SAND2022-2292C

Model Based Control of Microstructure for Additively Manufactured 316L Stainless Steel

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Motivation

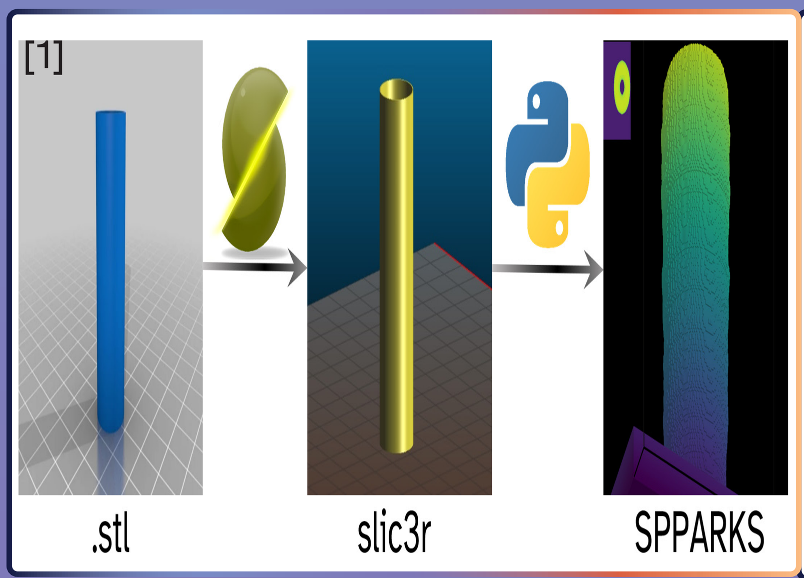
Microstructural properties such as grain size and eccentricity for additively manufactured parts is an important factor in determining mechanical strength, ductility, and fatigue life. To optimize and control both microstructure and mechanical properties there is a desire to:

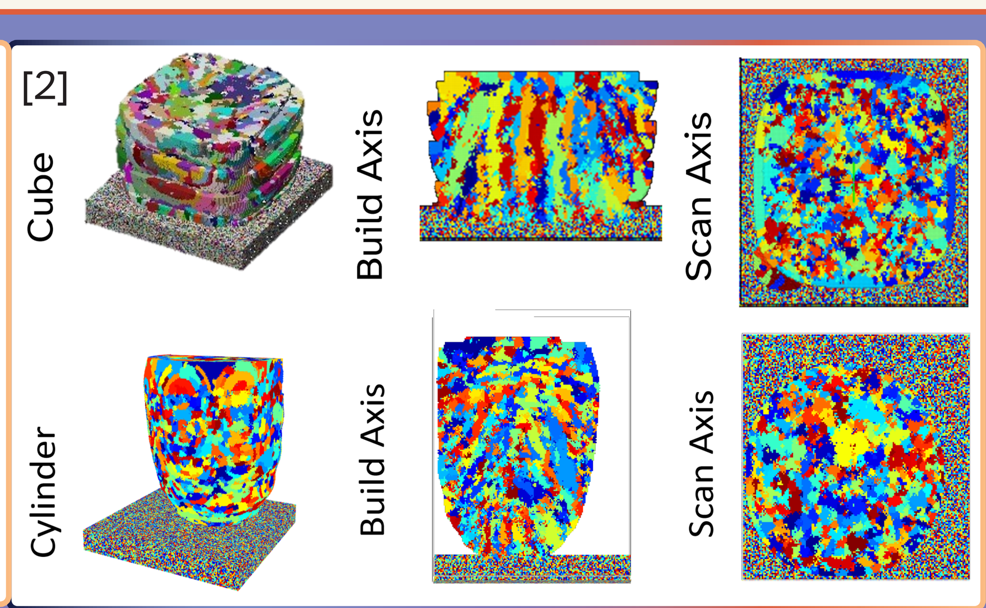
Develop a decision framework for microstructural properties through simulation model to optimize build settings and achieve desirable microstructural properties.

