SAND2017-7407C

*Exceptional service in the national interest*

Sandia National Laboratories

# Direct Numerical Simulations of Microstructure Effects during High-Rate Loading of Thermally Sprayed Ta

Corbett Battaile, Nathan Moore, and Steve Owen

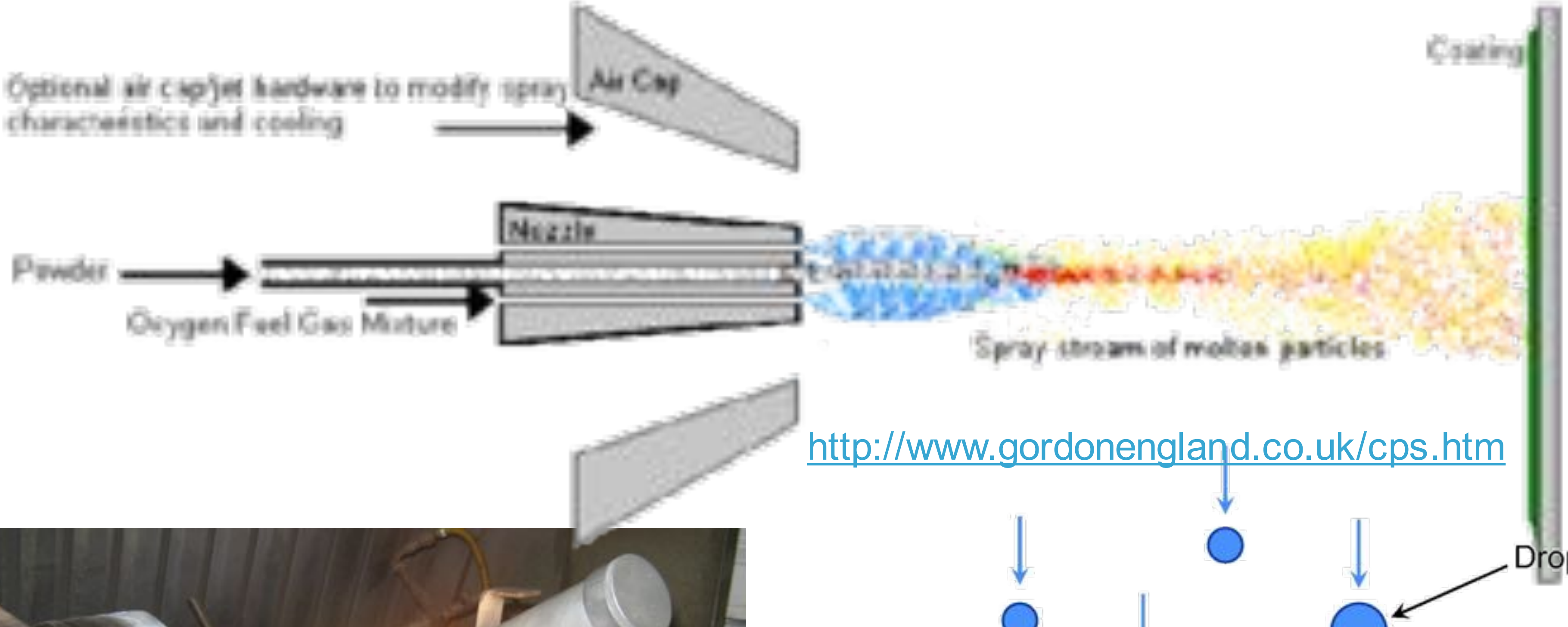
20th APS Conference on Shock Compression of Condensed Matter
Monday July 10, 2017

U.S. DEPARTMENT OF ENERGY  NNSA National Nuclear Security Administration  LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

