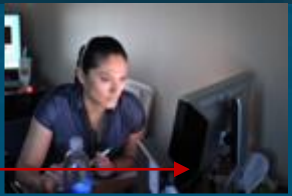
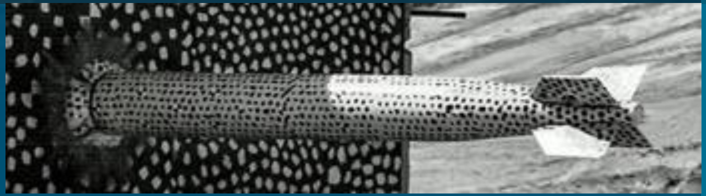
SAND2023-05347C

Sandia National Laboratories

Mesoscale model for spall in additively manufactured metals





Stewart A. Silling, David P. Adams, Brittany A. Branch, Paul A. Specht

23rd Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter

June 23, 2023
Chicago, IL

SANDxxx

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & 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.

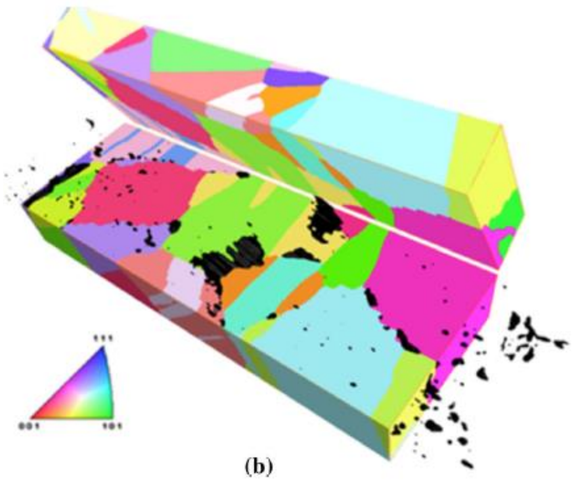
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Objective

- Develop a computational model for that
  - Includes realistic AM material features
  - Helps to relate free-surface velocities in plate impact tests to these AM features.
- We are not explicitly modeling microstructural features like voids, dislocations, precipitates, inclusions (although these are known to affect spall*).

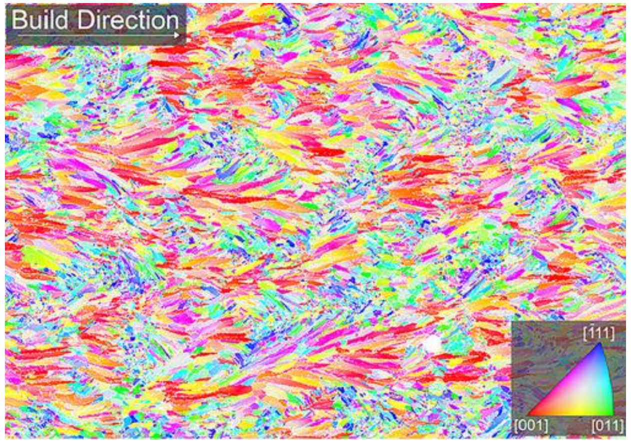
*Sample of work on spall at the microstructural scale

- Trumel et al., J. Mech. Phys. Solids (2009)
- Wayne et al., Scripta Mater. (2010)
- Krishnan et al., Metall. Mat. Trans. A (2014)
- Li et al., Mater. Sci. Eng. A (2016)
- Wang et al., J. Applied Phys. (2017)
- Li et al., Acta Mech. Solida Sinica (2018)
- Li et al., Mater. Sci. Eng. A (2019)
- Nguyen, Luscher, & Wilkerson, Acta Mat. (2019)
- Dongare, Mater. Sci. Eng. A (2019)
- Chiu, in progress (2023)



Microstructural scale
Image: Krishnan et al. (2014)

Length scale for this study



Mesoscale
Image: Specht & Brown (2021)

Outline

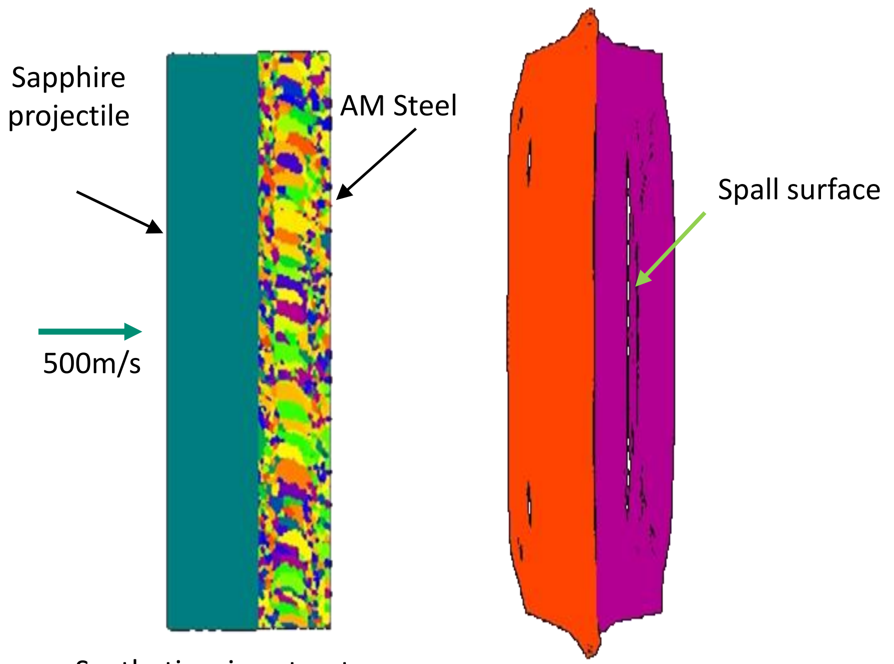
- Modeling methods
  - Peridynamics background.
  - Crystal plasticity model.
  - Spall kinetics model.
- Impact simulations and comparison with test data.

Acknowledgments

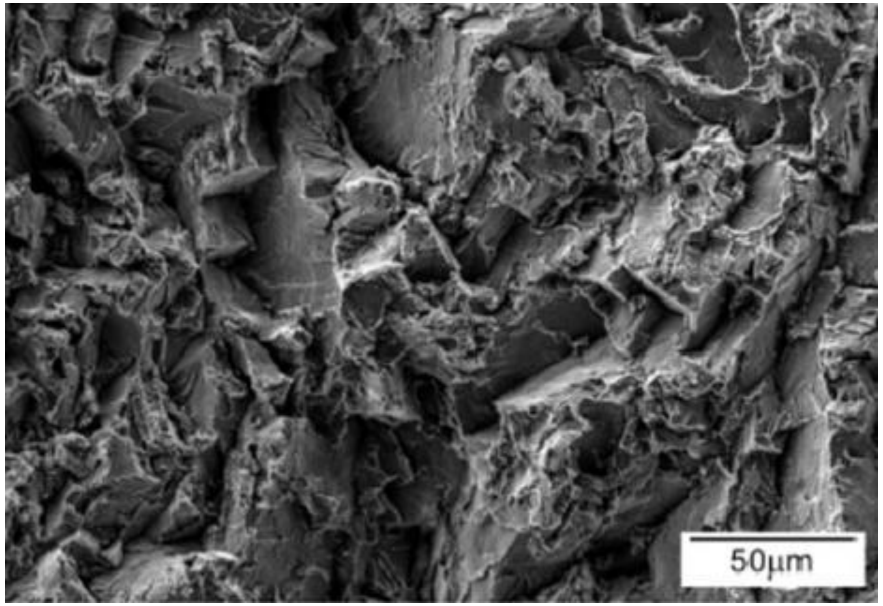
Justin Brown, Nathan Brown, John Mitchel

Failure of metals under impact loading

- Plate impact experiments are used in various configurations to measure dynamic material properties.
  - Equation of state data (Hugoniot and release).
  - Dynamic strength under high-rate tensile loading (~ 10^5 1/s)
  - Spall stress >> quasi-static tensile strength (typically > 3GPa for steel).
- Basic test data is the free surface velocity.



