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**DOE HQ:** Staci Brown

# Integrating Modeling and Experiments for Strength in Tantalum: A Tri-lab Effort

**J. Matthew D. Lane**
Sandia National Laboratories
APS March Meeting, Los Angeles, March 7th 2018

U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

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# Strength in materials

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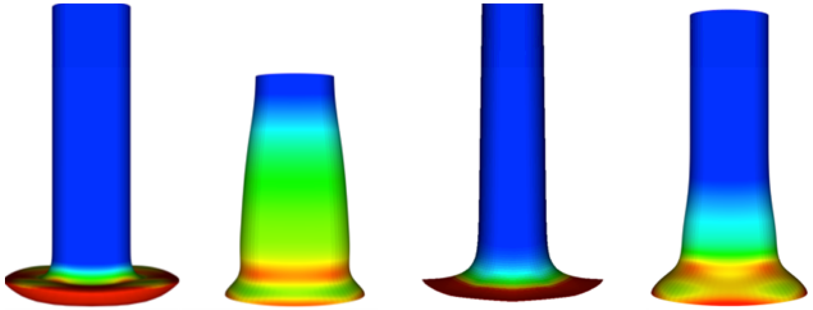
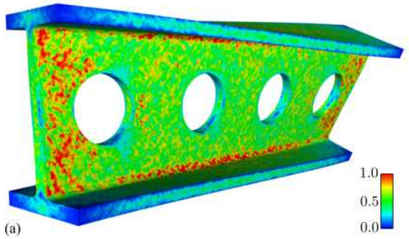


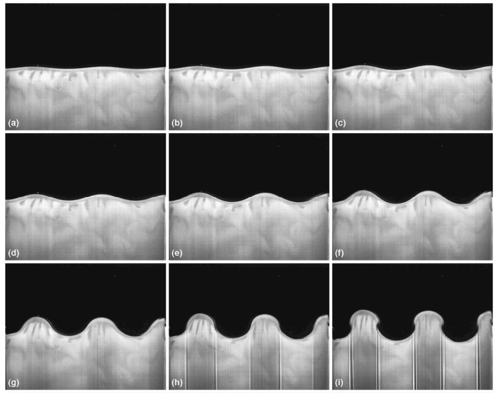


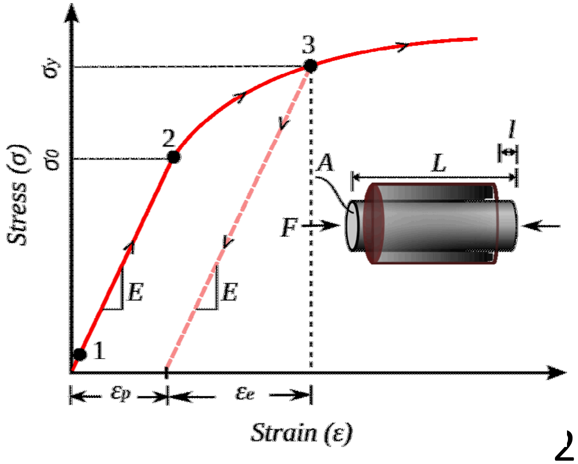

- **Strength** is a measure of a material's ability to sustain an applied load without failure or irreversible deformation.

- Strength response is "universal"
  **but** mechanisms are unique to each system.

- In the hydro code world,
  EOS → controls volume compression
  strength → controls deformability

- ## A few examples
  - Tensile yield stress in entangled polymers
  - Fracture strength in brittle glass
  - Spall
  - **Compressive plastic flow stress in textured polycrystalline metal (ignoring anisotropy)**





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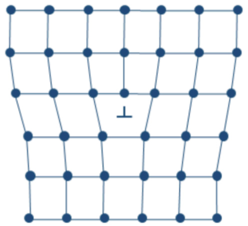
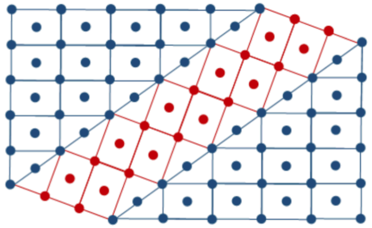
# Dynamic strength in the real world

**Models are complex and it is extremely easy to over generalize.  The devil is in the details.**

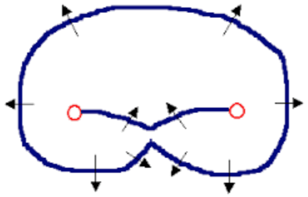

Dislocation

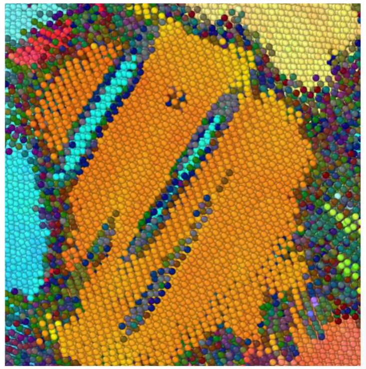

Twin

**Dynamic compression of metals**

Dislocation motion
Dislocation generation
Grain boundary motion
Twinning and stacking faults
Phase transition

Simple experimental measures are an illusion





**Microstructure**

Grain size
Grain orientation
Grain boundary orientation

**History and path dependence**



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# Dynamic strength in the real world

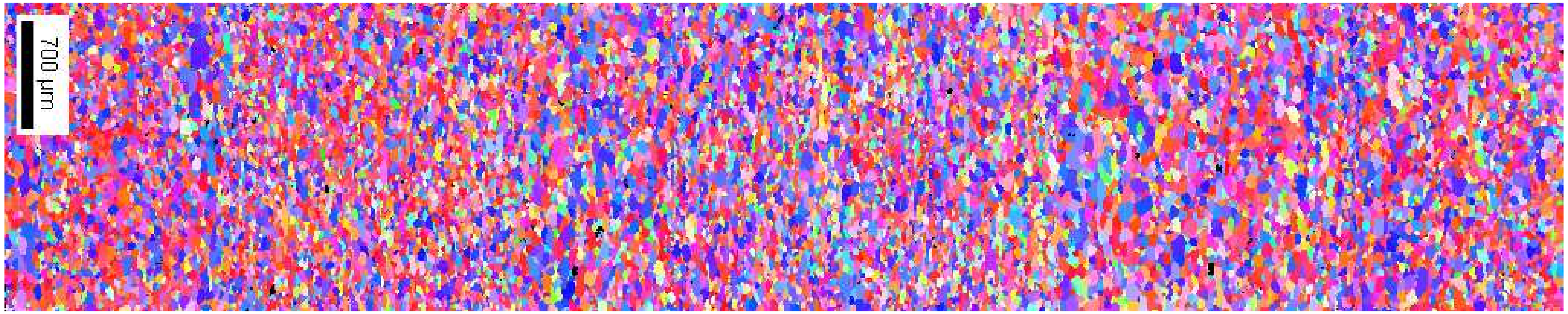
Models are complex and it is extremely easy to over generalize.  The devil is in the details.

**Simple experimental measures are an illusion**

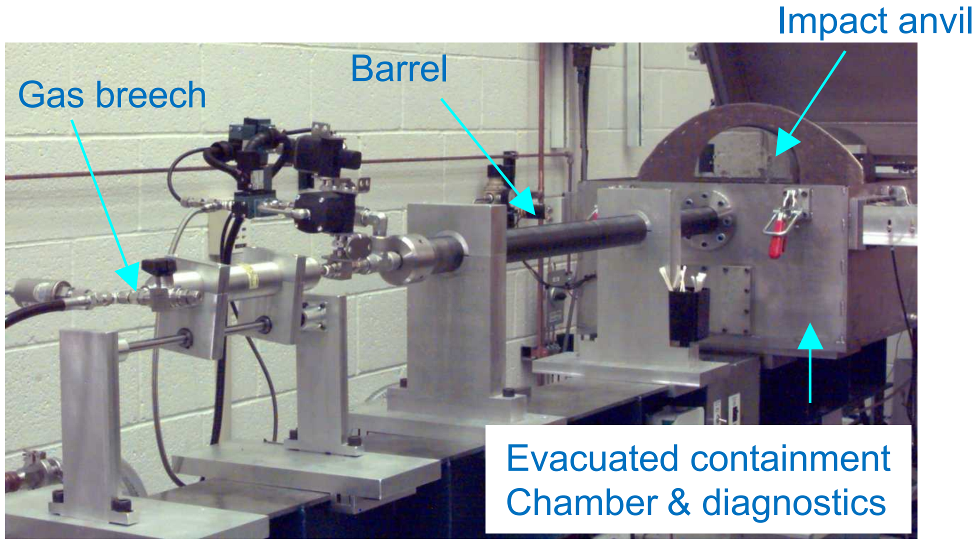
# Why tantalum is an interesting material

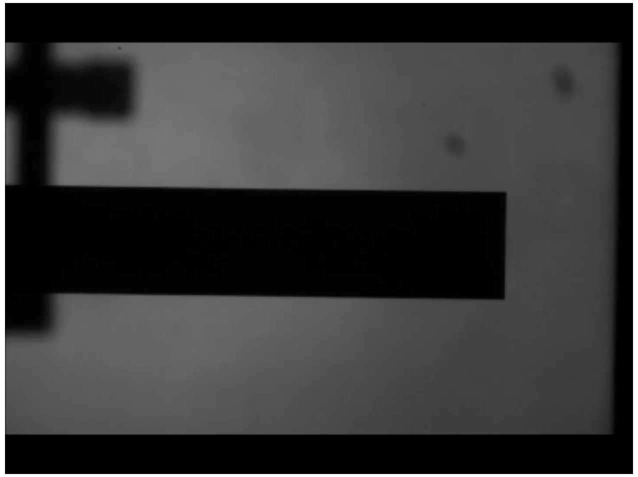
- Tantalum, as a high-Z **body-center-cubic (bcc) metal** with **no experimentally observed high-pressure phase transitions** up to 350 GPa, has potential use a standard for high-pressure studies.  But, its properties depend on poorly understood elastic/plastic and dislocation dynamics. High melt temperature of 3290 K.

- A number of recent papers have identified unusual shock and ramp wave response in tantalum, especially in extracting dynamic strength response
  - Strength in single-crystal - Comley, et al. PRL, 110 115501 (2013)
  - Strength at high-pressure and strain-rate -  Brown et al. JAP, 115 043530 (2014)
    Brown et al. JAP, 114 223518 (2013)
  - High-pressure ramp to 330 GPa - Davis et al. JAP, 116 204903 (2014)
  - Grain-size effects on plastic flow - Park et al. PRL, 114 065502 (2015)




# Taylor Impacts experiments



$V_0 = 146.2 m/s$

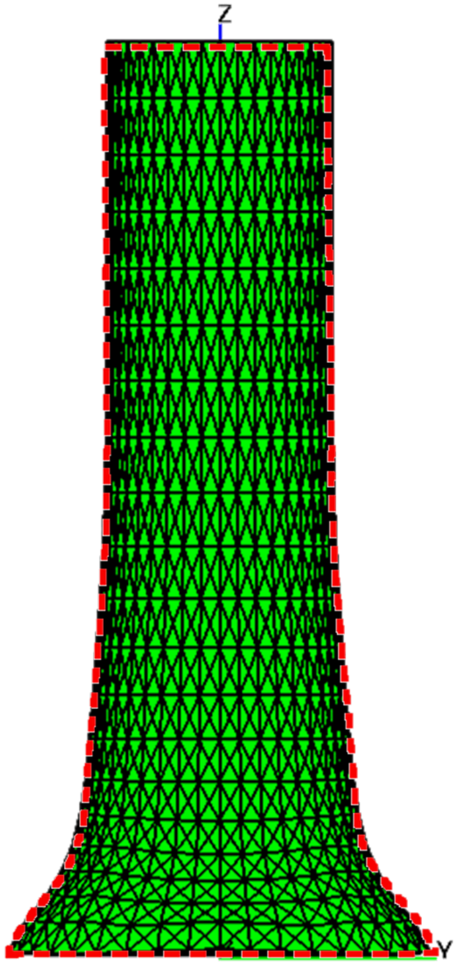
**Los Alamos National Lab**
Shuh-Rong Chen and Rusty Gray

| | |
|---|---|
| Peak pressure: | 1 to 3 GPa |
| Strain rate: | $10^4$ 1/s |

**Experiment Description:**
- Gas guns throw rod at a steel anvil at ~150 m/s

**Measurement:**
- The primary experiment output is the final shape of the rod.

**Strength Determination:**
Strength model validated by comparison with simulated final foot radius, rod height & deformed profile.



