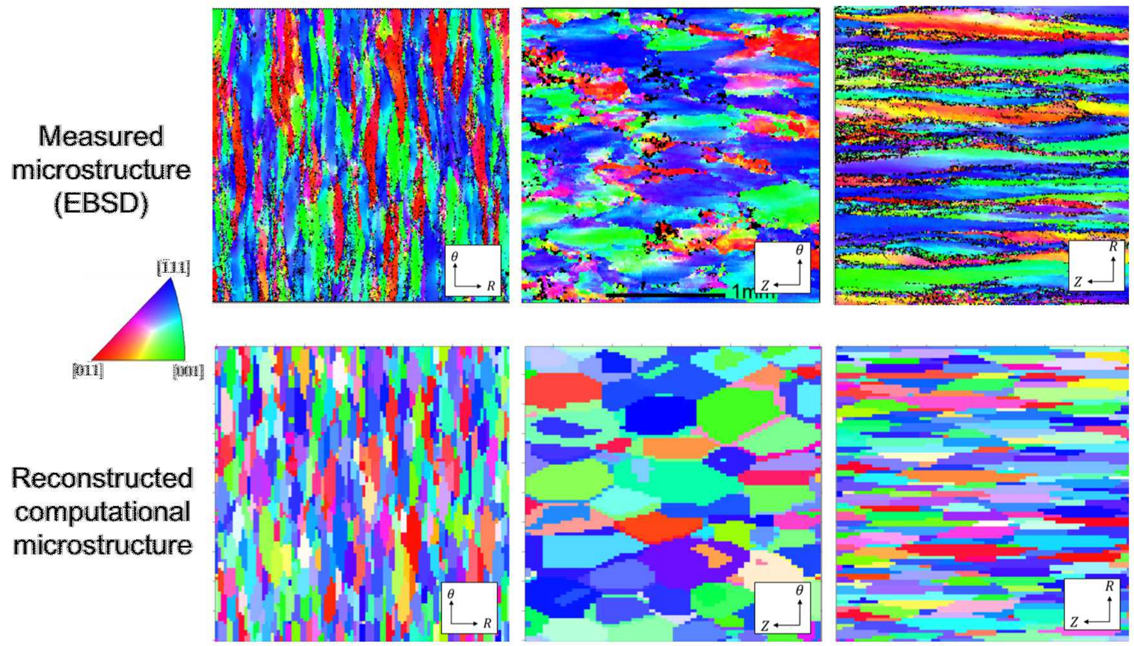


Fig 1: Measured and computational microstructures in various directions. Here, colors represent the orientations in θ direction.

- XRD and EBSD data are used to generate equivalent 3D microstructures, i.e. texture and grain morphology.
- Computational microstructure is then used to predict anisotropic mechanical behaviors of Al7079. Predicted anisotropic behavior agrees well with measured values.

