SAND2017-13370PE

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Predicting Micro-Scale Deformations During High-Rate Loading of (a Different Process for) Additively Manufactured Materials

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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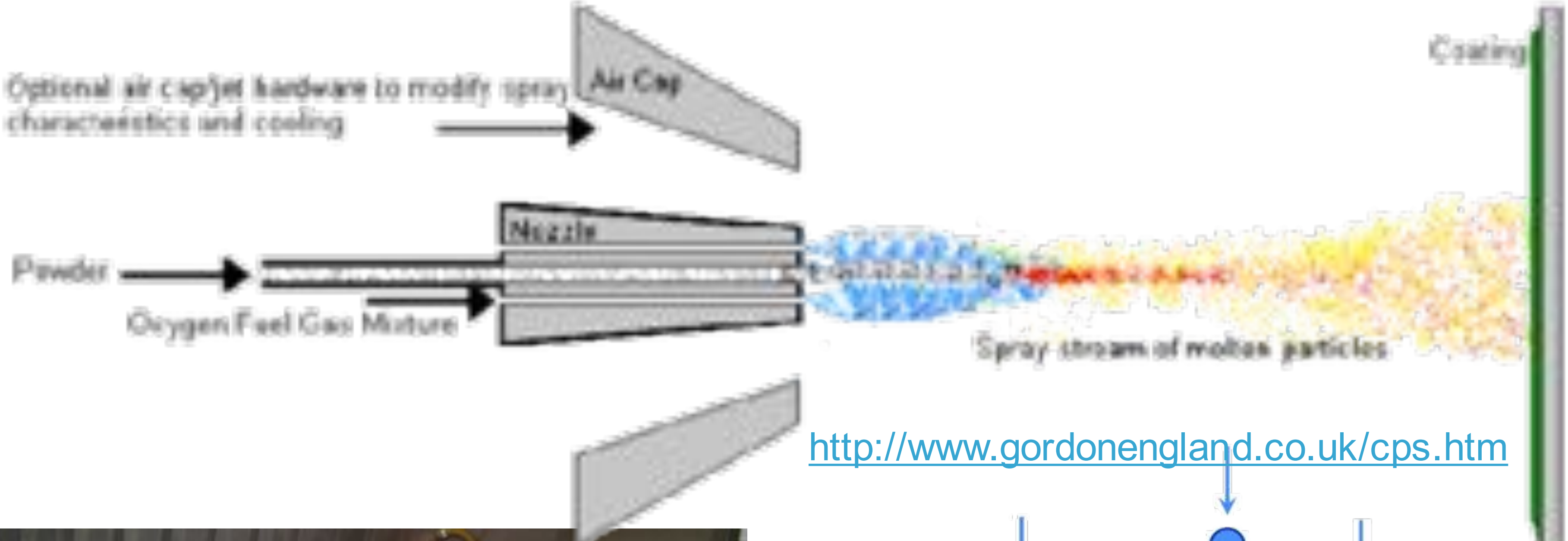
Introduction

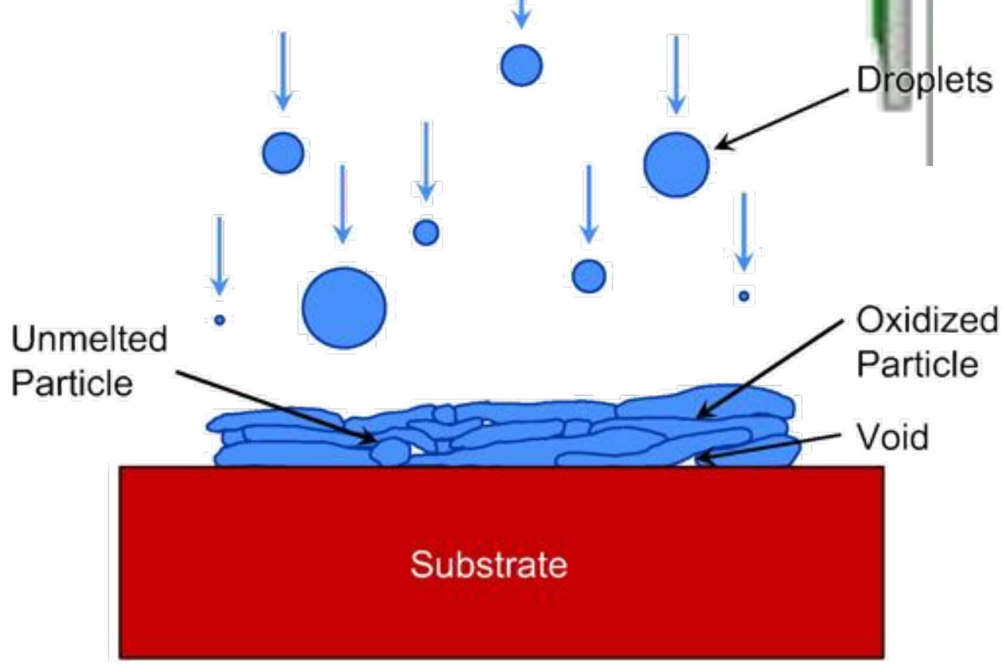
- To accomplish modeling- and simulation-assisted qualification and certification, and/or ICME, we need approaches for exploring the process-**structure-properties**-performance relationships.
- For the sake of variety, we'll take a look at a different (non-laser-based) additive technology: thermal spraying.
- We generally spray powders made of pure metals, and sometimes mixed multi-metal powders.
- Microstructural complexity and porosity defects are often desirable for the application requirements.
- The very same concepts presented here are being used to analyze high-rate properties of laser-based additive parts.