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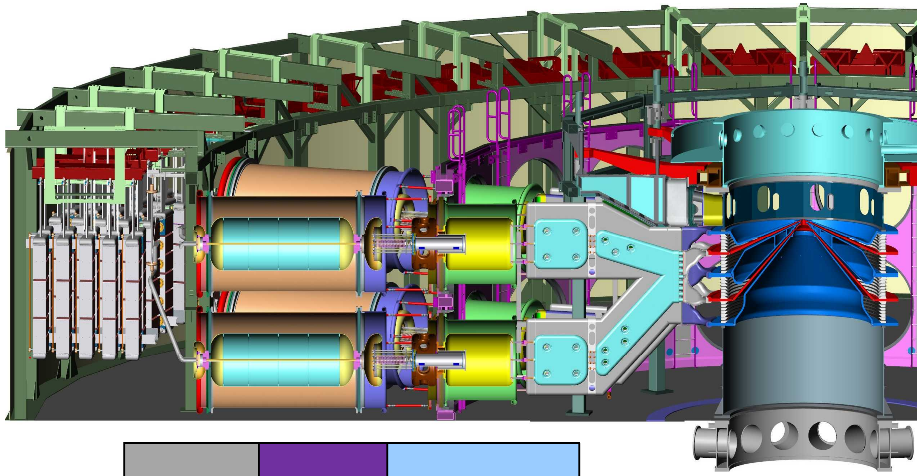
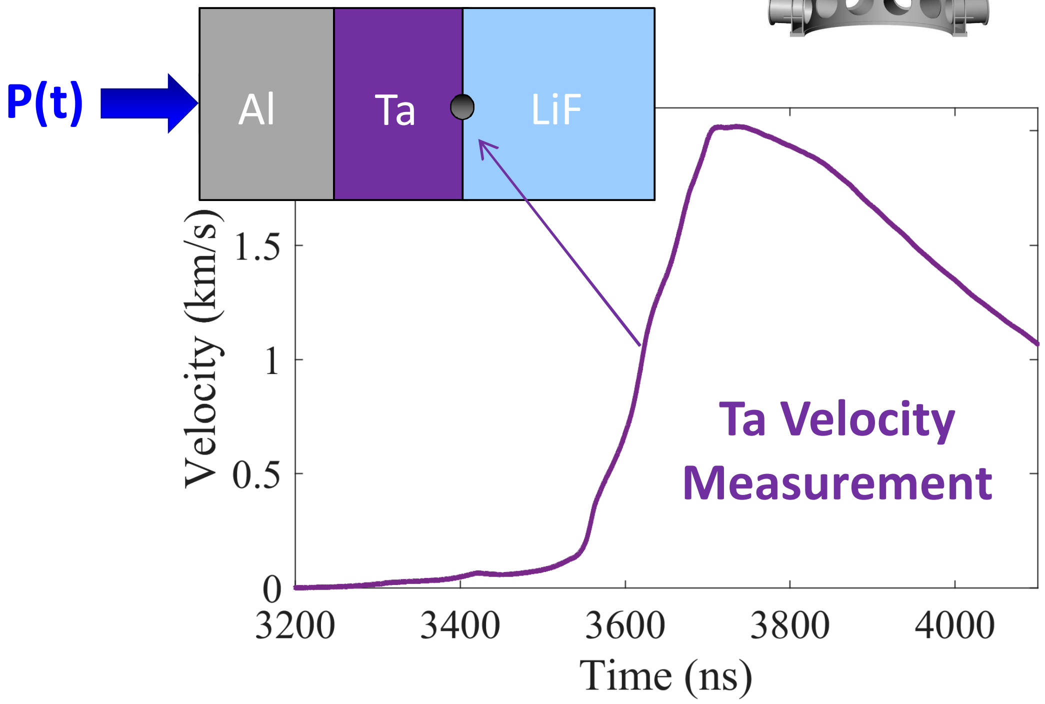
# Z machine ramp-release






**Sandia National Labs**
Justin Brown

| | |
|---|---|
| Peak pressure: | ~50 to 380 GPa |
| Strain rate: | $10^5$ 1/s |

**Experiment Description:**

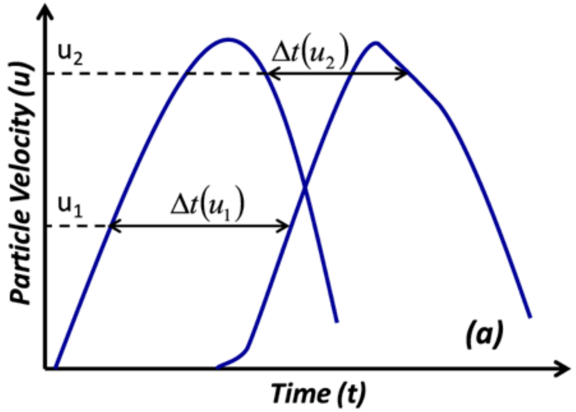
- Pulse-power driver 22 MA

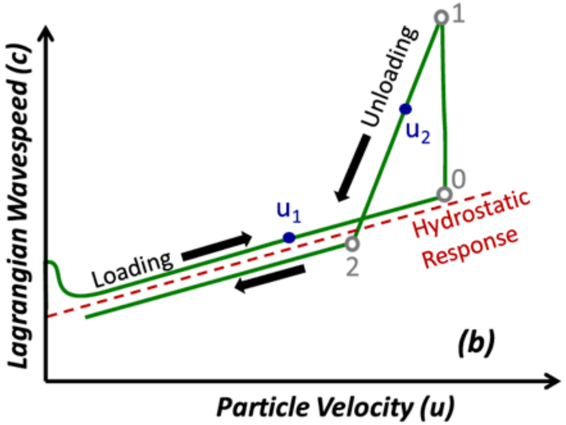
**Measurement:**

- The primary output is back surface time-resolved velocity profiles.

**Strength Determination:**

Strength model 1D wavespeed analysis to infer strength from the shear stress, $\tau$



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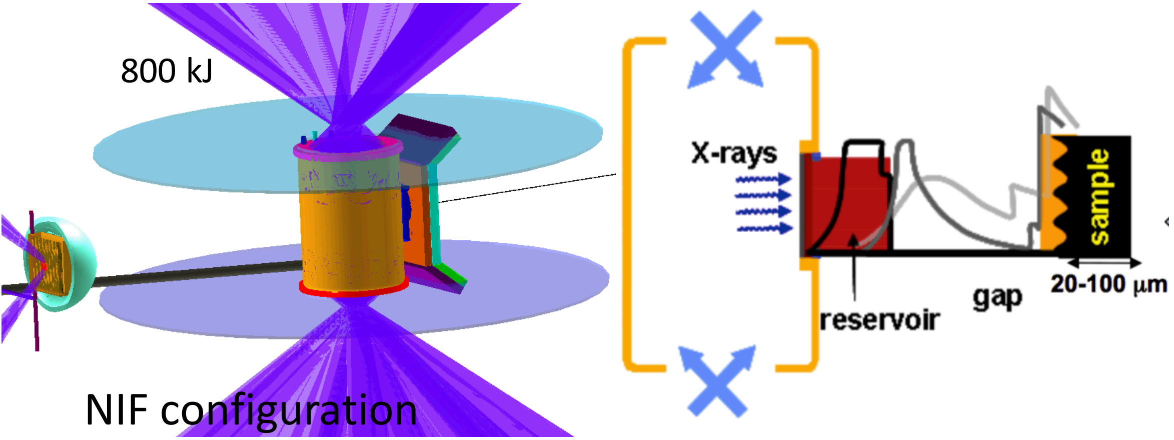
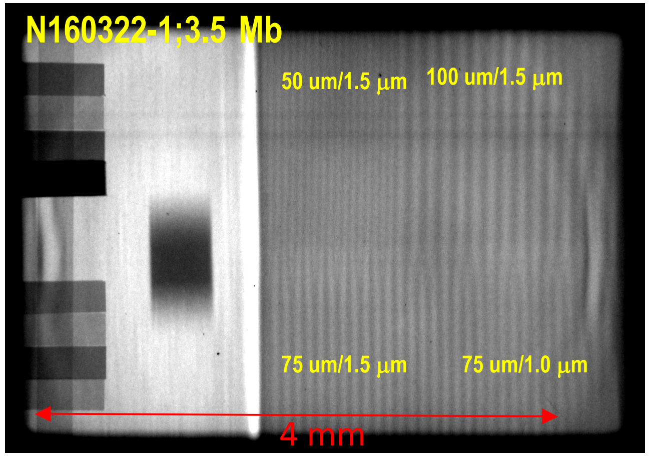
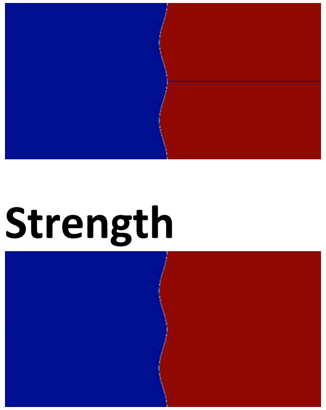
# Rayleigh-Taylor growth: NIF/Omega lasers




Strength will suppress RT growth

No Strength



Strength

Movies courtesy: http://gfs.sourceforge.net

**Lawrence Livermore National Lab**

Hye-Sook Park

| | Omega | NIF |
|---|---|---|
| P: | ~50-100 GPa | ~350-500> GPa |
| $\dot{\varepsilon}$ : | $10^7$ 1/s | $10^7$-$10^8$ 1/s |

**Experiment Description:**

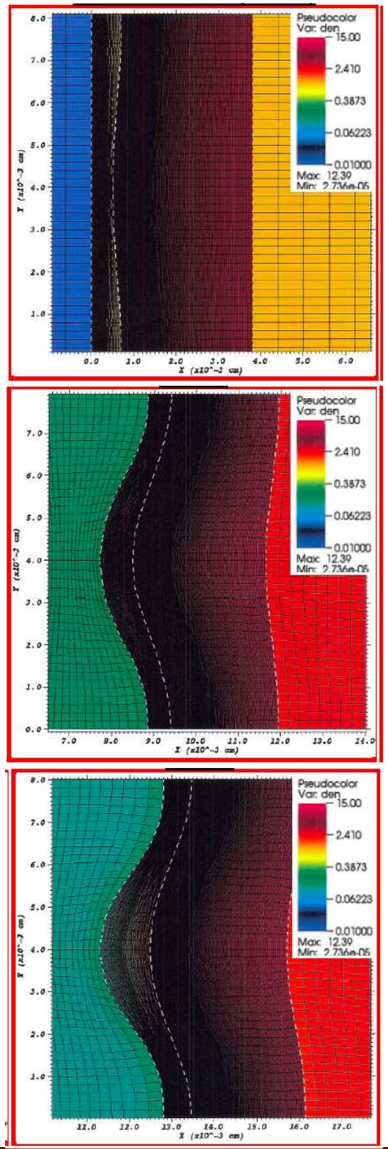
- 800 kJ of laser energy focused to a small cylinder X-ray hohlraum

**Measurement:**

- Experiments output is the face-on radiograph of the ripple

**Strength determination:**

Strength model validation by comparison with simulated growth factor.





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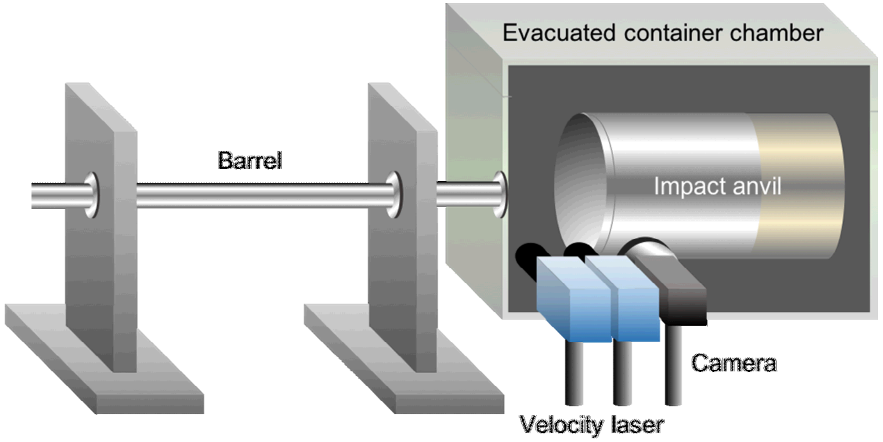
# Integrated modeling and experiment

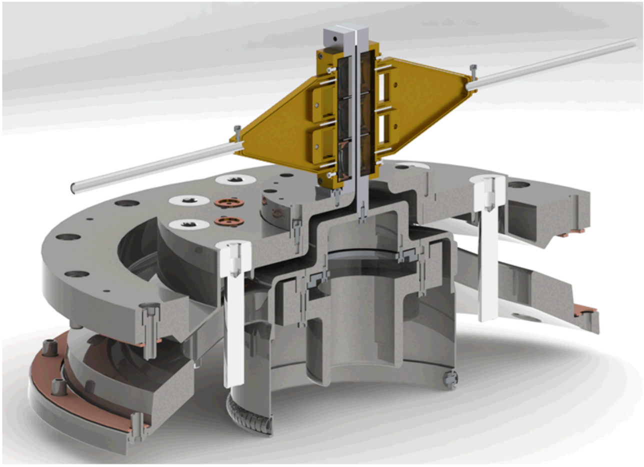
None of these experiments actually measure strength, directly. They allow us to test existing models and propose improvements through experience.

Three labs had at least three models which ran (sometimes exclusively) on each labs three hydro codes. Such that each was well suited to address the conditions found in each specific regime of pressure and strain-rate.

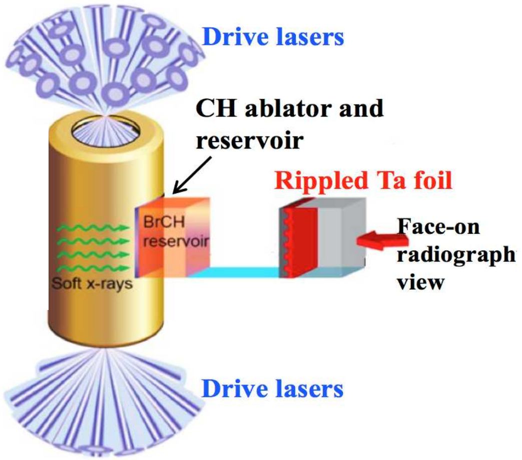
Taylor Impact (LANL)




Z ramp/shock (SNL)



NIF/Omega RT growth (LLNL)



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# Tri-Lab Ta Strength Collaboration

Sandia National Laboratories

Begun in FY17 and continuing into FY18, the group consists of a broad spectrum of experimentalists, modelers and managers from each of the three DOE NNSA labs.

Goals

1. Collect  and share experimental data across each platform
    - A single well-characterized material - eliminate microstructural variation
2. Jointly model each others experiments
    - Implement an improved common model (PTW Common Model)
3. Work to improve connections and overlap for robust cross-platform comparisons
    - New experiments in the pressure and strain rate ranges between drivers



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# Strength models, old and new

**SG** (Steinberg-Guinan, 1980) – A : incorporates strain-rate, and pressure dependence through the shear modulus

**SGL** (Steinberg-Guinan-Lund, 1989) – Extension of SG model to incorporate low strain-rates and bcc materials

**PTW** (Preston, Tonks, Wallace, 2003) – A phenomenological model: incorporates work ha e law at lower strain rates; above $10^9$ 1/s u shocks to calculate flow stress rate dependence.