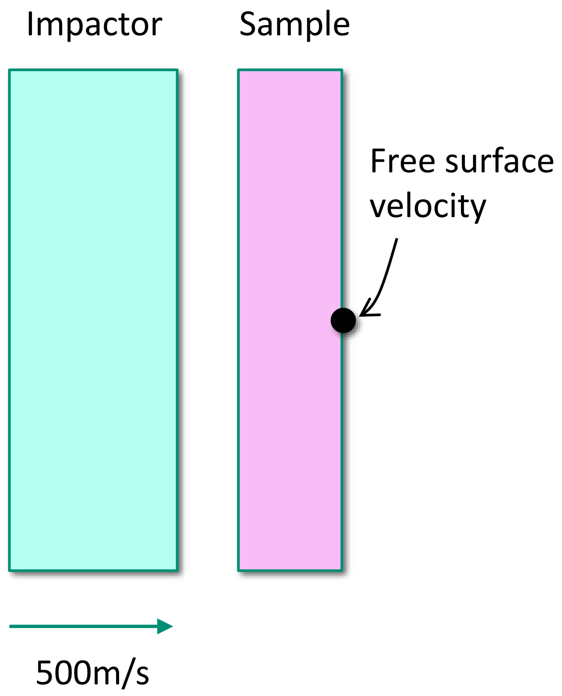
Synthetic microstructure

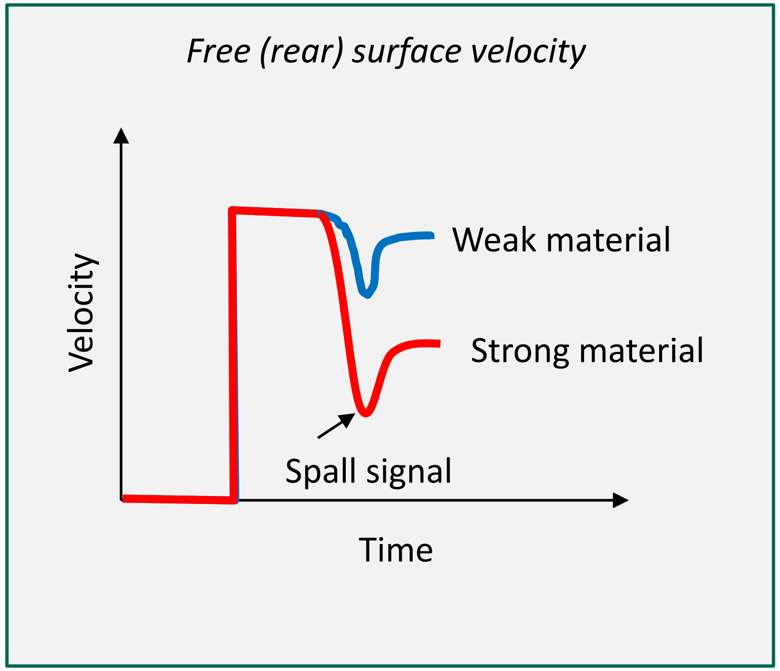


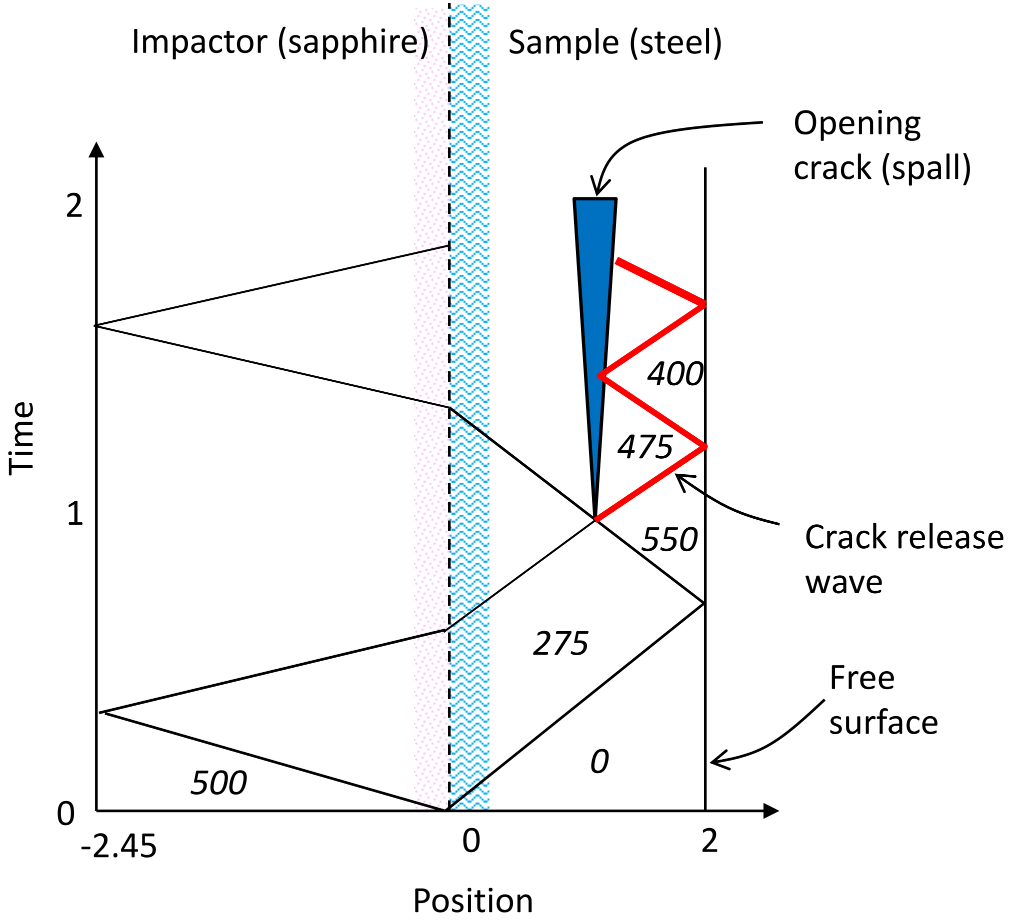
Spall surfaces can be irregular*

*Image: E. Svabenska et al., "Effect of shock wave on microstructure of silicon steel", Surfaces & Interfaces (2020).

Wave reflections lead to strong tension



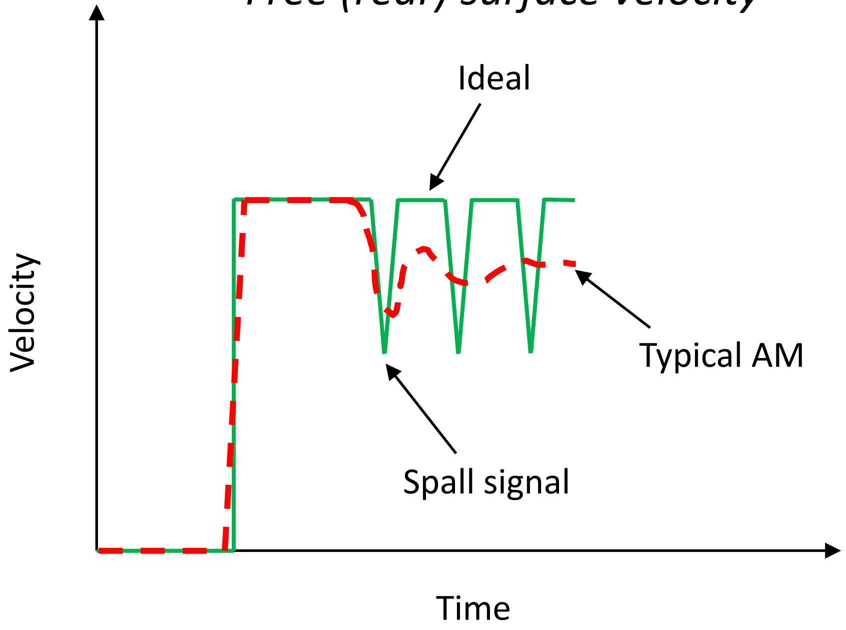


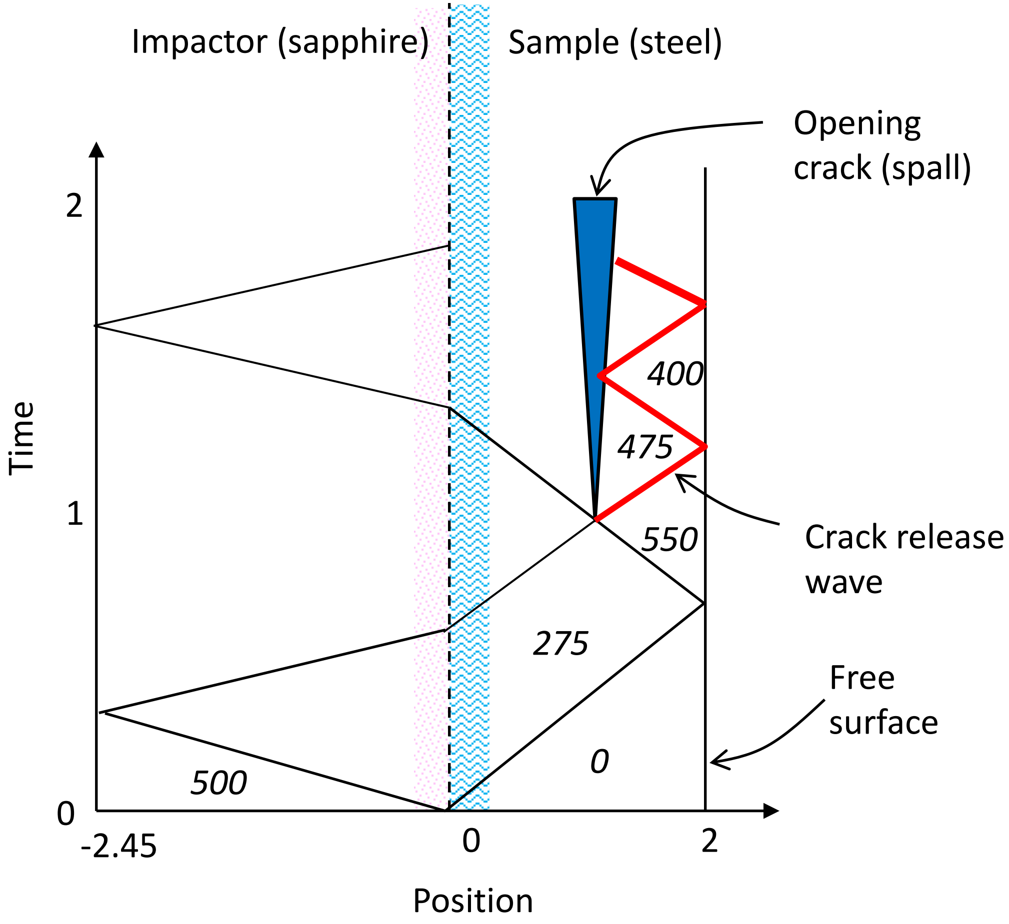


Ideal vs. observed AM spall response

- Ideal:
  - Instantaneous, straight fracture
  - No wave dispersion
- Typically observed:
  - Fracture at a finite rate, complex surface
  - Dispersive shock and reflected waves