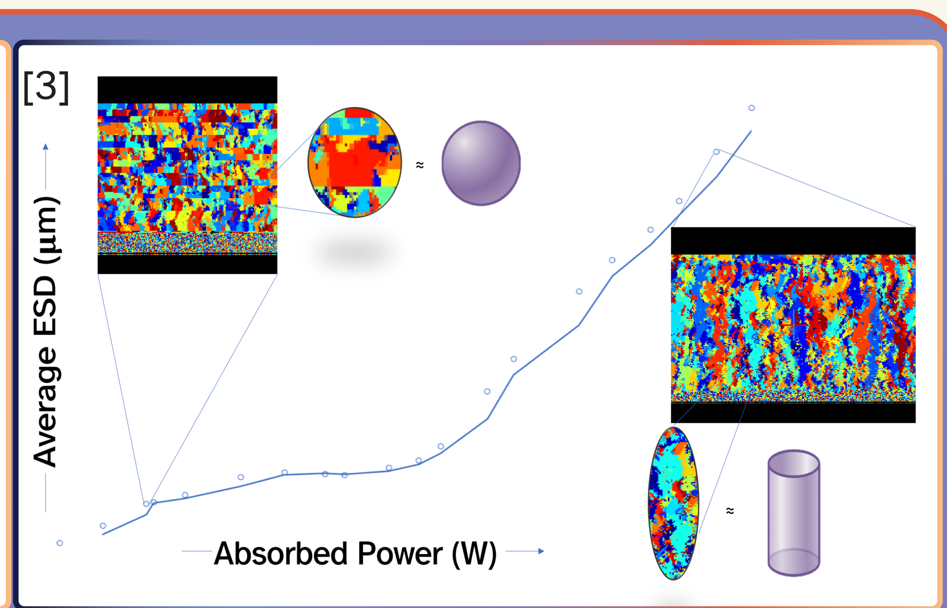
Methods of Simulation

- kinetic Monte-Carlo (kMC) simulations were performed with the Stochastic Parallel PARticle Simulator (**SPPARKS**) Thermal package, with simulations being 250x150x120 voxels and each voxel being 125 μm^3 for a total domain size of 0.5625 mm^3.
- Post-processing in Python calculated: (i) the average equivalent spherical diameter (ESD), where ESD is the diameter of a sphere equal to the volume of the grain. (ii) the average grain eccentricity where each grain eccentricity is defined by unity minus the ratio between the longest and shortest axis.

Fig 1 (left) SPPARKS geometires were developed through .stl files which are converted into slic3r files. This produces gcode which is then modified to create SPPARKS geometires.
Fig 2 (middle) Cube and cylinder geometries were used to observe grain size. The cube was chosen for it's simple geometry and the cylinder was chosen as it showcased high eccentricity grains that were much less prevalent within the cube geometry. Isometric, build axis, and laser scan axis are shown for both geometries.
Fig 3 (right) Sensitivity analyses, optimizations, and process parameter scans were done over the full experimental conduction mode range. The line plots the trend of laser power and it's relation to grain size over the simulation range.