Common Model

**KP** (Kink-pair Lim, et al. 2016) – A model b ation-based crystal plasticity model describing temperat rate dependent flow stresses in BCC metals. The kink-pair the e stress required to move a screw dislocation over the Peierls iginated in low strain rate regime.

**LMS** (Livermore Mul l, Barton et al., 2011,2013) – A physics-based model which integrat tronic structure calculations, molecular dynamics, dislocation dynamics, and polycrystal homogenization to inform functional forms and parameters for continuum-scale models. Developed in high rate regime.

Lab-specific Models

$$\sigma_y^{SGL} = \frac{\mu(P,T)}{\mu_0}\left(\sigma_T(\dot{\epsilon},T) + \sigma_A f(\epsilon)\right)$$

$$\dot{\epsilon}_p = \left\{\frac{1}{C_1}\exp\left[\frac{2U_K}{kT}\left(1-\frac{Y_T}{Y_P}\right)^2\right] + \frac{C_2}{Y_T}\right\}$$

$$\sigma_y^{PTW} = \hat{\tau}_s + \frac{1}{p}(s_0 - \hat{\tau}_y)\ln\left[1 - \left[1 - \exp\left(-p\frac{\hat{\tau}_s - \hat{\tau}_y}{s_0 - \hat{\tau}_y}\right)\right] \times \exp\left\{-\frac{p\theta\psi}{(s_0 - \hat{\tau}_y)\left[\exp\left(p\frac{\hat{\tau}_s - \hat{\tau}_y}{s_0 - \hat{\tau}_y}\right) - 1\right]}\right\}\right]$$

$$\sigma_y^{KP} = M\left(\min\left(\tau_{EI}^*, \tau_{LT}^*\right) + \bar{\tau}\right)$$



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# Combining platforms

| Platform/ loading | Taylor Cylinder* | Gun (FS13) Shock-release | Gun (FS18) Shock-release | Z (2516)* Ramp Release | Omega* RT | Z (2488) Shock-Ramp Release | Z (3103)* Ramp Release | NIF* Ramp Release |
|---|---|---|---|---|---|---|---|---|
| Peak Pressure (GPa) | 3 | 52 | 101 | 106 | 130 | 240 | 380 | 350 |
| Sample Temperature (K) | 305 | 700 | 1800 | 640 | 1200 | 900 | 1200 | 3800 |
| strain rate (1/s) | $5x10^4$ | $1x10^6$ | $1x10^6$ | $3x10^5$ | $1x10^7$ | $3x10^5$ | $3x10^5$ | $1x10^7$ |

Ambient melt temperature at 3290 K



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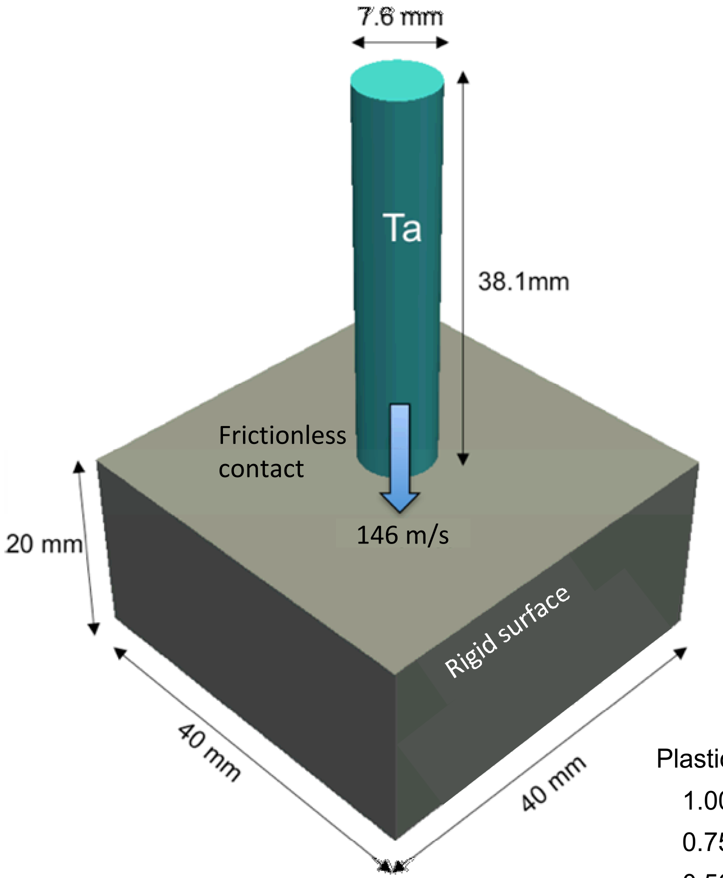
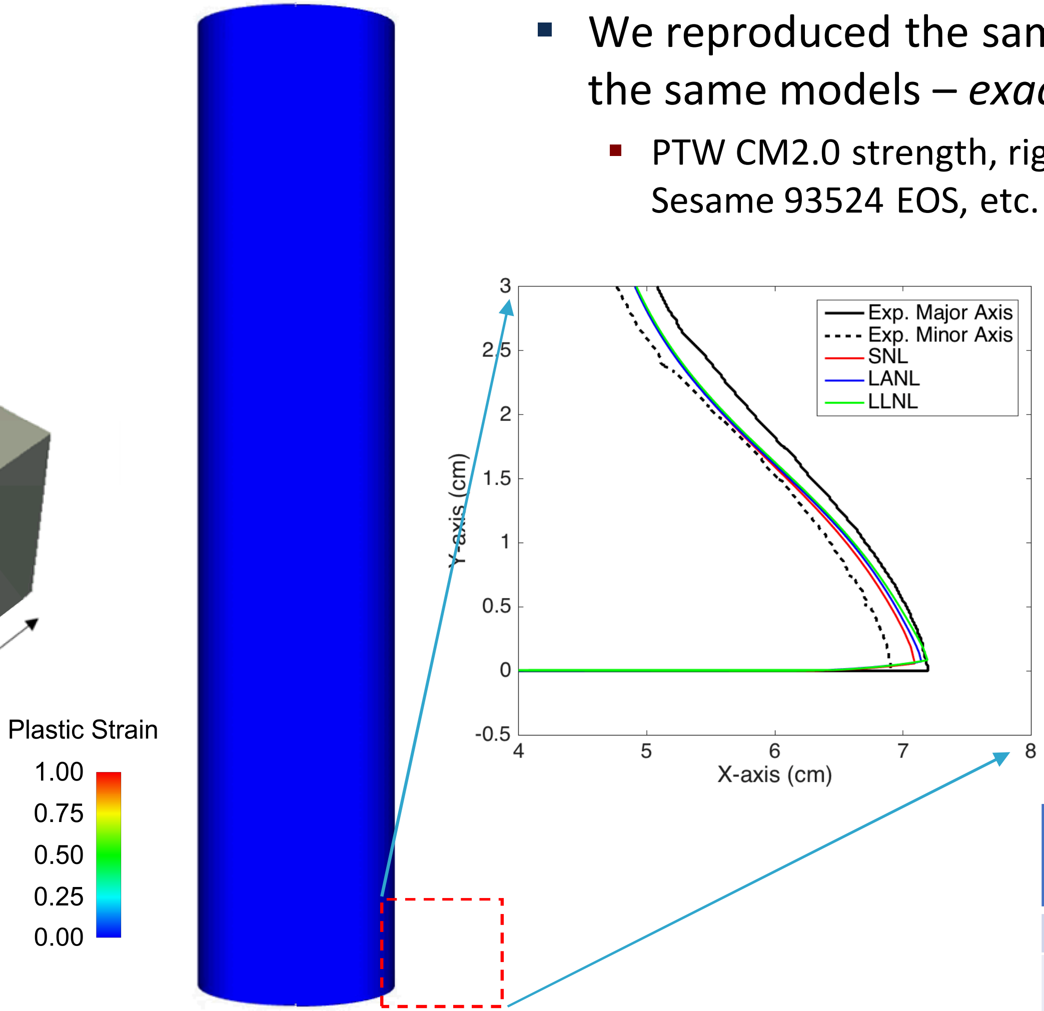
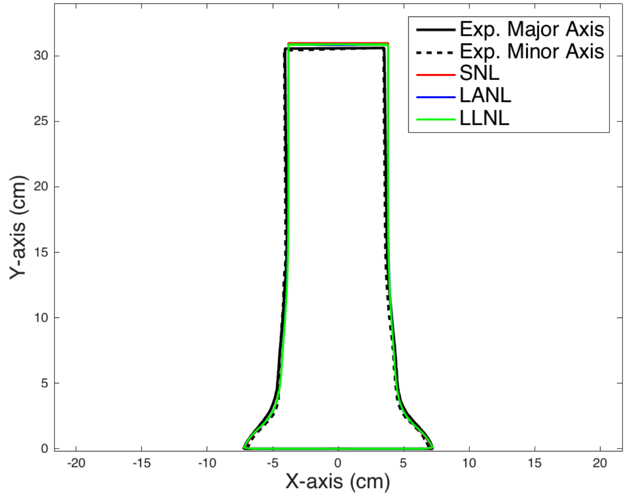
# Common model comparison: Taylor impact




- We reproduced the same results when all codes used the same models – *exactly the same models*
  - PTW CM2.0 strength, rigid anvil, no friction, artificial viscosity, Sesame 93524 EOS, etc. *No anisotropy*




| (unit: cm) | Exp. (major axis) | Exp. (minor axis) | SNL | LANL | LLNL |
|---|---|---|---|---|---|
| Foot radius | 7.19 | 6.90 | 7.09 | 7.14 | 7.19 |
| Rod height | 30.60 | 30.60 | 30.97 | 30.84 | 30.89 |



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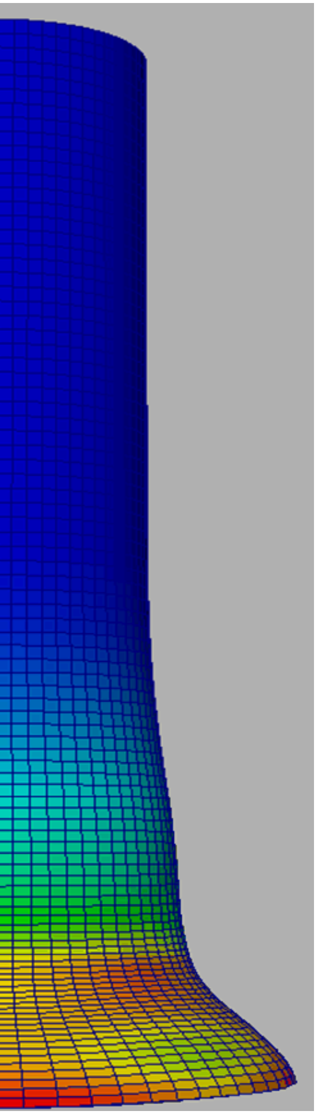
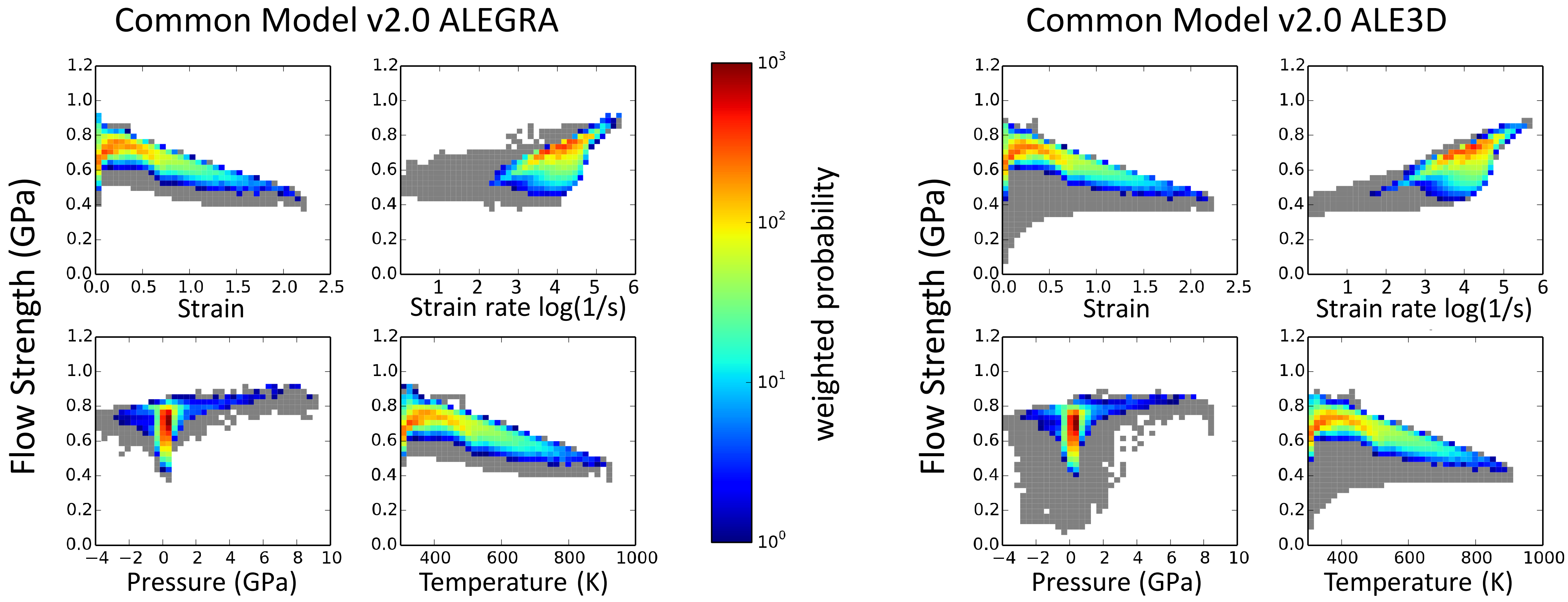
# Common model comparison: Taylor impact



Nathan Barton (LLNL) produced **histograms from temporal and spatial tracer points of Flow Strength probability** weighted by the equivalent plastic strain aggregated.