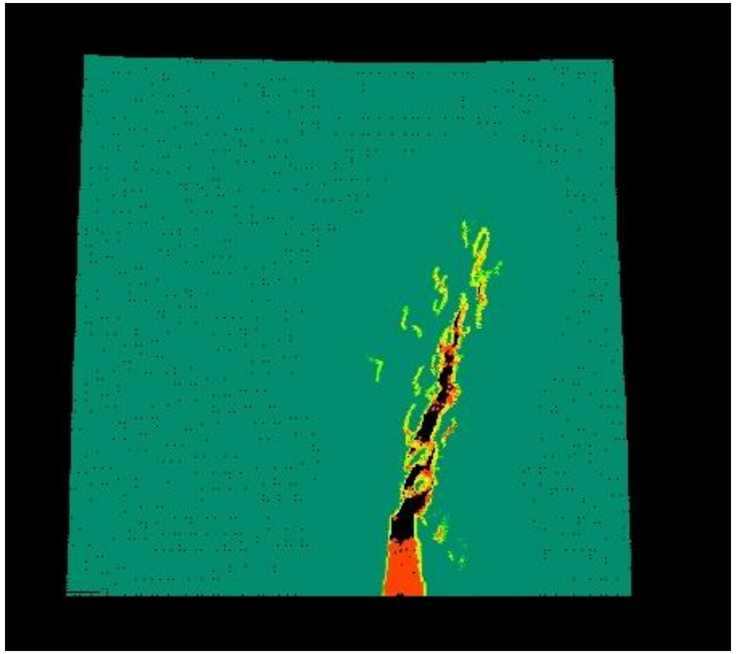
Free (rear) surface velocity



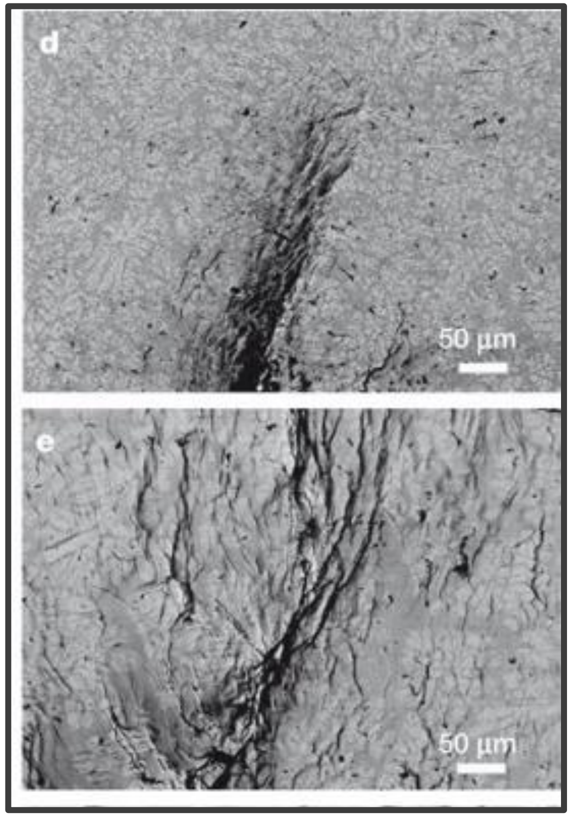


Peridynamics: What it is

- It is a theory of solid mechanics that allows for discontinuities within the basic equations.
- It also allows for long-range forces.



Peridynamic simulation



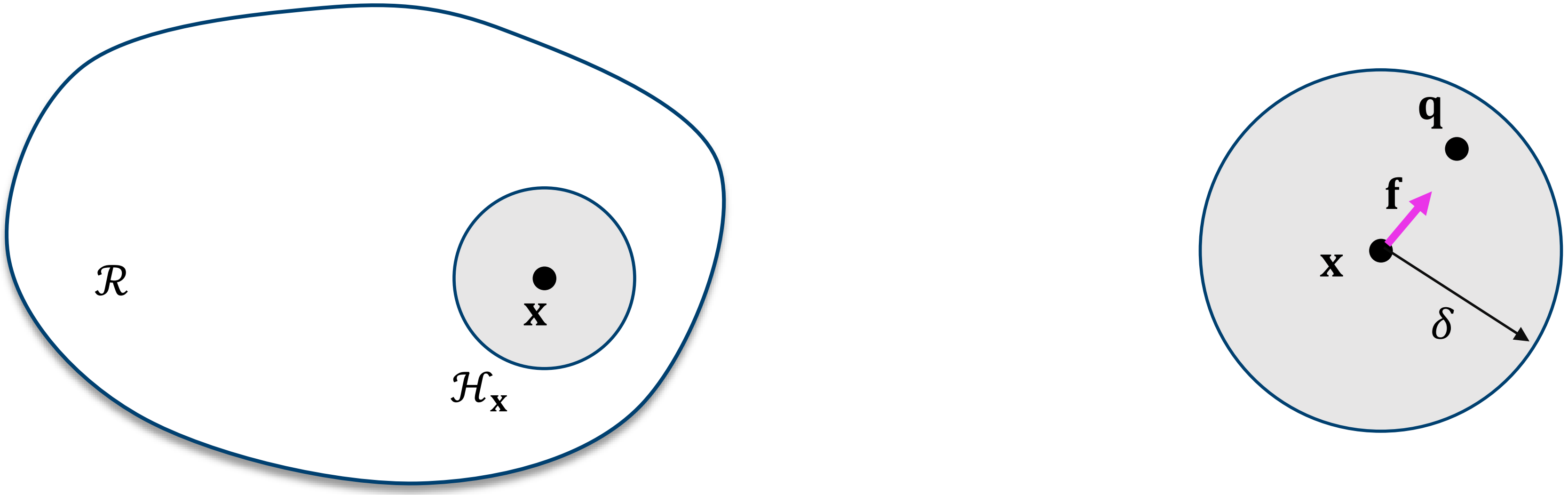
Metallic glass crack tip
Images: Hofmann et al, 2008

Peridynamics background

- Peridynamic momentum balance in 3D:

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{\mathcal{H}_\mathbf{x}} \mathbf{f}(\mathbf{q},\mathbf{x},t)\,\mathrm{d}\mathbf{q} + \mathbf{b}(\mathbf{x},t) \qquad \forall \mathbf{x} \in \mathcal{R},\ t \geq 0.$$

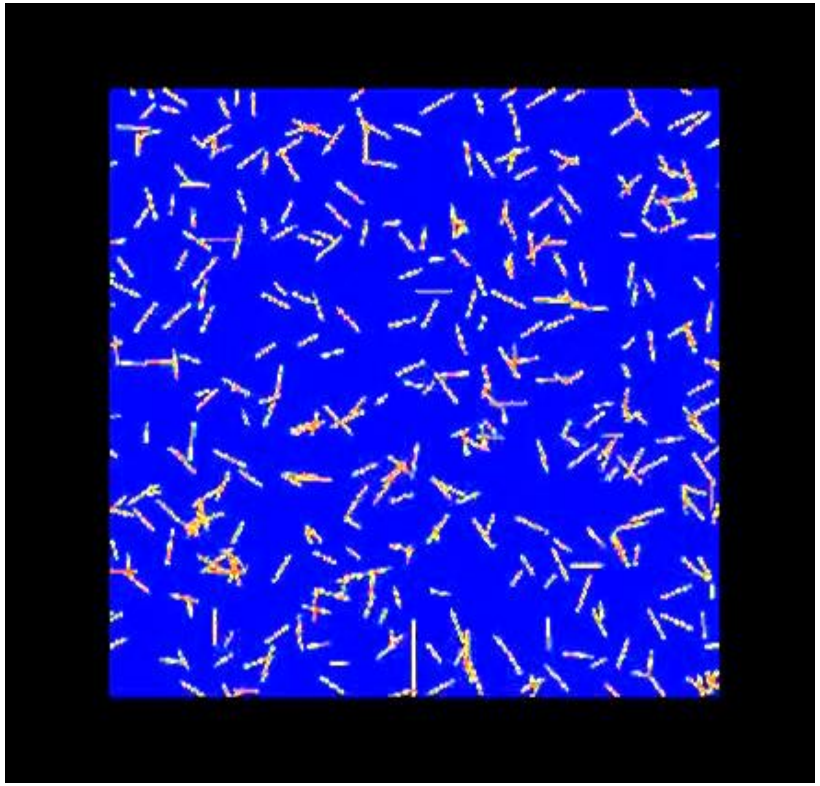
- $\mathbf{f}$ is the *pairwise bond force density* of the *bond* from $\mathbf{q}$ to $\mathbf{x}$.