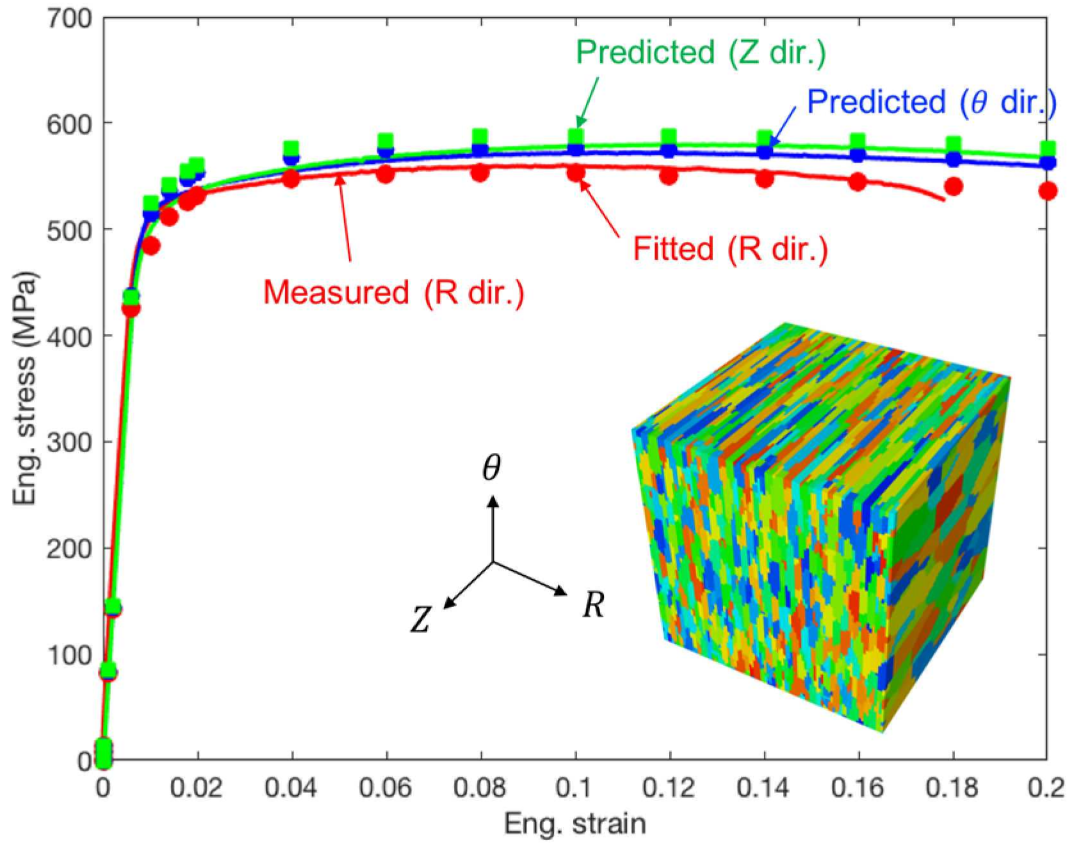
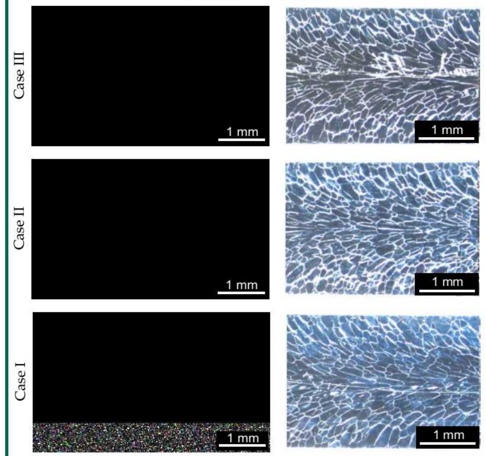


Fig 2: Measured and predicted stress-strain responses of polycrystalline Al7079. Here, mechanical response along R direction is fitted and Z direction is predicted.

- These results support validity of using crystal plasticity models informed from EBSD to understand the anisotropy of polycrystalline metals. The current approach enables characterization of plastic anisotropy without extensive mechanical tests. Furthermore, microstructure informed simulations provide a more physically-based approach that enables investigation of microstructural effects and variability to target optimum microstructures and properties.

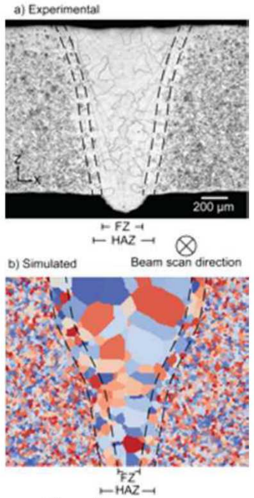
SPPARKS framework for mesoscale microstructure simulation