The thermal spray process

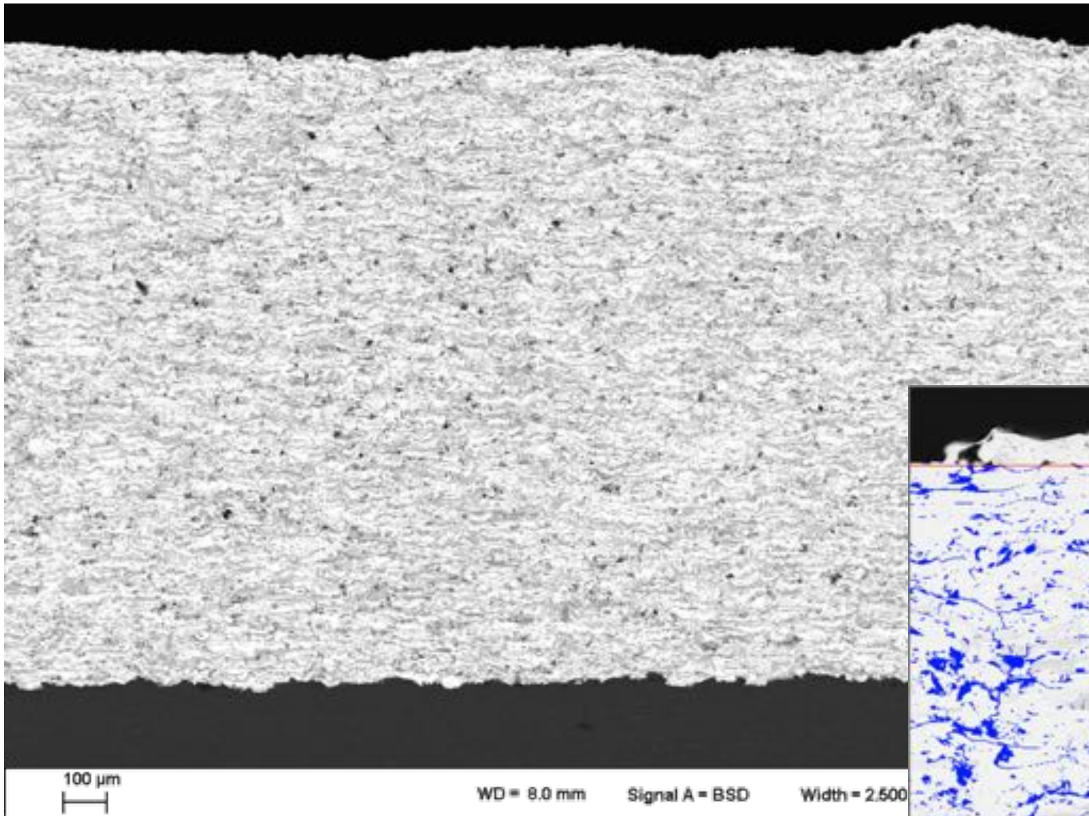


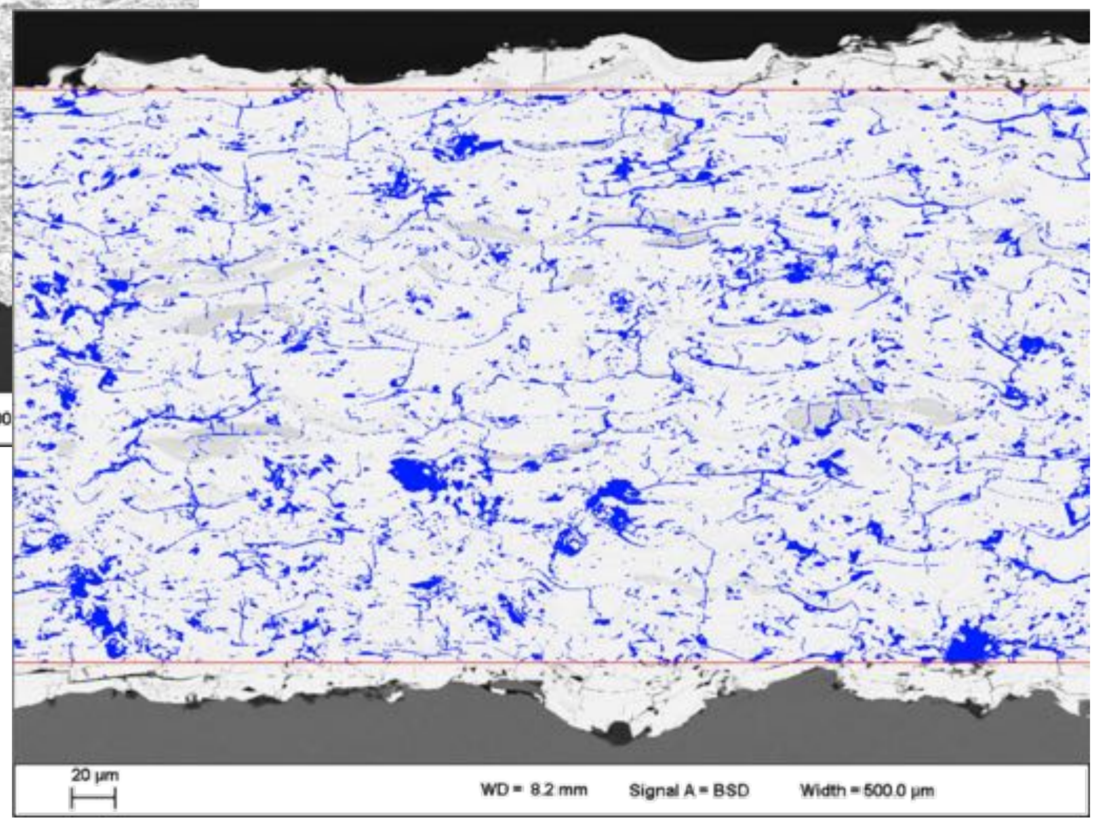
http://www.gordonengland.co.uk/cps.htm

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



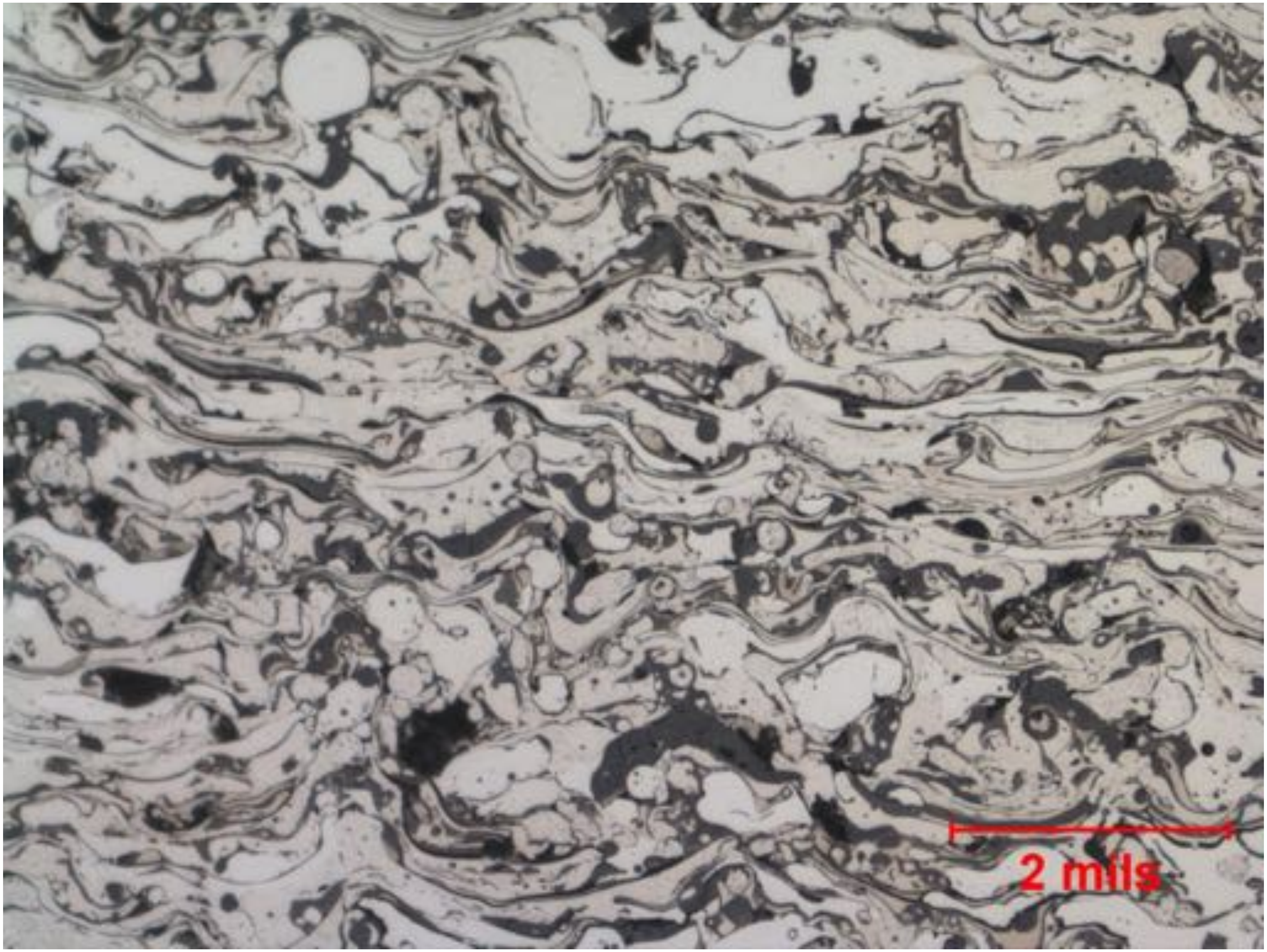
Sprayed materials are very complex



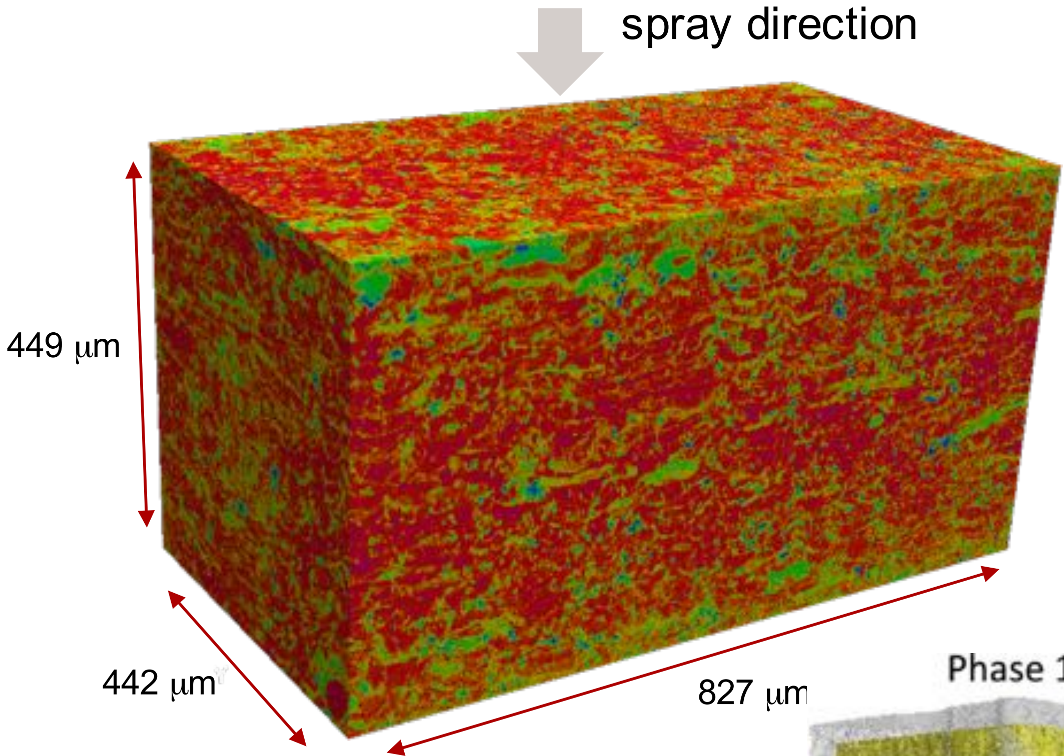


Tantalum

Sprayed materials are very complex

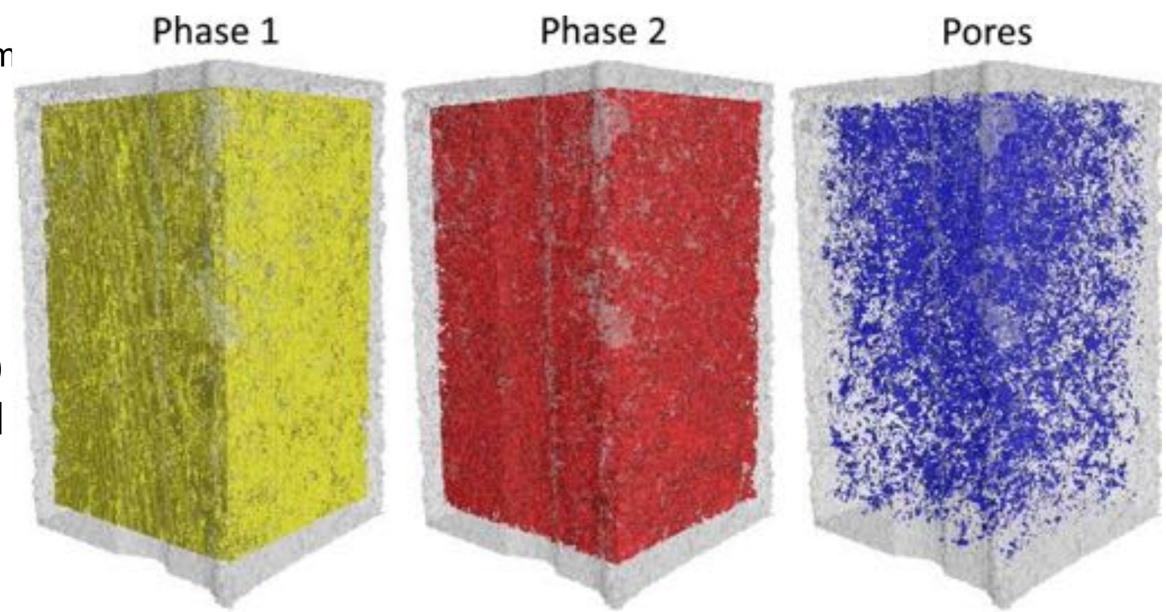


Sprayed materials are very complex



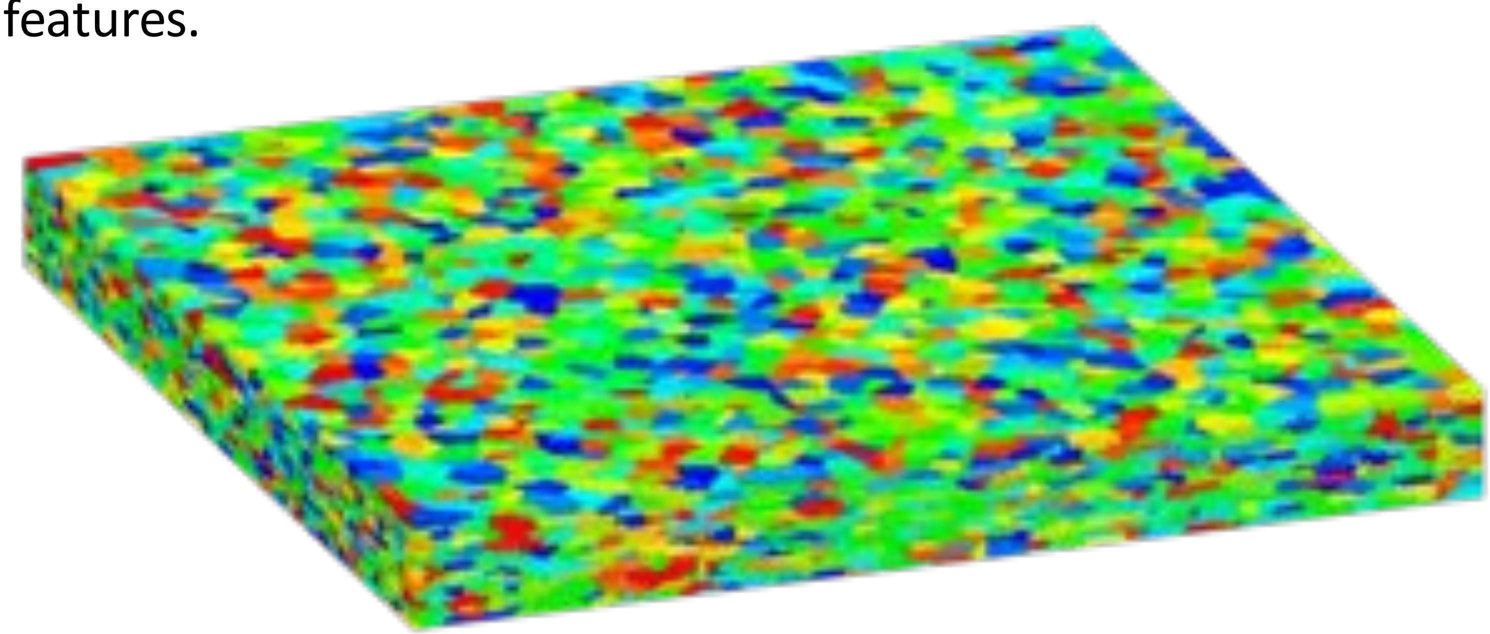
3D density map from x-ray tomography (Advanced Photon Source, ANL) at ~0.8-µm resolution performed on rectangular specimens cut from a second batch of material produced with the same spray conditions. A subset of the data is shown for clarity.

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



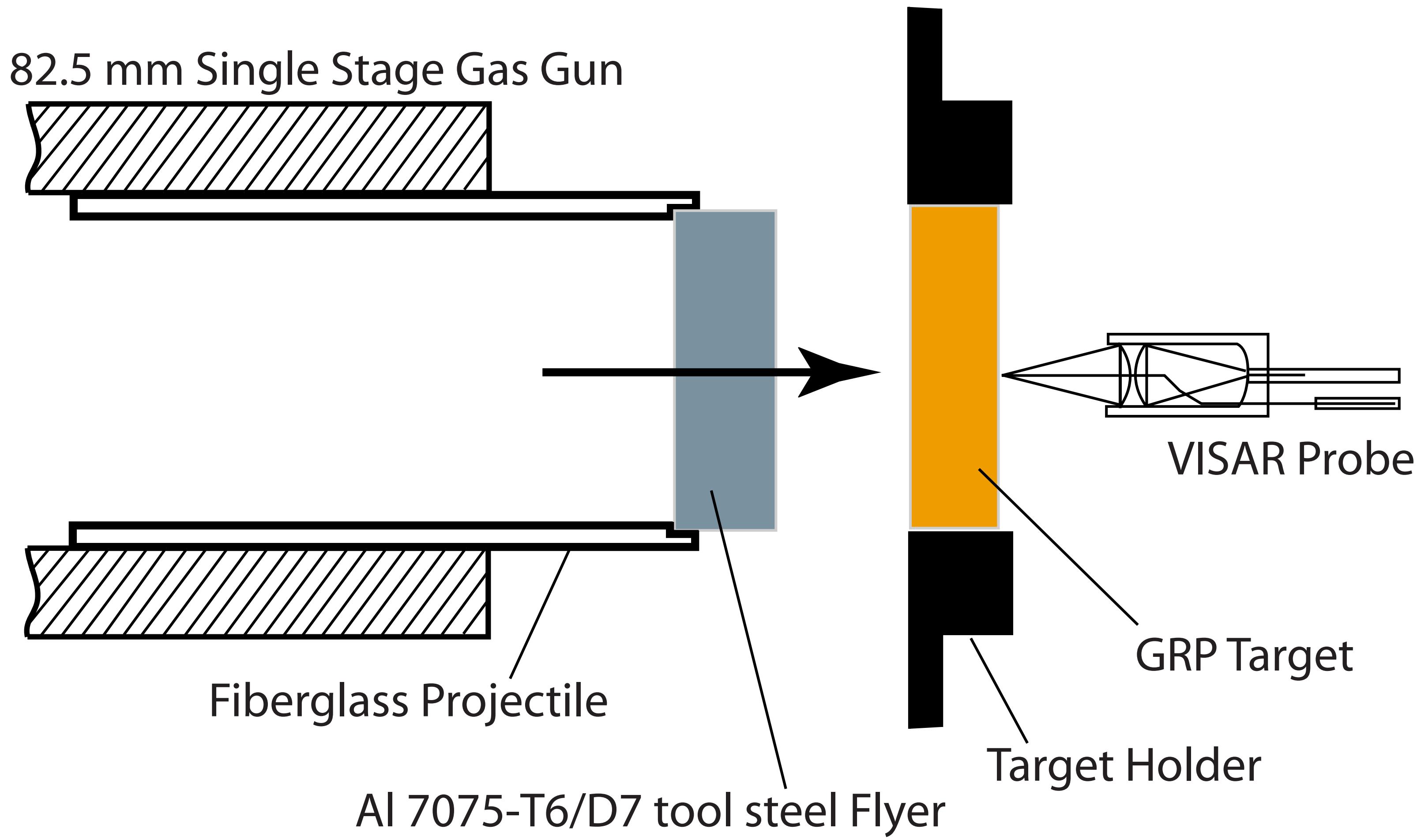
Microstructure creation

- 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 plate impact



L. Tsai, F. Yuan, V. Prakash, and D.P. Dandekar, *J. Appl. Phys.* **105** (2009) 093526.

Flyer simulation geometry creation

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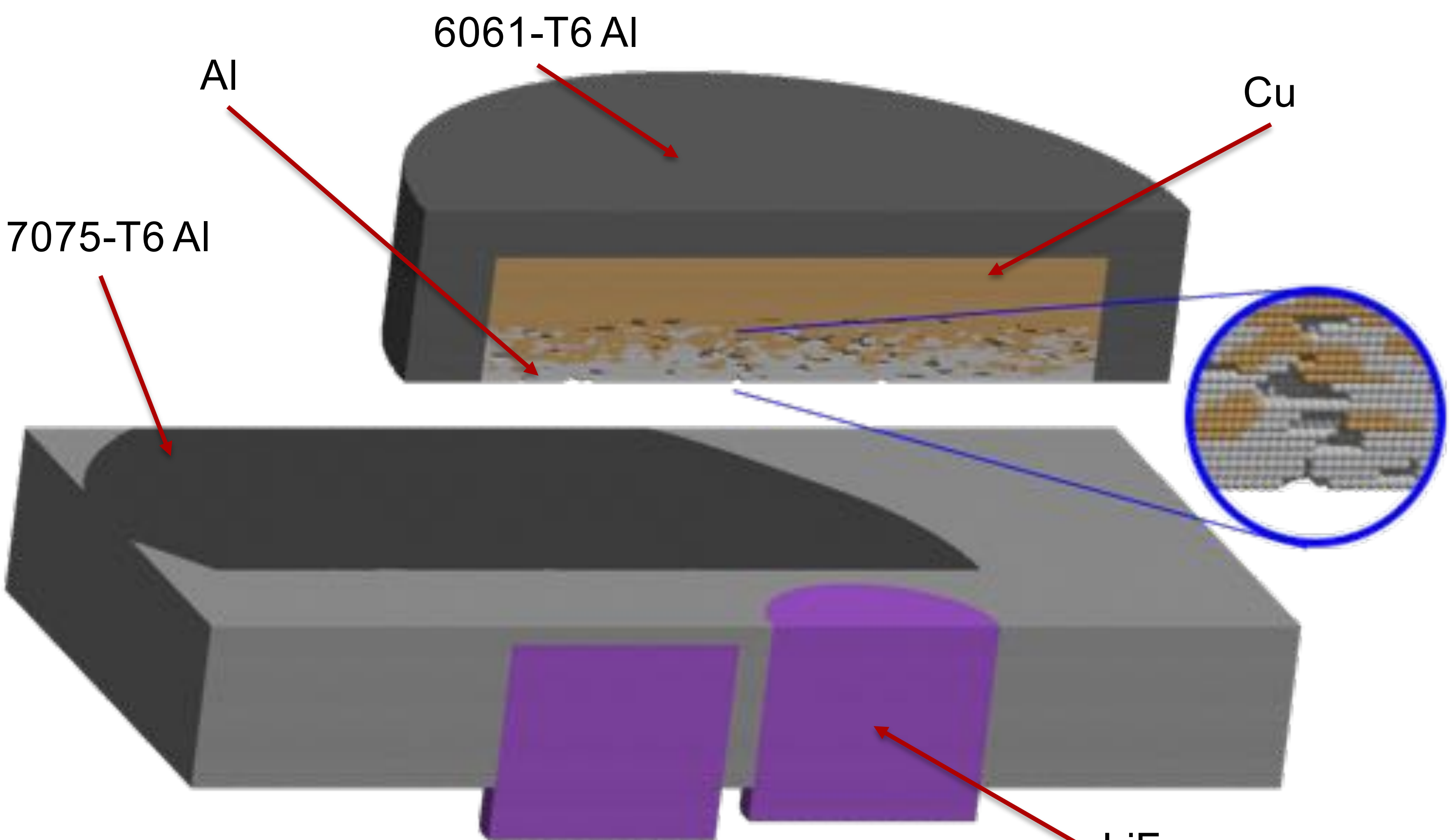
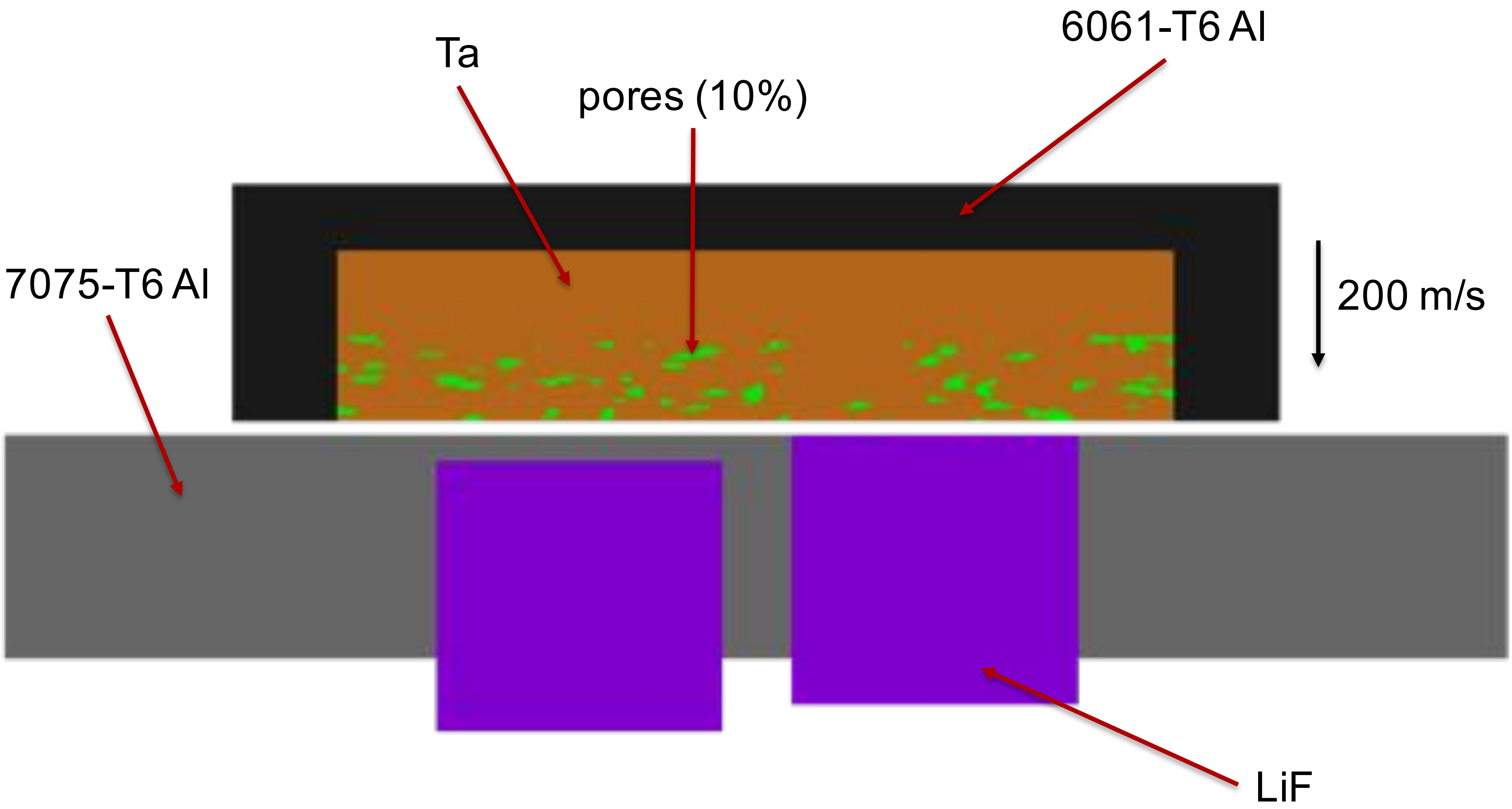
- The corners of the microstructure model are cut off to create a disc of porous “material.”
- The disc is enclosed on two of the three sides (“top” and circumference) by another material.
- On the opposing (“bottom”) side, a target plate (rectangular in cross-section) with one buffered and one unbuffered 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