Peridynamics allows fractures to appear spontaneously

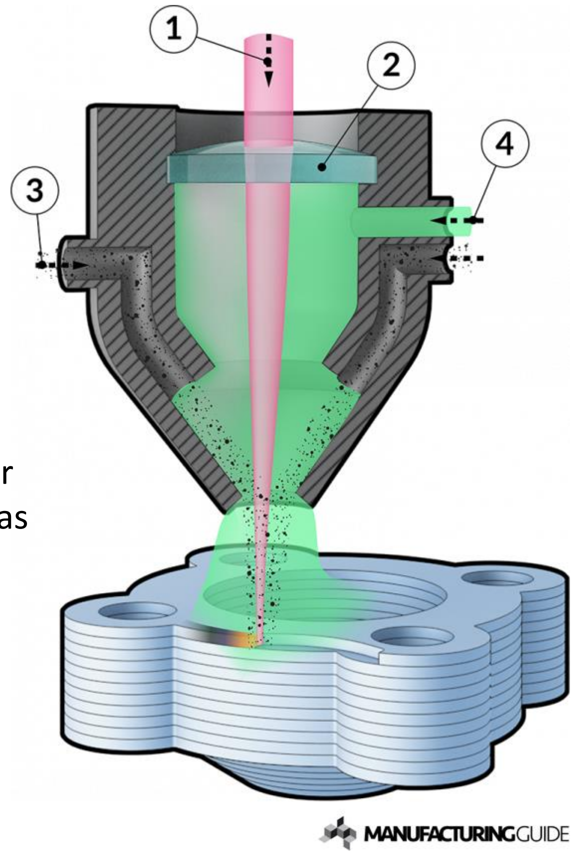
- Integral equations: no need to try to differentiate on a singularity.
- Meshless discretization allows grains to be defined in any shape without a FE mesh.
- Bonds fail according to a damage criterion..
  - which in this case is supplied by the Spall Kinetics Model (more later).

Example of macroscopic failure in a sample with defects
VIDEO



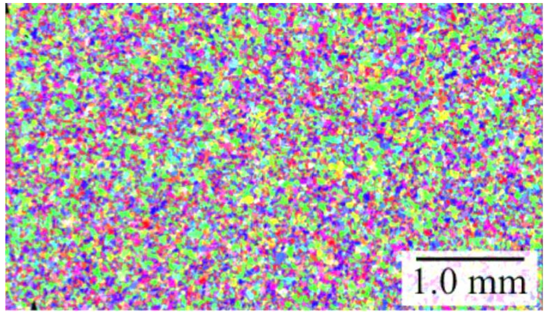
LENS process

- Large, elongated grains are typically formed
- Nonuniform thermal history

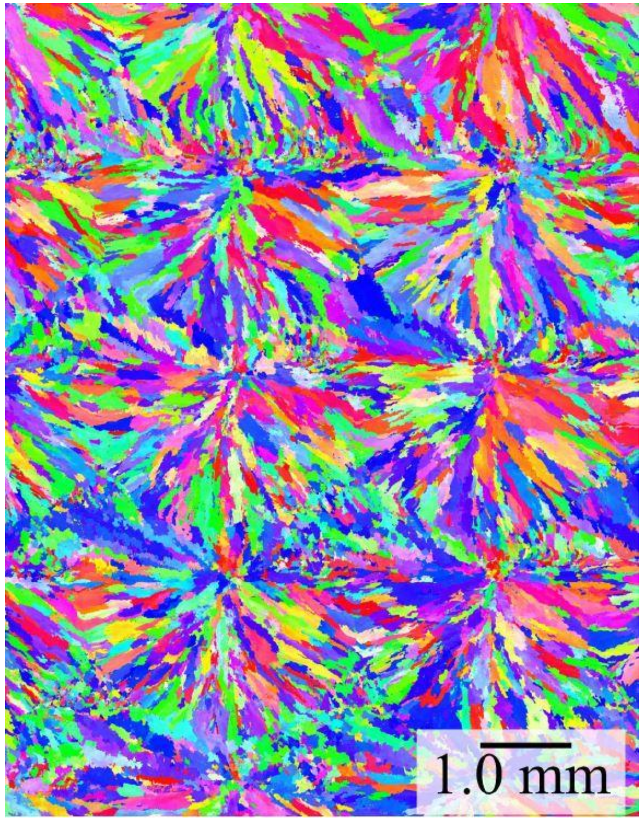


1. Laser
2. Lens
3. Powder
4. Inert gas

Wrought microstructure



Typical AM microstructure



Images:

- https://www.manufacturingguide.com/en/laser-engineered-net-shaping-lens-0
- D. Adams et al, SAND2019-7001 (2019)

Crystal plasticity implementation in peridynamics

- Need to capture:
  - Preferential flow directions determined by the slip planes.
  - Anisotropic elastic response.
- Previous work uses:
  - Correspondence approach to material modeling in peridynamics
  - Decomposition of the deformation gradient into sequential plastic and elastic parts:

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$$

❖ S. Sun & V. Sundararaghavan, *International Journal of Solids and Structures* (2014).
❖ J. Luo, A. Ramazani, & V. Sundararaghavan, *International Journal of Solids and Structures* (2018).
❖ X. Gu, Z. Qing, & E. Madenci, *Engineering Fracture Mechanics* (2019).
❖ A. Lakshmanan et al., *International Journal of Plasticity* (2021).

- Present work uses a simpler but less general approach.

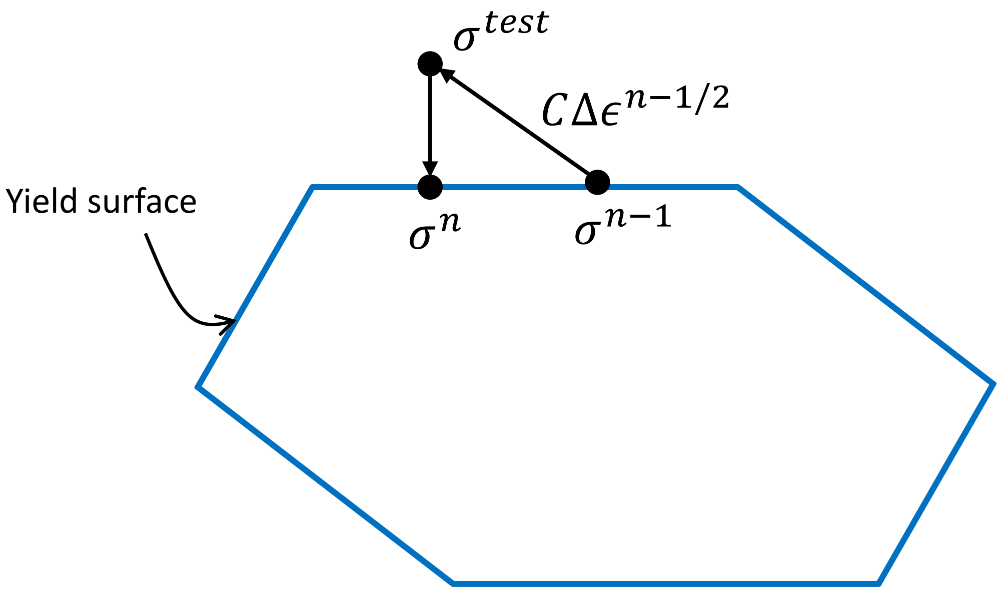
Crystal plasticity model*

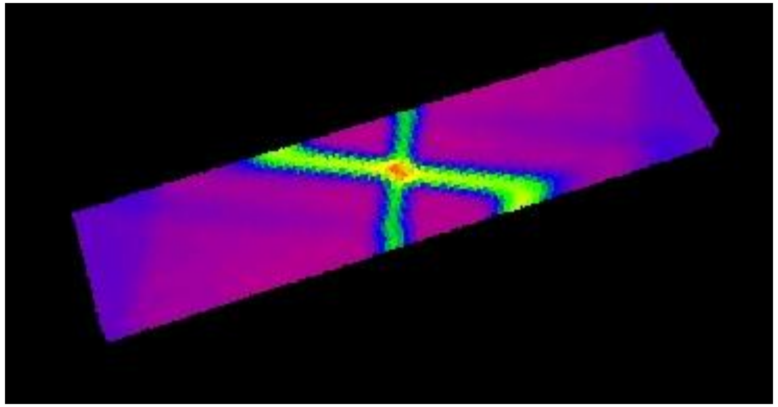
- Analogous to the radial return method
- The slip systems limit the deviatoric stress to a polyhedron in the space of deviatoric tensors.
- A test stress is found from the previous cycle stress and the current stress increment.

$$\sigma^{test} = \sigma^{n-1} + C\Delta\epsilon^{n-1/2}$$

where C is the anisotropic 4th order elasticity tensor.

- The new stress σ^n is the point on the surface closest to the test stress.