Potts/Weld



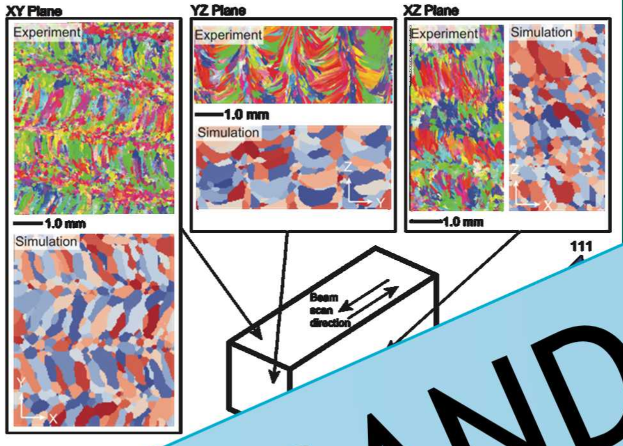
Rodgers et al., MSMSE 2017

Potts/Weld/JOM

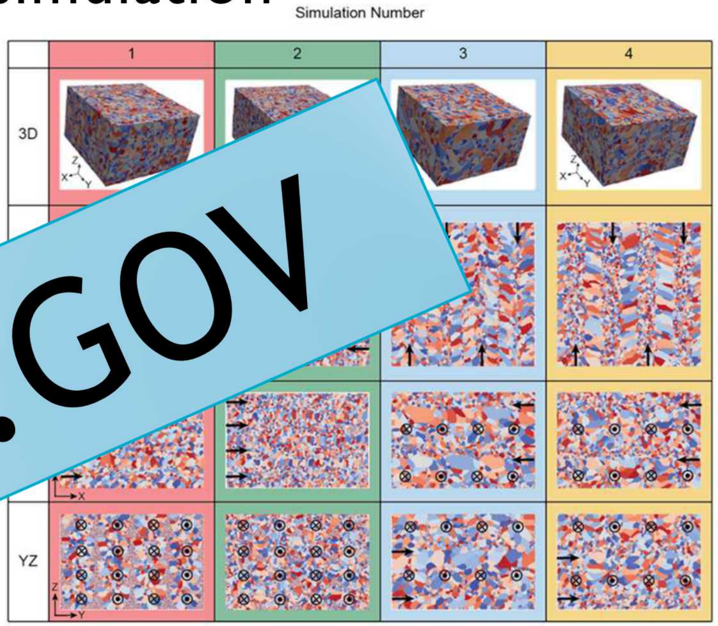


Rodgers et al., JOM 201

Potts/Additive

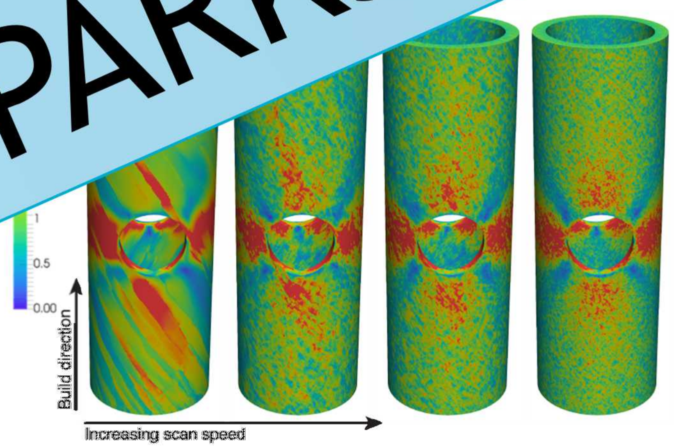


SPPARKS.SANDIA.GOV

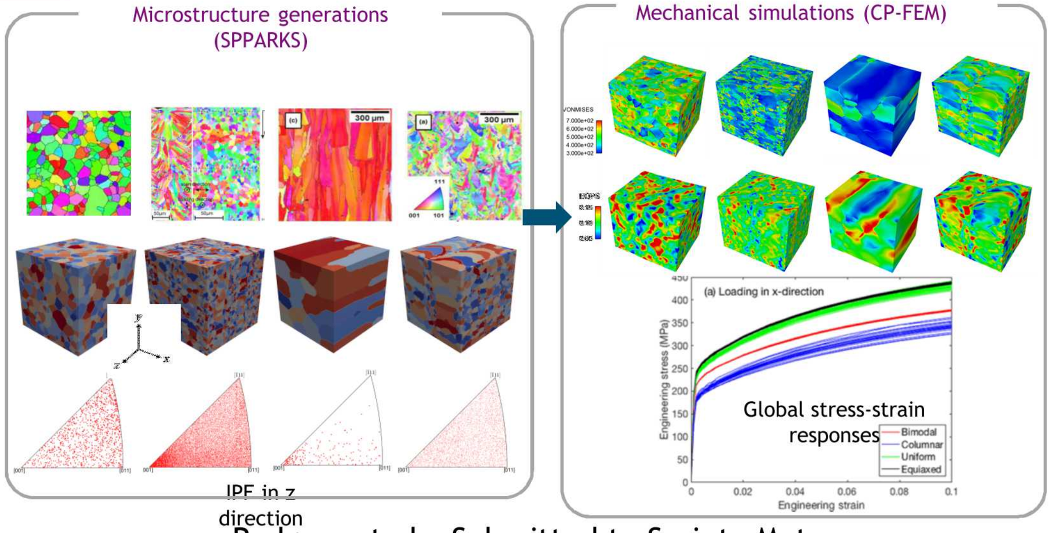


Popova et al. IMMI 2017

Johnson et al., Computational Mechanics 2018



Rodgers et al., MSMSE 2018