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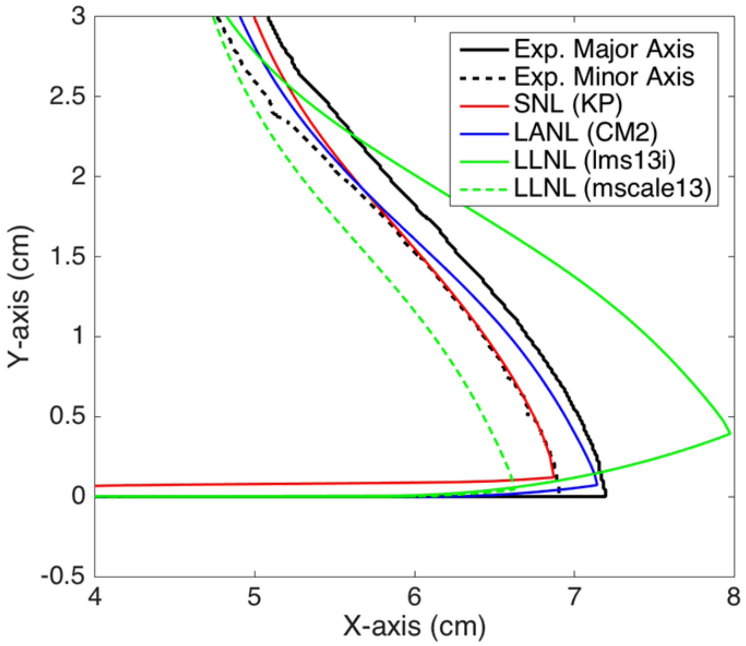
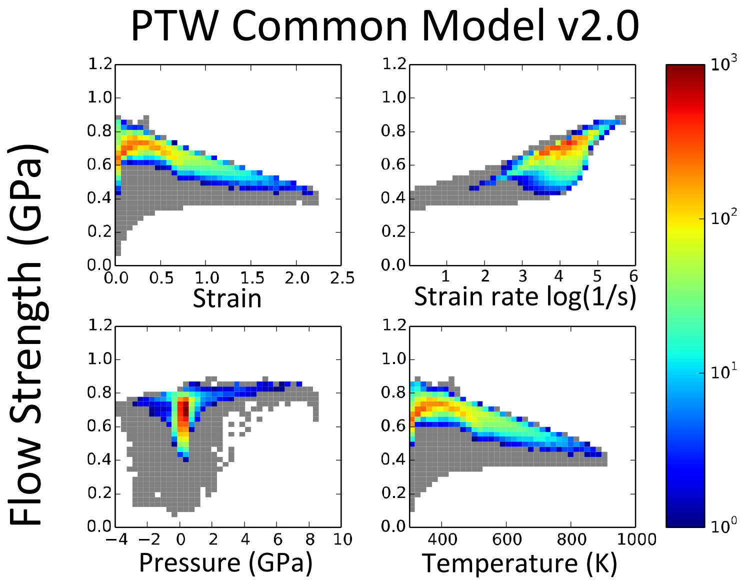
# Lab-specific strength models

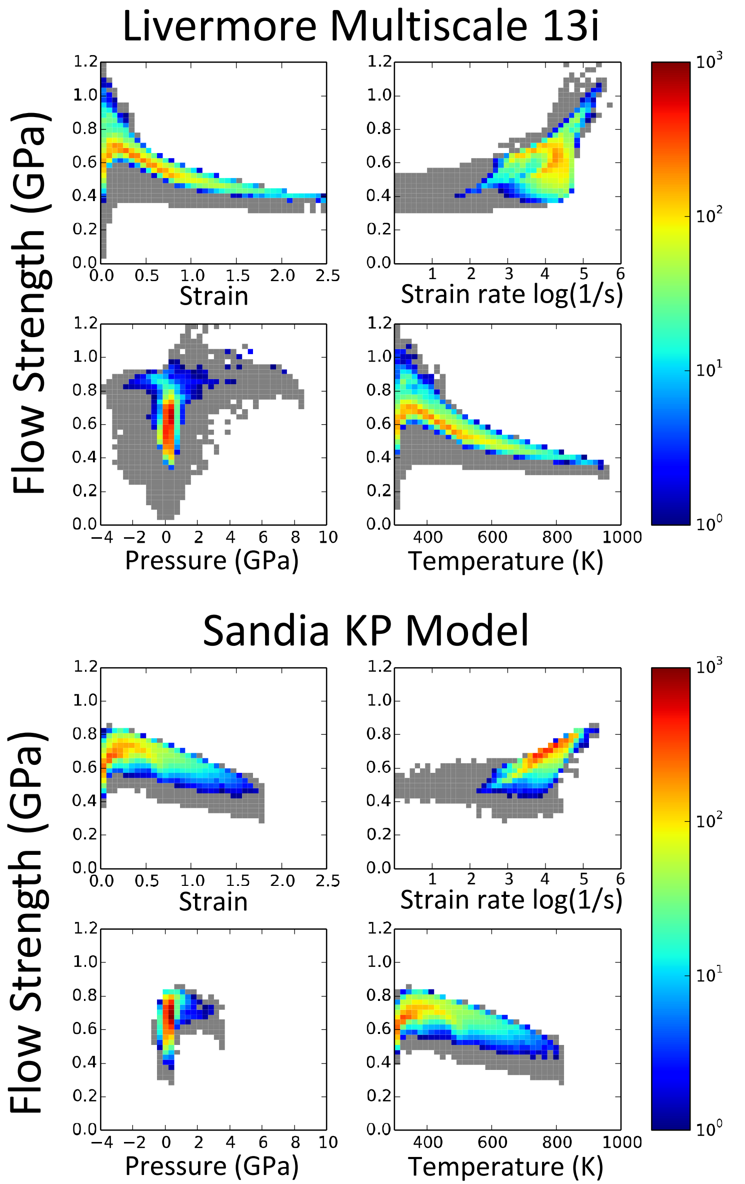
If we change **only** the strength model,

we compare the effect of each lab-specific model




Different models vs data - differences between models are larger than between codes



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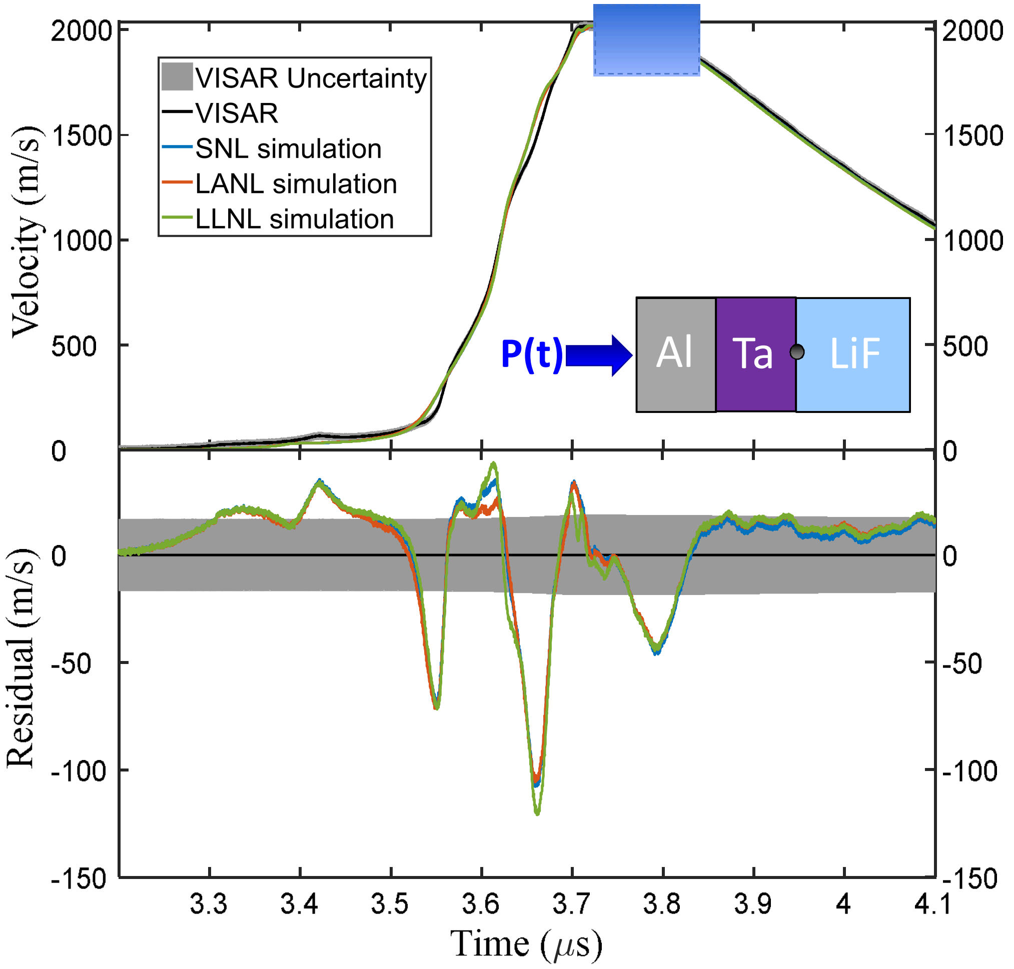
# Strength Modeling: Z ramp-release

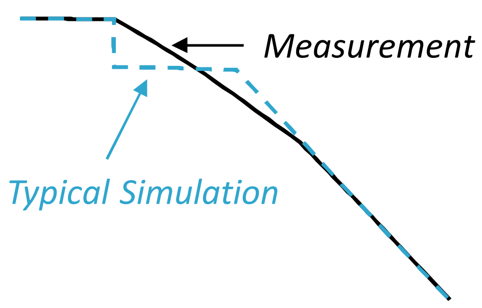
## Common Model Simulations: agrees to 5 m/s

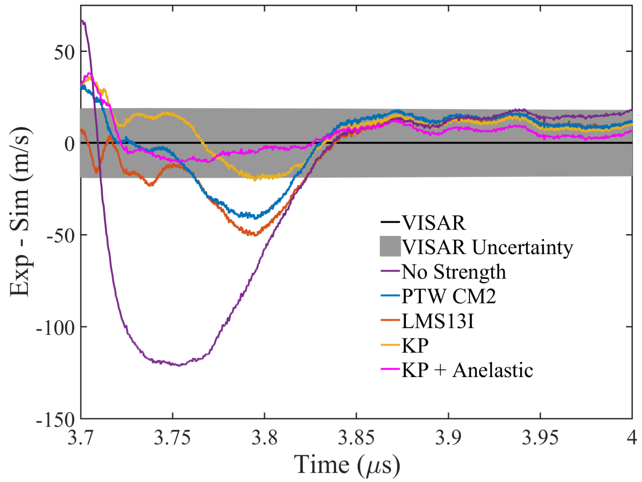
- Within the experimental uncertainties of 20 m/s



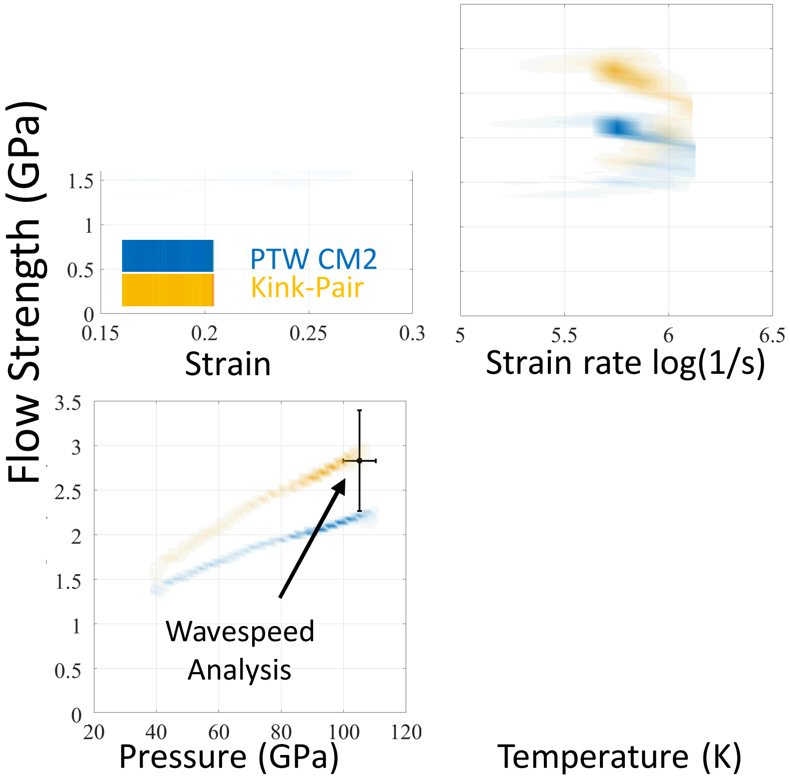

## Lab-specific Models:

1. all miss quasi-elastic release;




2. Models differ in this pressure/strain rate regime




Simulated histograms give insights into the relevant conditions related to strength



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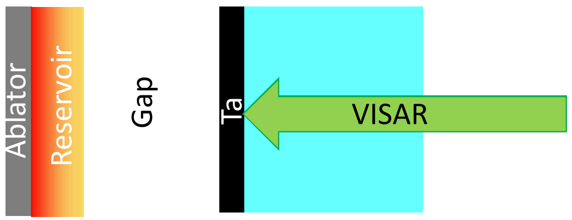
# Strength modeling: NIF/Omega RT growth

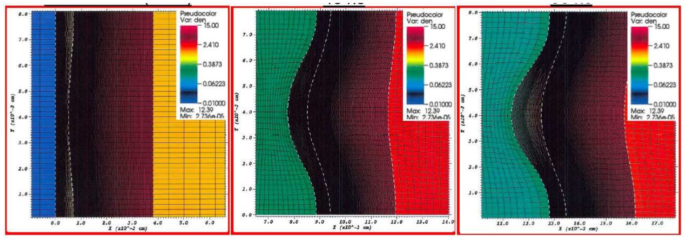
Common Model Simulations:

- Drive and back surface measures

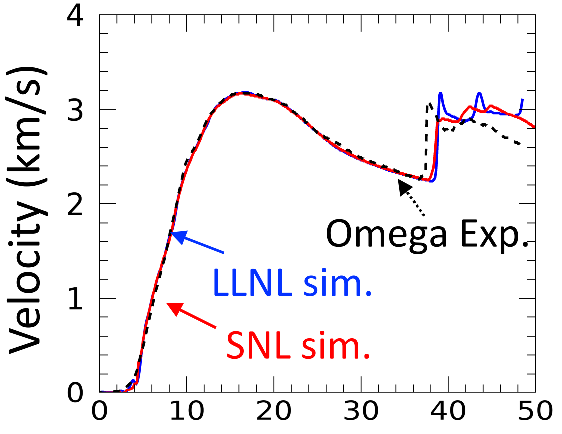



Common Model Simulations:

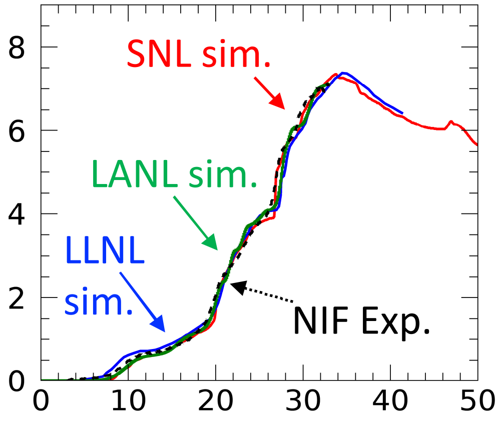
- Growth factor



Omega drive simulation

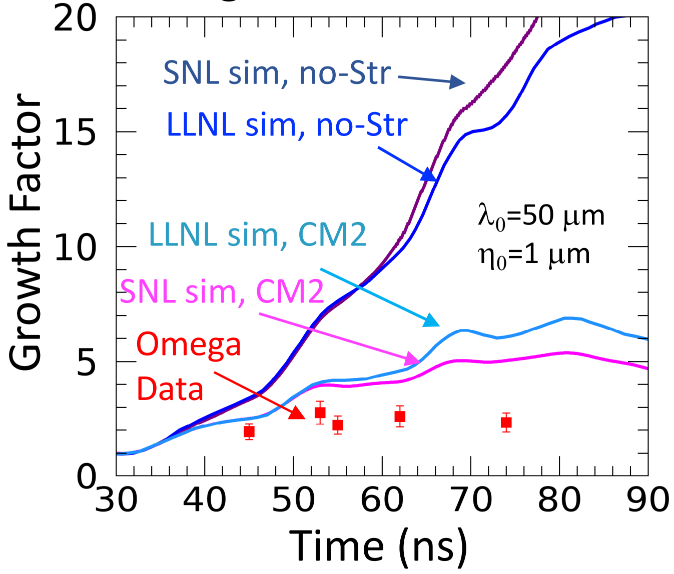



NIF drive simulation

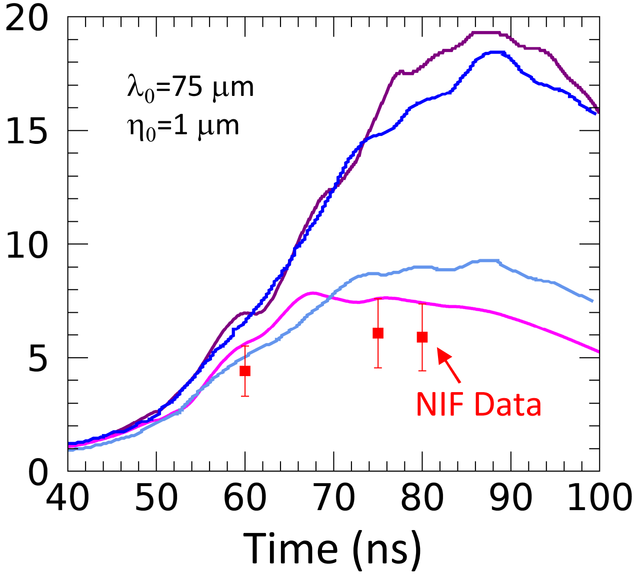



The plasma drive simulations agree well between SNL, LANL and LLNL codes except 1 ns timing shift

Omega GF simulation




NIF GF simulation




Difference in GF sims. may be due to strength in tamper

3 ns shift between SNL/LLNL simulations



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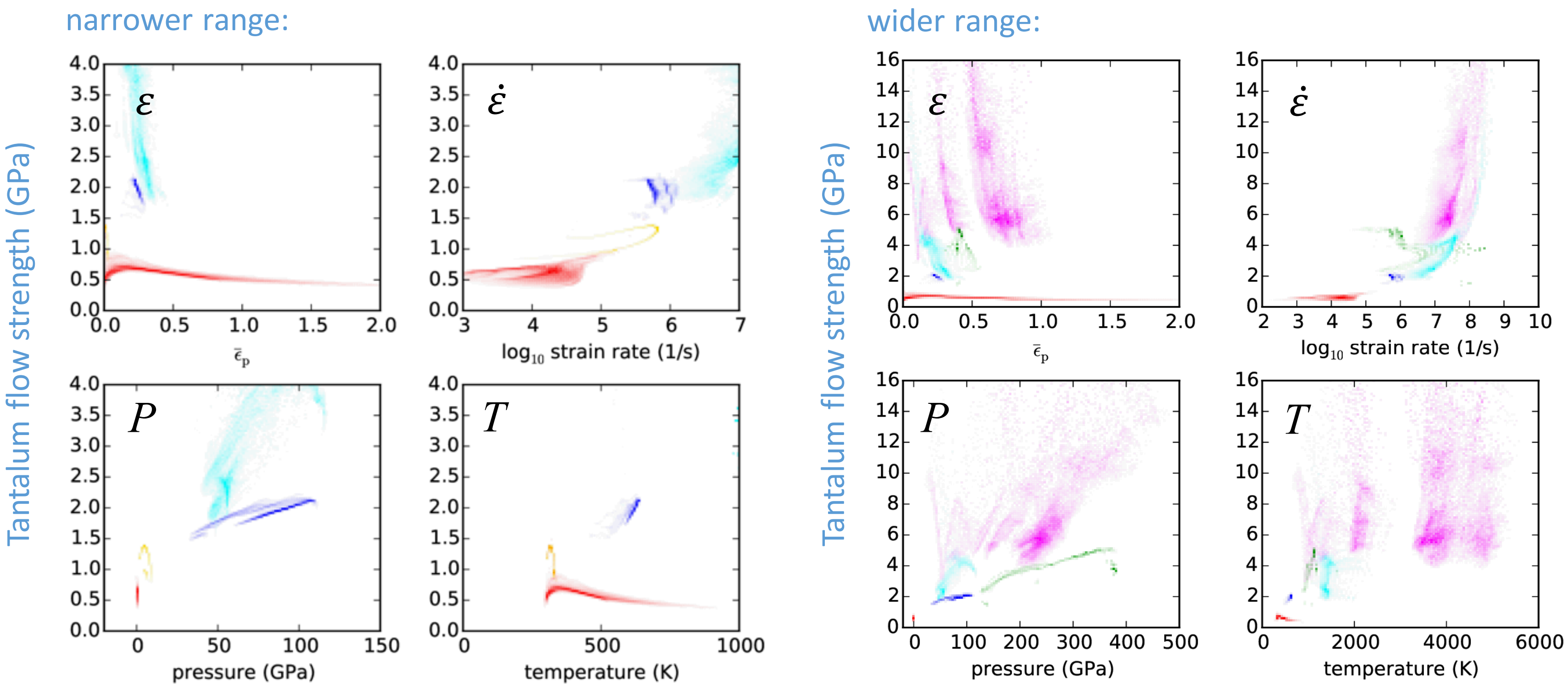
# Putting it all together: Tantalum strength

Histograms of simulation points from TC (red), gun (orange), Z1Mbar (blue), Z3.5Mbar (green), Omega (cyan), NIF (magenta)




- The platforms are complimentary: minimal overlap in conditions
- Experiments accessing higher pressure tend to sample a wider range of conditions
- Compact set for Z1Mbar may facilitate use as calibration data



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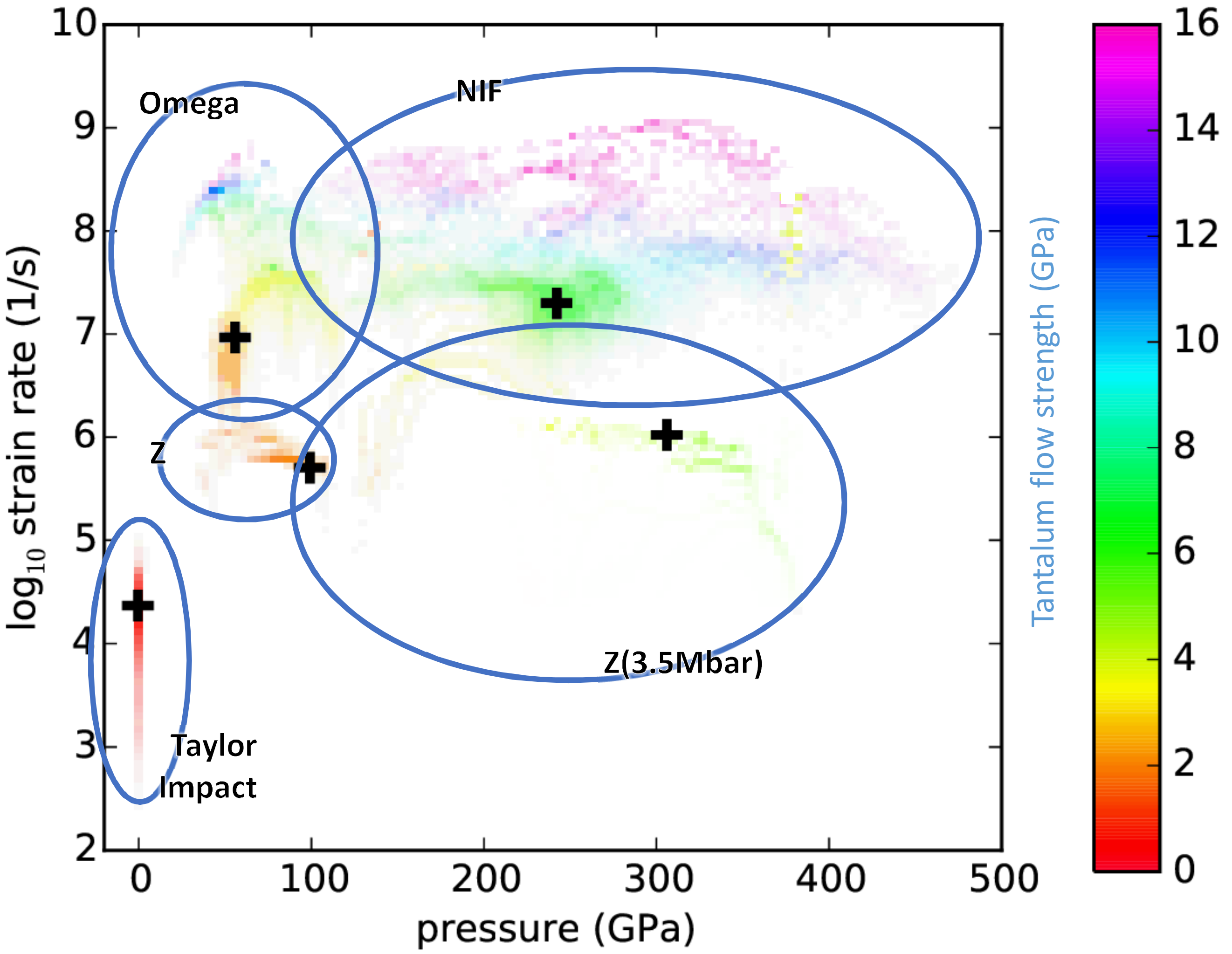
# Cross-platform trends: pressure, strain rate

- Overall trends make sense – strength increases with both pressure and rate
- Shows dependence on other quantities – and path dependence
- Strength isn't a single-value
- Different models are being used in these simulations of the experiments!