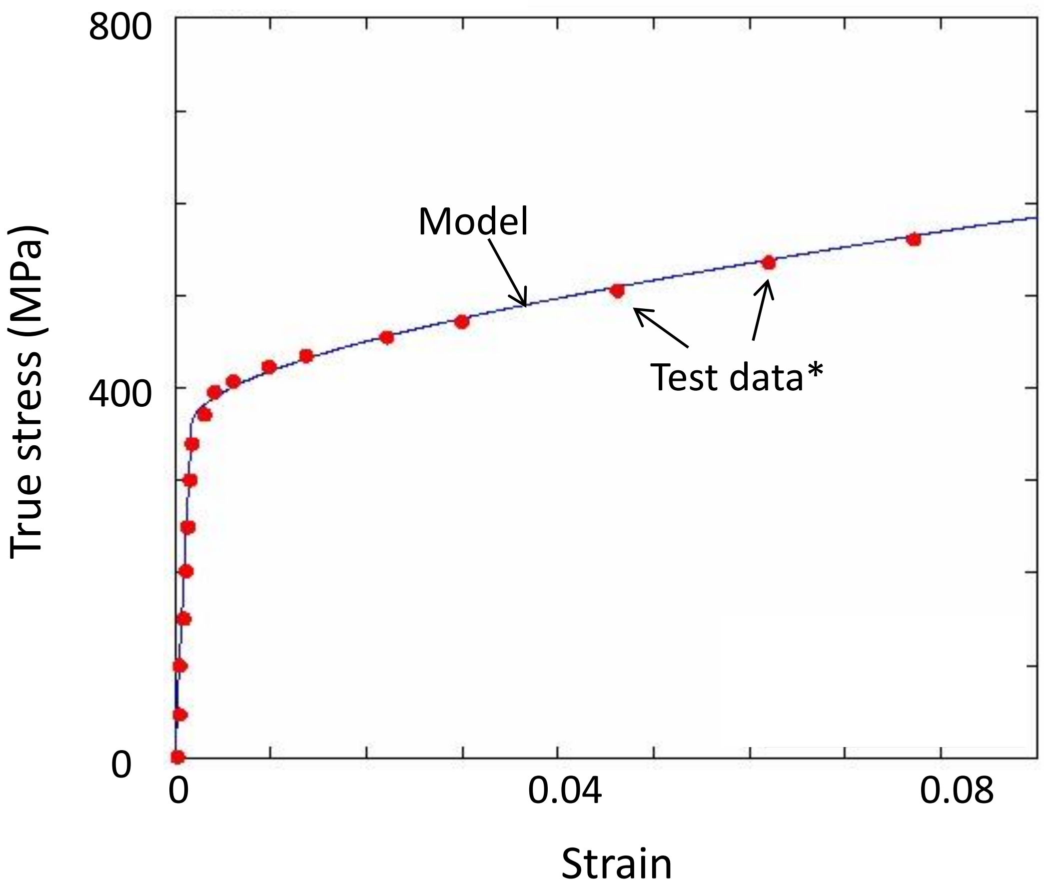


Stretching of a bar with one slip system
Colors show equivalent plastic strain

* P. Maudlin and S. Schiferl, *Computer Methods in Applied Mechanics and Engineering* (1996)

Fit to quasi-static stress-strain data for AM 304L stainless steel

- Sample was additively manufactured with the Laser Engineered Net Shaping (LENS) process.
- The model also contains temperature and strain rate dependence.

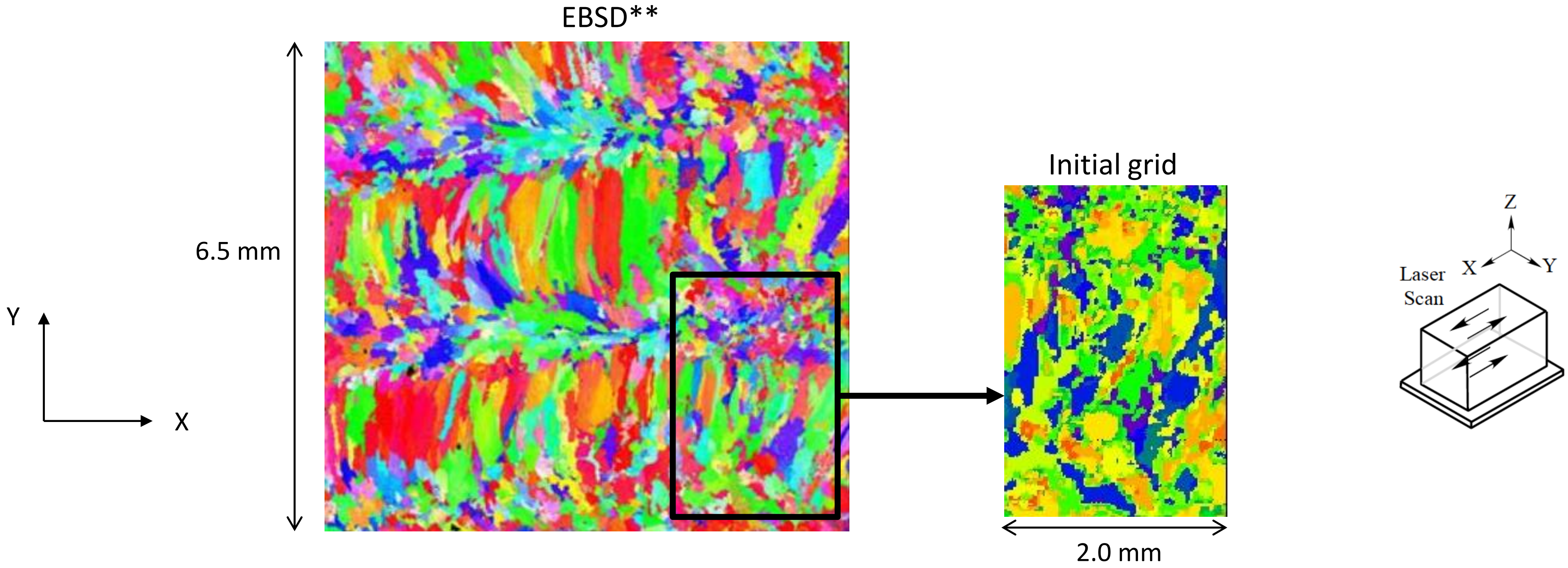


* D. P. Adams et al., Sandia tech report SAND2019-7001 (2019)

Assignment of lattice orientations

- Grains are imported into the model from electron backscatter diffraction (EBSD) images.
- Lattice orientations are assigned randomly using Euler angles.
- These are combined with published anisotropic crystal elasticity data* for 304L SS to compute C for each grain.

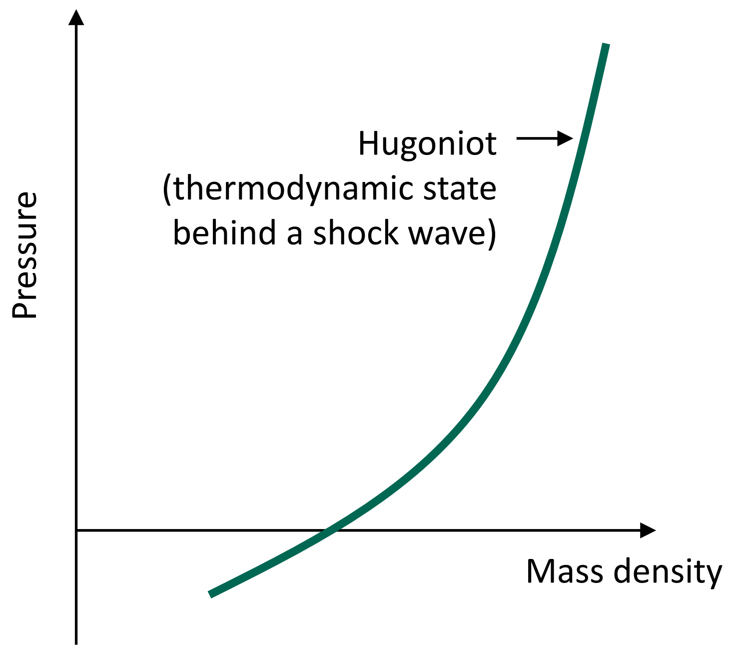
$$C_{11} = 209\text{GPa} \qquad C_{12} = 133\text{GPa} \qquad C_{44} = 121\text{GPa}$$

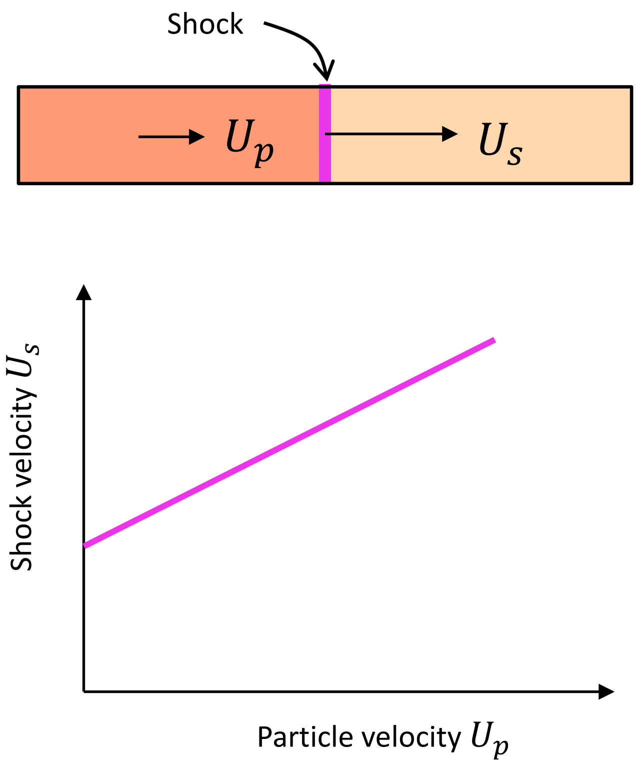


*H. Ledbetter, Physica B+C (1985)
**Image: T. Ruggles

Equation of state

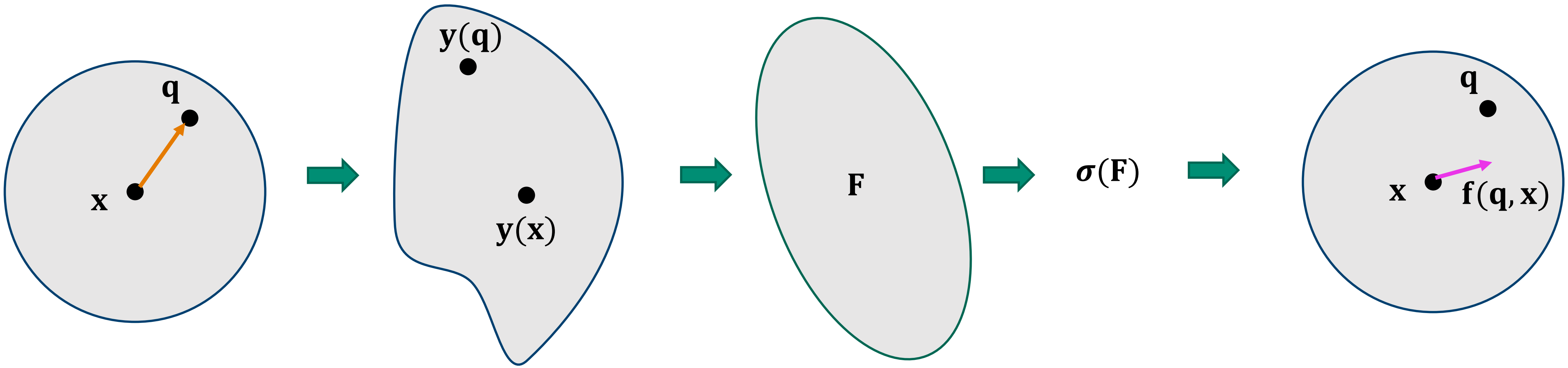
- Add a pressure term to the deviatoric stress found from the crystal plasticity model.
- Mie-Gruneisen EOS:
  - Input: Internal energy density, mass density
  - Output: Pressure, temperature
  - Shock velocity is a linear function of particle velocity behind the shock.
  - Same EOS for all grains