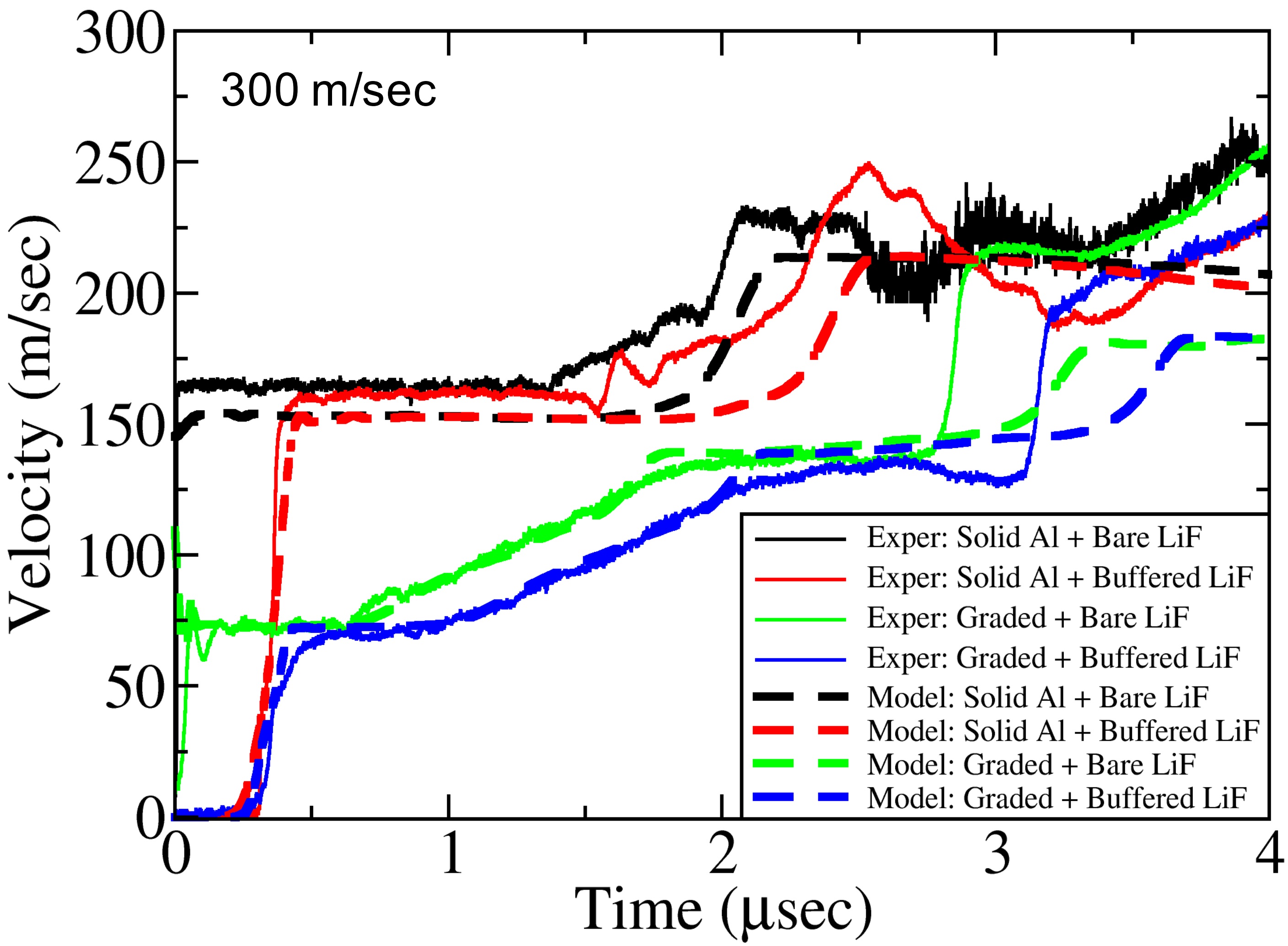


~ 20M finite elements

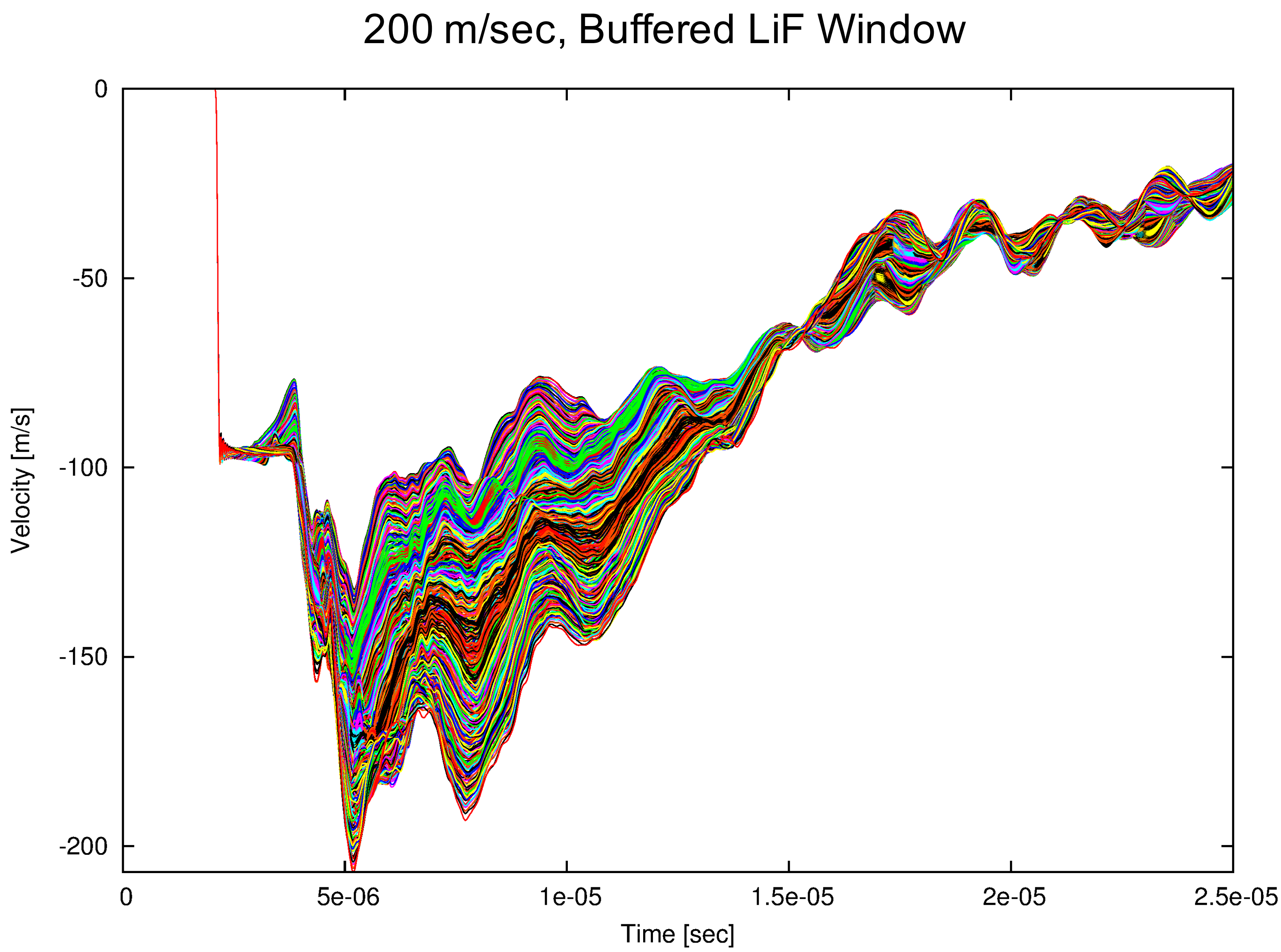
Cross-section of Ta flyer model



Validation VISAR on AlCu flyer plates



Simulated VISAR in Al w/ no pores



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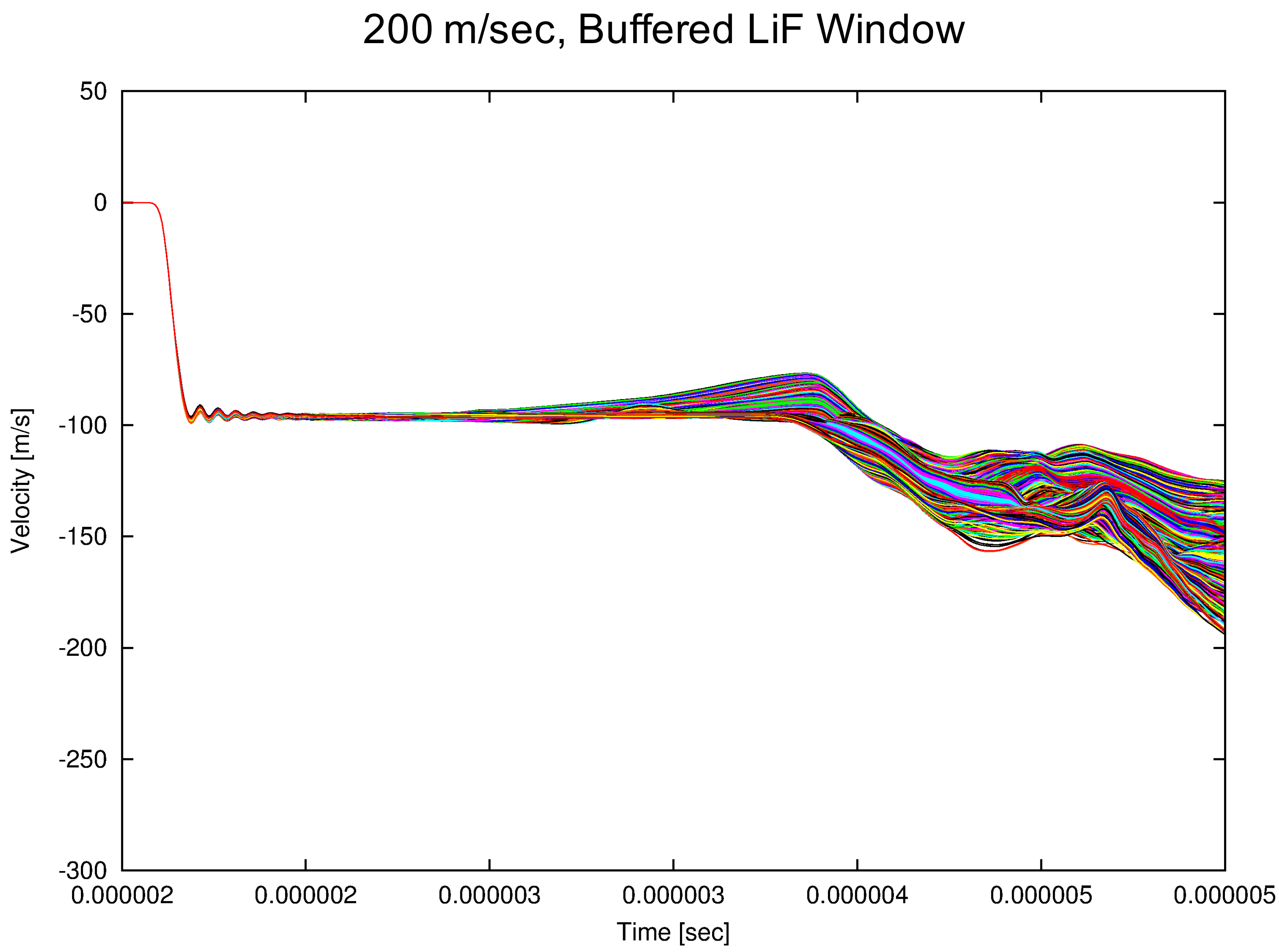
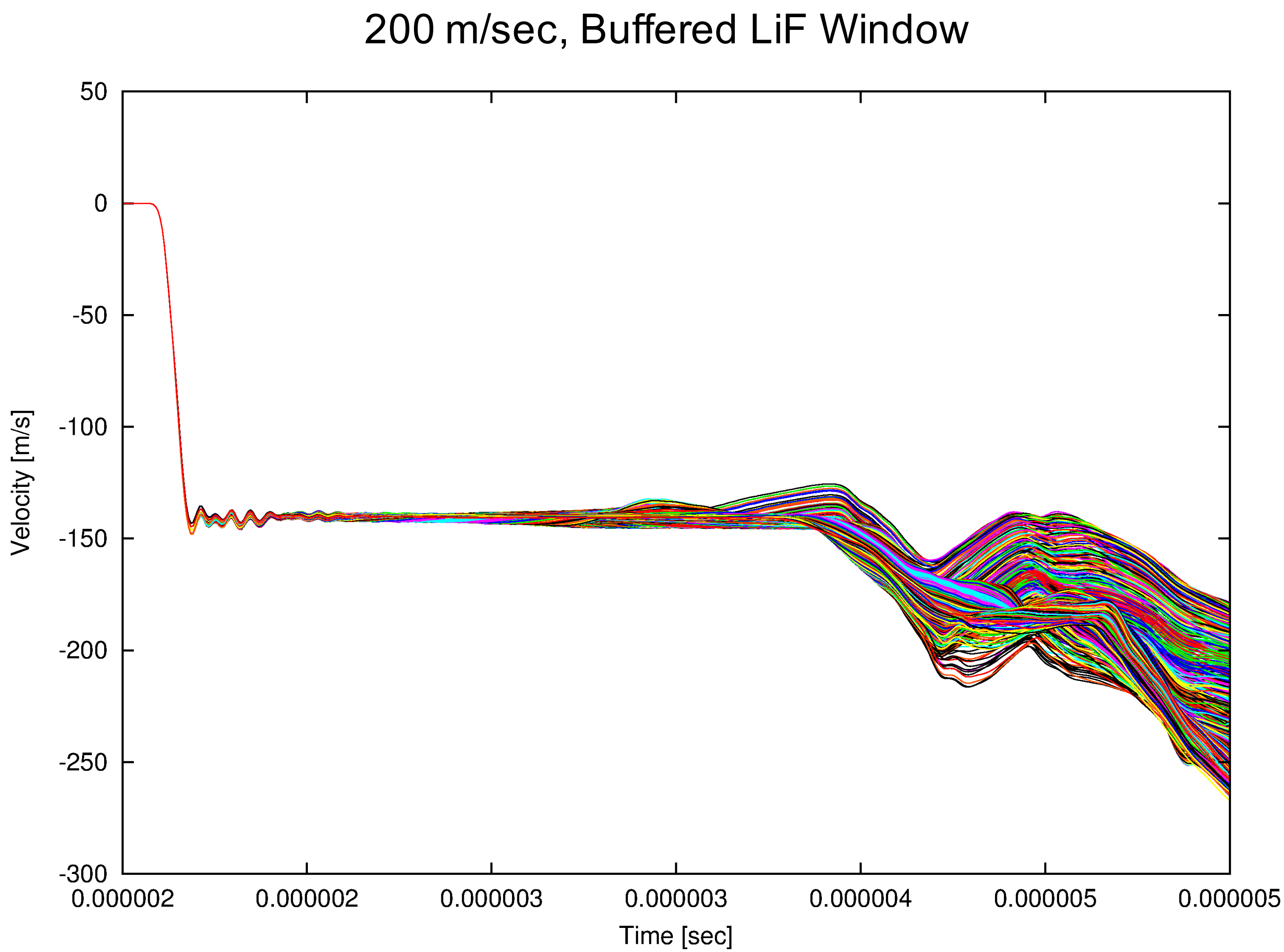
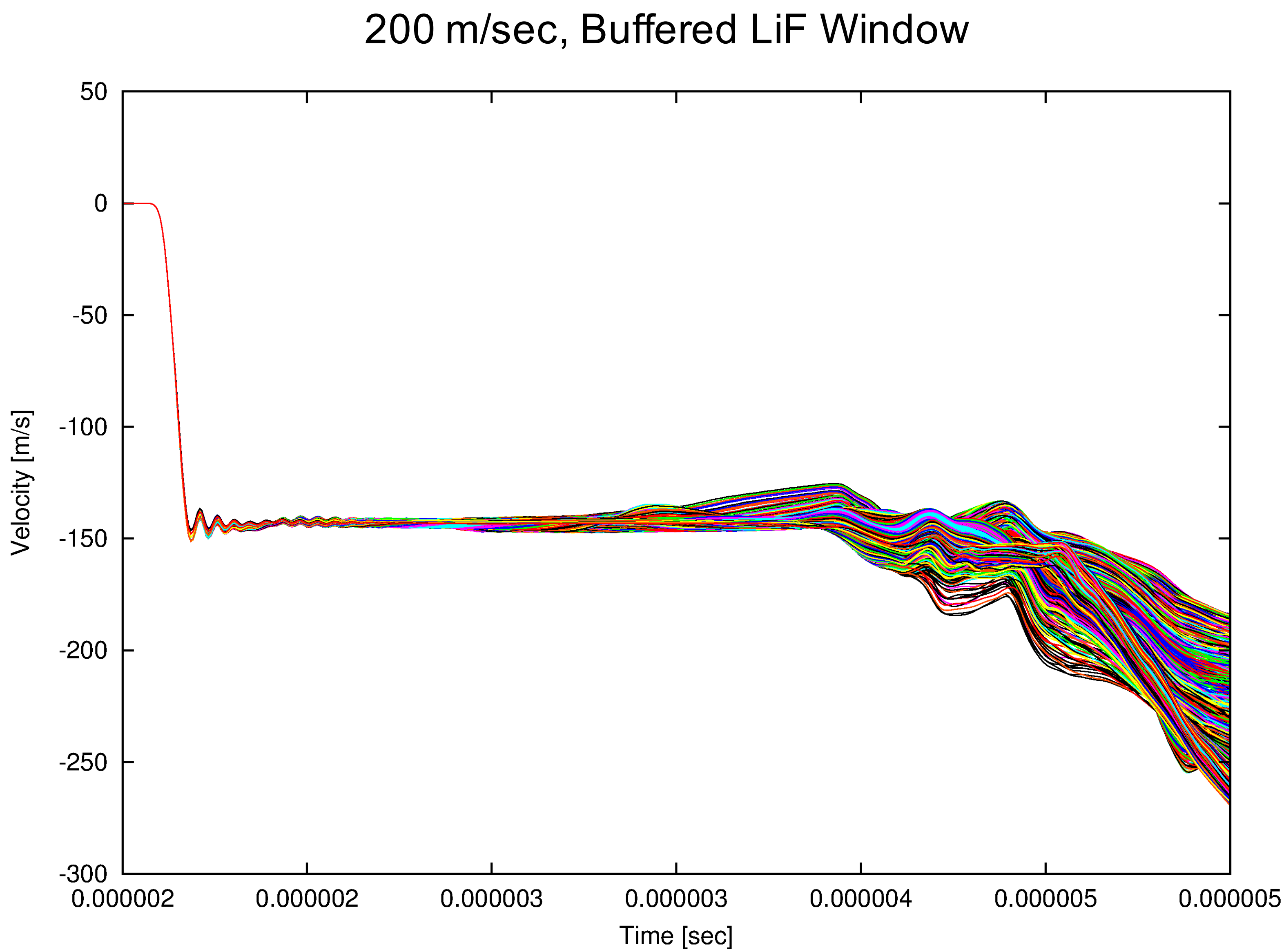
Simulated VISAR in Al w/ no pores