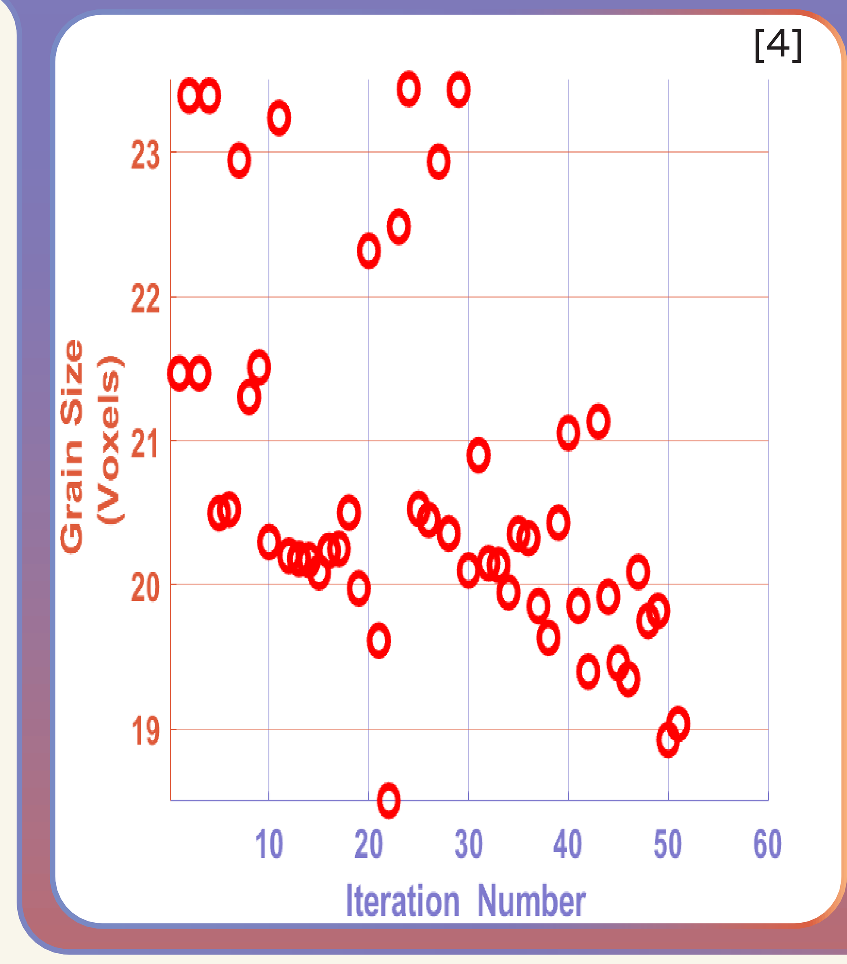


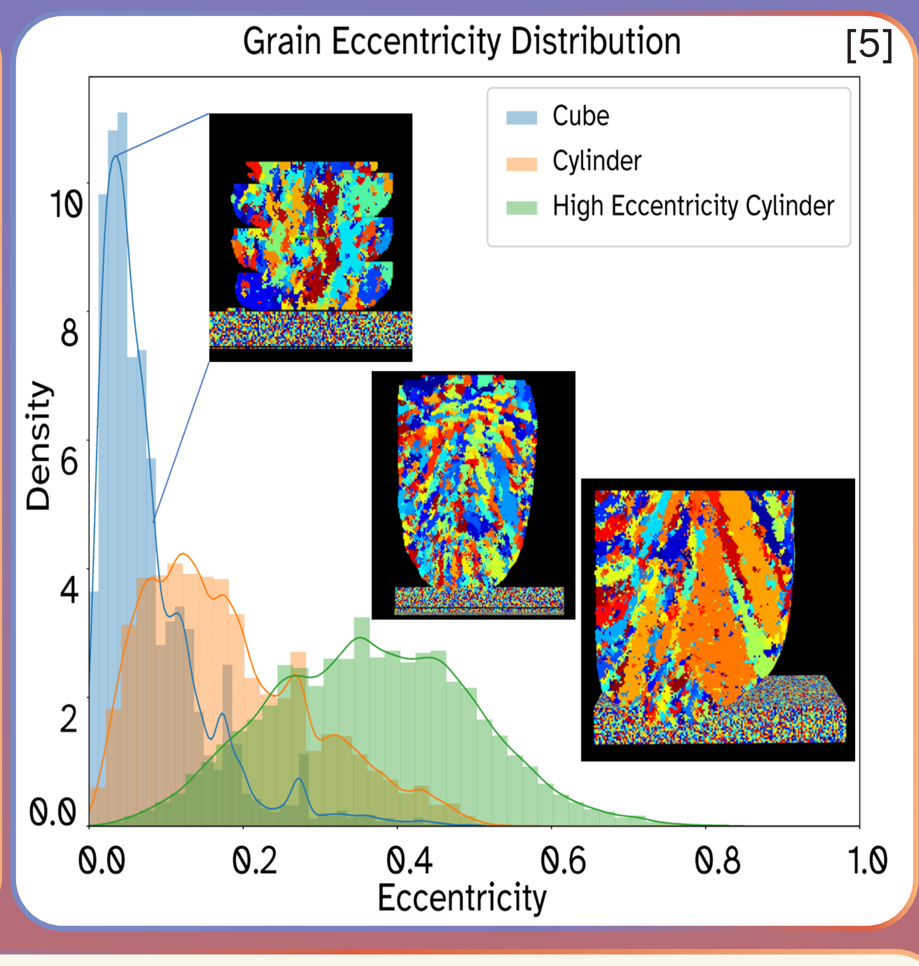




Optimization & Control

Using Dakota, simulations are processed in parallel with a multi-objective DIviding RECTangles (DIRECT) optimization method. Objectives were grain size, eccentricity, and accuracy to original geometry. Future work will be focused on controlling mechanical properties for a material such as minimizing the stress distribution.