Correspondence material models

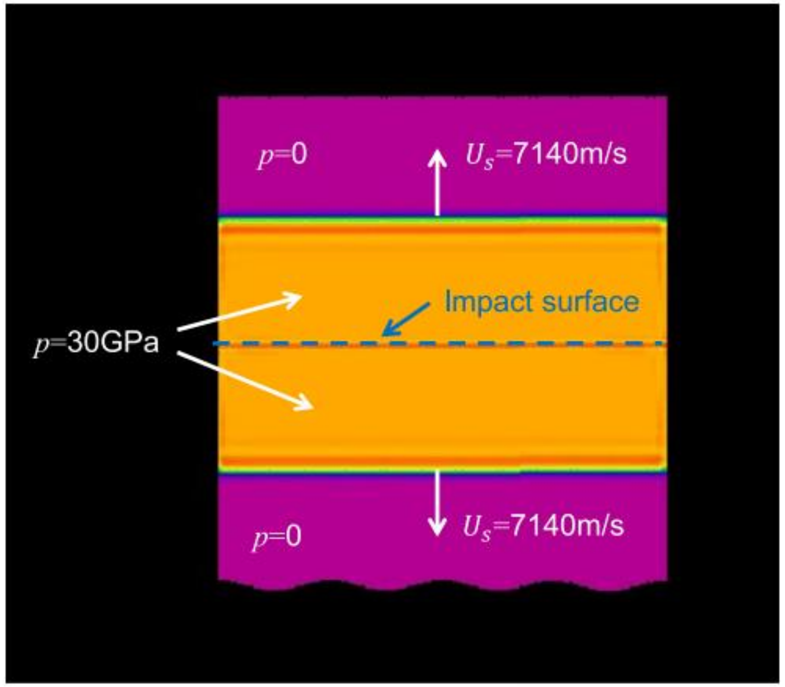
- The above material models are implemented using the correspondence framework.
- This adapts a local material model to the peridynamic framework.
    - The deformation of a family is mapped to an approximate deformation gradient tensor $\mathbf{F}$.
    - A stress tensor $\boldsymbol{\sigma}$ is found from a stress-strain relation.
    - The stress tensor is mapped onto the bonds to provide the bond forces $\mathbf{f}(\mathbf{q}, \mathbf{x})$.



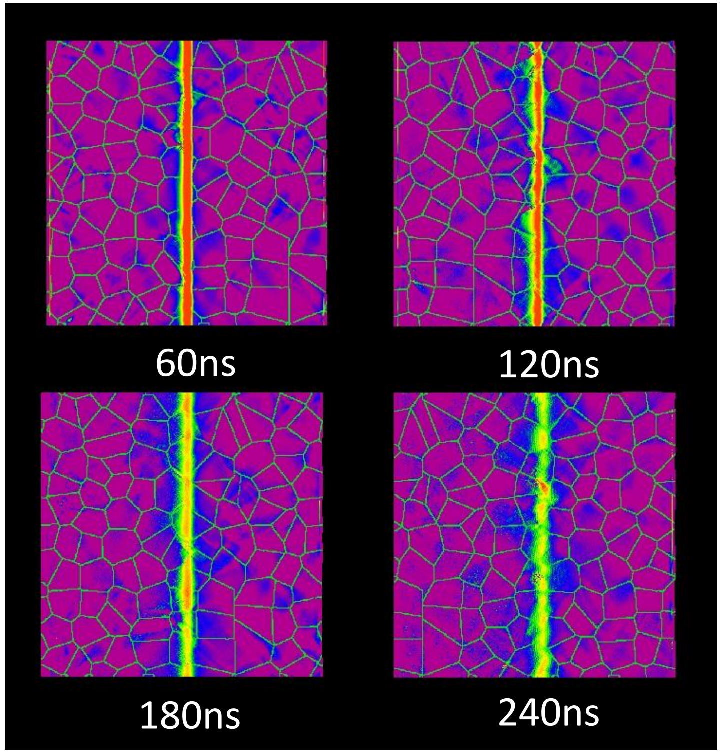
Modeling shock waves in peridynamics

- Von Neumann artificial viscosity is needed.
- Energy balance is treated using a nonlocal version of the first law of thermodynamics.
- For very large deformations, an Eulerian material model formulation is needed.
    - Not used in the present application.

Aluminum impact at 3km/s
Colors show pressure



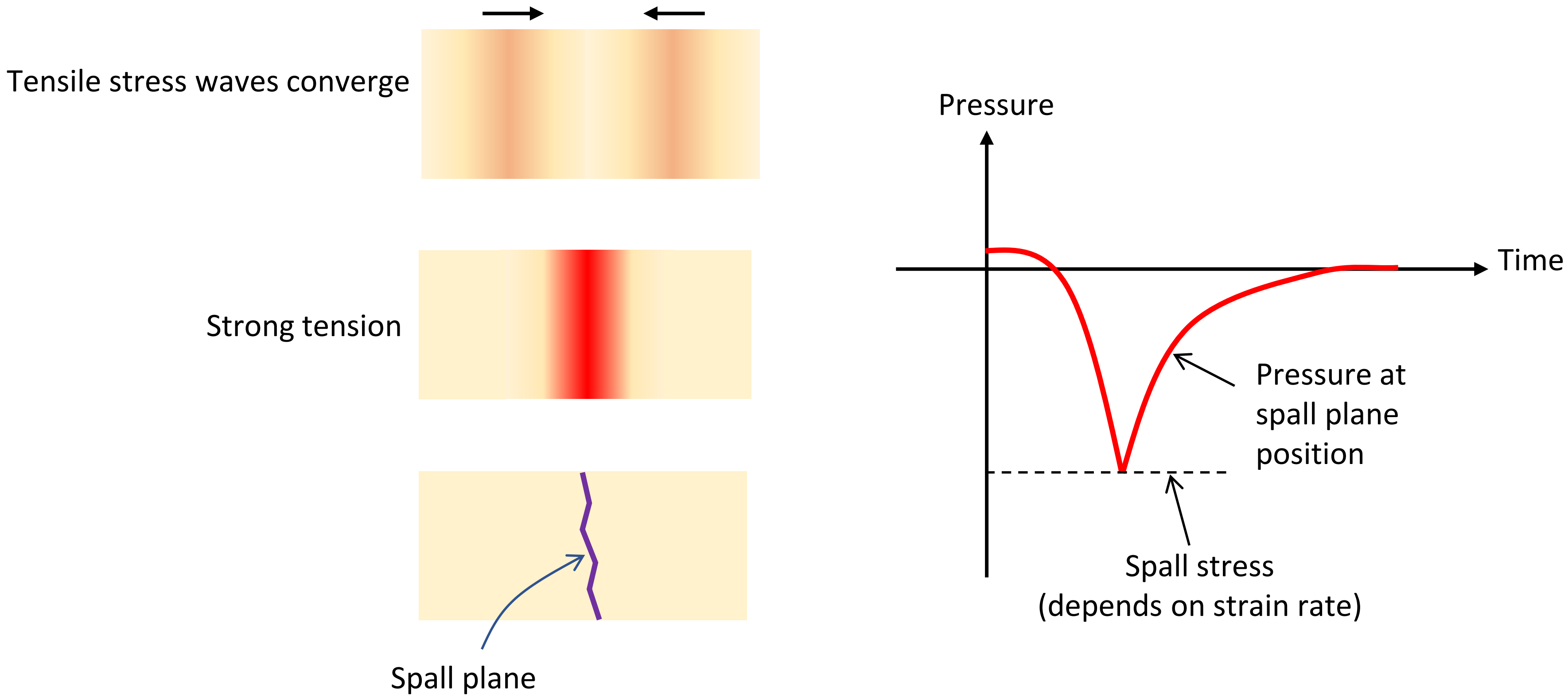
Shock wave in a polycrystal
Colors show strain rate



- SS et al, Modeling shockwaves and impact phenomena with Eulerian peridynamics, *Intl J Impact Engin* (2017)

Spall kinetics model

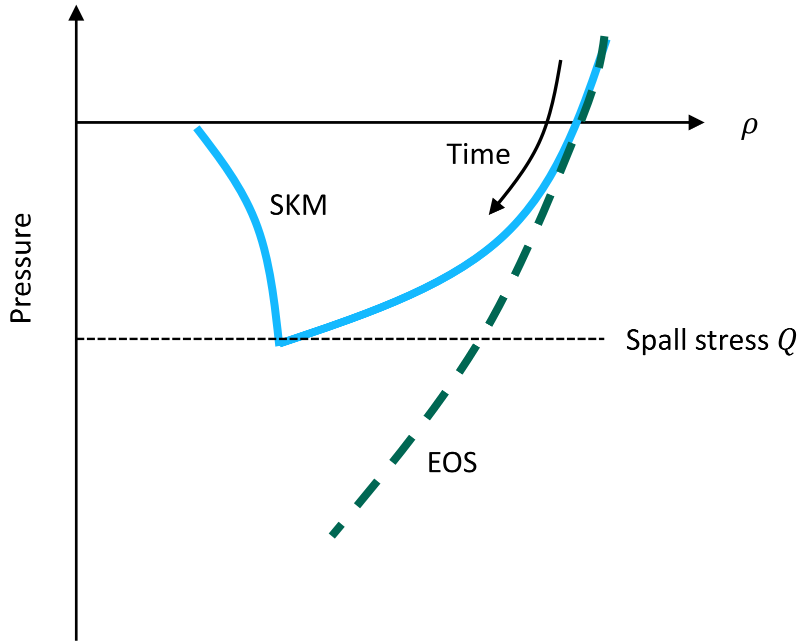
- Failure occurs over a finite period of time.
- The rate of failure depends on the peak tensile stress and strain rate.