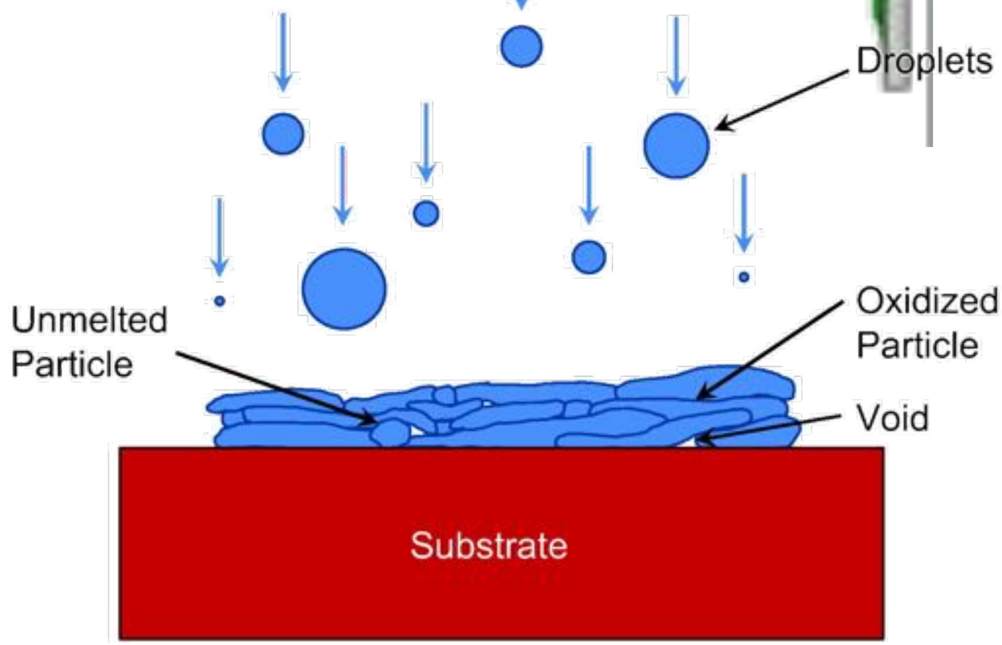
# The thermal spray process

Sandia National Laboratories



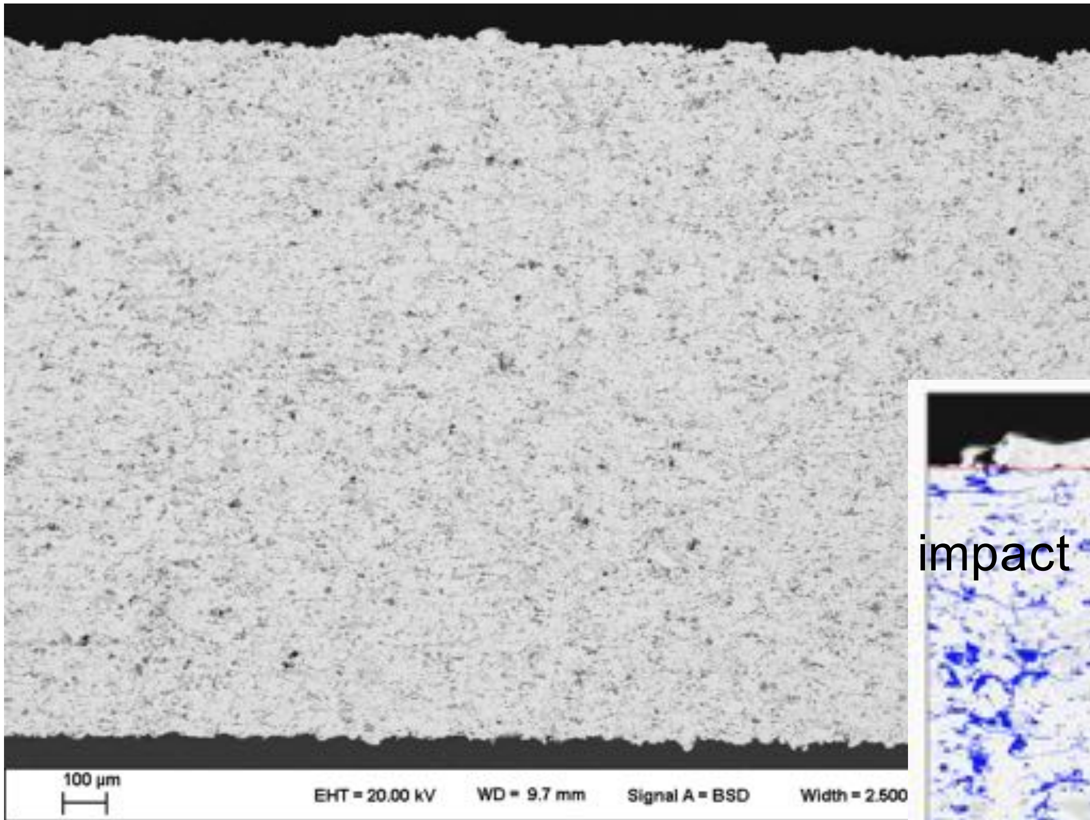

http://www.gordonengland.co.uk/cps.htm

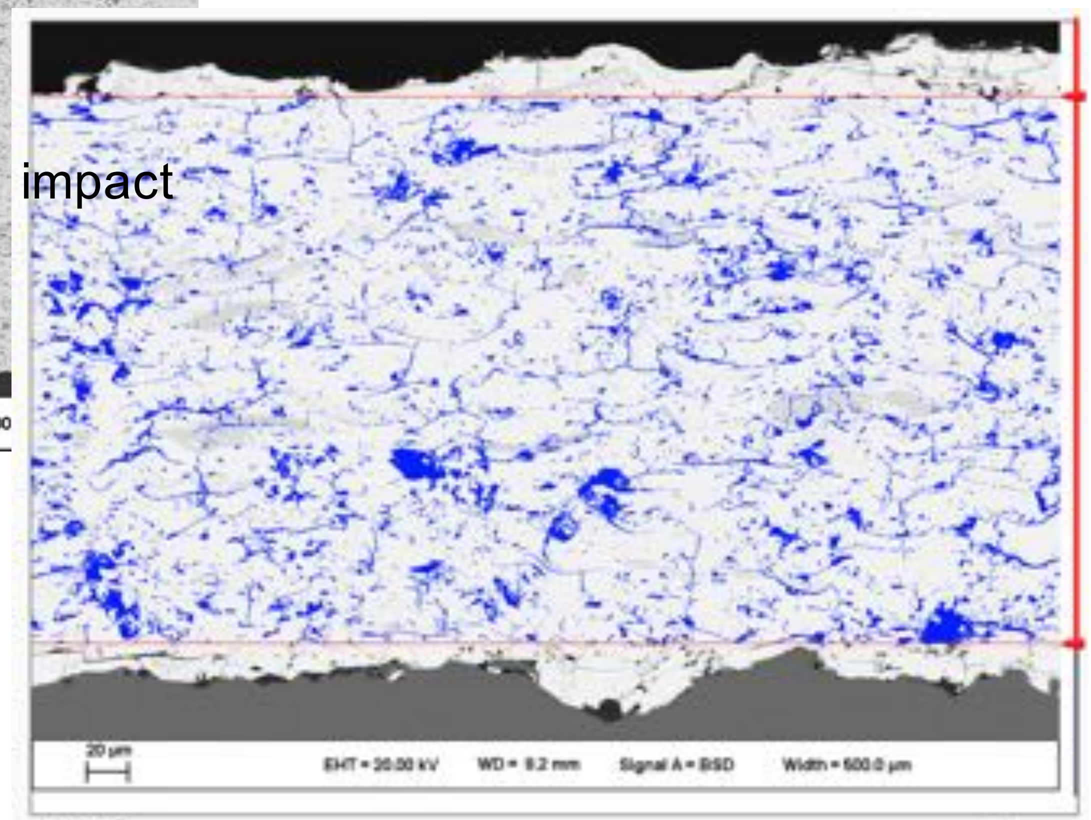
http://www.ust.com.au/thermal-spray.htm



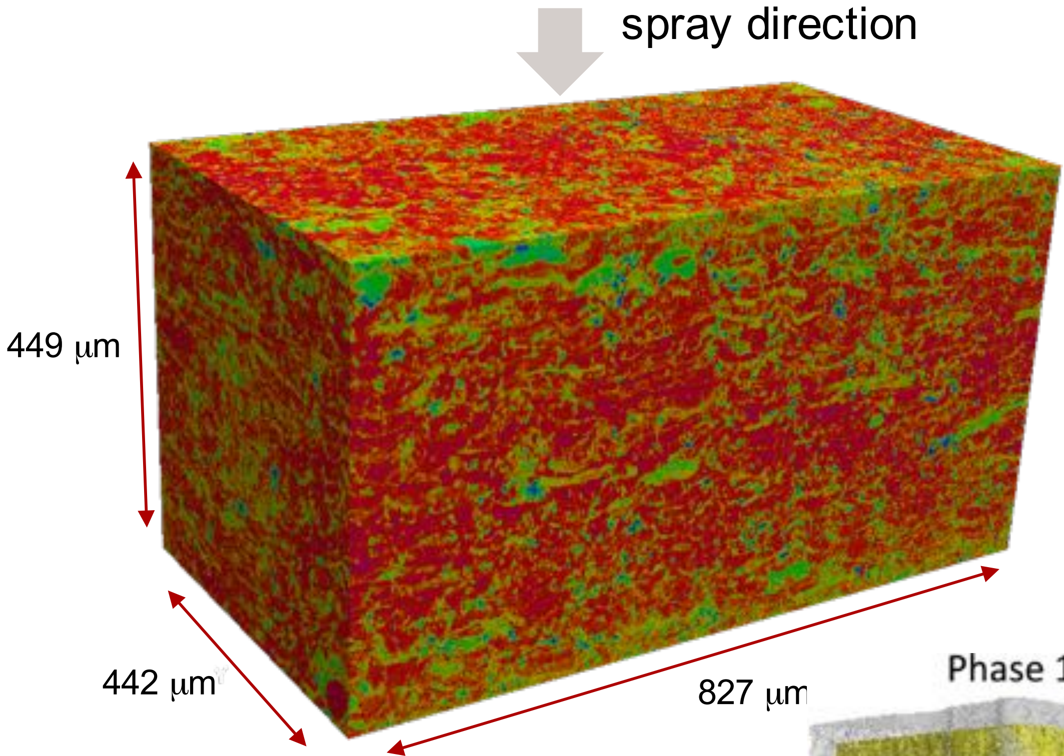

M.R.W. Brake et al, Surf. Coat. Tech. **310** (2017) 70.

