SAND2018-2600C

Improving High Strain-Rate Strength Models of Tantalum using Molecular Dynamics

Alexander P. Moore, Hojun Lim, Justin Brown, **J. Matthew D. Lane**

Sandia National Laboratories
TMS Annual Meeting, Phoenix, March 13th 2018

SAND2018-

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Compressive strength in materials

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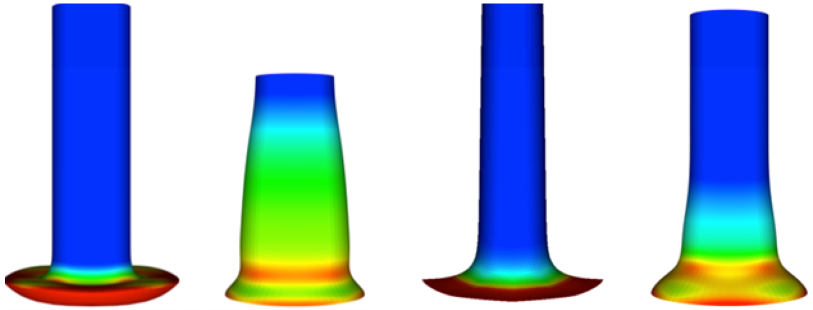
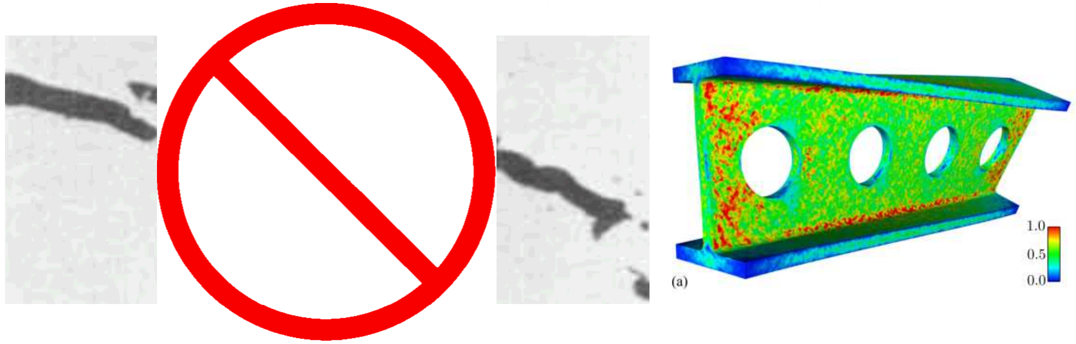
- **Strength** is a measure of a material's ability to sustain an applied load without failure or irreversible deformation.
  - **Compressive plastic flow stress in textured polycrystalline metal (ignoring anisotropy)**

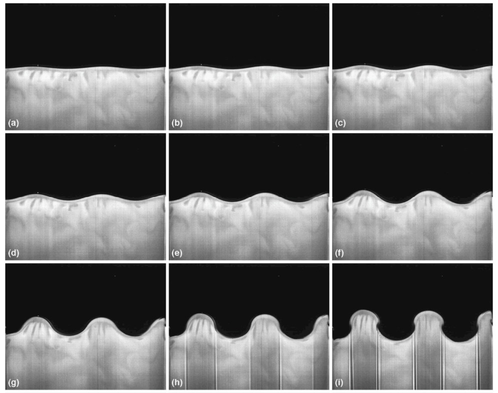
- Strength response is "universal"
  but mechanisms are unique to each system.

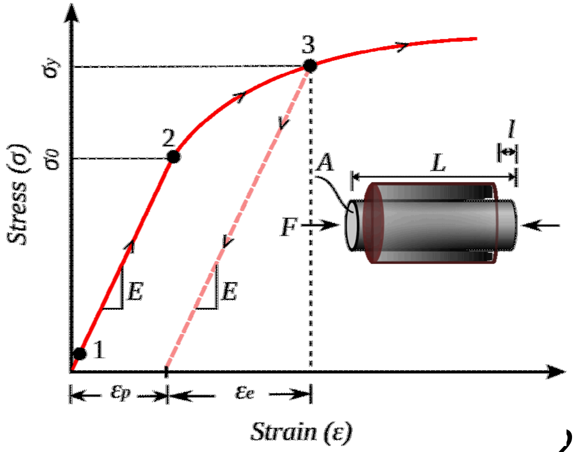
- In the hydro code world,
  EOS → controls volume compression
  strength → controls deformability

- Tantalum, as a high-Z **body-center-cubic (bcc) metal** with **no experimentally observed high-pressure phase transitions** up to 350 GPa. High melt temperature of 3290 K.