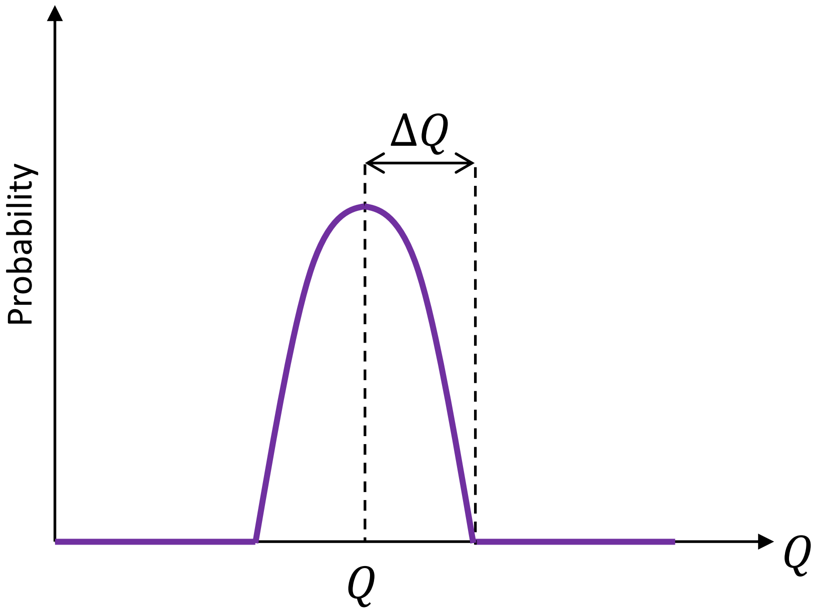
Spall kinetics model: softening and variability

- The EOS is modified to include softening as the critical stress for failure is approached.
- Each grain (from EBSD) is randomly assigned a value of spall stress.

Softening and failure during expansion



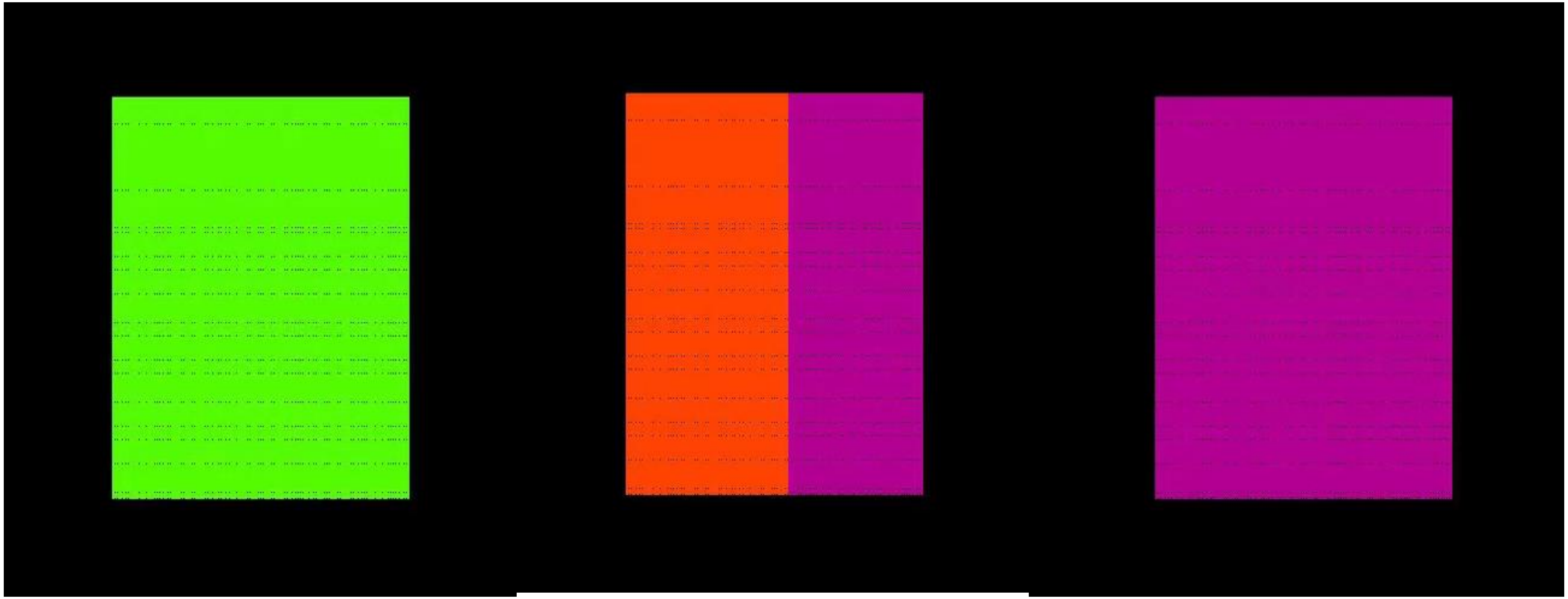
Grain-to-grain variability in spall stress



Impact on AM steel at 247m/s: Videos

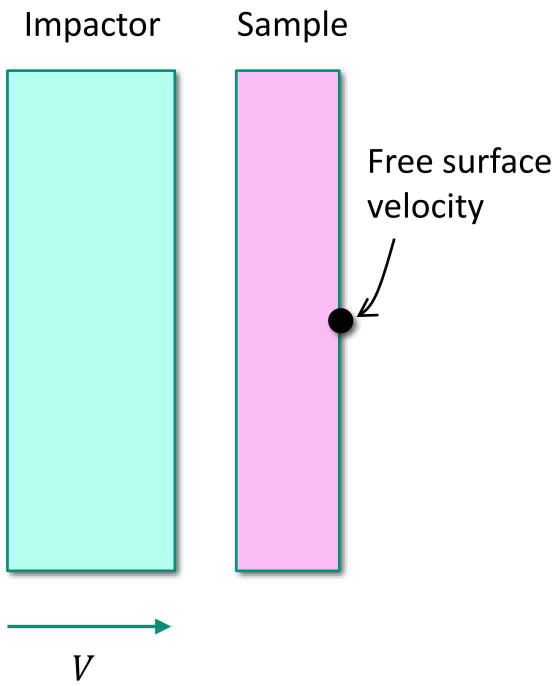
- Total time simulated is 1.8μs.

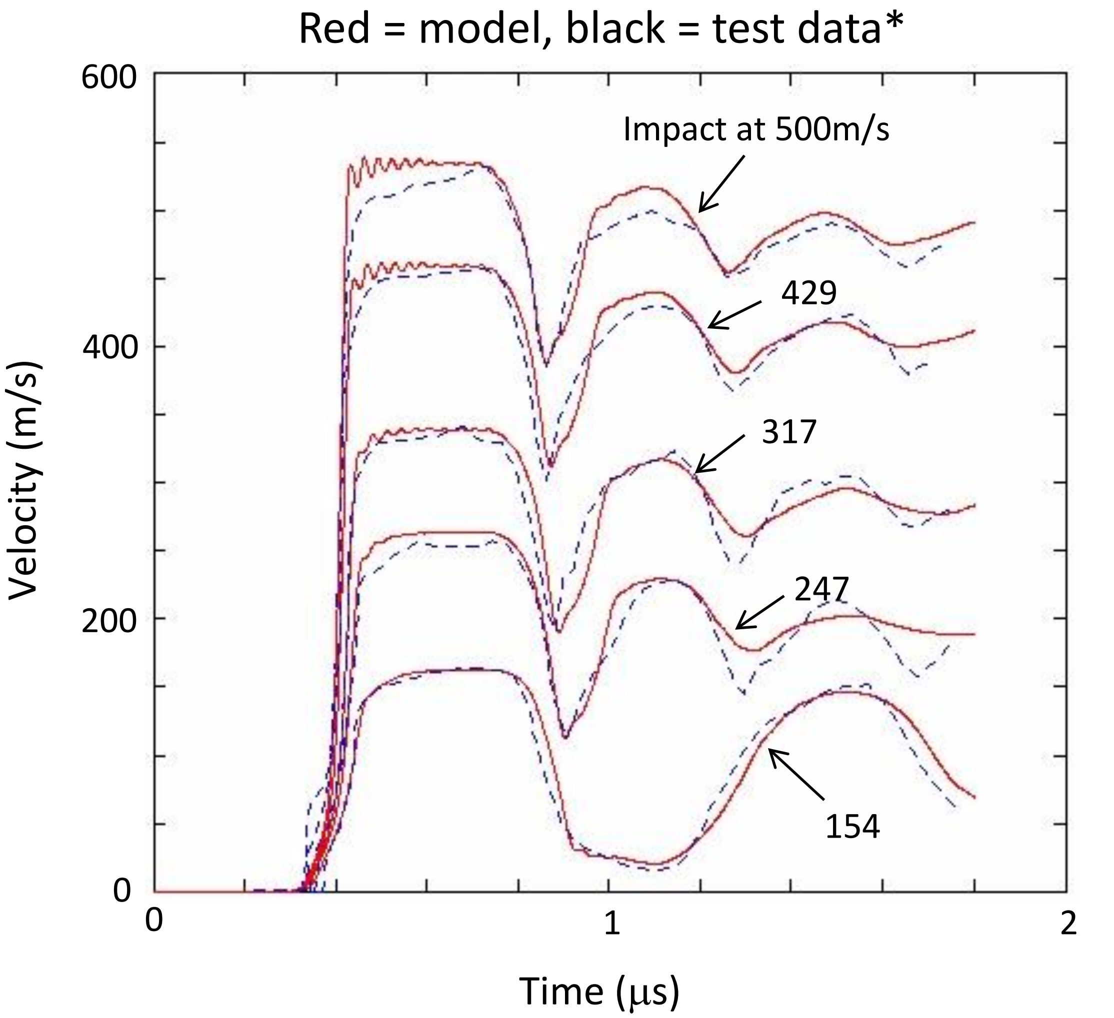
Pressure	X-Velocity	X-Displacement
Red > 4GPa	Red > 250m/s	Red > 0.27mm
Purple < -4GPa	Purple < 0	Purple < 0