# Sprayed materials are very complex



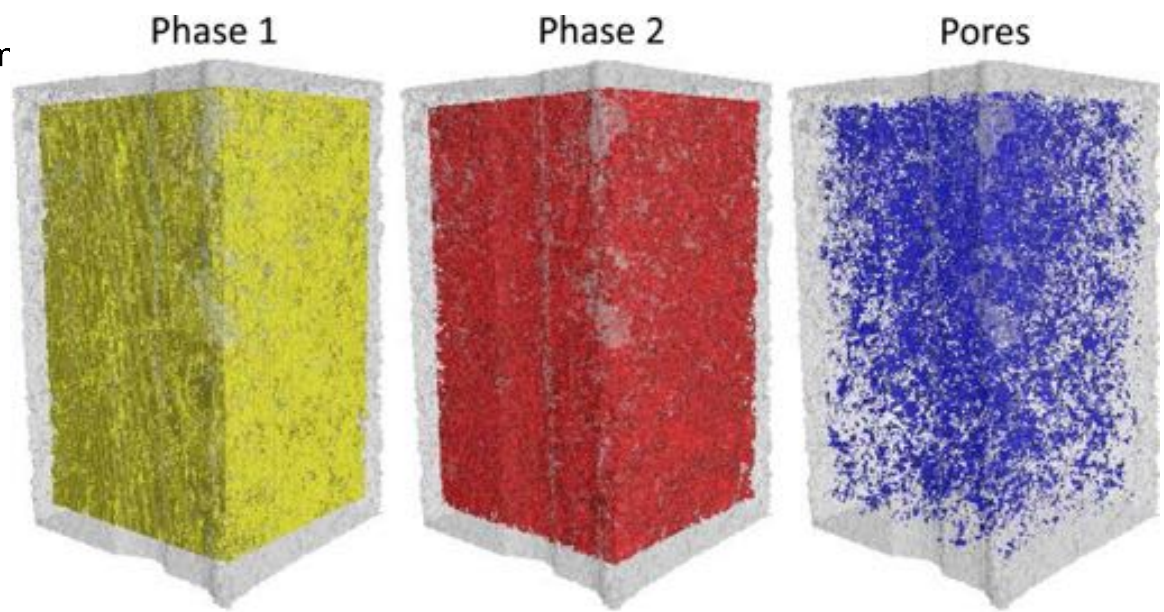



# Sprayed materials are very complex



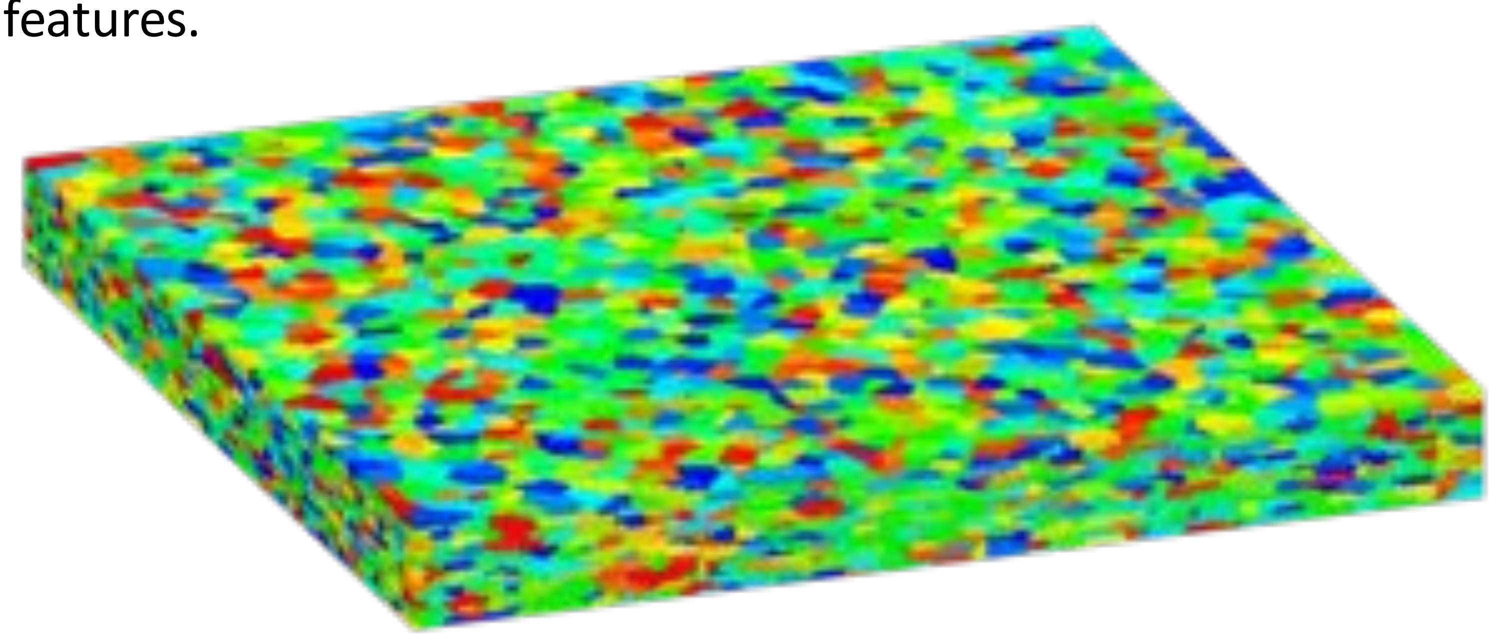

3D density map from x-ray tomography (Advanced Photon Source, ANL) at ~0.8-µm resolution performed on rectangular specimens cut from a second batch of material produced with the same spray conditions. A subset of the data is shown for clarity.

Ta (1) and Ta-oxide (2) phases are distinguished from pores.



# Microstructure creation

- Porous microstructures were created using a simple space-filling algorithm.
  - Place “seeds” at the centroid of each splat to achieve desired average feature size.
  - Grow seeds radially until all space is filled.
  - Bias the rates of growth in each direction to achieve elongated features.