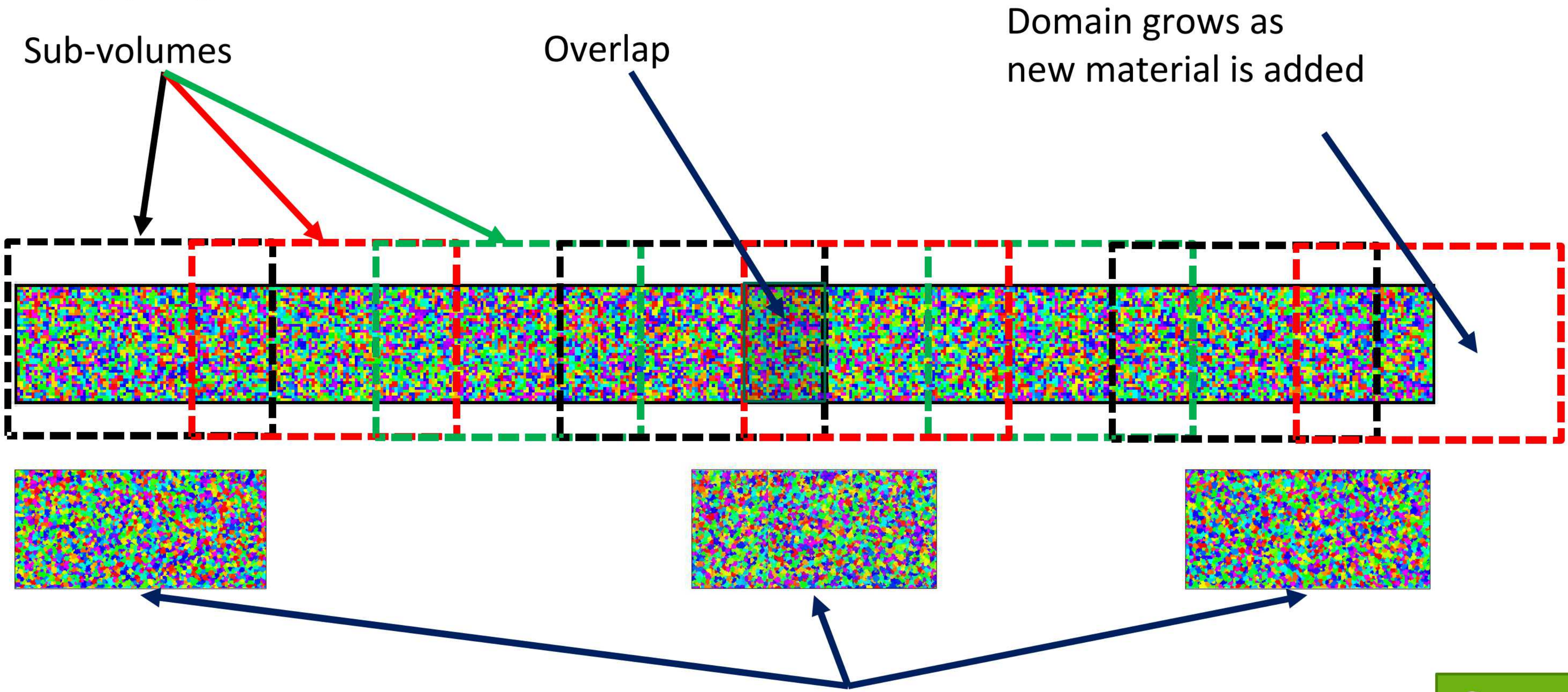


Rodgers et al., Submitted to Scripta Mat.

Matching part-length scales with STITCH

John Mitchell

Laser welding across a large domain is simulated using a series of smaller overlapping sub-volumes.



Post-process, visualize and analyze on arbitrary sub-volumes and arbitrary times

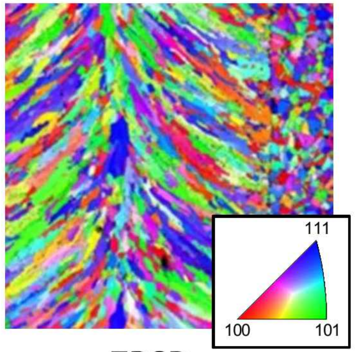
Open source library release this year!