Results: Free surface velocity

- Figure compares model results with test data.



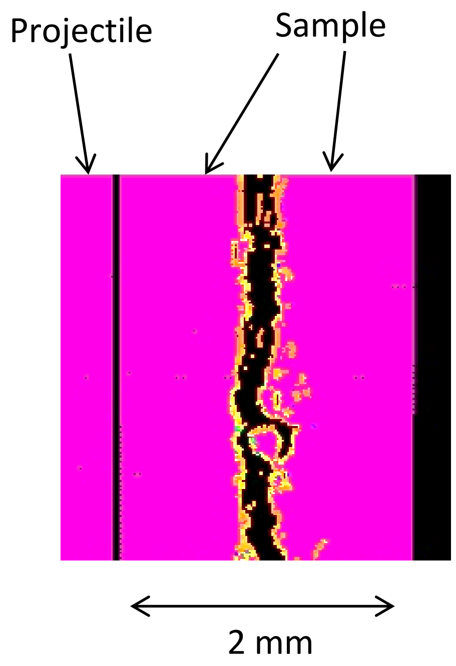


* J. L. Wise et al., AIP Conference Proceedings (2017)
P. E. Specht et al., Sandia tech report SAND2019-12275 (2019)

Spall surface condition

$$V = 317\mathrm{m/s}$$

Experiment*

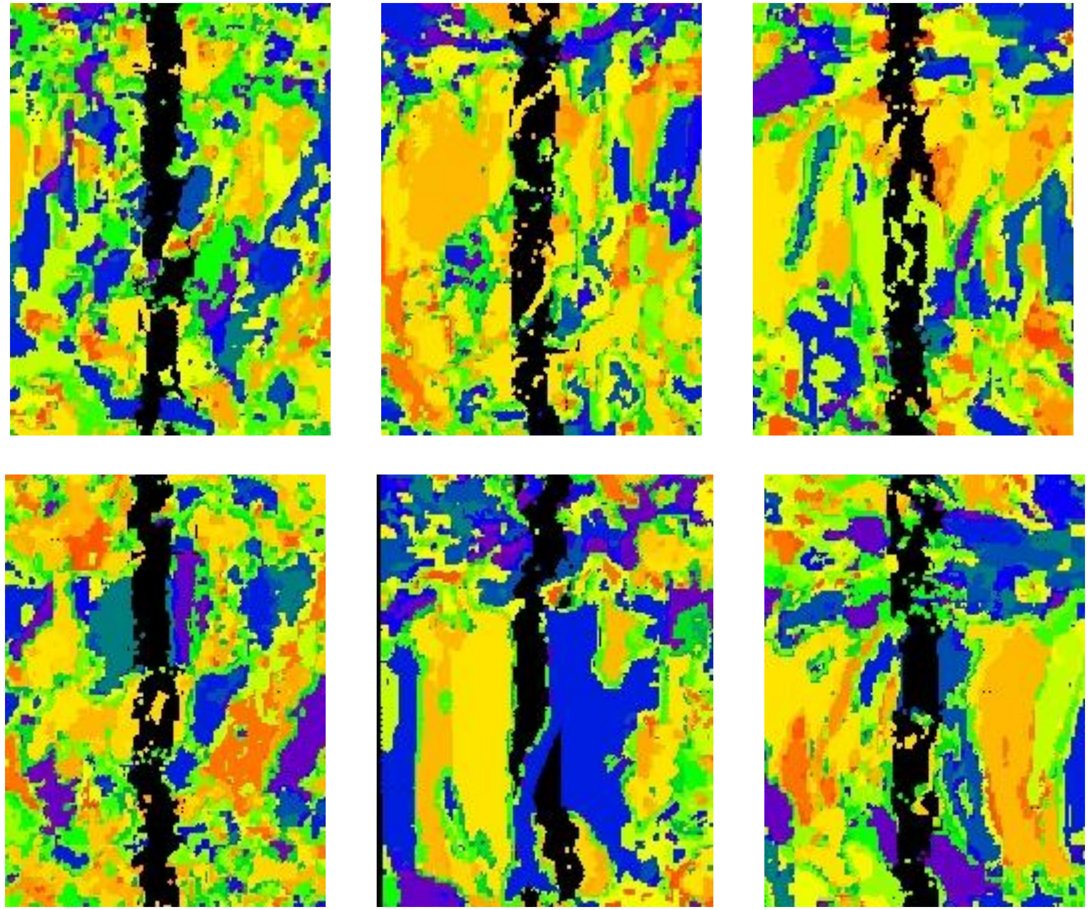


Model
(Colors show damage)

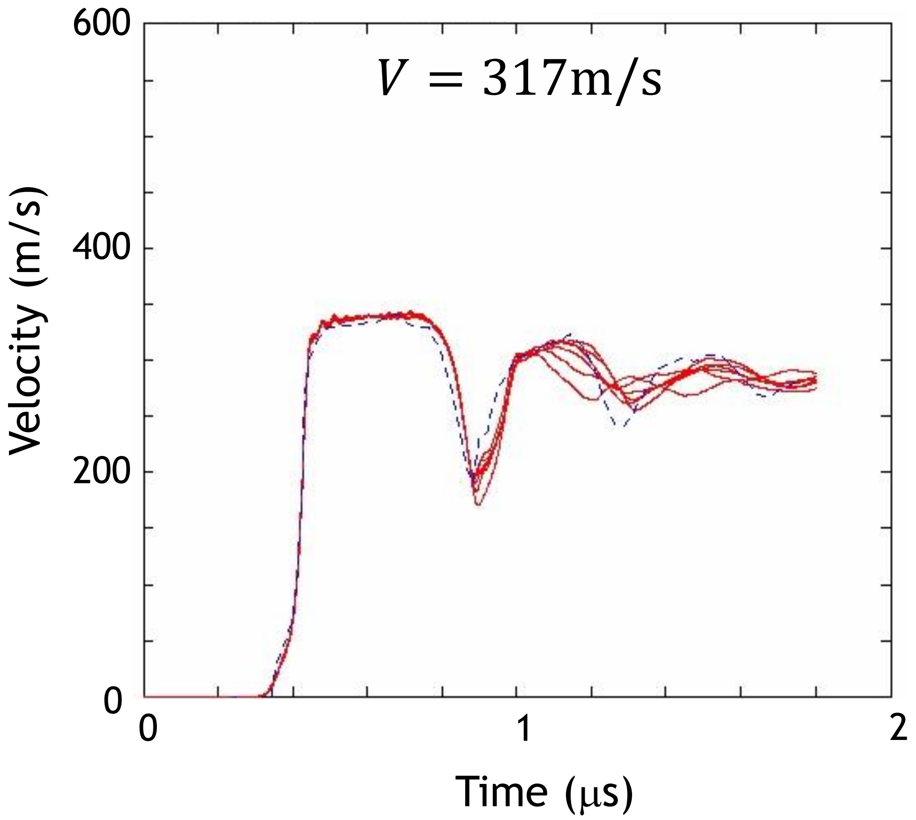
* D. P. Adams et al., Sandia tech report SAND2019-7001 (2019)

Effect of microstructure

- What is the effect of extracting different samples from within the EBSD image?
- Makes some difference at intermediate impact velocities.



Free surface velocity for the 6 samples, all X-cut



Discussion

- The large and distorted grain shapes with AM materials affect the dynamic failure properties.
- A number of new capabilities have been implemented in peridynamics:
  - Crystal plasticity
  - Importing microstructures
  - Spall kinetics model
  - Material variability
- The resulting model reproduces the main features of the test data over a range of impact velocities.

This work: S. Silling, D. Adams, and B. Branch, “Mesoscale Model for Spall in Additively Manufactured 304L Stainless Steel”, *International Journal for Multiscale Computational Engineering* (2023)