Simulated VISAR in Cu w/ no pores



Simulated VISAR in 304L w/ no pores



Simulated VISAR in Ta w/ no pores

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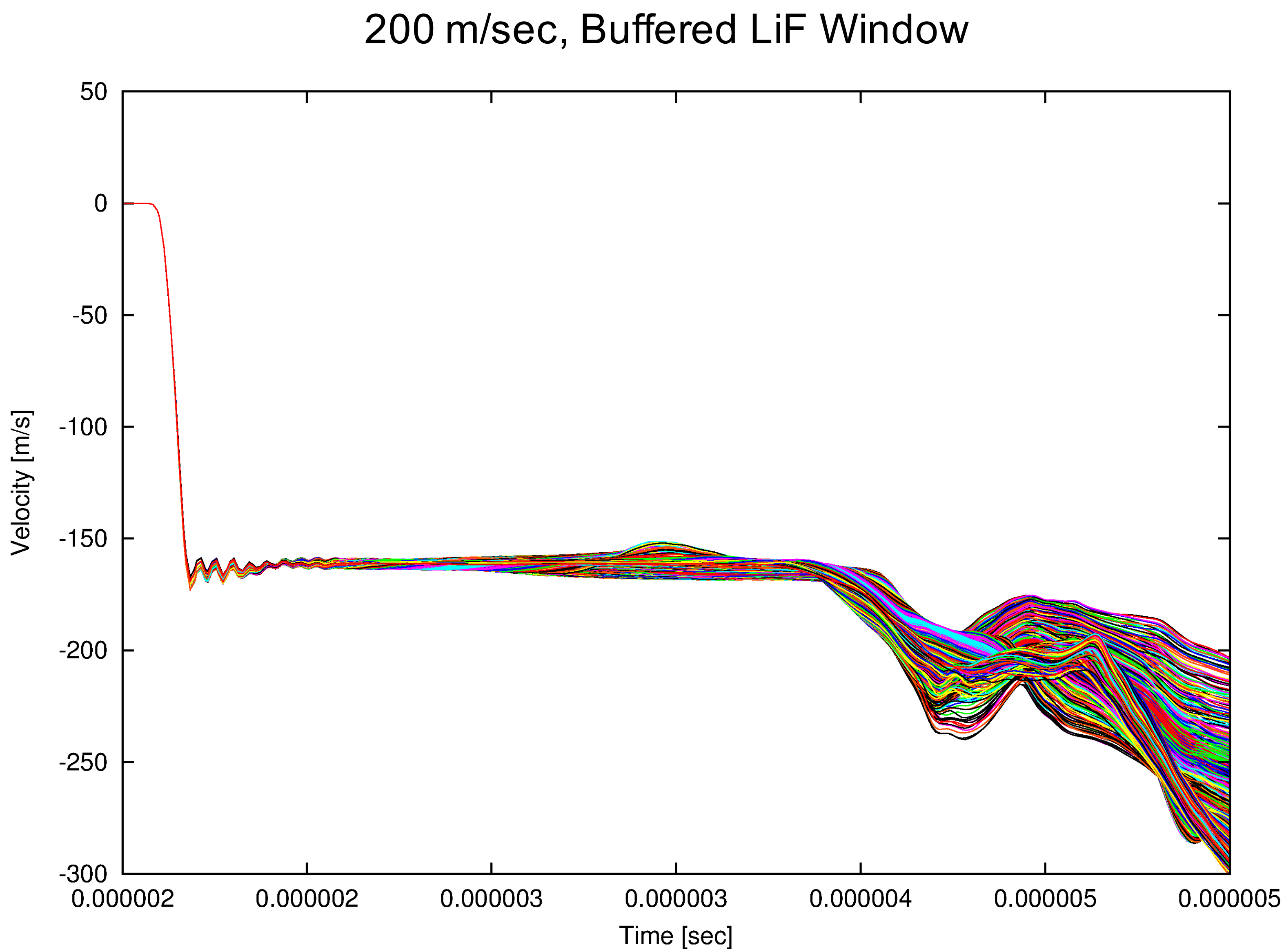
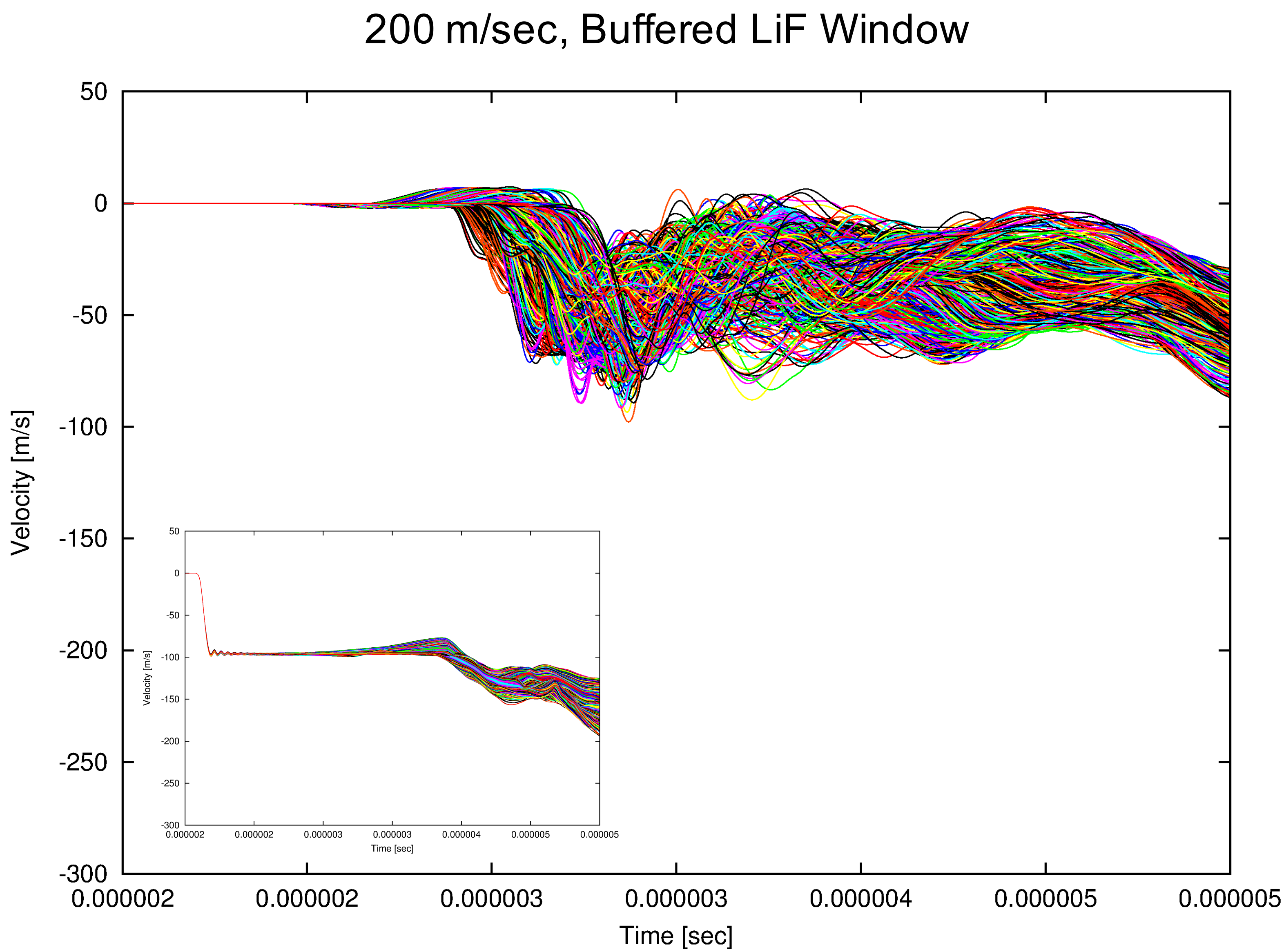
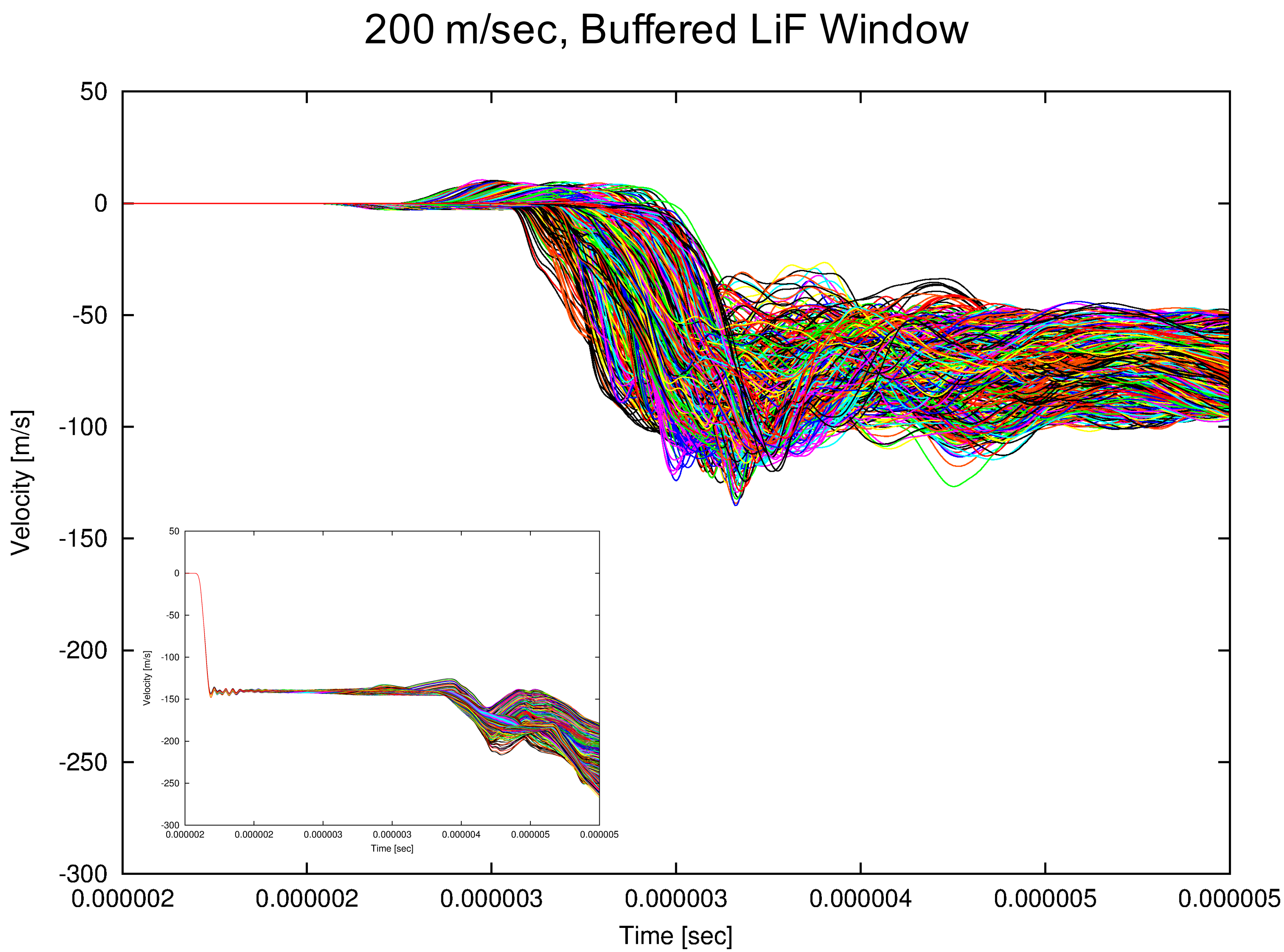