TC, Z1Mbar, Z3.5Mbar, Omega1Mbar, NIF3.5Mbar



# Strength in collaboration

- Tightly integrating modeling with experiment across *platforms* is giving *invaluable* insight into the multivariate (pressure, strain rate, T) behavior of strength in extreme conditions

- Each experimental platform provides unique capabilities in complimentary conditions
  - **Taylor impact** measures of **large deformation** at low pressures and a focused range of strain rates
  - **Z ramp-release** allows **precise strength extraction** at a given pressure but requires material release treatment in models for full mod-sim interpretation
  - **NIF/Omega RT** **probes a large range of deformation conditions** in a single shot and reaches very high pressures. However, sensitivity to the surrounding target material requires further study

- Modeling capability testing
  - Sensitivity to the hydrocode can be controlled
  - No single model appears to span low pressure/low strain rate and high pressure/high strain rate experiments



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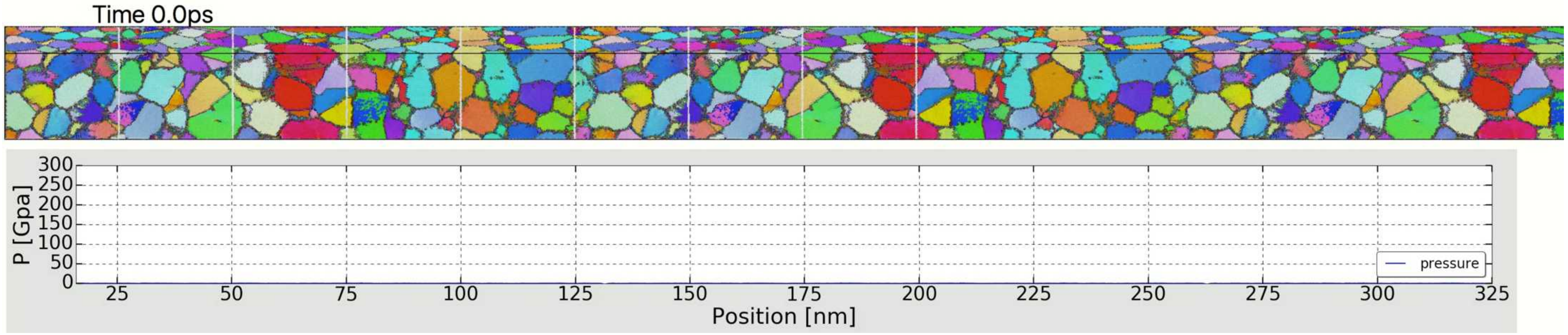
# Atomistic simulations for microstructures

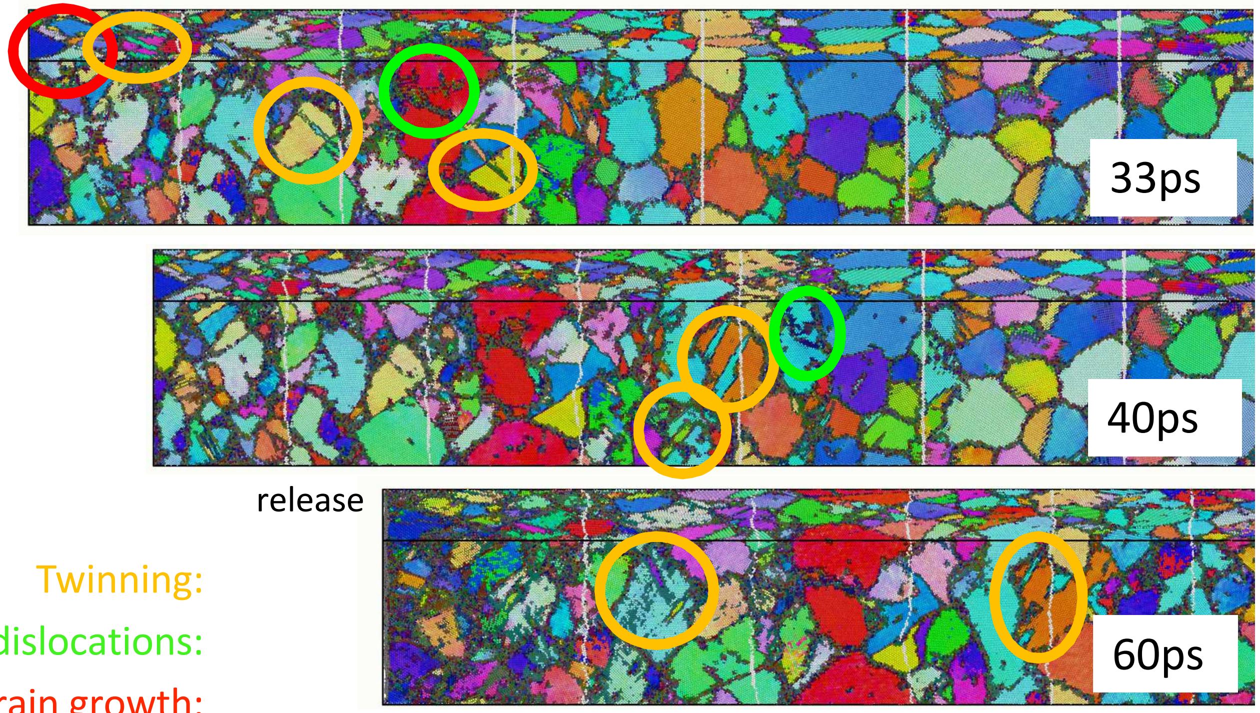



## Compression:

- Stacking faults and dislocations emitted from GBs.
- Some stacking faults grow to become twins.
- Grain growth is observed.

## Release:

- Most compression twins disappear and new release twins form and grow.
- Significant grain reorientation is observed.

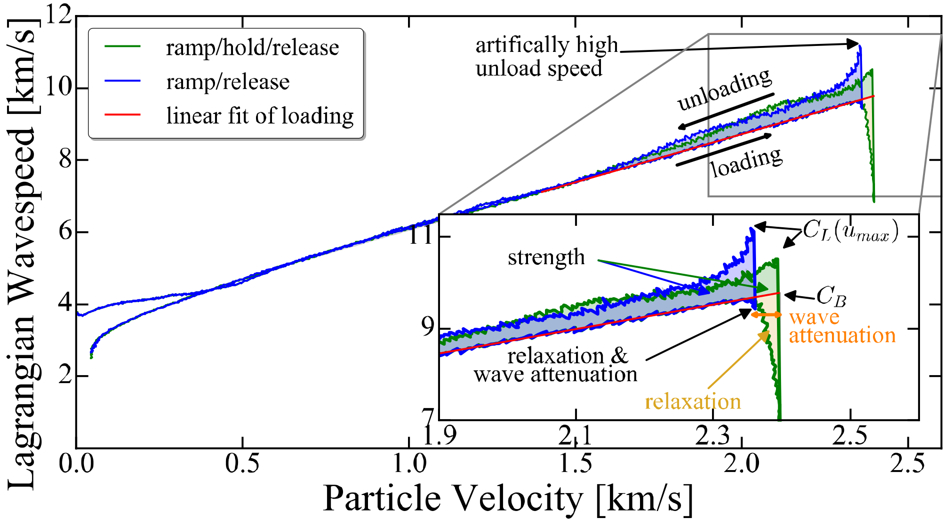



Twinning:

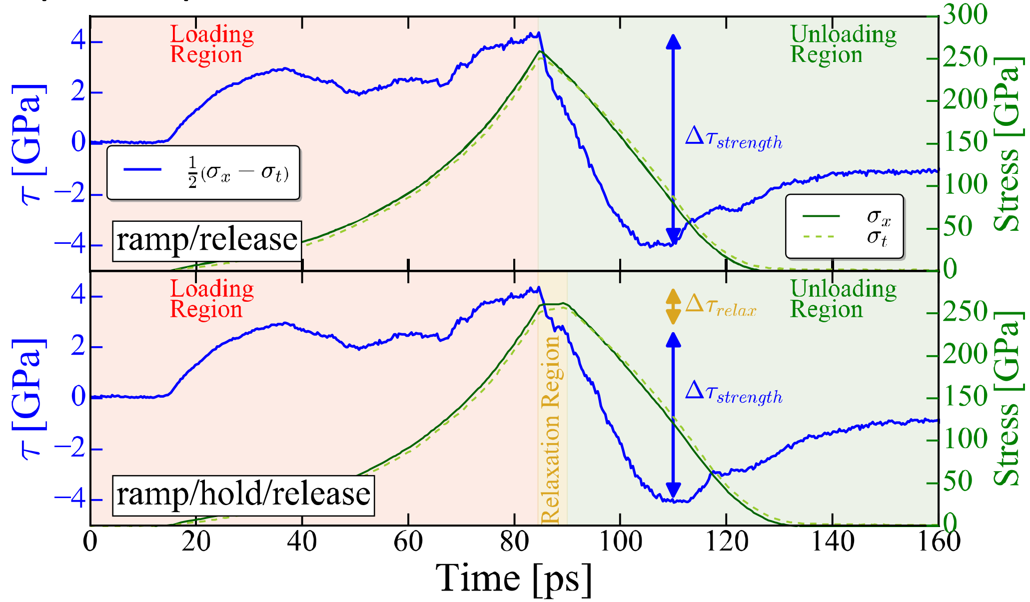
Stacking faults & dislocations:

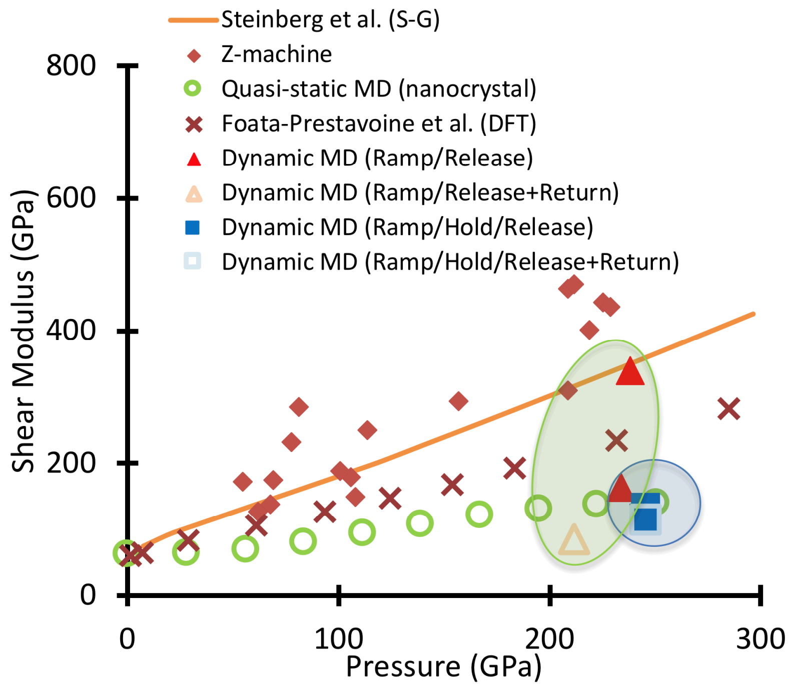
Grain growth:

# Atomistic for wave analysis improvements




Time profiles of pressure tensor and shear stress.




Ramp/hold/release profile in the hold region, showing relaxation via additional plasticity.

Motivate new ramp-hold experiments on Sandia's Thor



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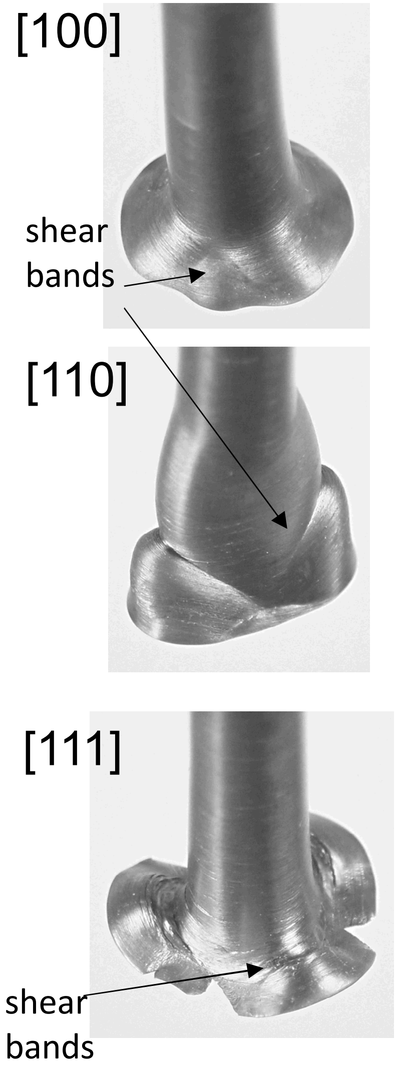
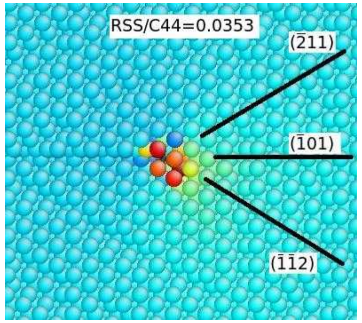
# Crystal Plasticity Methods

Hojun Lim (Sandia)

- Crystal plasticity = Grain-level (mesoscale) approach to materials modeling using multiscale strategies
- Explicitly model discrete grains and slip systems (anisotropy, texture evolution,…)



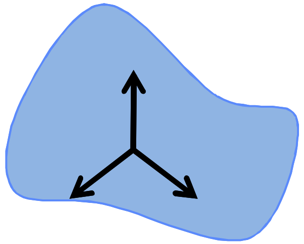

**Atomic phenomenology:**
**Fundamental mechanisms**




Yield criterion:

$$\sigma_{cr}^{app}[a_0\mathbf{m}^{(s)}\mathbf{n}^{(s)} + a_1\mathbf{m}^{(s)}\mathbf{n}^{(s')} + a_2\left(\mathbf{n}^{(s)} \times \mathbf{m}^{(s)}\right)\mathbf{n}^{(s)} + a_3\left(\mathbf{n}^{(s)} \times \mathbf{m}^{(s)}\right)\mathbf{n}^{(s')}] = \tau_{cr}$$

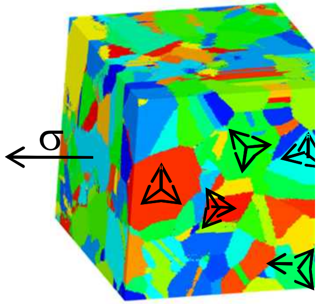
**Single crystal plasticity:**
**Deformation one crystal**

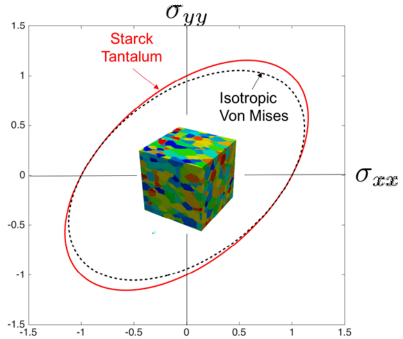


Constitutive law:

$$\dot{\gamma}^{(s)} = \frac{\tau^{(s)}}{\tau_{cr}}\left|\frac{\tau^{(s)}}{\tau_{cr}}\right|^{\frac{1}{m}-1}$$

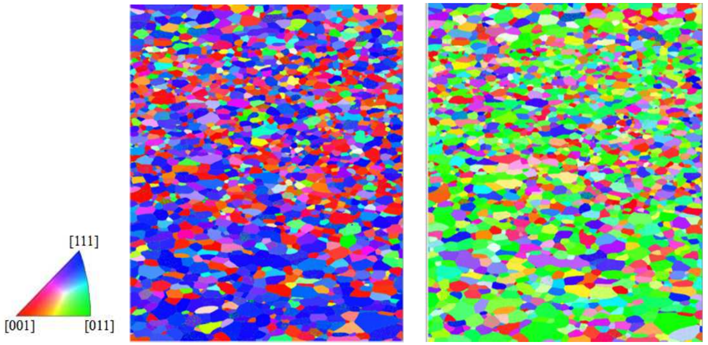
**Polycrystal plasticity:**
**Assemble polycrystalline ensemble**




Predict collective behavior.