Stitch: radical new approach to I/O

Applications of SCULPT technology

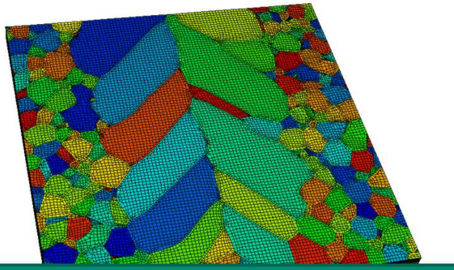
Steve Owen, Hojun Lim, Fadi Abdeljawad, Judith Brown

Laser Engineered Net Shaping (LENS®), Additively manufactured 304L SS

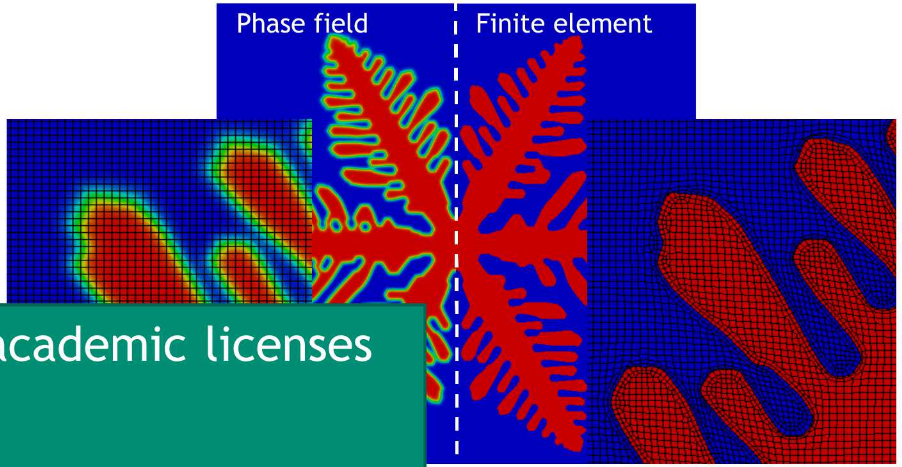


EBSD
(Adams et al., 2016)

S
(Rodg



Dendritic microstructure



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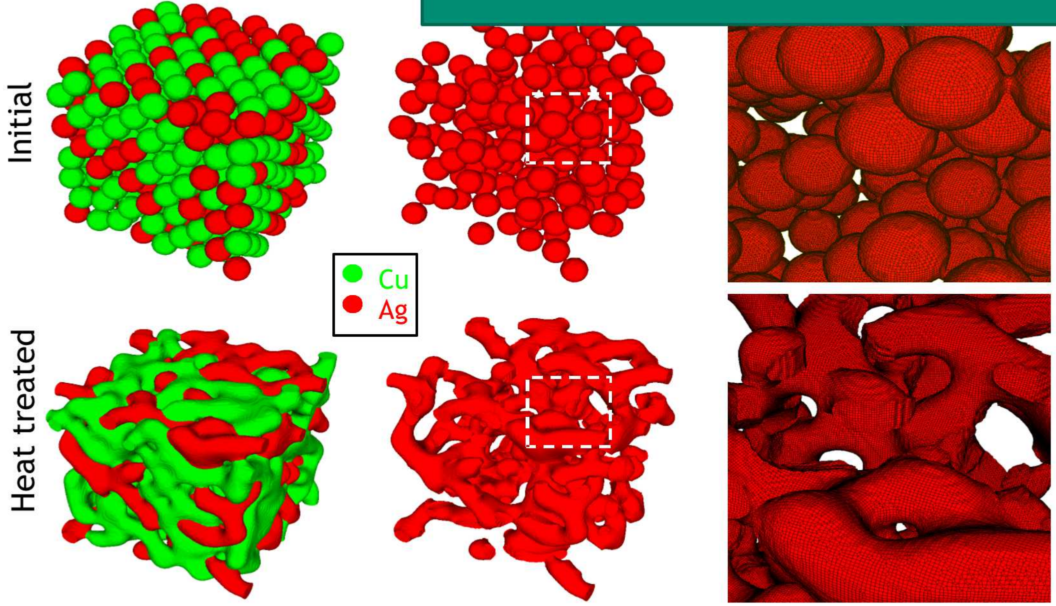
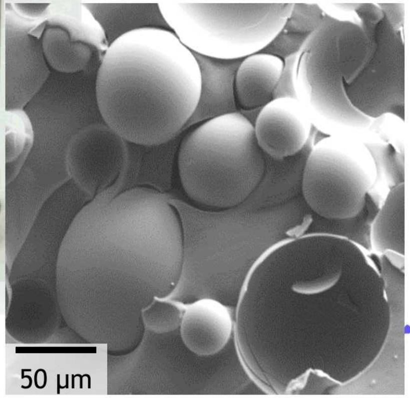
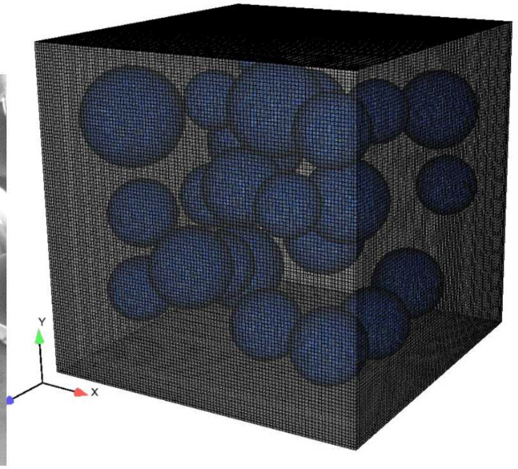
Multi-phase microstruct