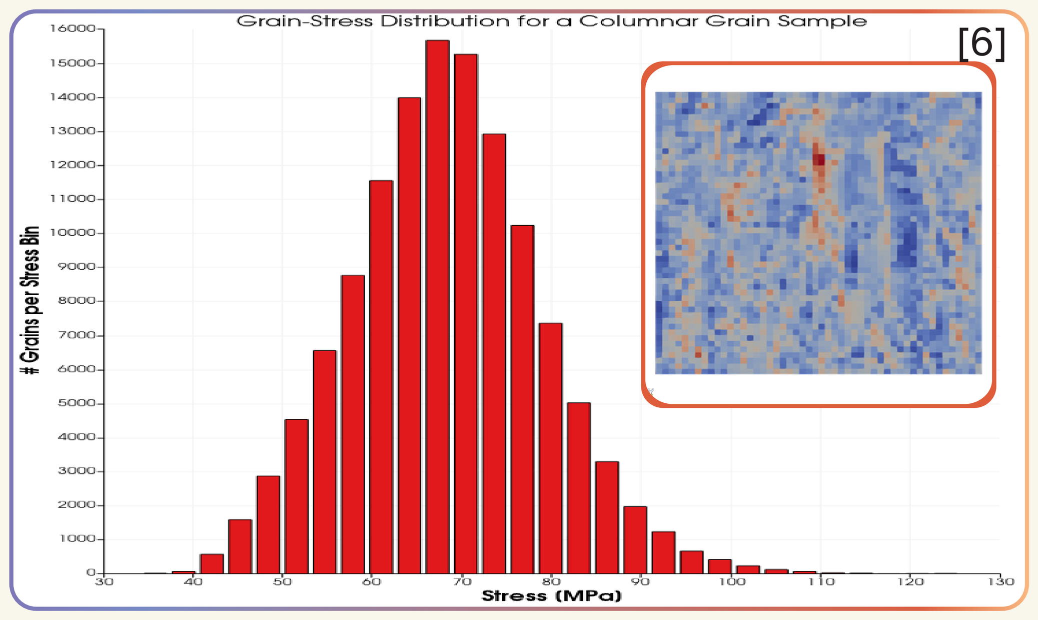
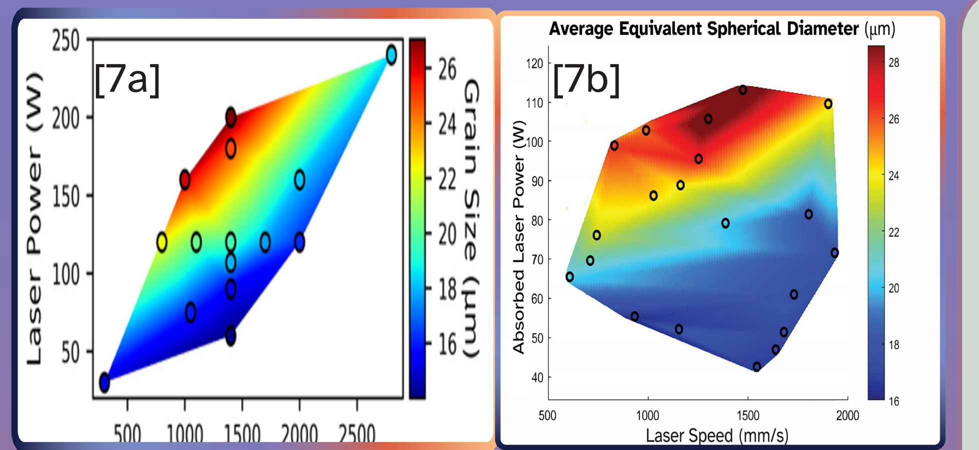


Fig 4 (above left) The average grain size based on equivalent spherical diameter (ESD) is plotted in relation to the iteration count for the simulation set. 51 simulations took place, with the minimum occuring spuriously at the 18th iteration. The optimization framework rapidly converges after the 30th iteration.
Fig 5 (above right) Eccentricity histograms and KDE plots for a cube, cylinder, and a cylinder with maximized eccentricity using the optimization framework. The eccentricity of a cube sets a reference for both cylinders, and it is observed that between the two cylinders, the optimized cylinder with a maximal eccentricity has a 72% larger average eccentricity and a more even proportion of high eccentricity grains to low eccentricity grains than the original cylinder simulated.
Fig 6 (left) Crystal Plasticity simulation performed using Sierra Mechanics can predict mechanical properties of a simulated grain structure that would not be present in a continuum setting. A 50x50x50 voxel columnar grain sample illustrates a stress distribution with a maximum stress (126 MPa) nearly twice that of the homogeneous stress (69 MPa).

Sensitivity Analysis

Latin Hypercube studies were performed for laser power, scan speed, and the wait time between hatches. Studies showed that laser power and laser speed had the most effect on microstructural properties such as grain size and grain eccentricity.