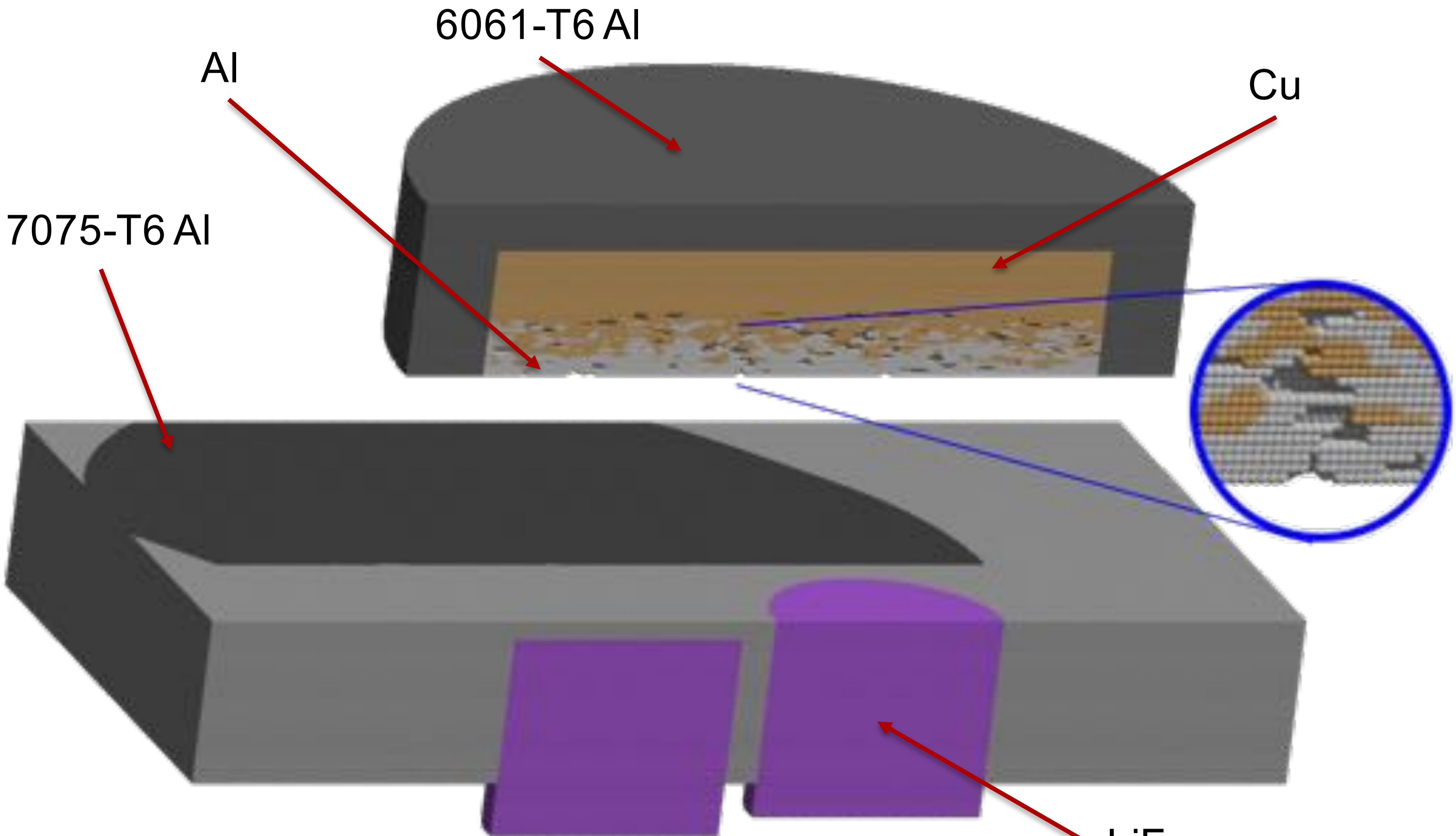


  - Remove some fraction of splats to achieve desired porosity (10%).

# Flyer simulation geometry creation

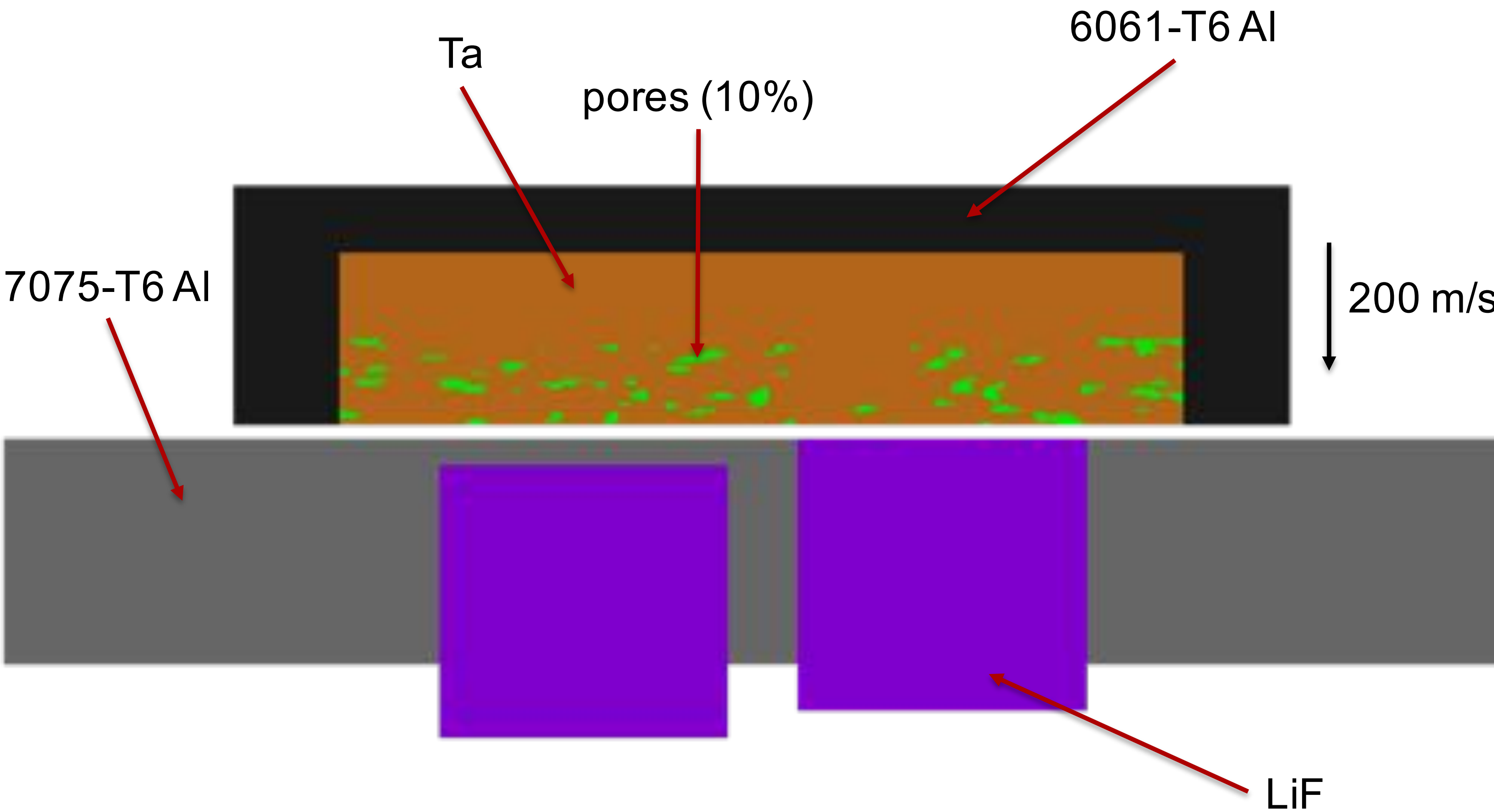
- The corners of the microstructure model are cut off to create a disc of porous “material.”
- The disc is enclosed on two of the three sides (“top” and circumference) by another material.
- On the opposing (“bottom”) side, a target plate (rectangular in cross-section) with one buffered and one unbuffered window material (cylindrical in shape) is inserted into the domain.
- The voxel domain is converted into a finite element model that has cubic elements.