Experiment
Texture measurement (EBSD)



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# Future collaboration and Sandia's models

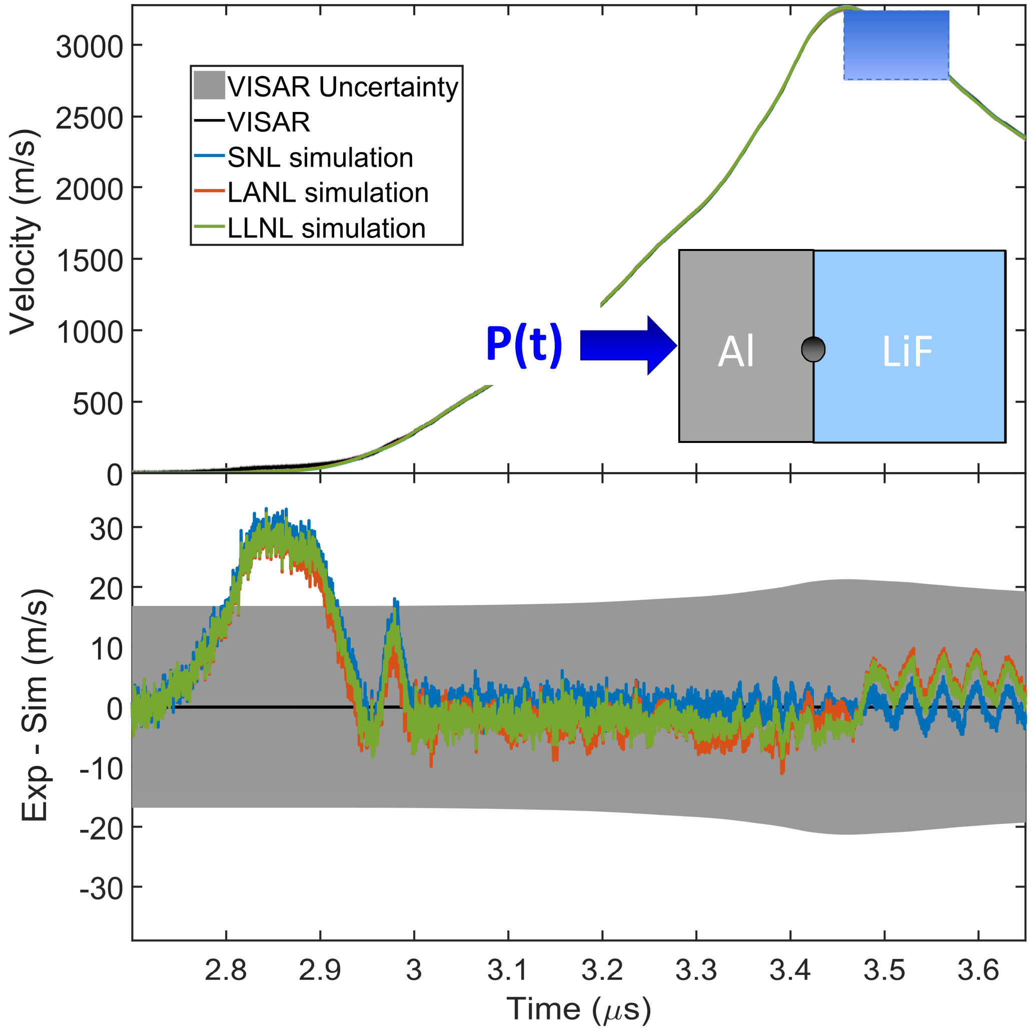
- Conduct experiments to increase overlap
  - NIF/Z comparison at 2.5Mbar
  - Double shock gun test at 1 Mbar
- Conduct experiments to further constrain models
  - Experiments on guns, DCS & Thor
  - High temperature Taylor Cylinder
  - High rate, low pressure (RMI) experiments
- Modeling & simulations to identify gaps in current models
  - Complete analysis of Omega/NIF experiments
  - Calibrate new PTW model incorporating higher pressure Z data
  - Broaden the range of each lab-specific models
    - Sandia: Work to engage atomistic and mesoscale modeling to improve

End

# Strength Modeling: Z ramp-release

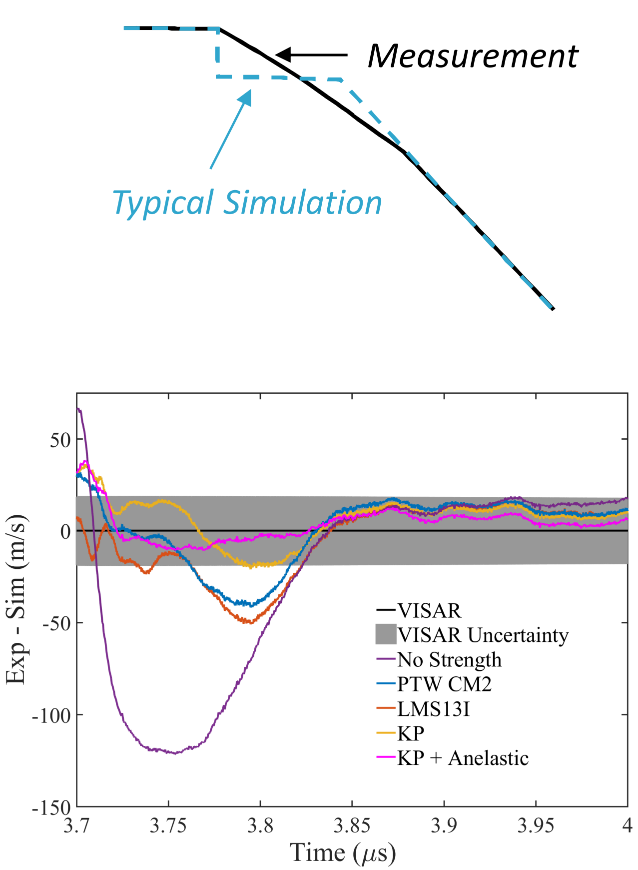
## Common Model Simulations: agree within 5 m/s

- Well within the experimental uncertainties of 20 m/s

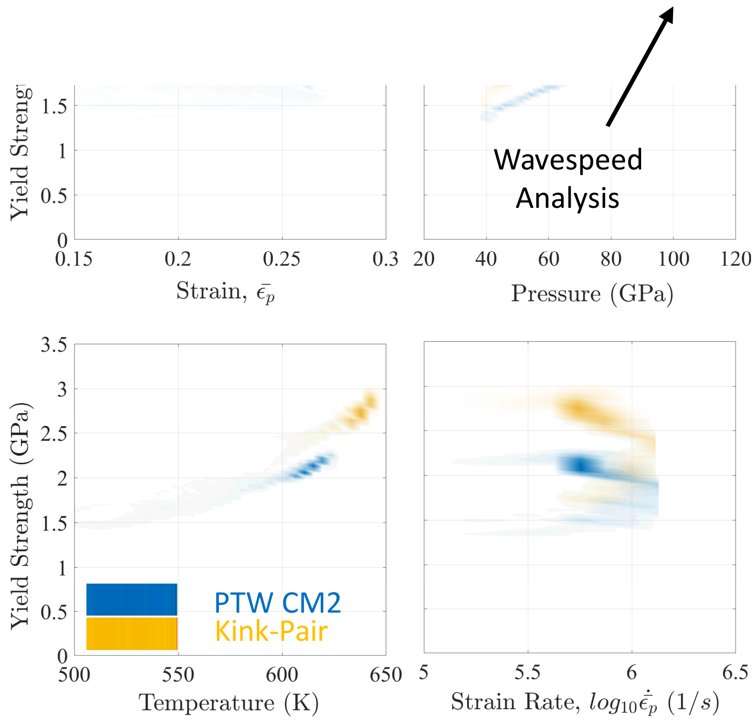



## Lab-specific Models:

1. all miss quasi-elastic release;




2. Models differ in this pressure/strain rate regime




Simulated histograms give insights into the relevant conditions related to strength



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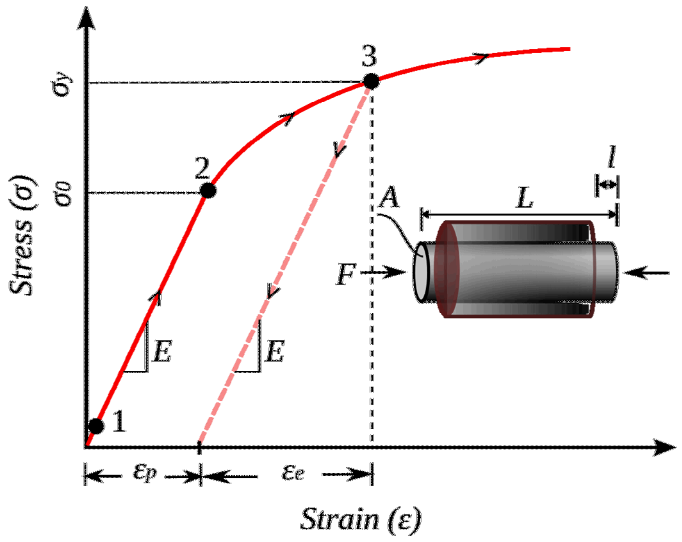
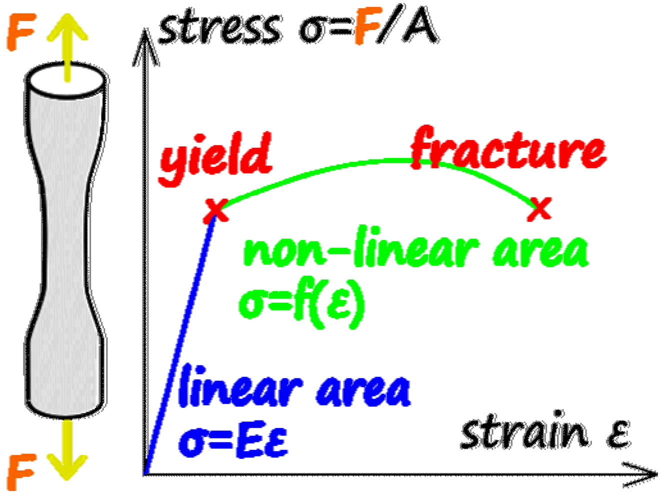
# Dynamic strength in the real world

1. **Strength has many definitions and contexts**

2. Models are complex and it is extremely easy to over generalize. The devil is in the details.

3. Simple experimental measures are an illusion



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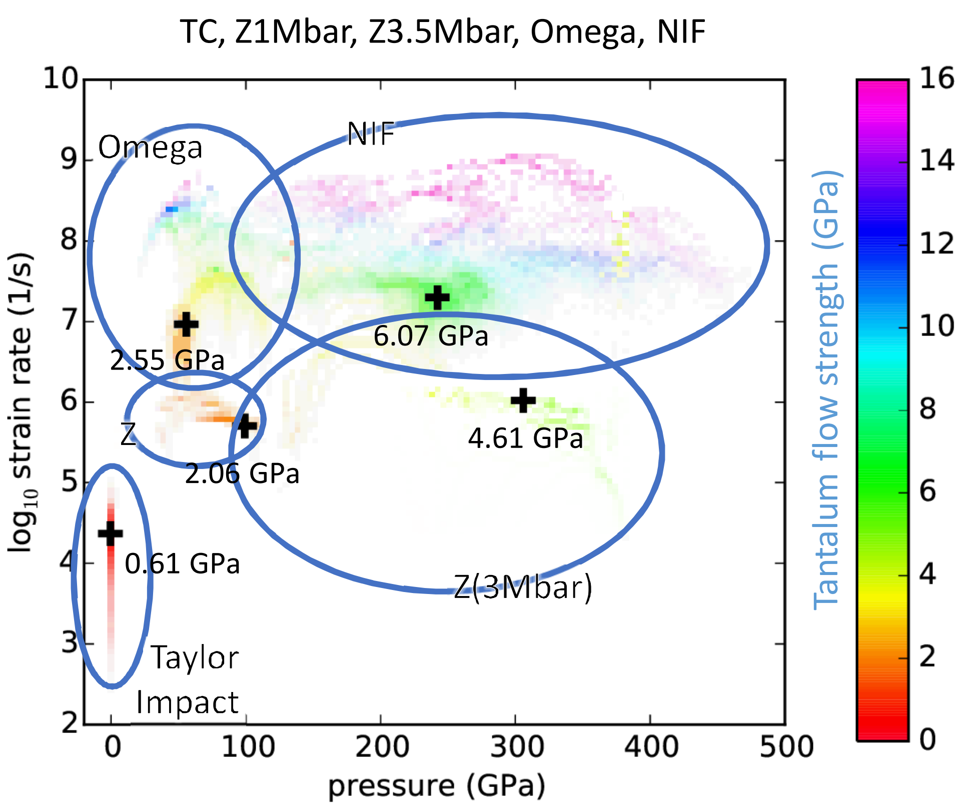
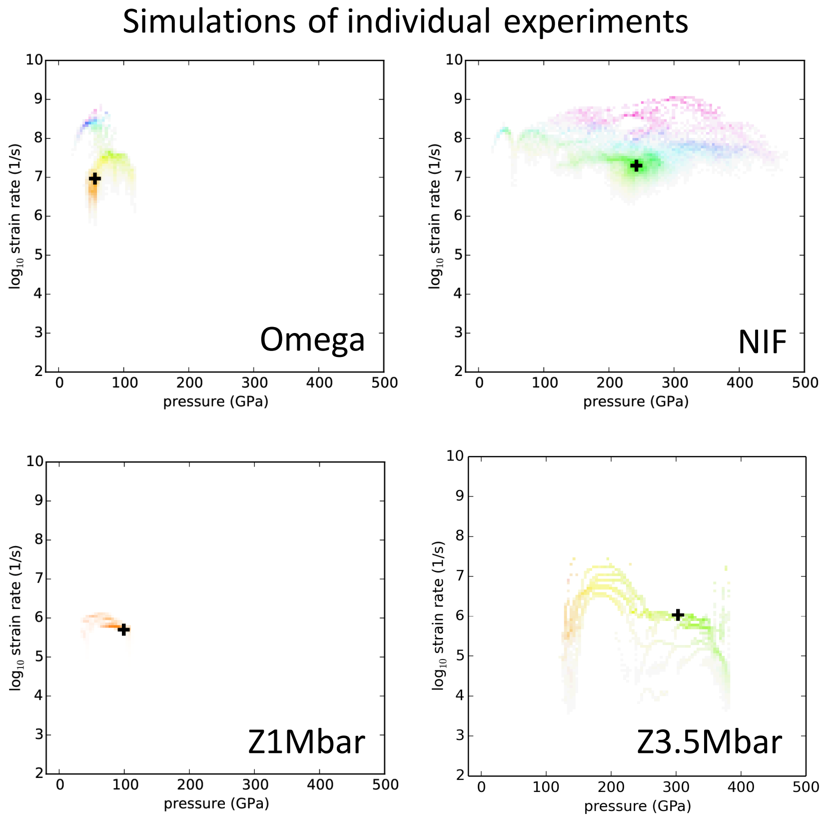
# Cross-platform trends: pressure, strain rate




- Overall trends make sense – strength increases with both pressure and rate
- Results in this projection need not align
  - Shows dependence on other quantities – and path dependence
- Different models are being used in these simulations of the experiments!