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Tri-Lab effort in experiments & modeling

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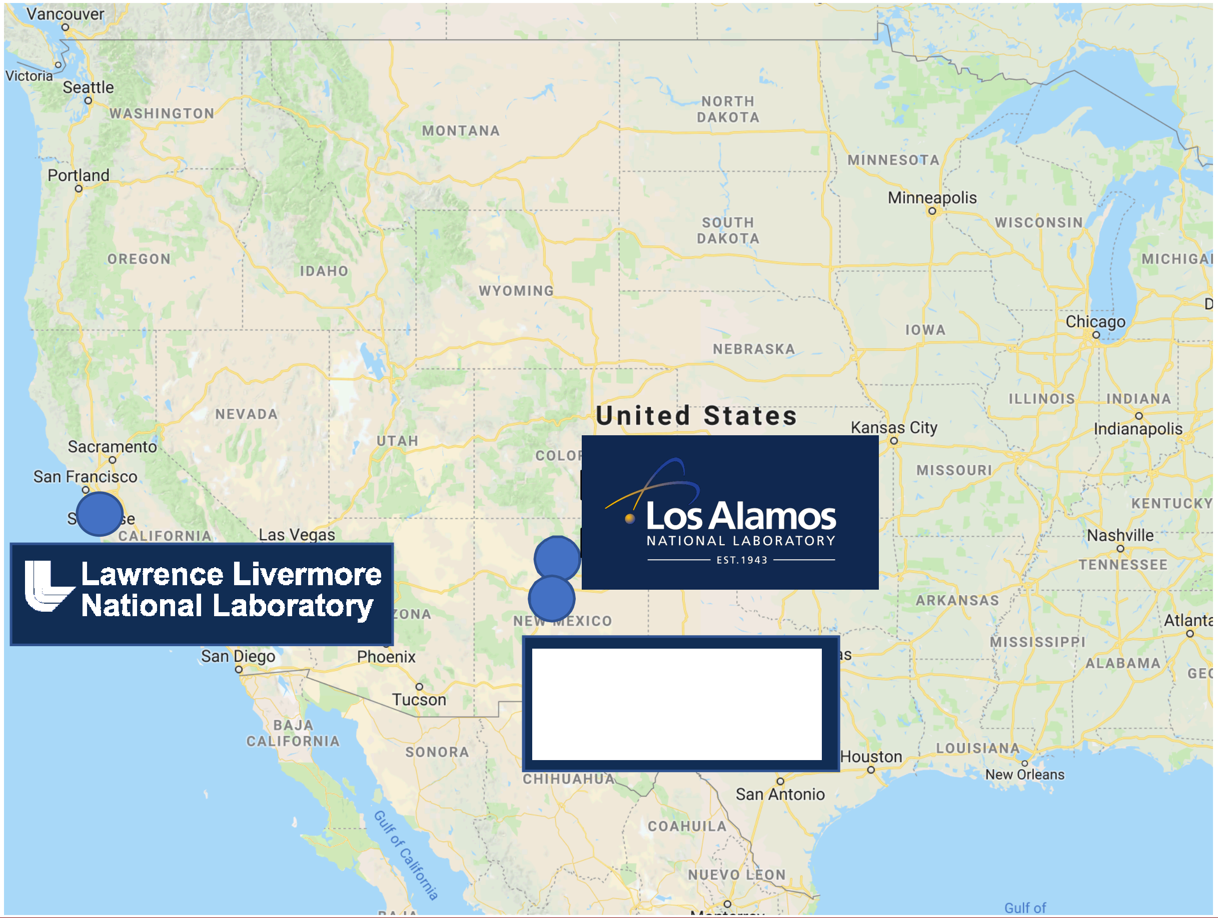
LANL: George T. Gray III, Shuh-Rong Chen, Curt Bronkhorst, Mark W. Schraad, Michael B. Prime, D.J. Luscher, Sayu Fensin, Dana Dattelbaum

LLNL: Tom Arsenlis, Hye-Sook Park, Shon Prisbrey, Dennis McNabb, Nathan R. Barton, Damian C. Swift, Ryan Austin, Bruce Remington

SNL: Dawn Flicker, Thomas Mattsson, Matthew Lane, Justin L. Brown, John F. Benage, Corbett Battaile, Alex Moore, Hojun Lim