Sylgard® with A-16 Glass Microballoon Fillers

Ahmadi et al., 2014





Conclusions & Comments

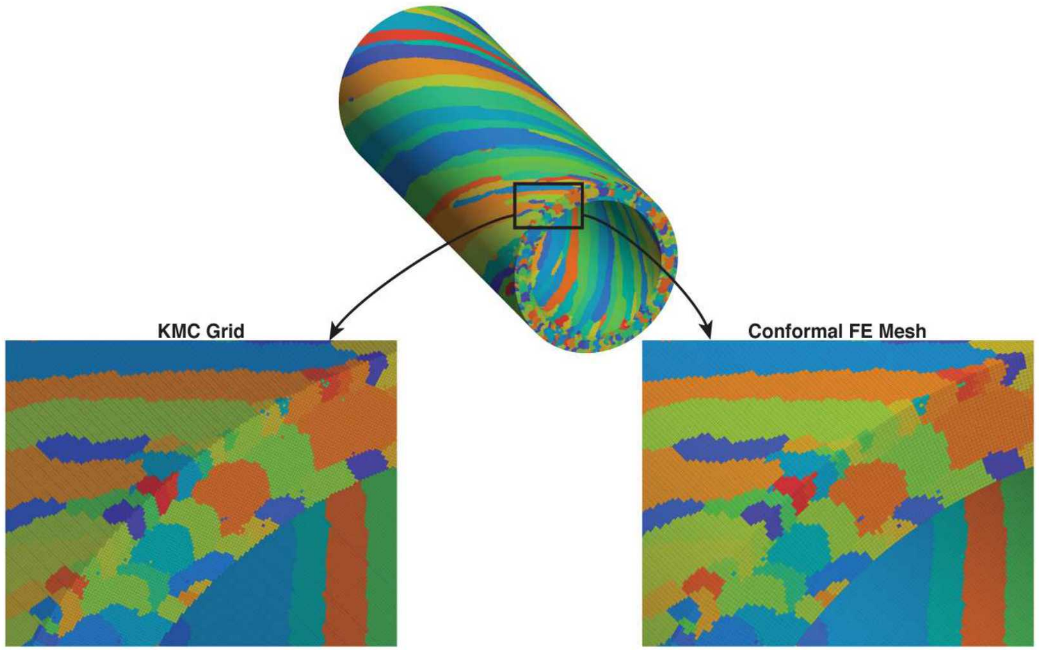
- Computational Materials methods are evolving to address heterogeneities introduced by advanced manufacturing processes.

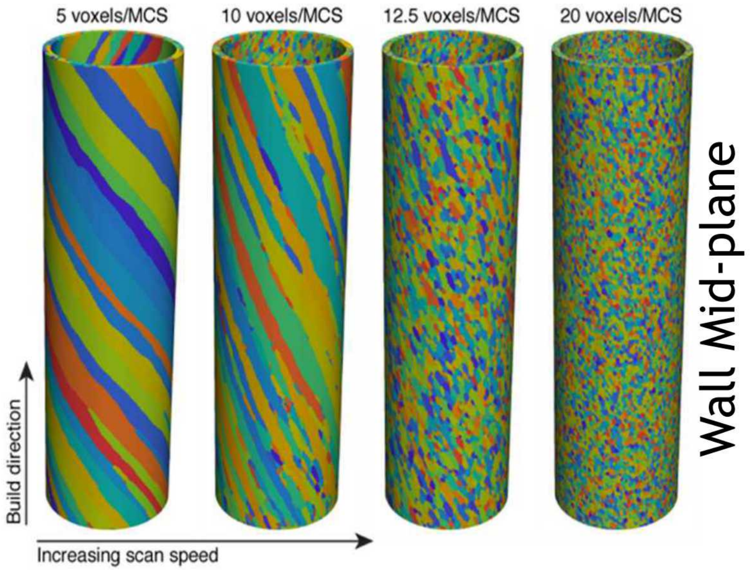
- Progress is ongoing to incorporate the effects of polycrystalline microstructure, residual stresses, and porosity into continuum material models.