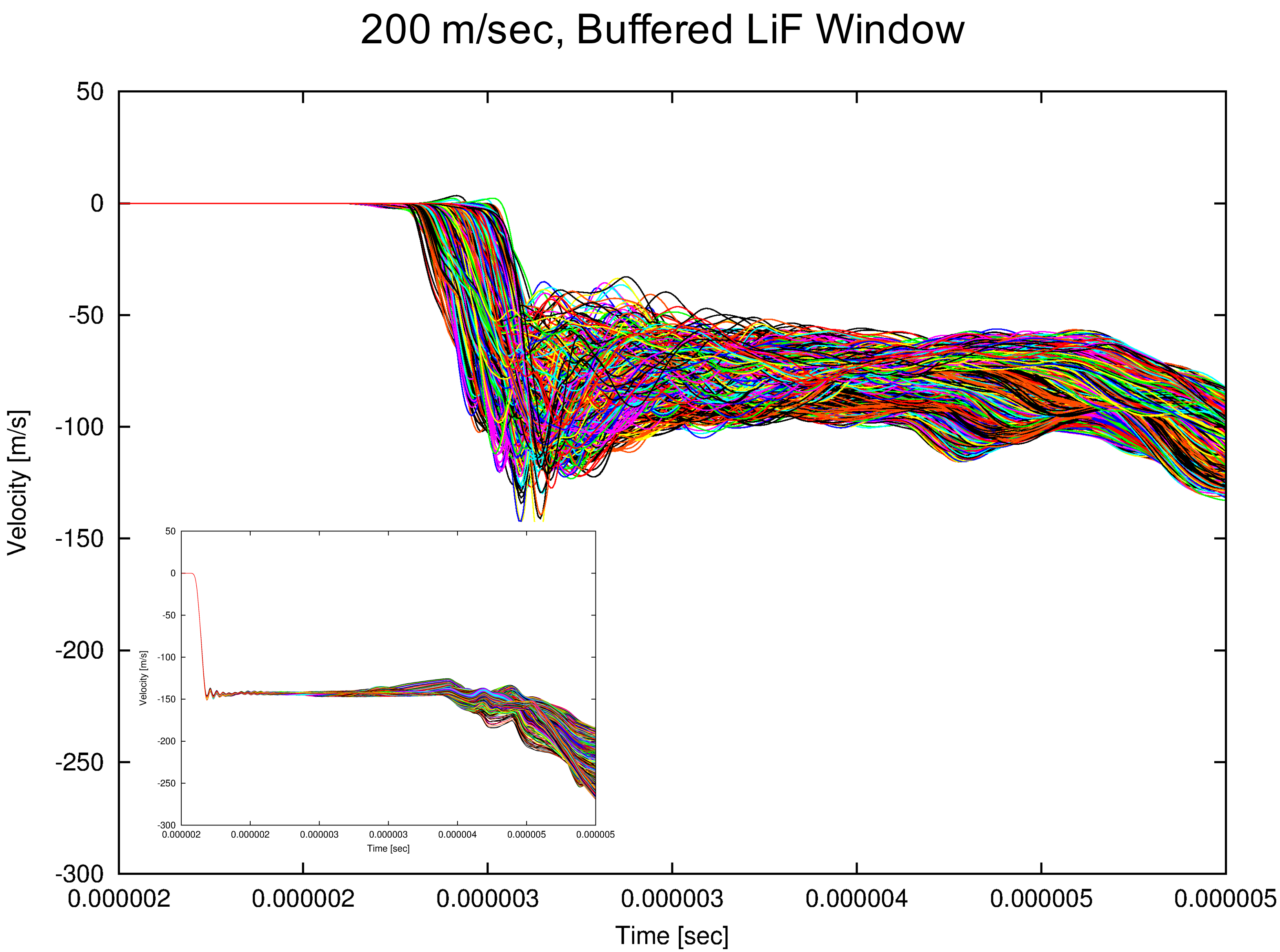
Simulated VISAR in Al w/ 10% pores



Simulated VISAR in Cu w/ 10% pores



Simulated VISAR in 304L w/ 10% pores



Simulated VISAR in Ta w/ 10% pores

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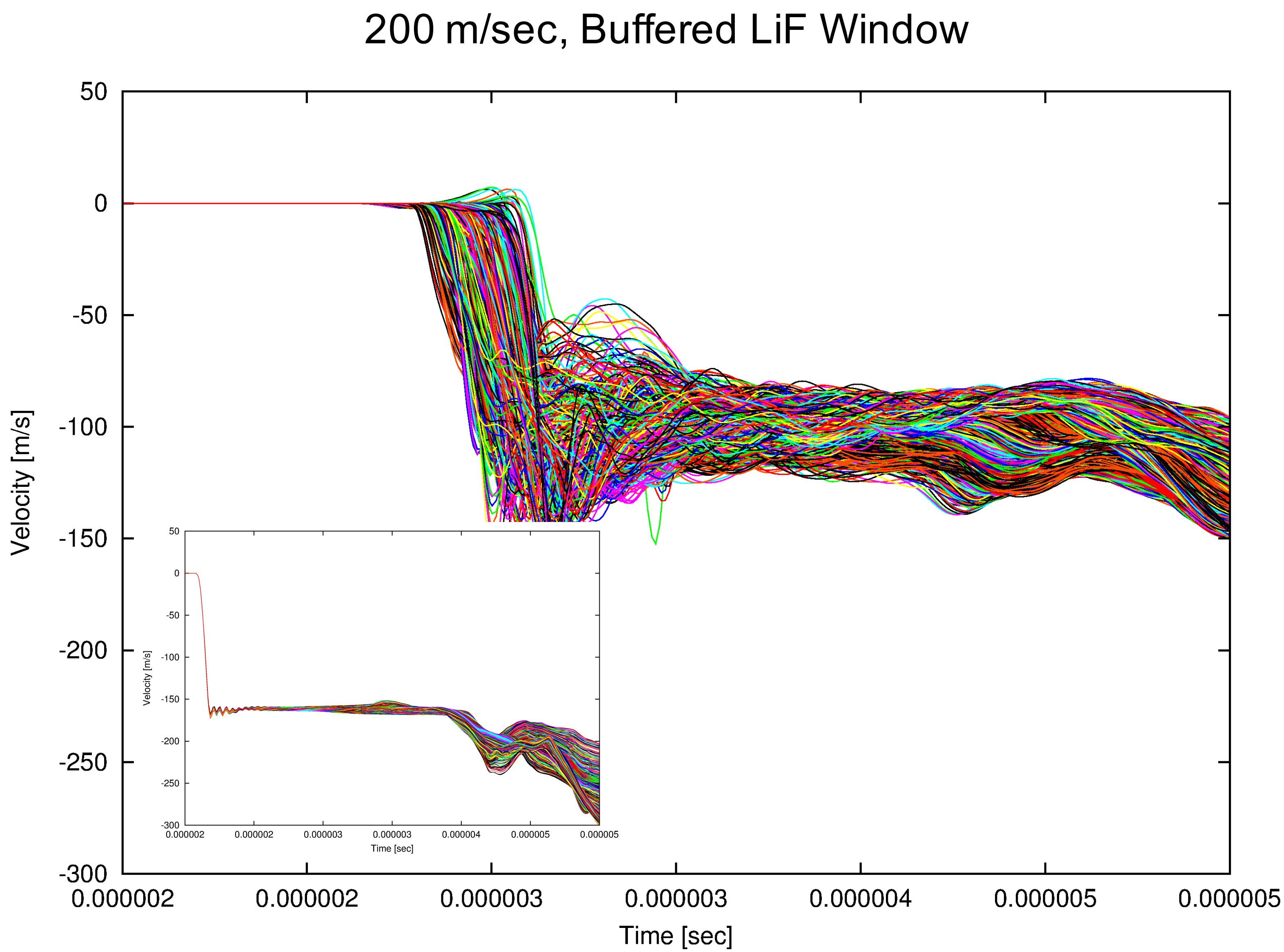
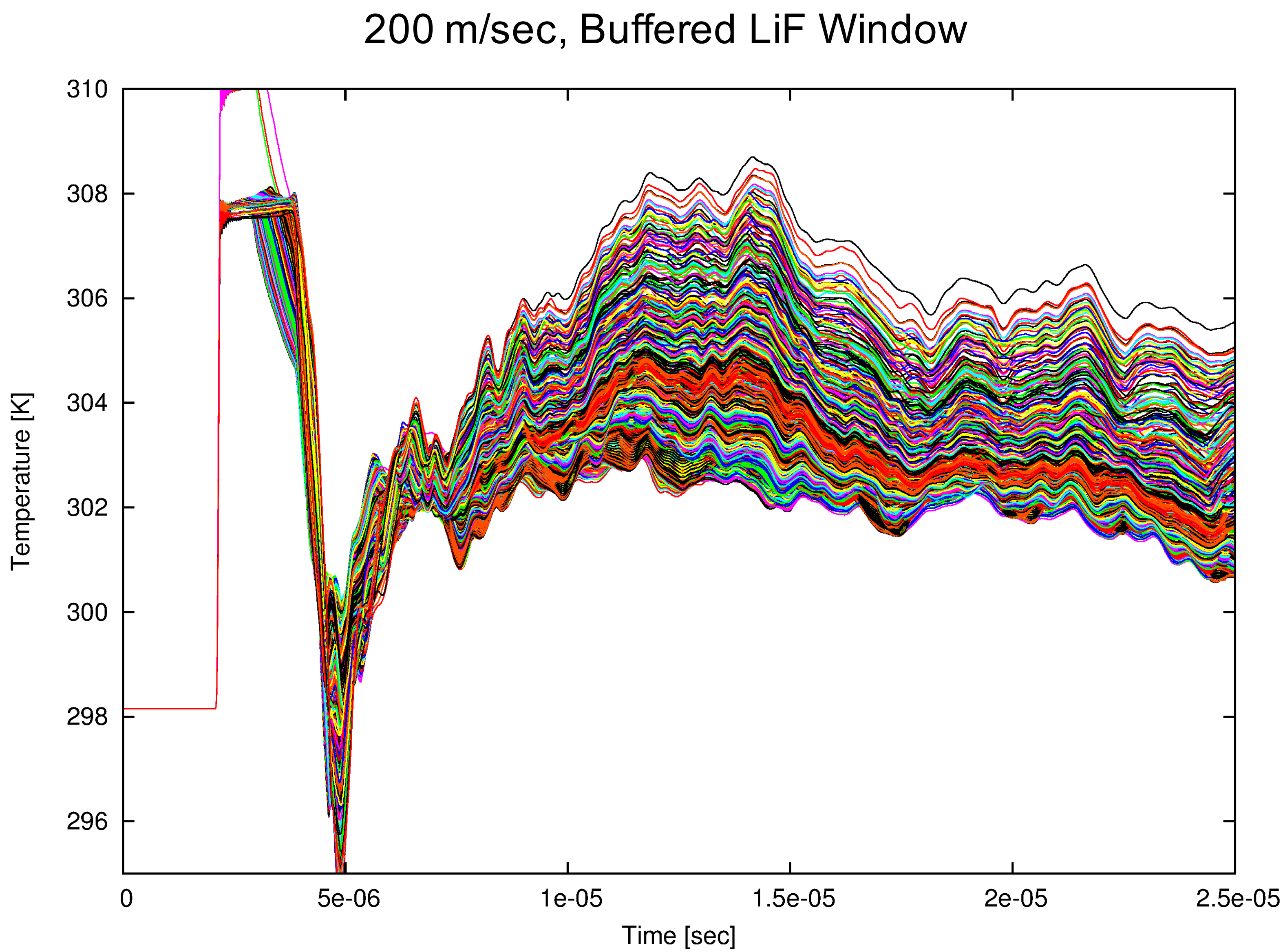
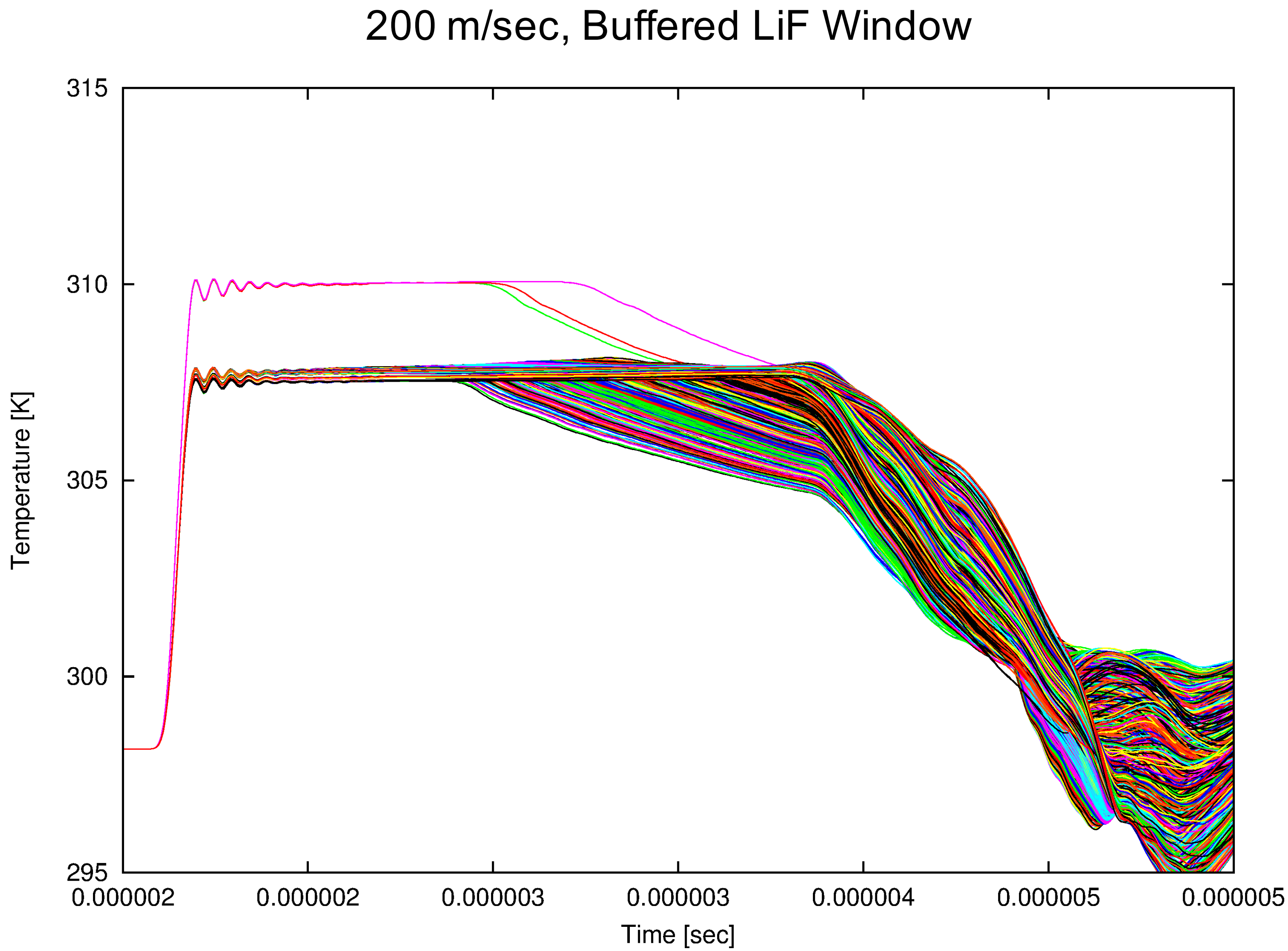