# Lagrangian Wave Analysis

- X is the Lagrangian coordinate.
- For isentropic flow of simple waves, the Lagrangian wave speed "c" can be calculated using the particle velocity histories at different locations.

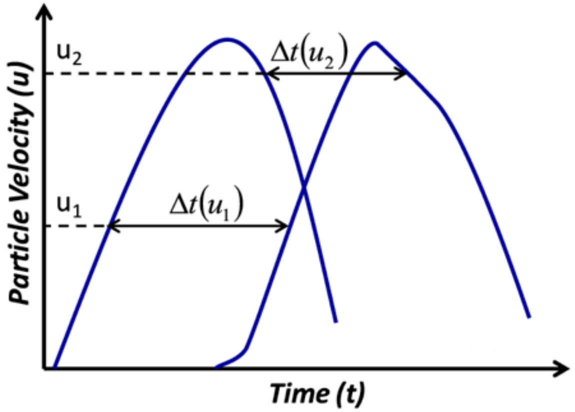
$$C_u = c_L\left(u_p\right) = (\partial X/\partial t)_u = \frac{\Delta X}{\Delta t}_u$$

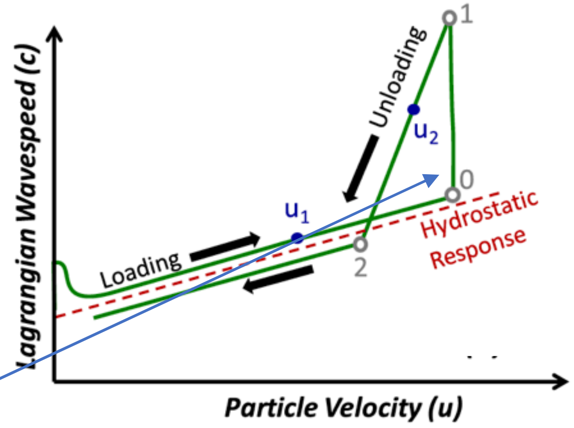
- The Lagrangian wavespeed can then be used to determine changes in the shear stress at pressure.

$$\sigma_x = \bar{\sigma} + (4/3)\tau \rightarrow \frac{d\sigma_x}{d\varepsilon} = \frac{d\bar{\sigma}}{d\varepsilon} + \frac{4}{3}\frac{d\tau}{d\varepsilon}$$

$$d\varepsilon = \frac{du}{c(u)} \rightarrow \rho_0 c^2 = \frac{d\sigma_x}{d\varepsilon} \leftarrow d\sigma_x = \rho_0 c(u) du$$

$$\tau(u_1) - \tau(u_2) = \frac{3}{4}\rho_0 \int_{u_2}^{u_1} [c^2(u) - c_B^2(u)] \frac{du}{c(u)}$$




*Brown, et al., J. Appl. Phys. 114, 223518 (2013).*



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# Calculation of Dynamic Properties



$$\tau(u_1) - \tau(u_2) = \frac{3}{4}\rho_0 \int_{u_2}^{u_1} [c^2(u) - c_B^2(u)] \frac{du}{c(u)}$$

↓

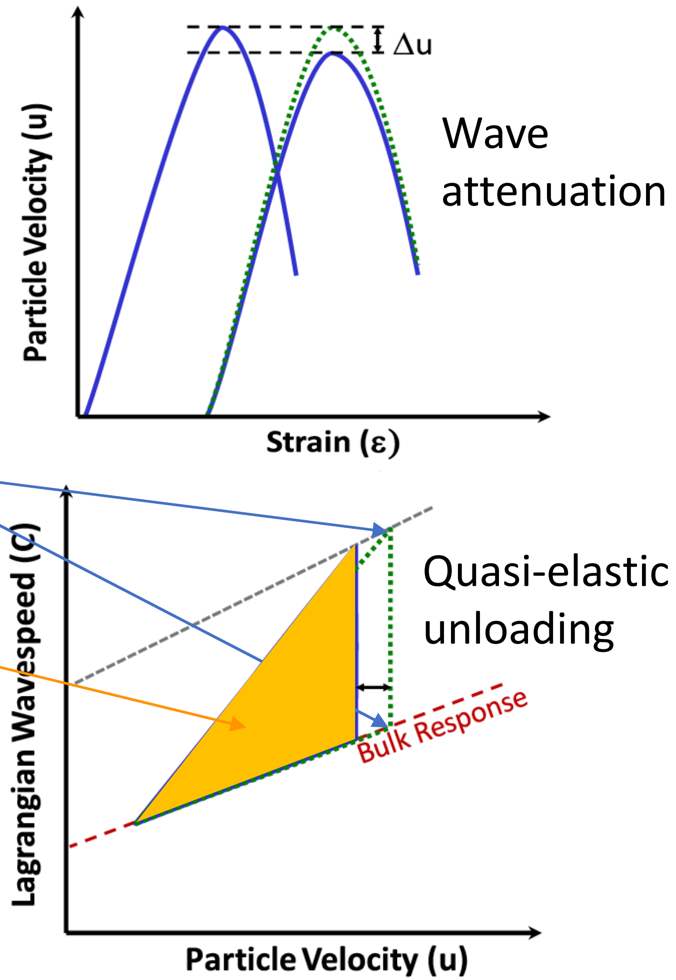
$$C_L = C_B \sqrt{1 + \left(4/3\right)\left(\partial\tau/\partial P\right)}$$

↓

$$G = \rho_0(1 - \varepsilon_{max} - \varepsilon_{attenuation}) \sqrt{\frac{3}{4}(c_L^2 - c_B^2)}$$

↓

$$Y = \int_{\varepsilon_{trans}}^{\varepsilon_{max}} G_{eff}\, d\varepsilon$$



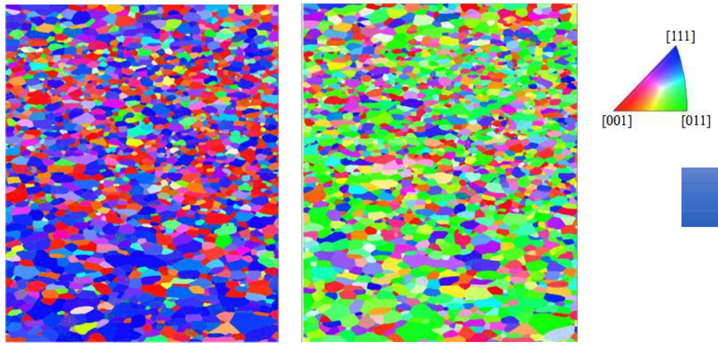

Attenuation of the peak particle velocity or pressure occurs when the rarefaction wave overtakes the compression wave.

$$K = \rho_0(1 - \varepsilon_{max} - \varepsilon_{atten})C_b^2 \qquad \nu = \frac{3C_b^2 - C_l^2}{3C_b^2 + C_l^2}$$

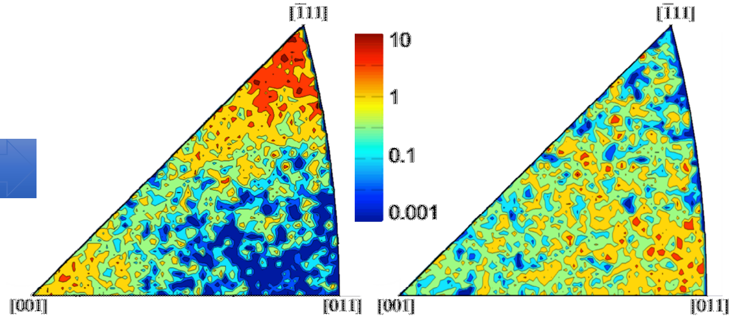
***Brown, et al., J. Appl. Phys. 114, 223518 (2013).***

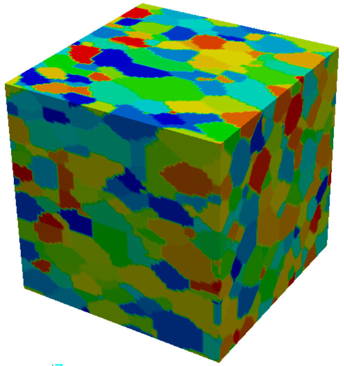
# Addressing anisotropic yield at mesoscale

Experiment
Texture measurement (EBSD)

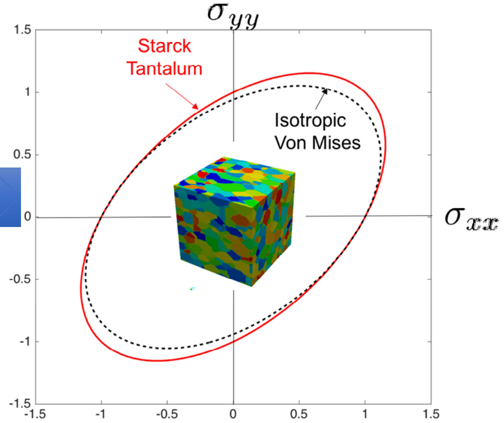



Modeling
Crystal plasticity finite element model



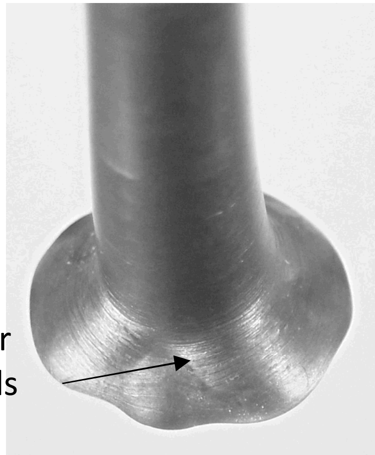



Modeling
Continuum anisotropic yield model

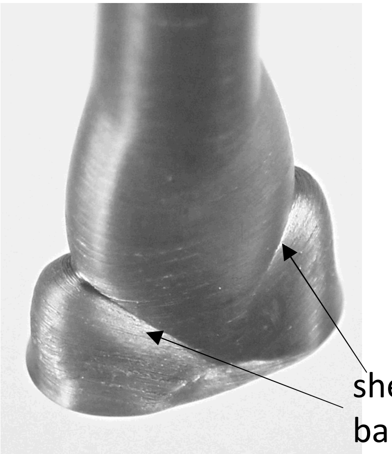



$$\phi = F\left(\sigma_{yy}-\sigma_{zz}\right)^2 + G\left(\sigma_{zz}-\sigma_{xx}\right)^2 + H\left(\sigma_{xx}-\sigma_{yy}\right)^2 + 2L\sigma_{yz}^2 + 2M\sigma_{zx}^2 + 2N\sigma_{xy}^2 = \bar{\sigma}^2$$

shear bands

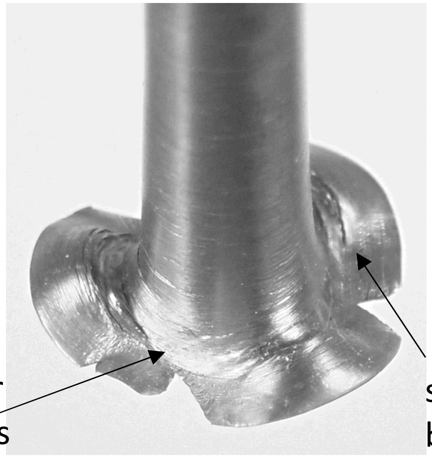


[100] single crystal



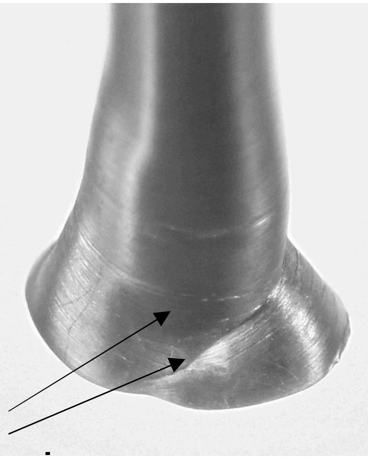
[110] single crystal

shear bands



[111] single crystal

shear bands



[149] single crystal



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