- Additional work is needed to understand multi-phase materials, grain-scale residual stress, and dislocation densities.

BACKUP SLIDES

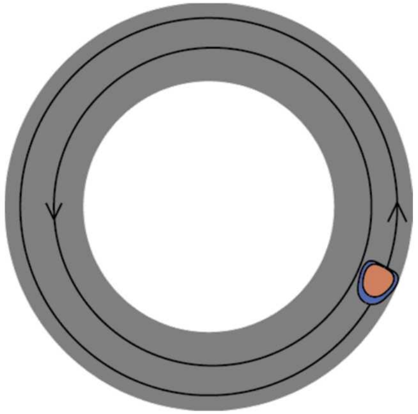
Direct Numerical Simulation on large-scale additive microstructures



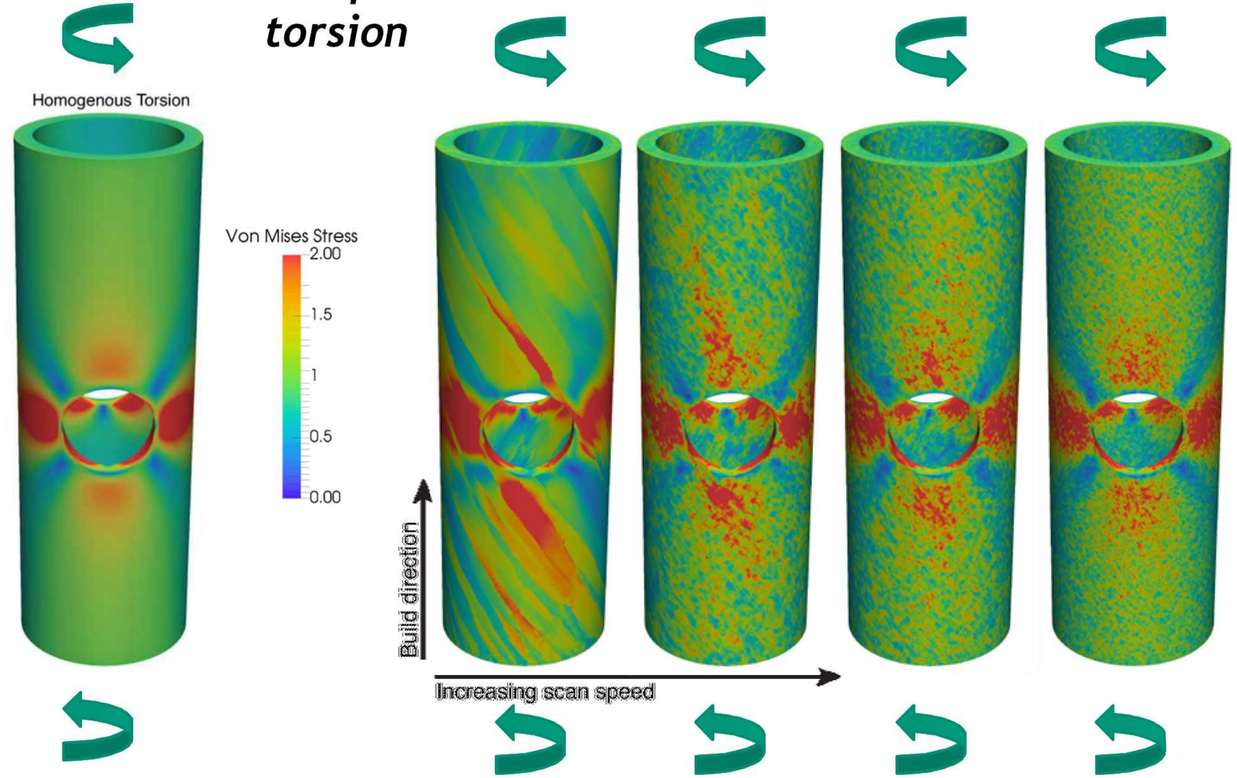


Synthetic AM builds

- 4 scan velocities.
- 2 concentric circular scan paths per layer.
- Idealized molten pool
- Significant microstructure variation w.r.t. scan velocities and w.r.t. wall thickness.