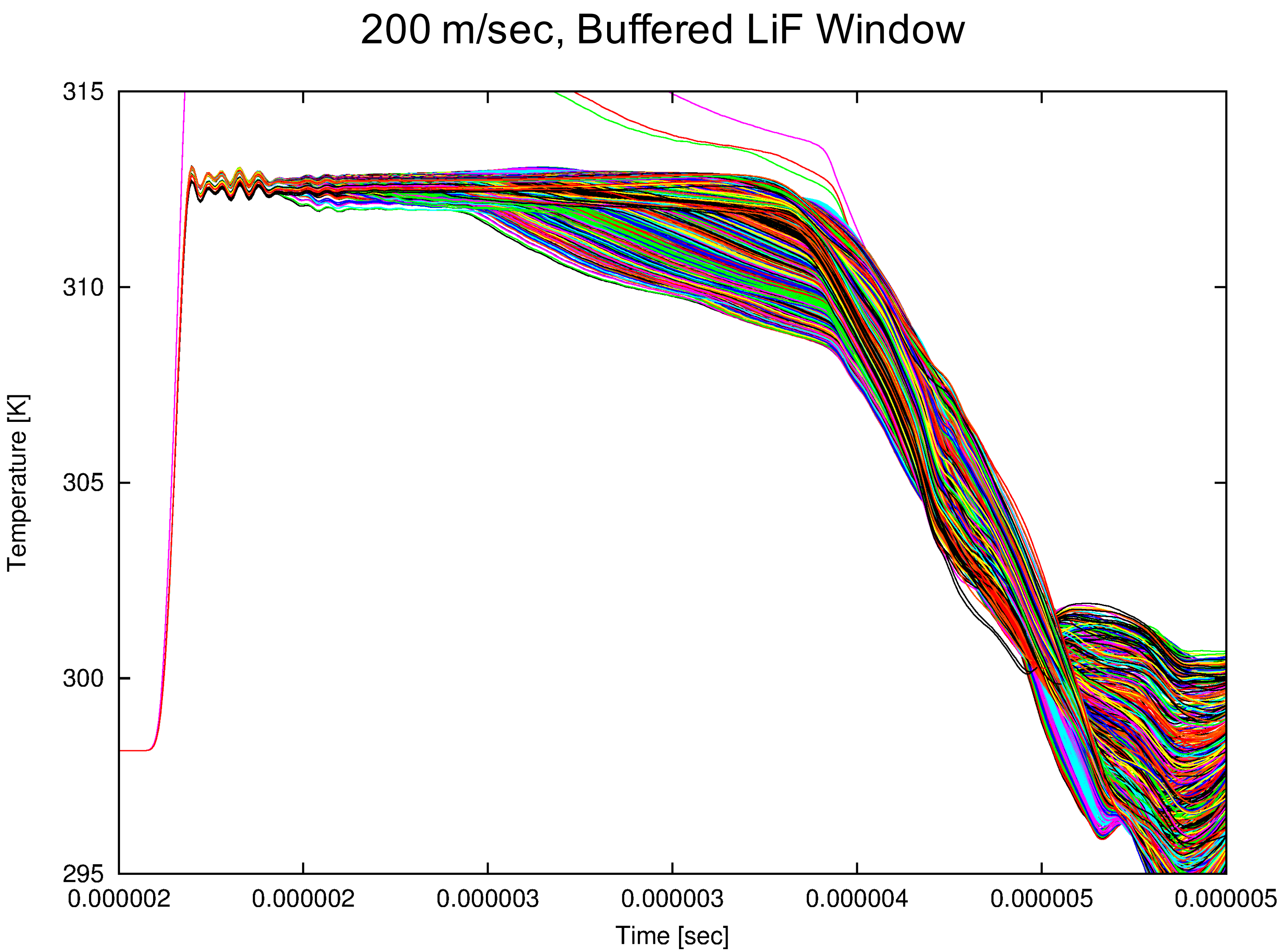
Simulated T in Al w/ no pores



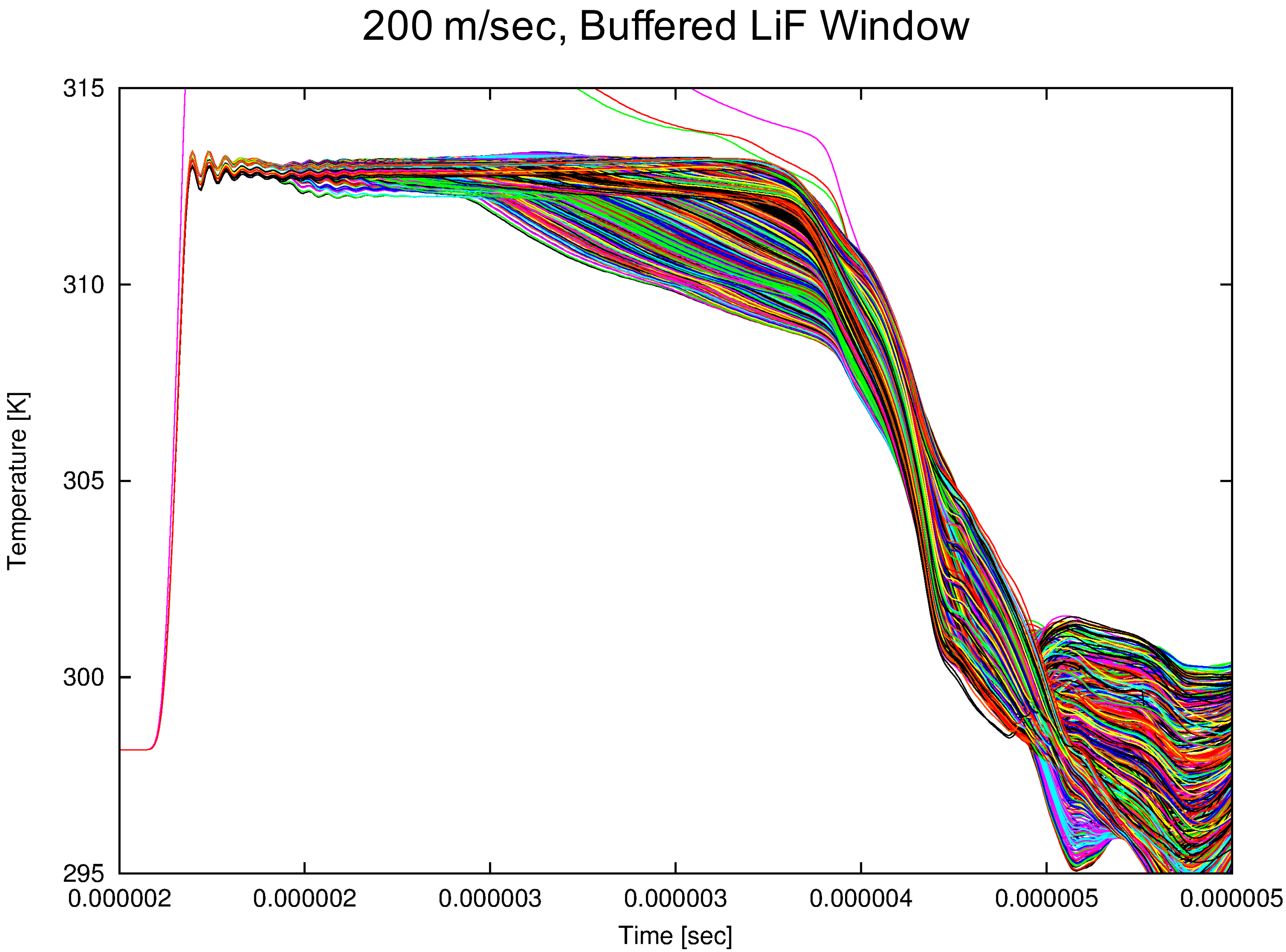
Simulated T in Al w/ no pores



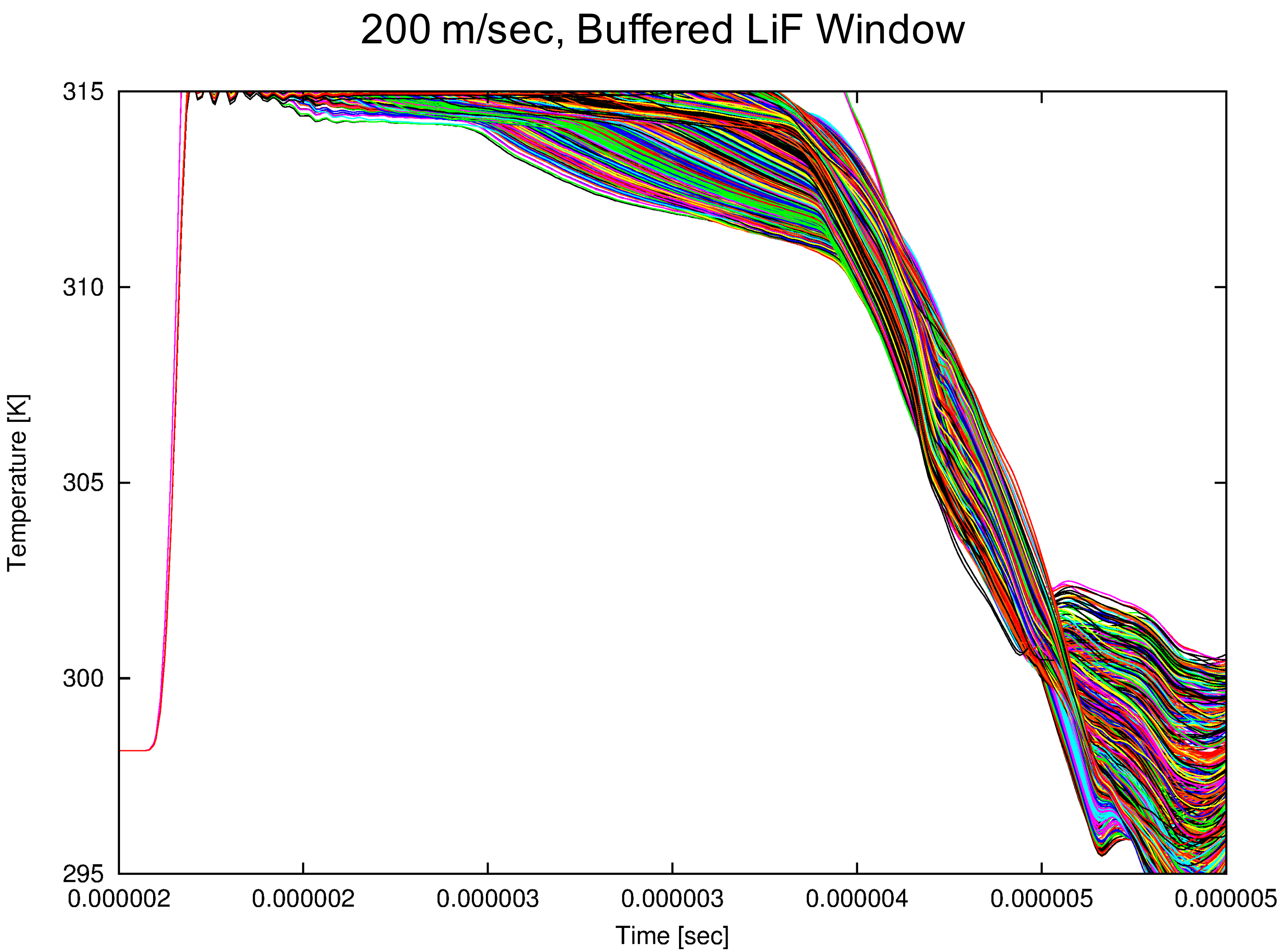
Simulated T in Cu w/ no pores



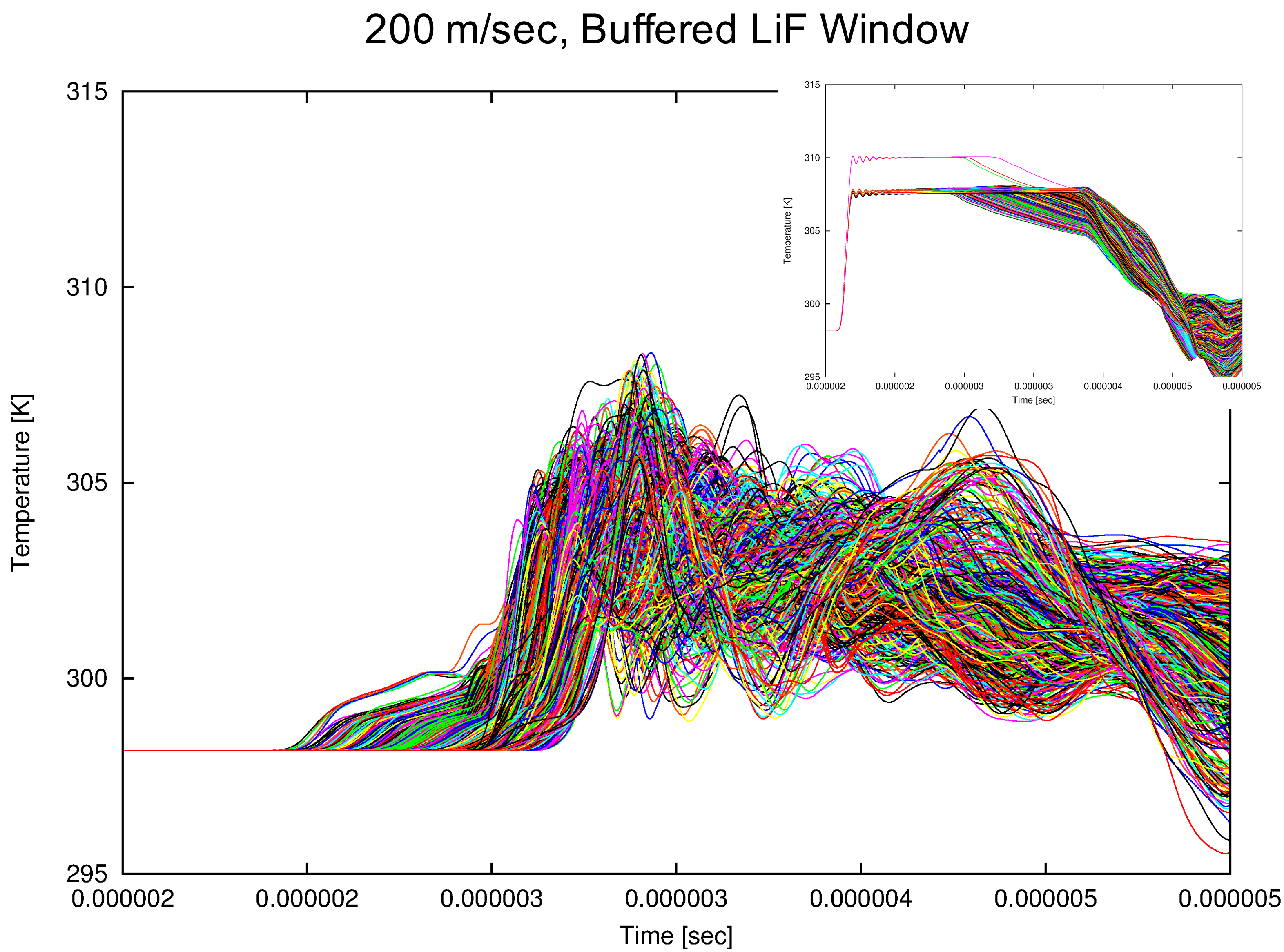
Simulated T in 304L SS w/ no pores



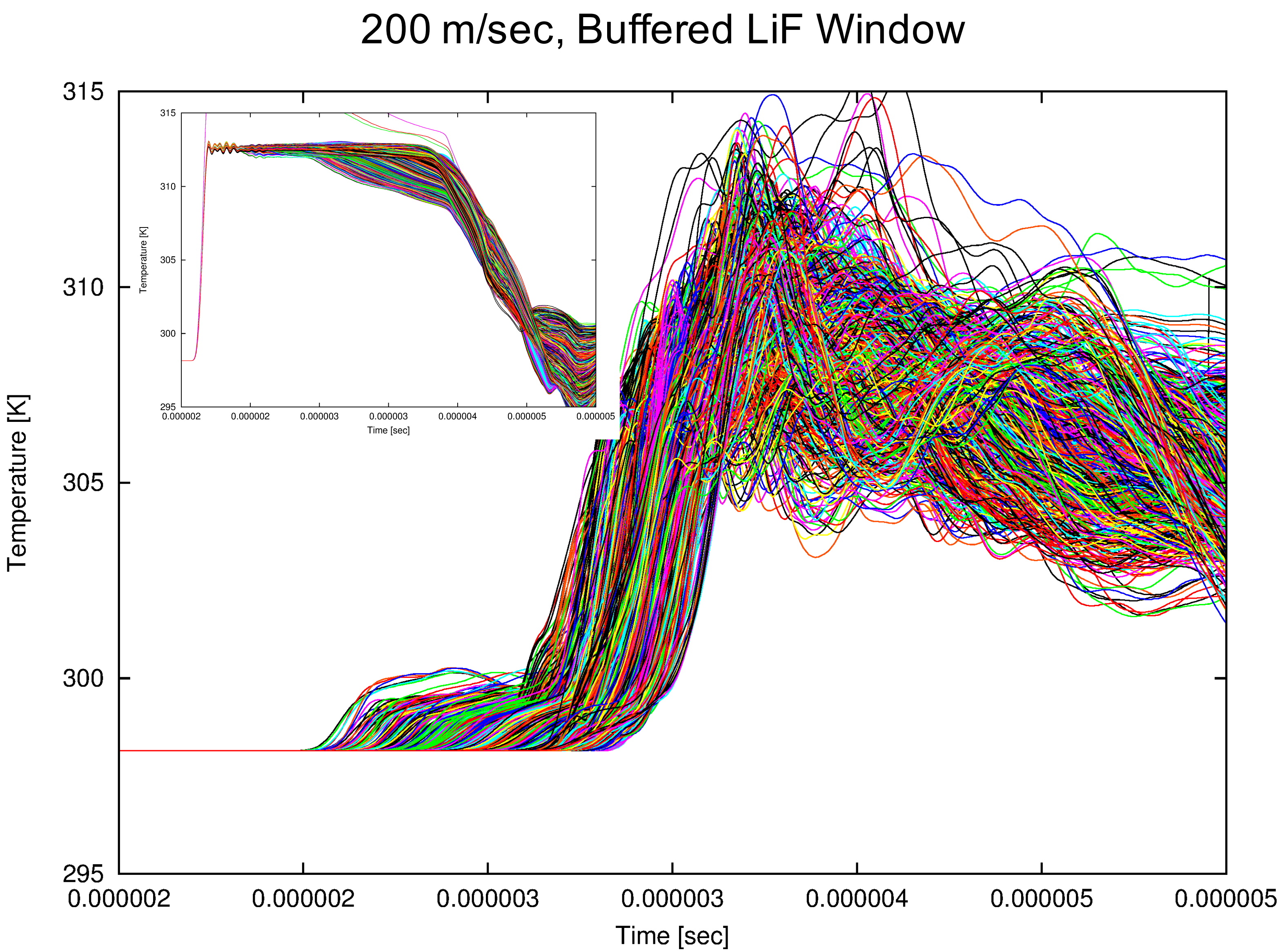
Simulated T in Ta w/ no pores



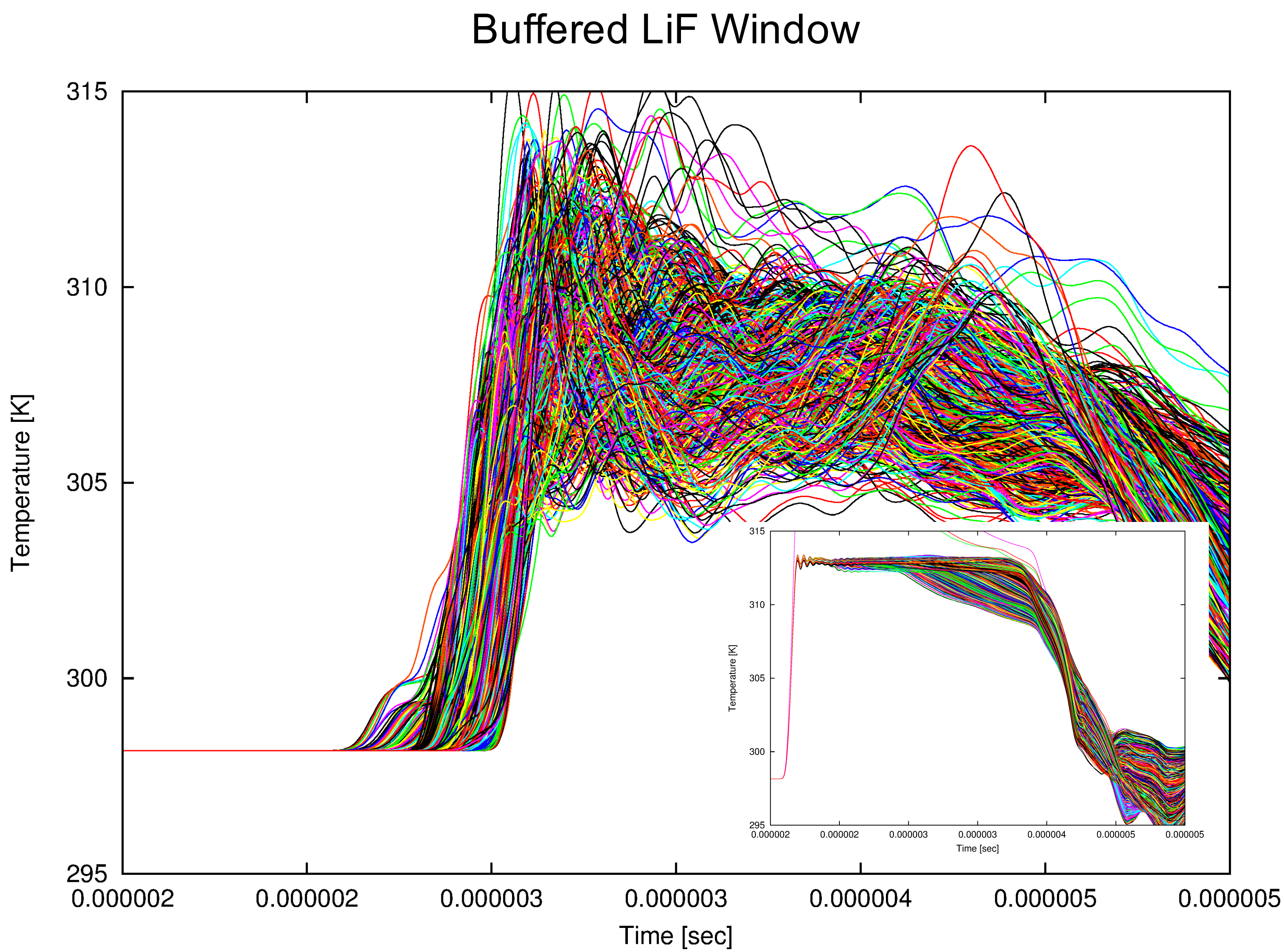
Simulated T in Al w/ 10% pores



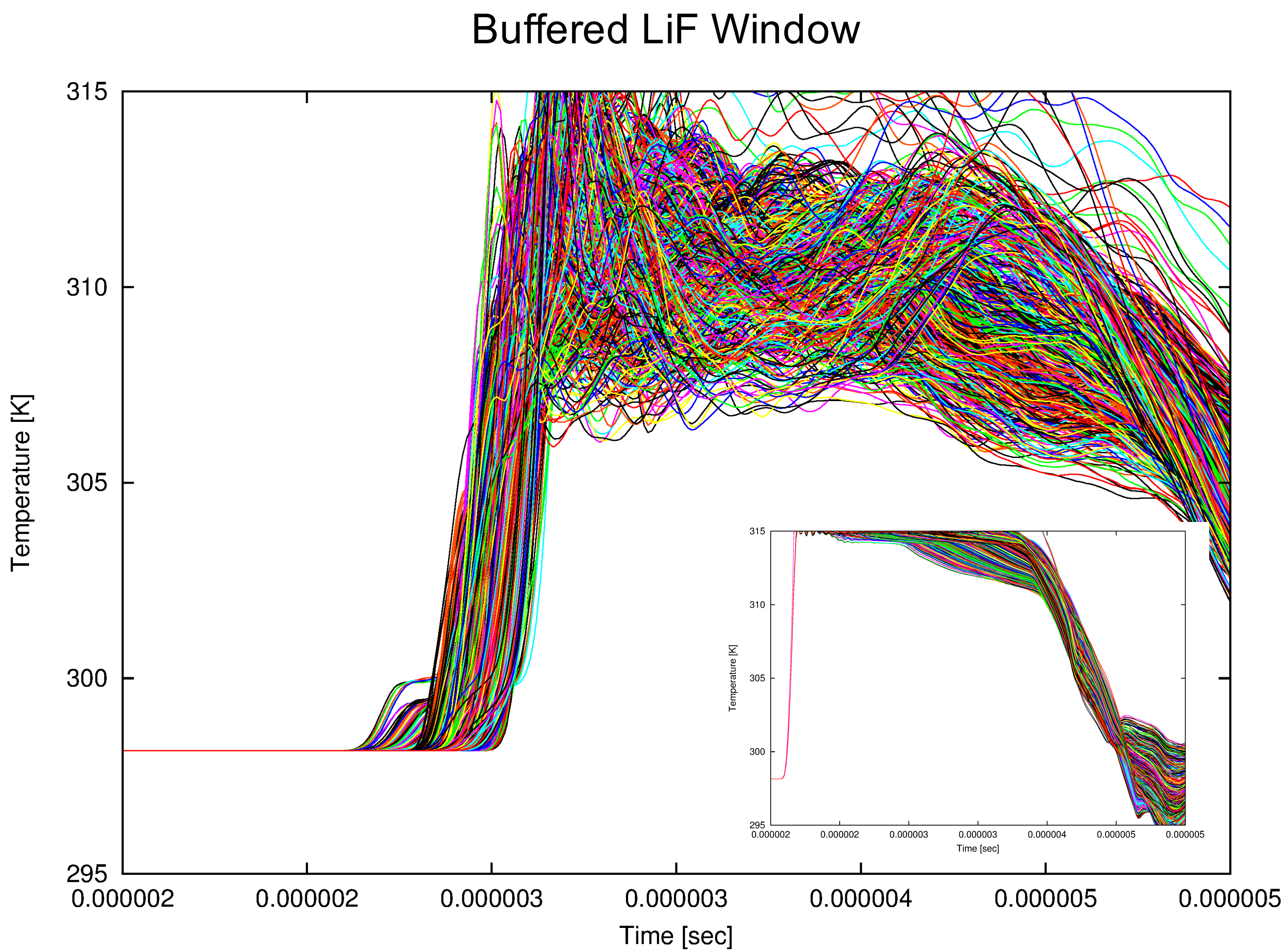
Simulated T in Cu w/ 10% pores



Simulated T in 304L SS w/ 10% pores