# Graded AlCu flyer model

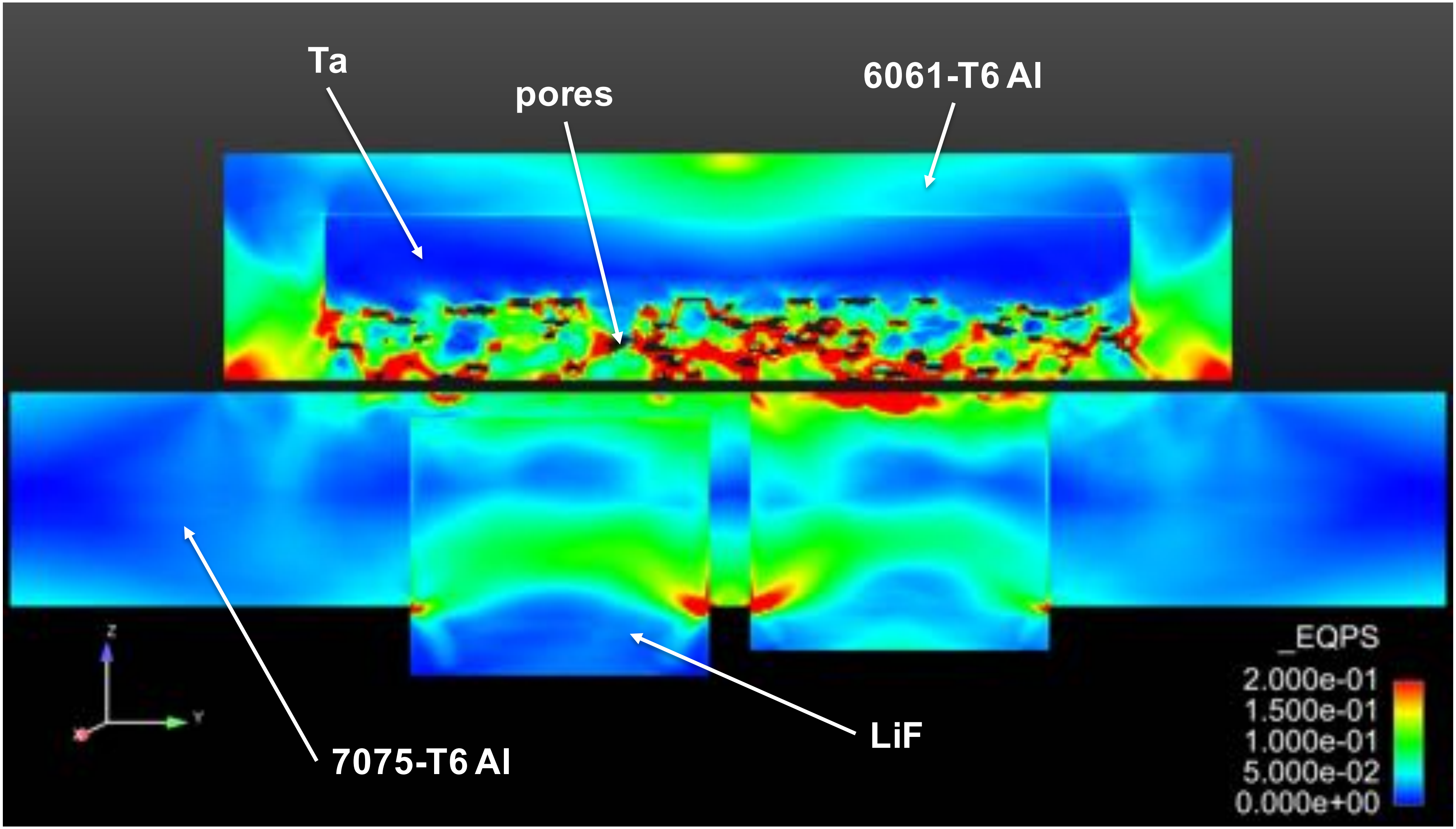



~ 20M finite elements

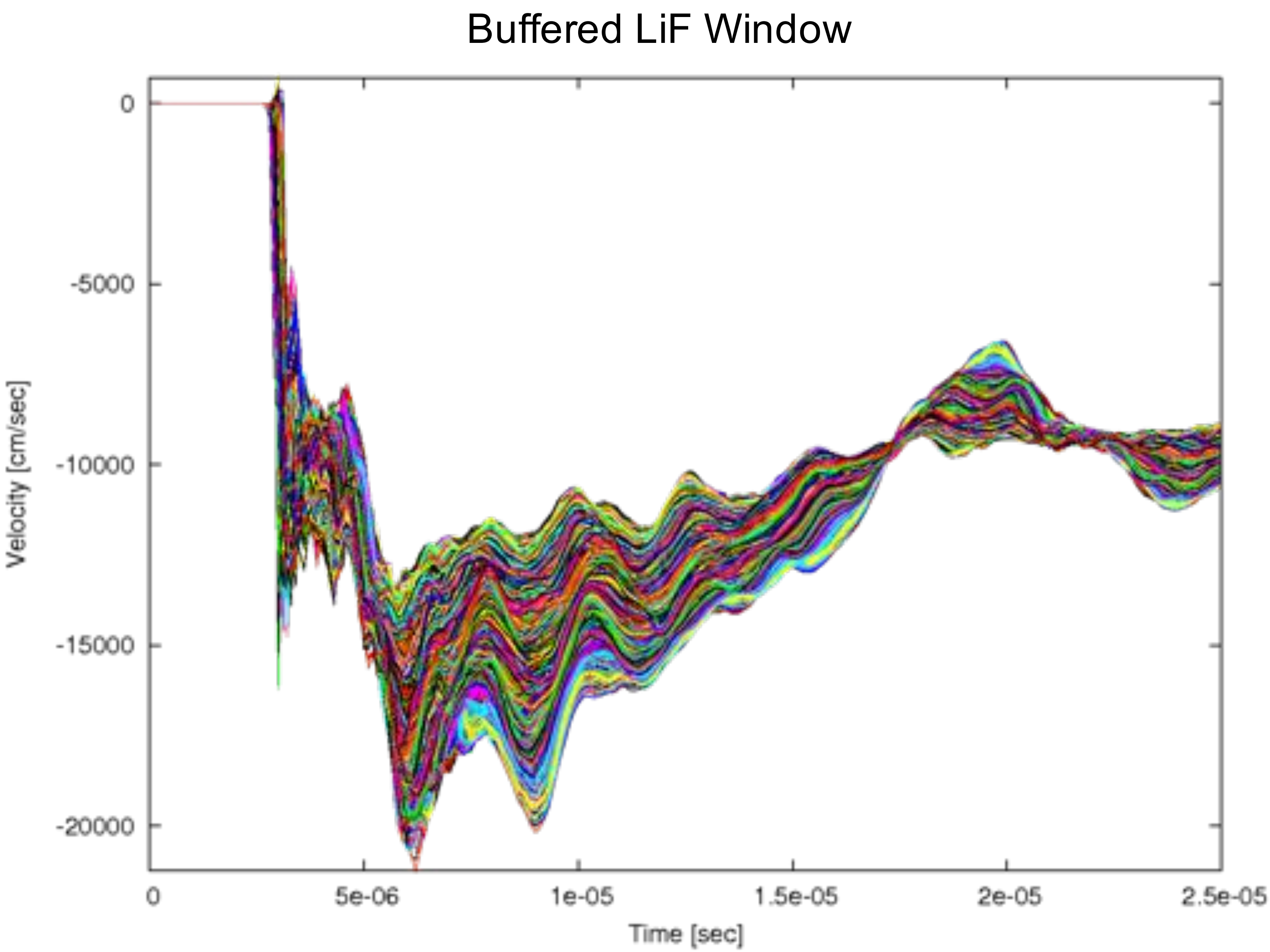
# Cross-section of Ta flyer model



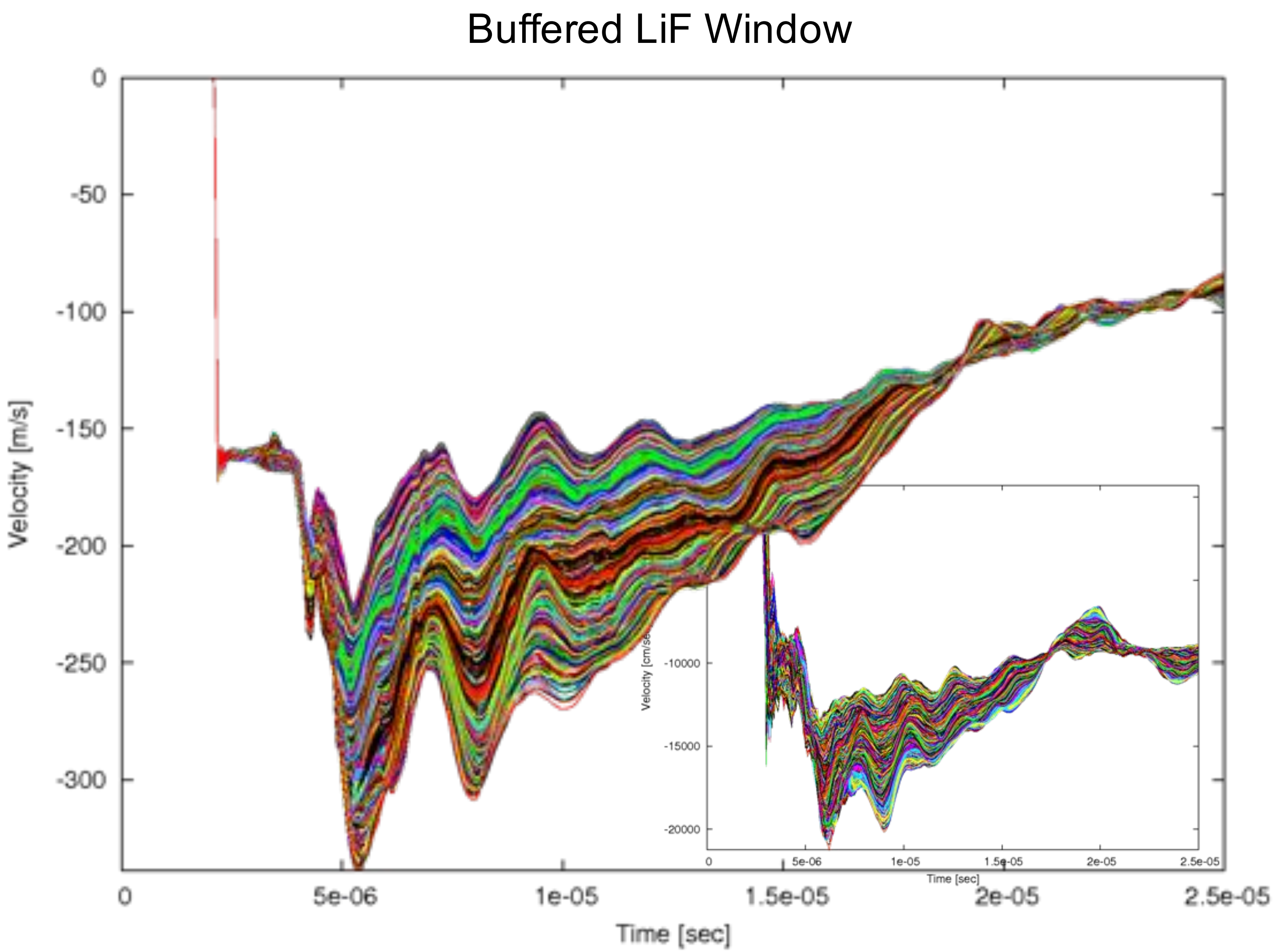
# Plastic strain in Ta w/ 10% pores



# Simulated VISAR in Ta w/ 10% pores

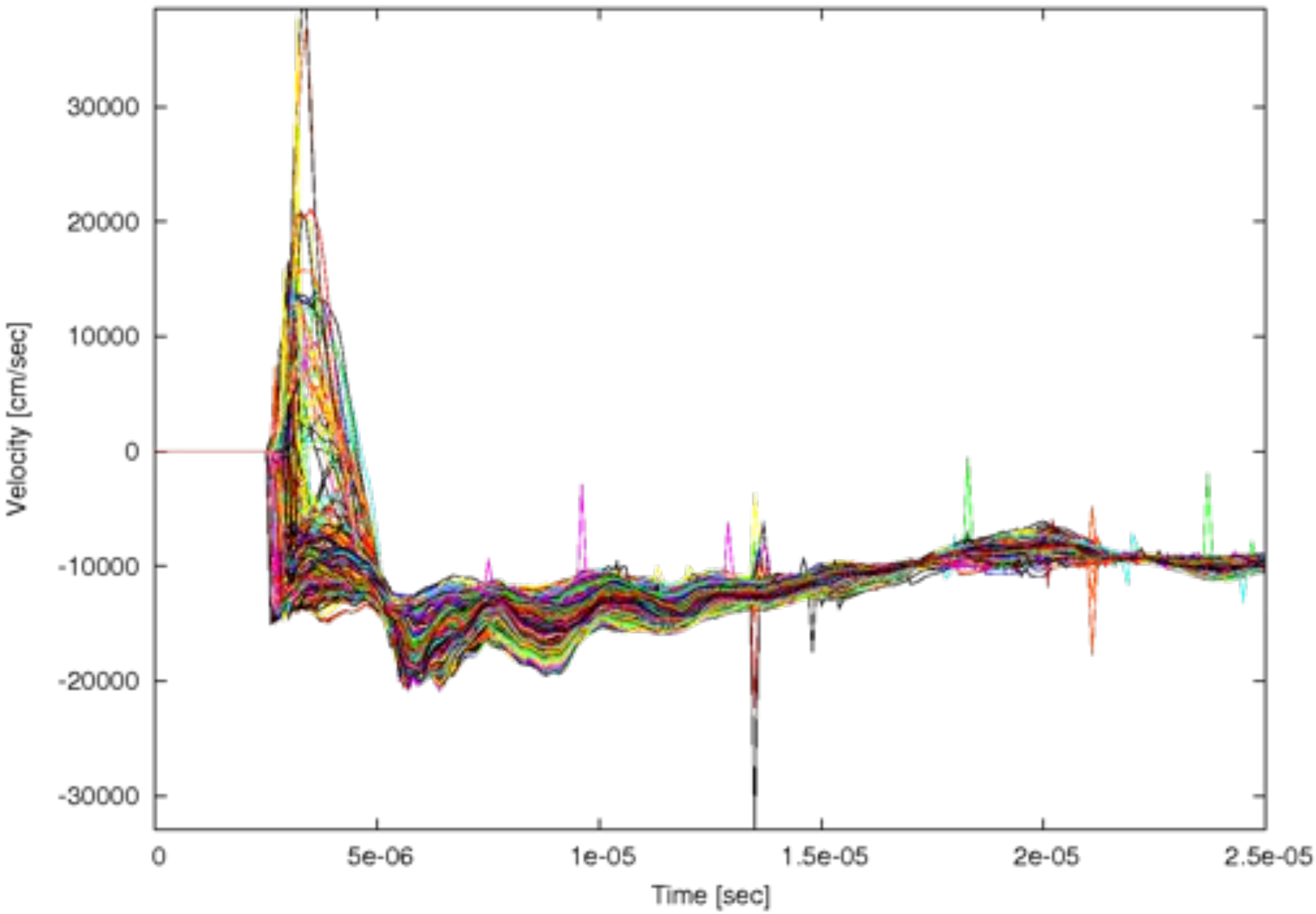


# Simulated VISAR in Ta w/ no pores

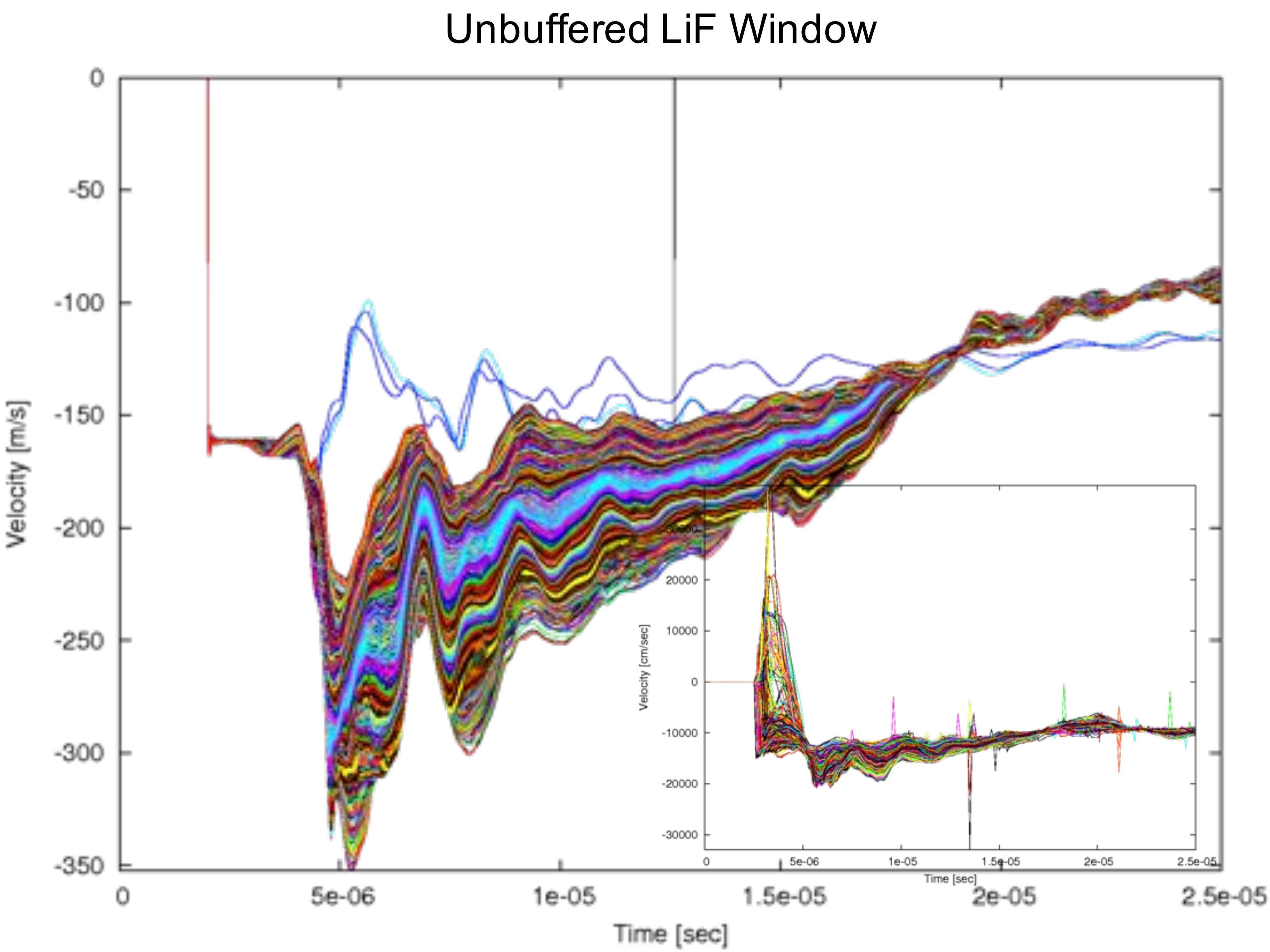


# Simulated VISAR in Ta w/ 10% pores

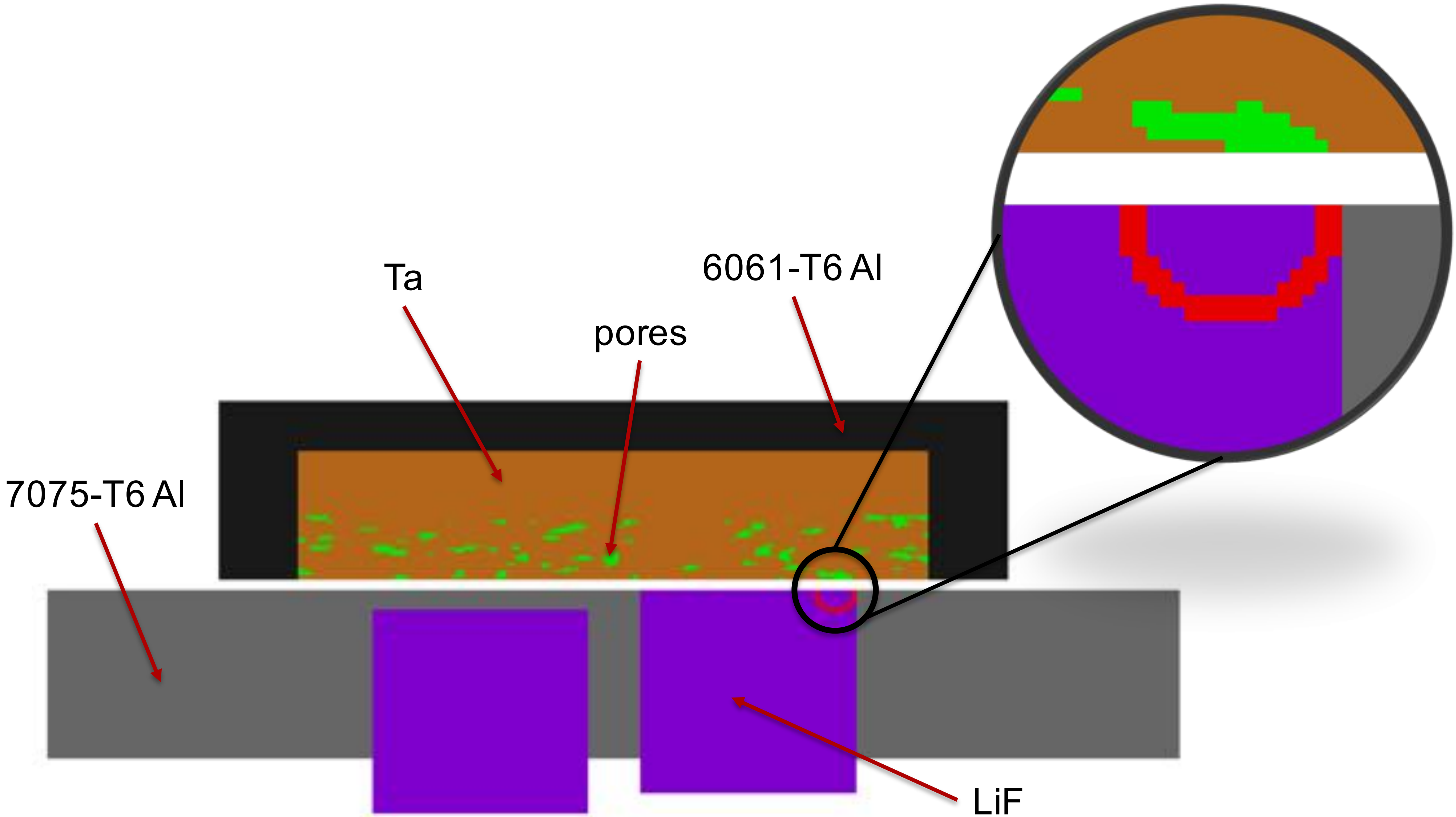