Stress response in torsion

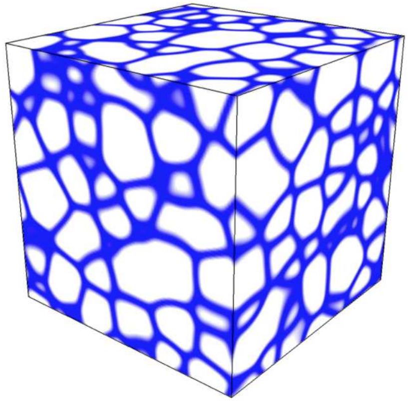


Constructing interface-conformal polycrystal FE mesh

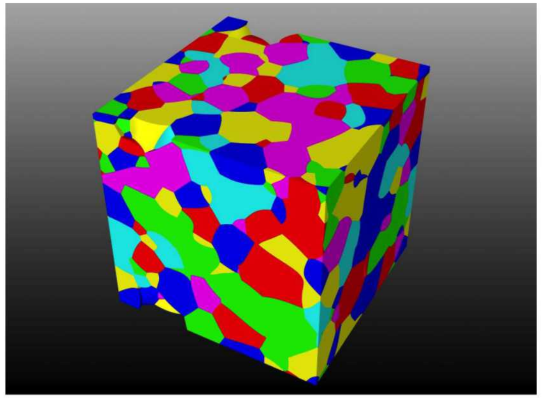
Fadi Abdeljawad, Hojun Lim, Steve Owen

Grain Growth Simulation → Polycrystalline FE mesh

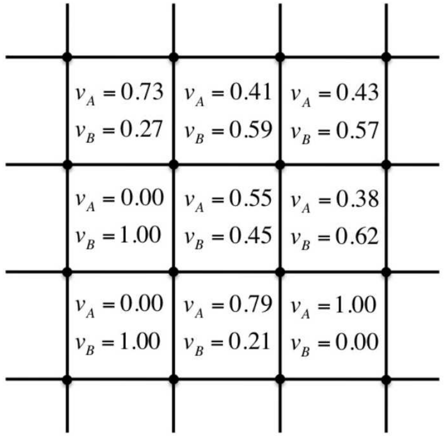
Cubit 'Sculpt'



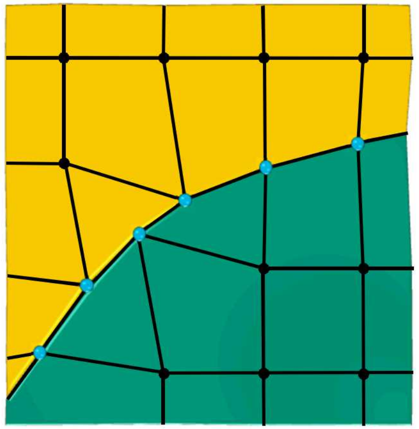
Realistic 3D microstructure
Conformal hex mesh at GB



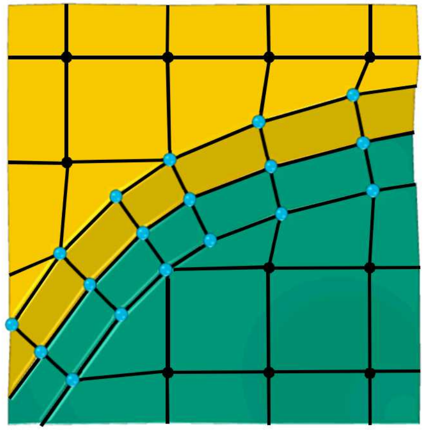
Volume fractions representing percent of grains for each cell



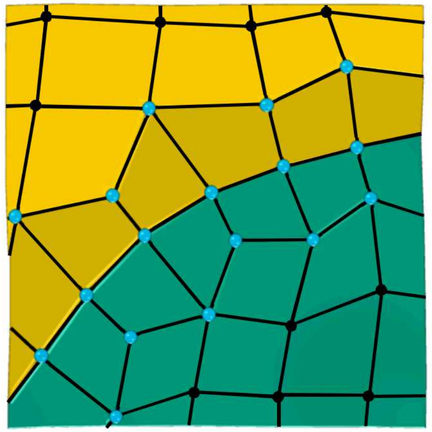
Resolve grain interfaces and project nodes to surfaces



Insert layer of hex elements at interfaces



Perform smoothing and pillowing to improve the mesh quality.



Lim et al., MSMSE (2016)

Top view of build

Absorbed laser power