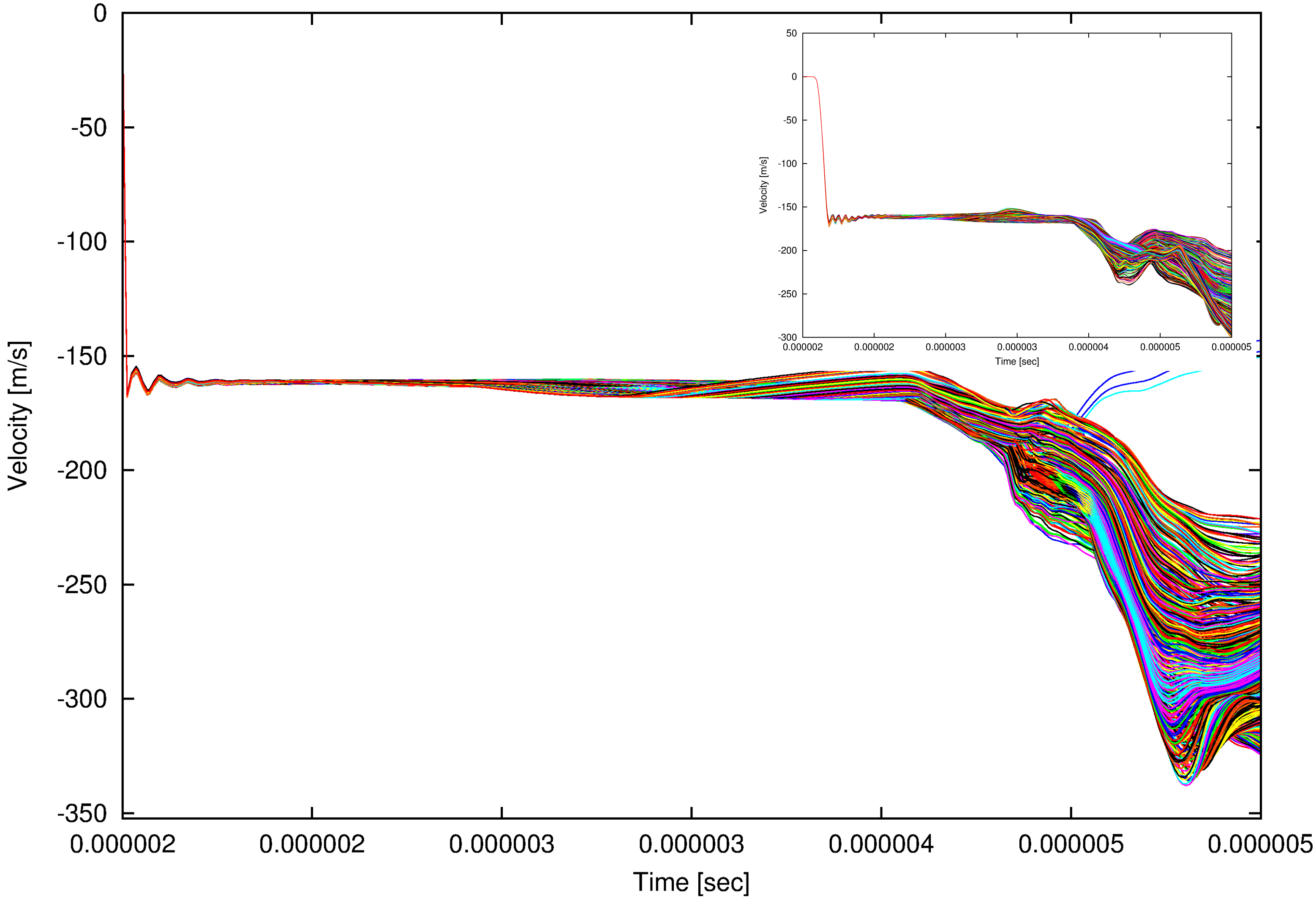


Simulated T in Ta w/ 10% pores



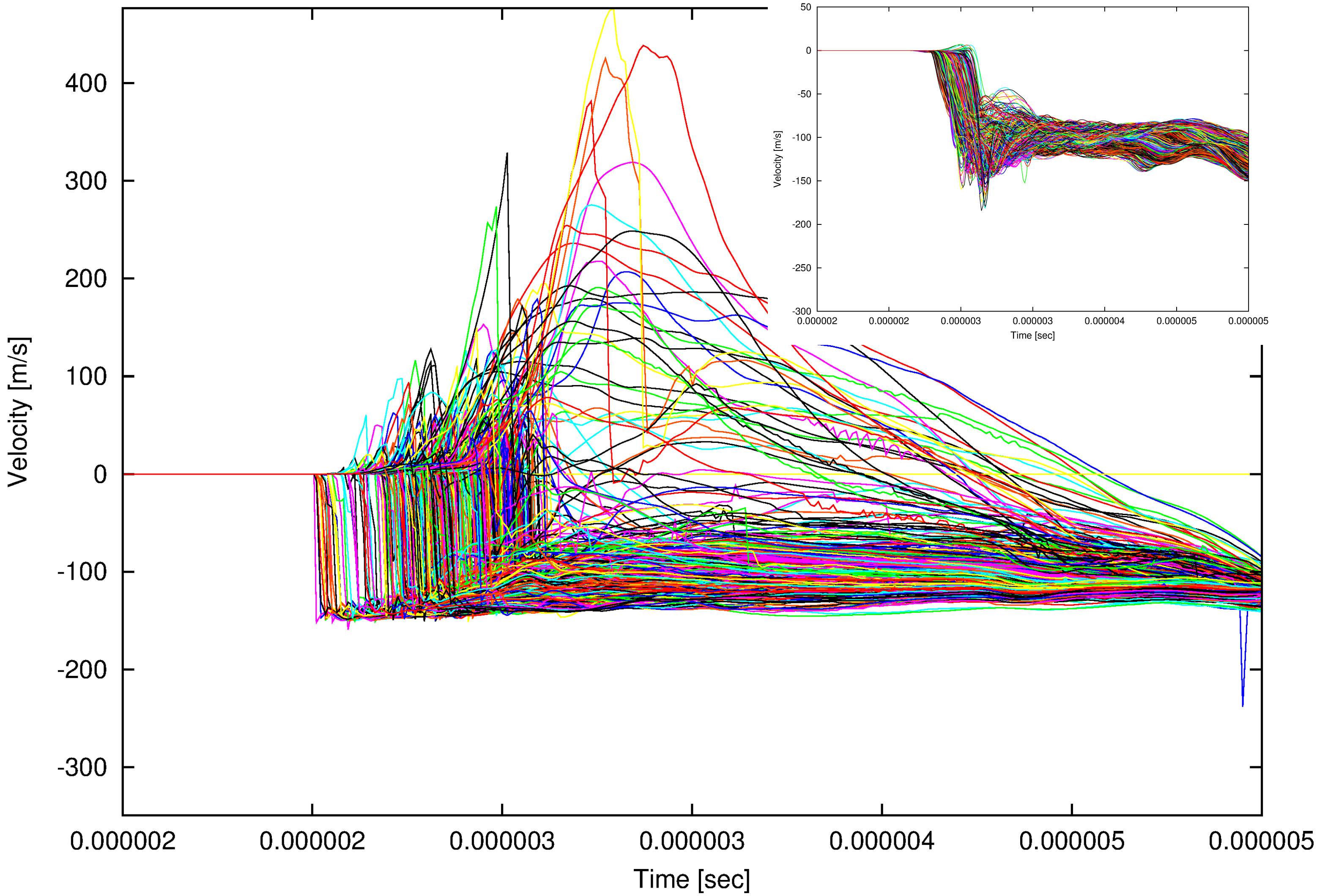
Simulated VISAR in Ta w/ no pores

200 m/sec, Unbuffered LiF Window



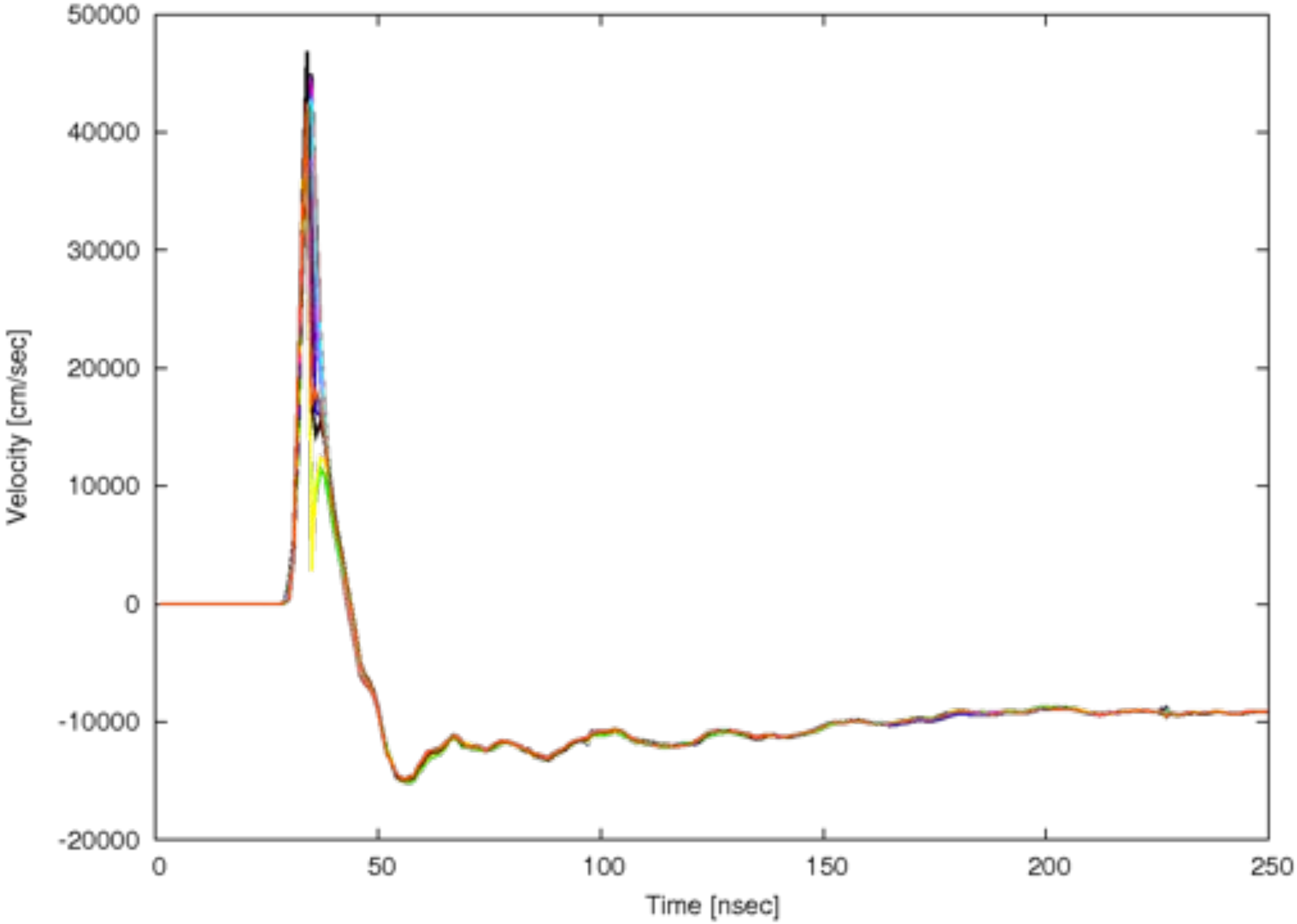
Simulated VISAR in Ta w/ 10% pores

200 m/sec, Unbuffered LiF Window

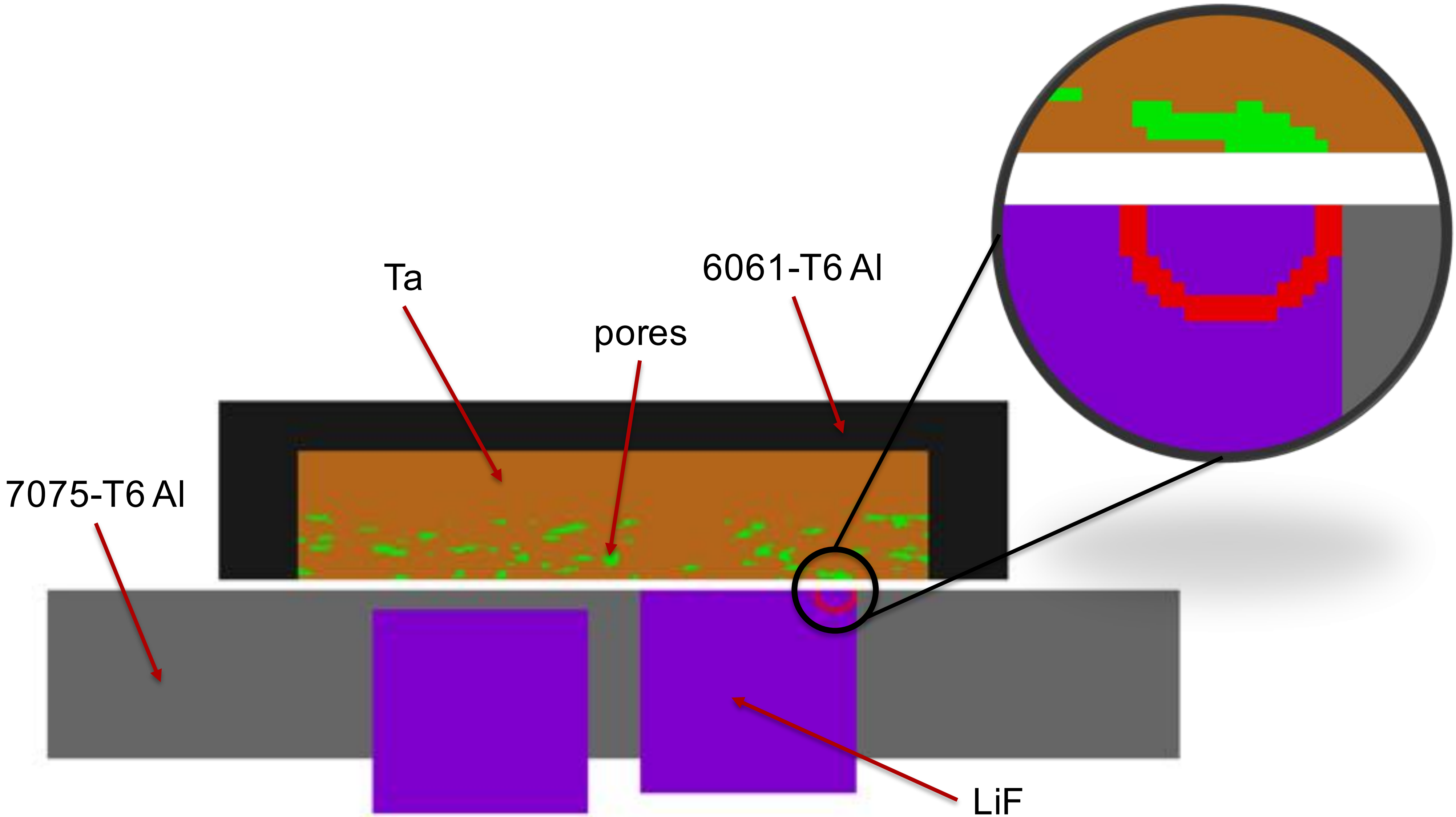


Ta VISAR: largest velocity excursions

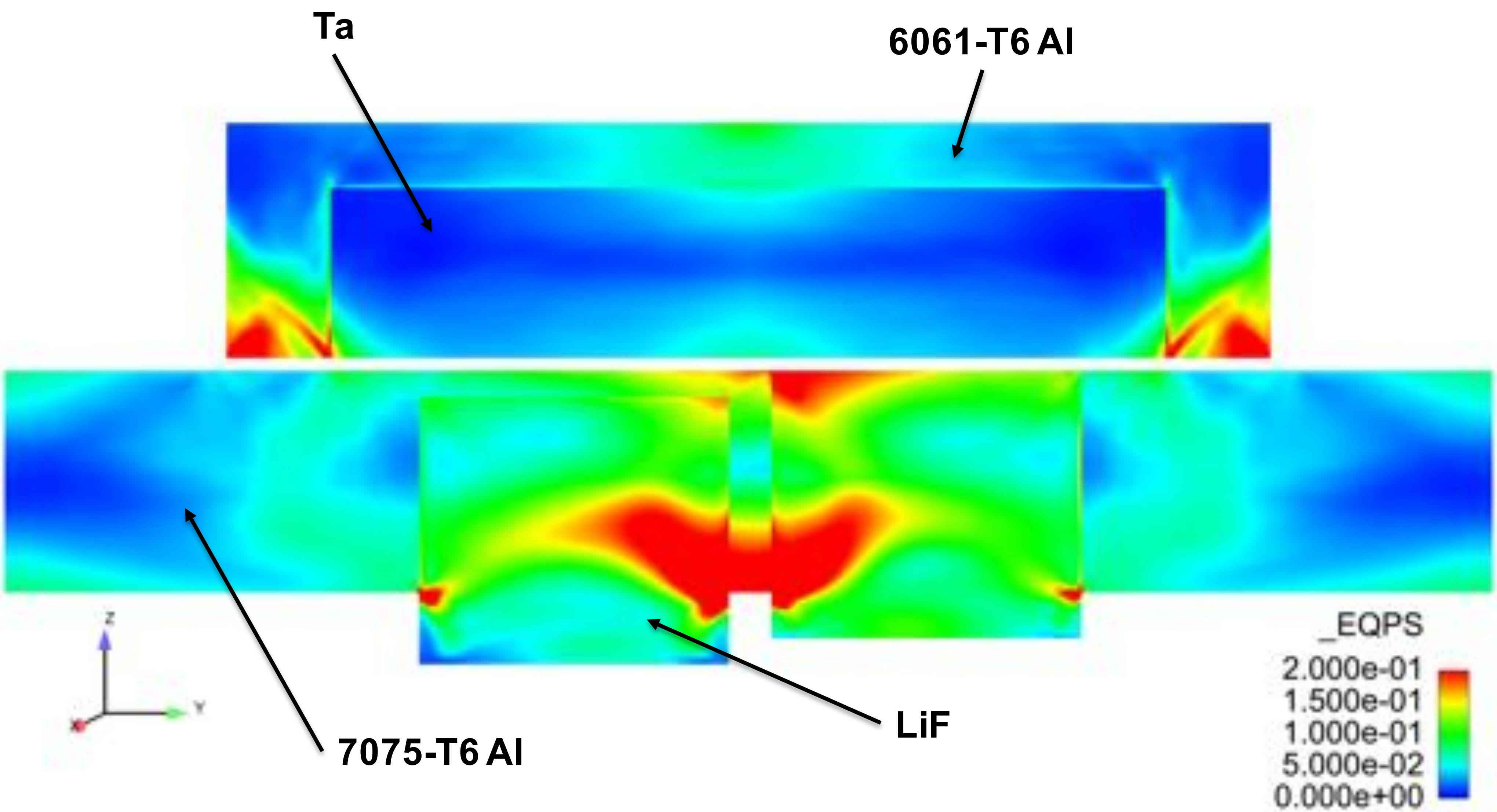
Unbuffered LiF Window



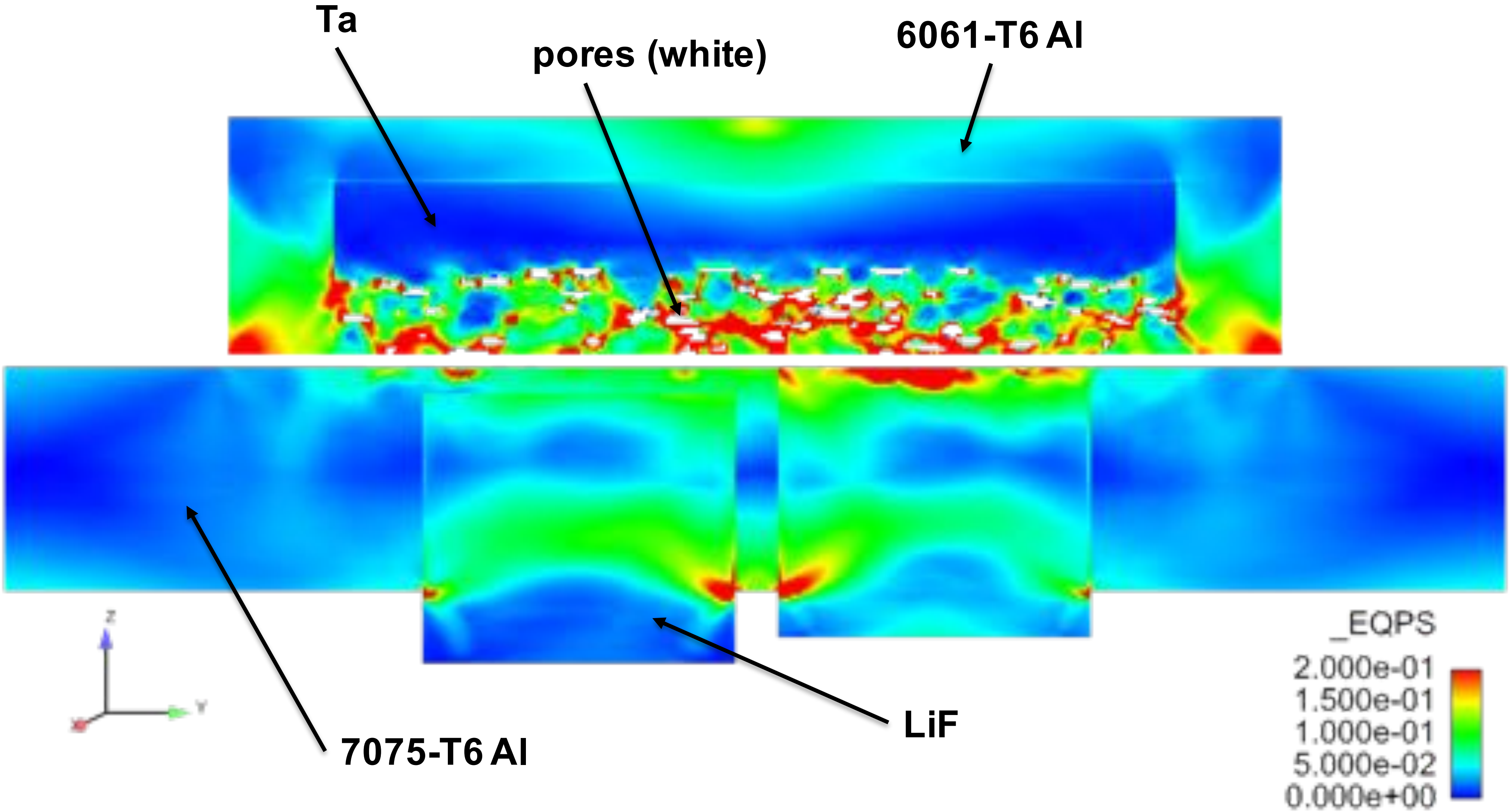
Excursions arise near surface pores



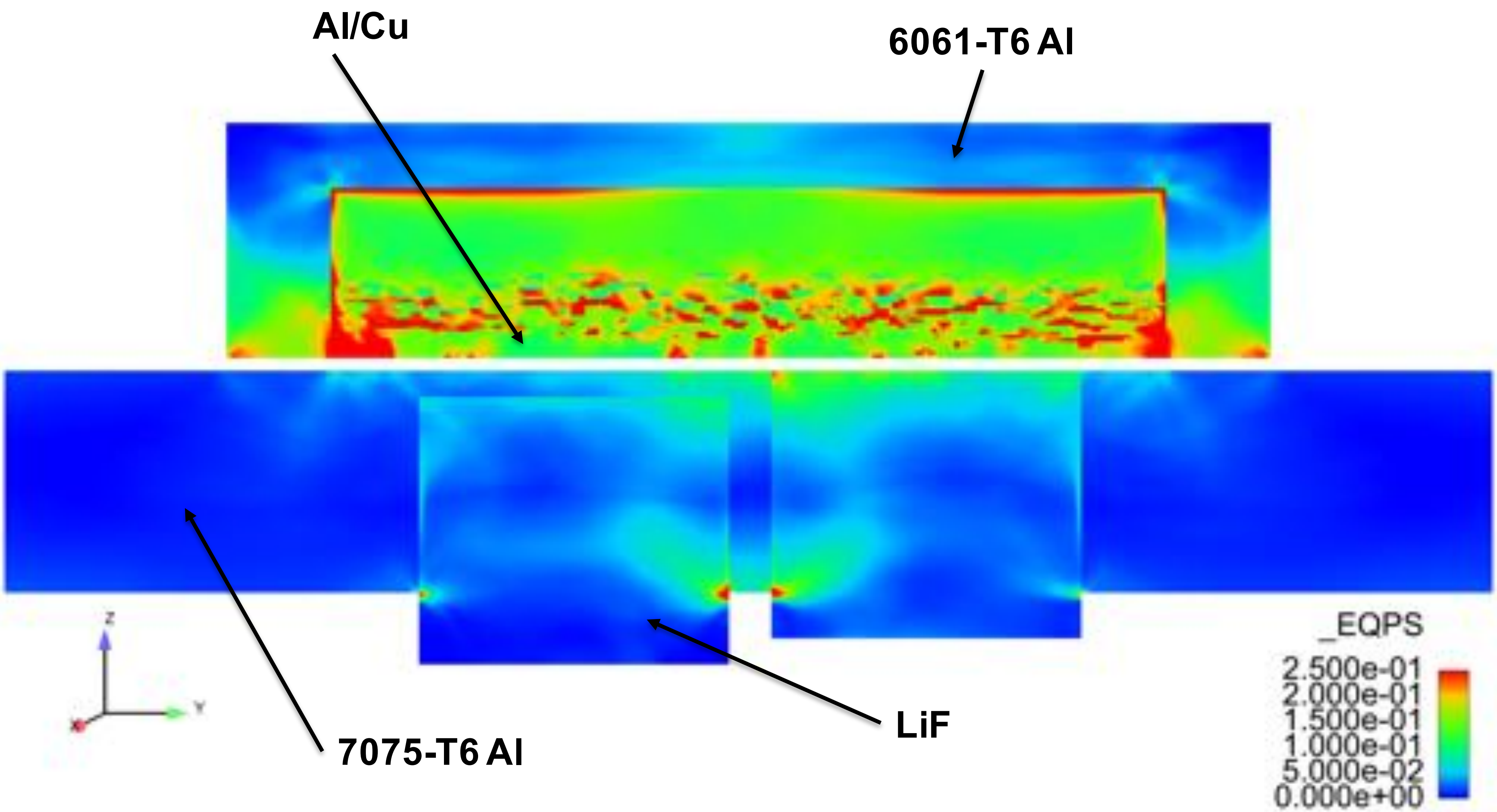