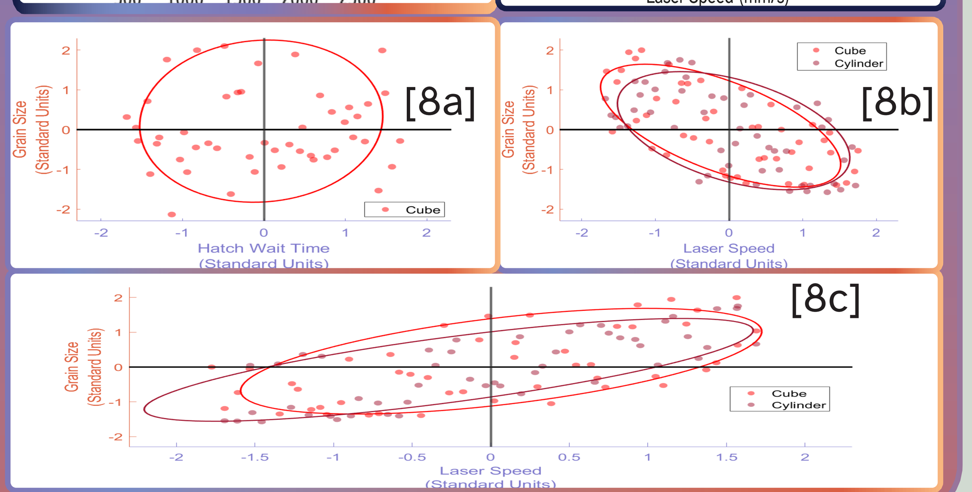
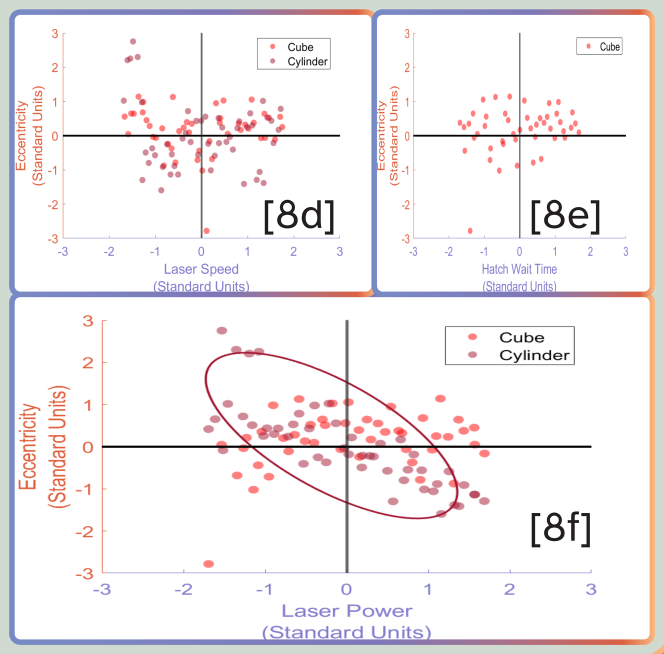


Fig 7 (above) a) Experimental data from M.J. Heiden et. al. (2022) illustrating how grain size is affected by laser power and laser speed. **b)** Comparison from a Latin Hypercube Study of 25 simulations. The simulated model displays similar trends to the experimental model for how grain size is affected by both laser power and laser speed.
Fig 8 (below,right) Sensitivity scatter plots show that: **a,e)** Hatch wait time does not affect grain size or eccentricity. **b,f)** Laser speed inversely correlates with grain size and eccentricity for a cylindrical geometry. However, for a cube geometry, grain size is inversely correlated. **c,d)** Laser power only directly correlates to grain size for both geometries.



Acknowledgements

The authors would like to thank the Sandia National Labratories for supporting and funding this research. As well, Tony Megofna and Al Davis for their continued support throughout the research.

Conclusion

A parallel multi-software framework using kMC simulations was developed for the optimization, control, and modeling of microstructure in 316L Stainless Steel. Sensitivity analysis shows that laser power has a strong positive and no correlation to grain size and eccentricity respectively. Laser speed shows a strong negative and no correlation. Wait time shows no strong correlations. The minimization of grain size converged to a process parameter set that resulted in a grain size 25% smaller than that of the starting process parameters. The maximization of eccentricity converged to a parameter set with a mean eccentricity 72% larger than that of the starting process parmaeters.

References

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