Unbuffered LiF Window



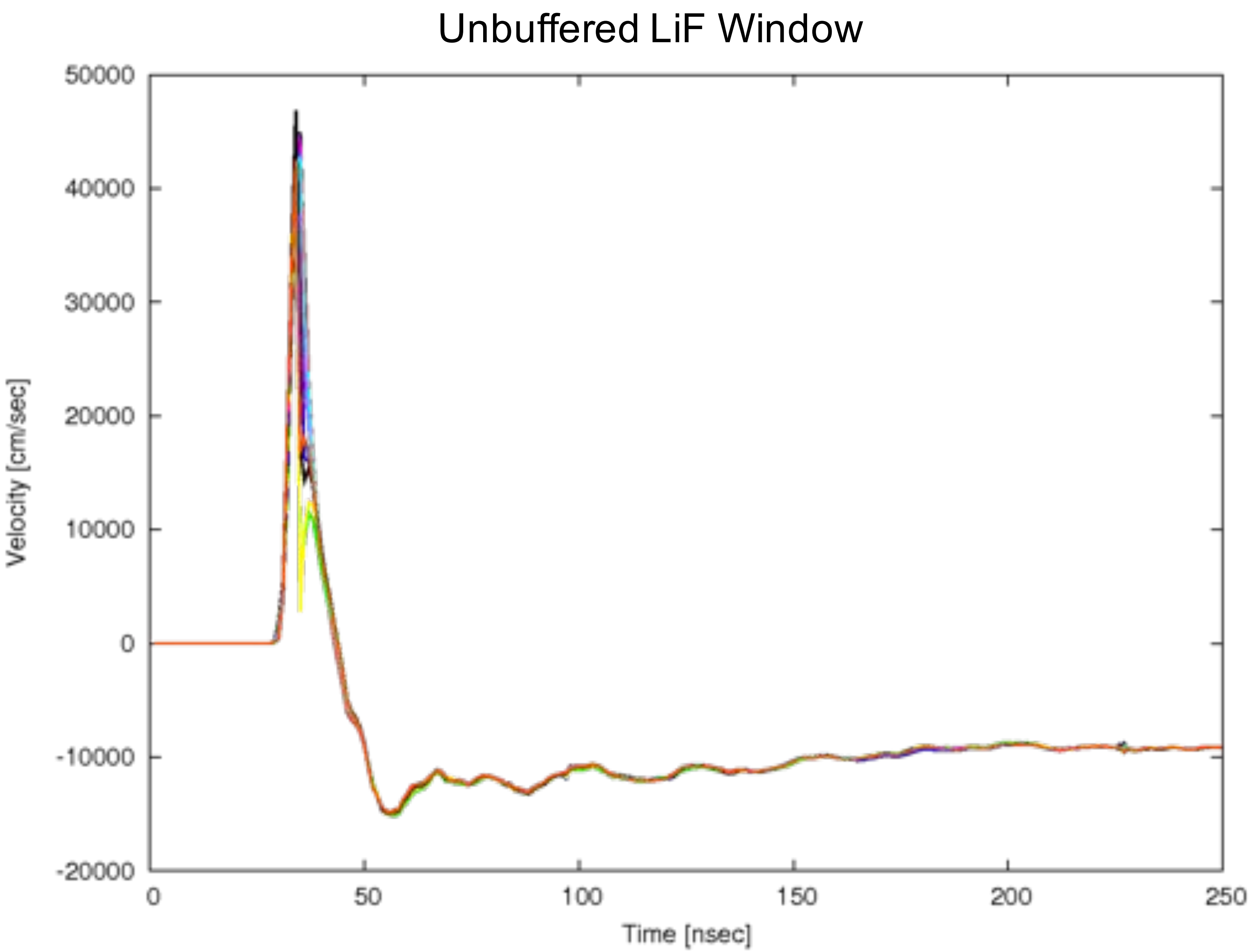
# Simulated VISAR in Ta w/ no pores



# Excursions arise at surface pores

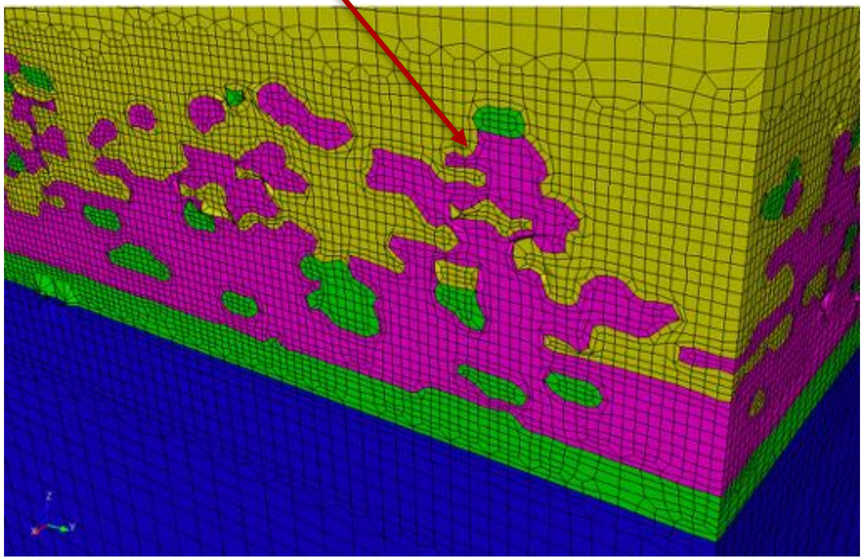


# Simulated VISAR near large pore



# Toward conformal interfaces …

Conformal ("smooth") Interfaces



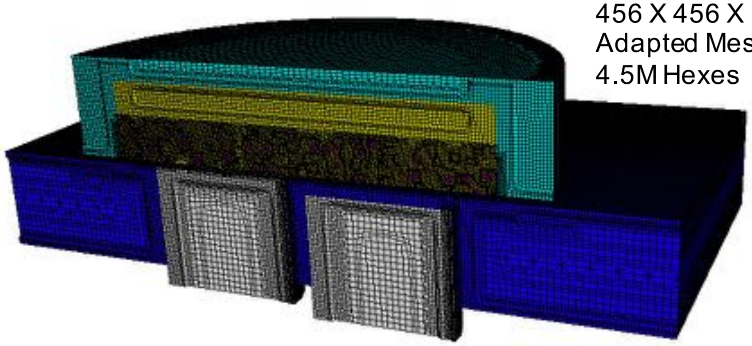
## Mesh Generation for Microstructures

Capabilities

- Parallel Conformal All-hex with Sculpt
- Dense Cartesian grid input
- Builds coarsened adaptive mesh from Cartesian data
  - Reduces element count by order of magnitude
- Filters microstructure mesh
  - removes non-manifold, small volumes, protrusions

Challenges

- Representing increased geometric complexity of microstructures with conformal hexes
- Robust Parallel Implementation
- Representing selected surfaces and interfaces (non-microstructures) with sharp features
- Plan B– build microstructure faceted model in Sculpt… Build tet mesh in Cubit



Initial Cartesian Grid
456 X 456 X 116 = 34.5M Hexes
Adapted Mesh w/Sculpt
4.5M Hexes

# Summary

- We have performed "direct numerical simulations" of flyer plate impact of thermally sprayed Ta. These simulations include a spatially explicit representation of porosity.
- Simulated velocimetry depends strongly on the details of the microstructure near the probe location.
- We are developing a conformal, hexahedral meshing capability to "smooth out" voxellated interfaces and eliminate the artifacts they can produce.