Plastic strain in Ta w/ no pores



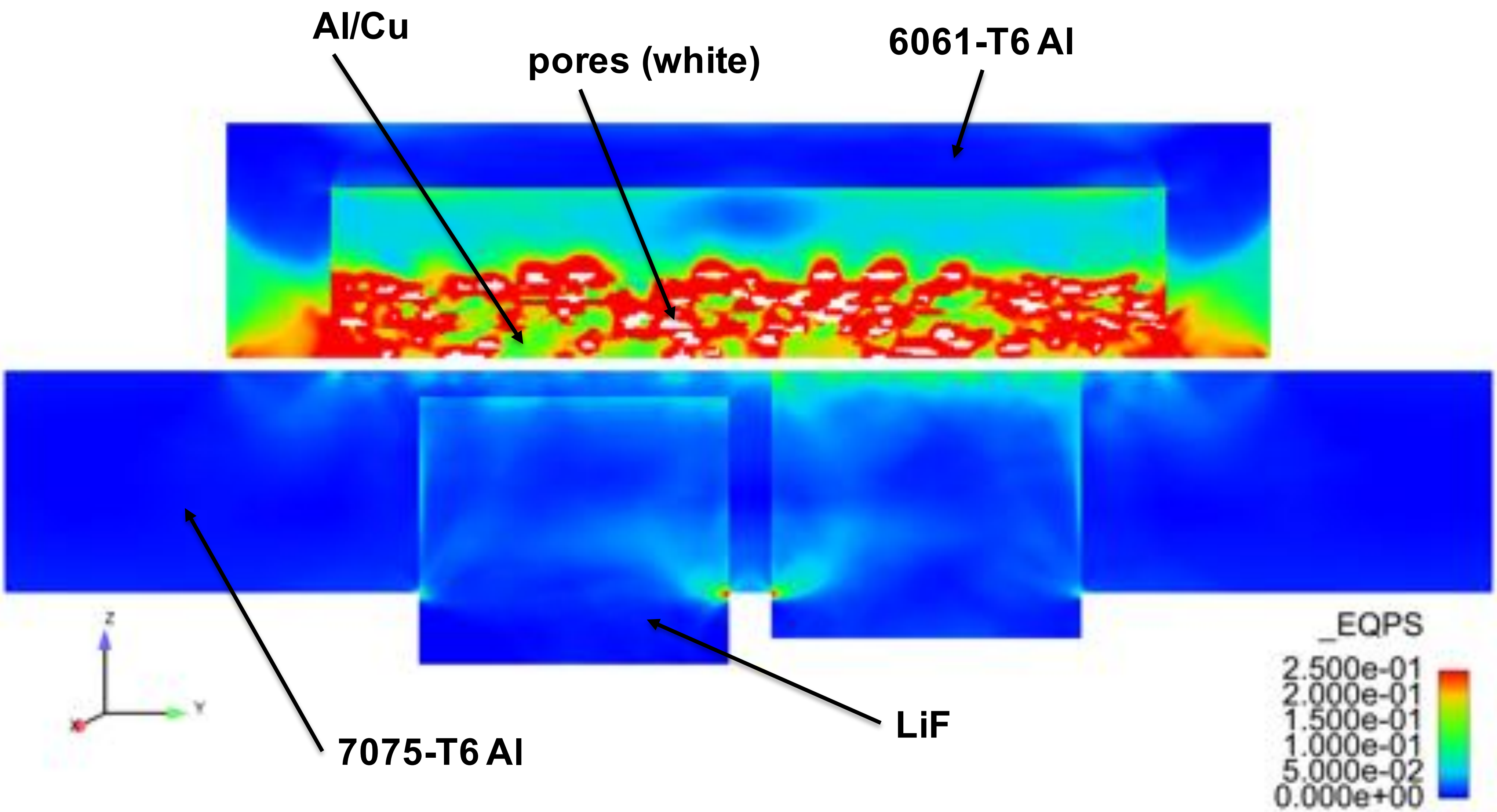
Plastic strain in Ta w/ 10% pores



Plastic strain in AlCu w/ no pores

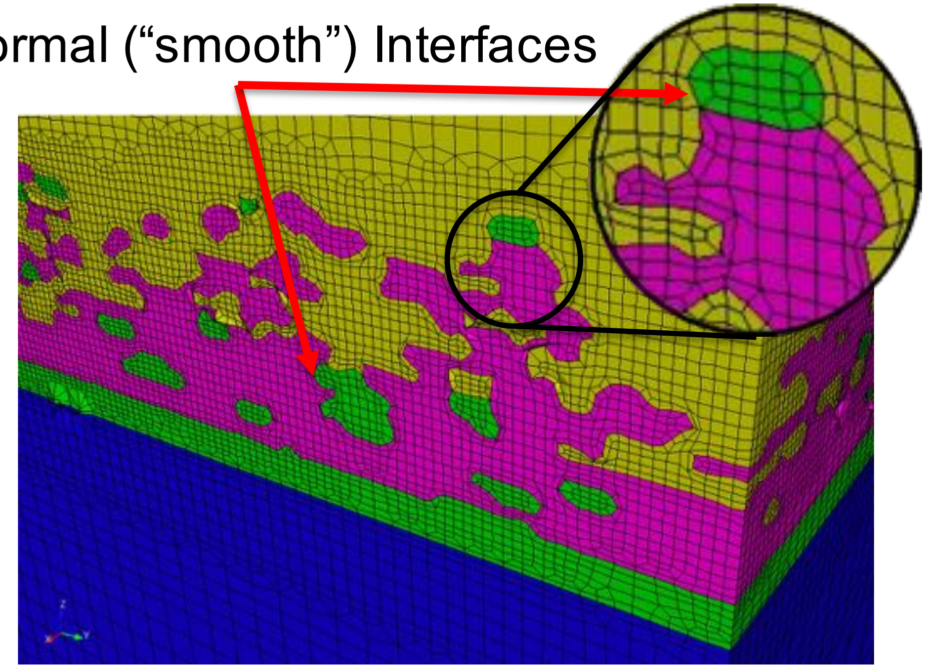


Plastic strain in AlCu w/ 10% pores



Toward conformal interfaces …

Conformal ("smooth") Interfaces



Mesh Generation for Microstructures

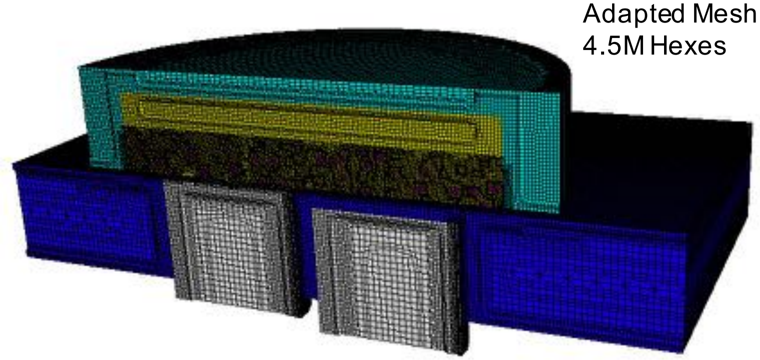
Capabilities

- 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, DREAM.3D, …

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



Summary

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