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

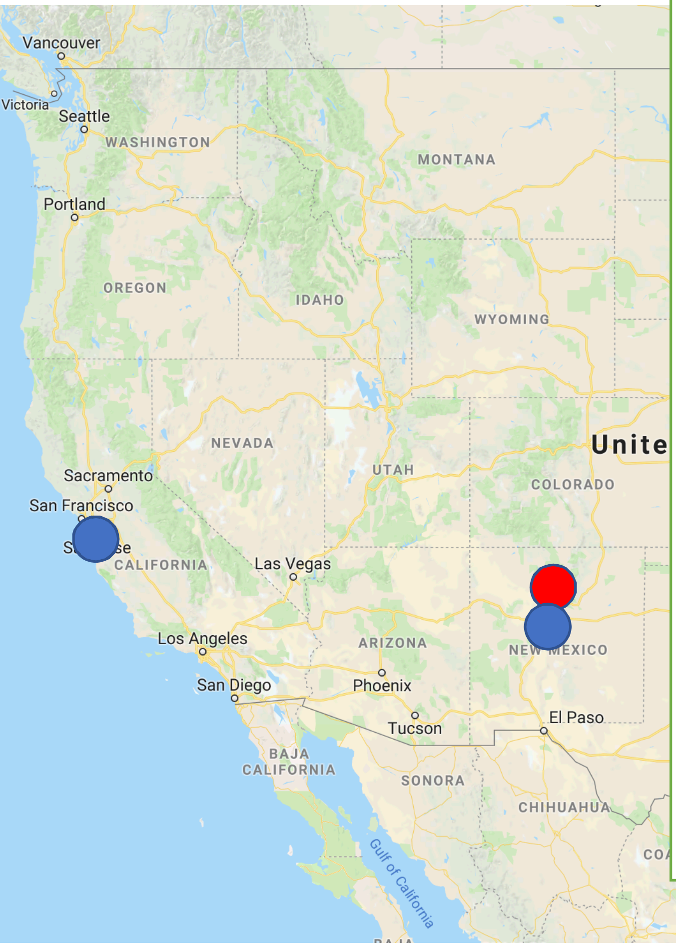
   A single well-characterized material - eliminate microstructural variation

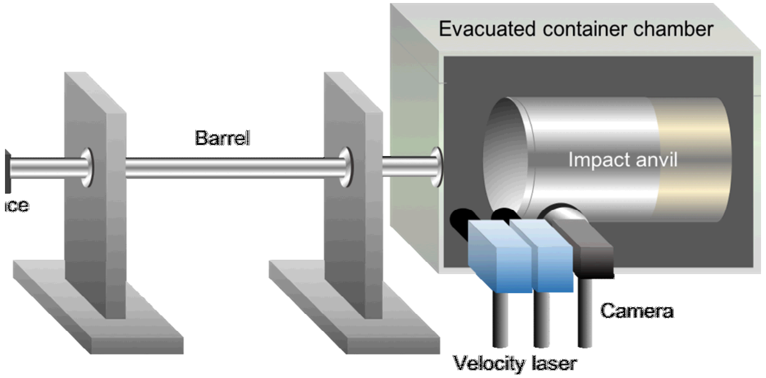
2. Jointly model each others experiments

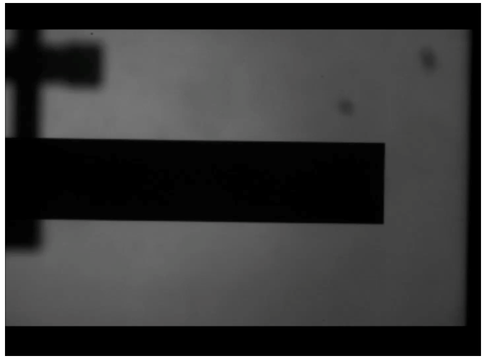
   Implement an improved common model (PTW Common Model)

3. Work to improve connections and overlap for robust cross-platform comparisons
   New experiments in the pressure and strain rate ranges between drivers

Taylor Cylinder Impact (LANL)







V_0 = 146.2m/s

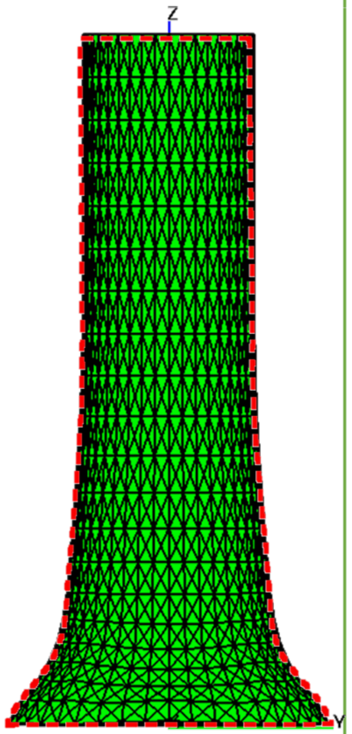
Los Alamos National Lab
Shuh-Rong Chen and Rusty Gray

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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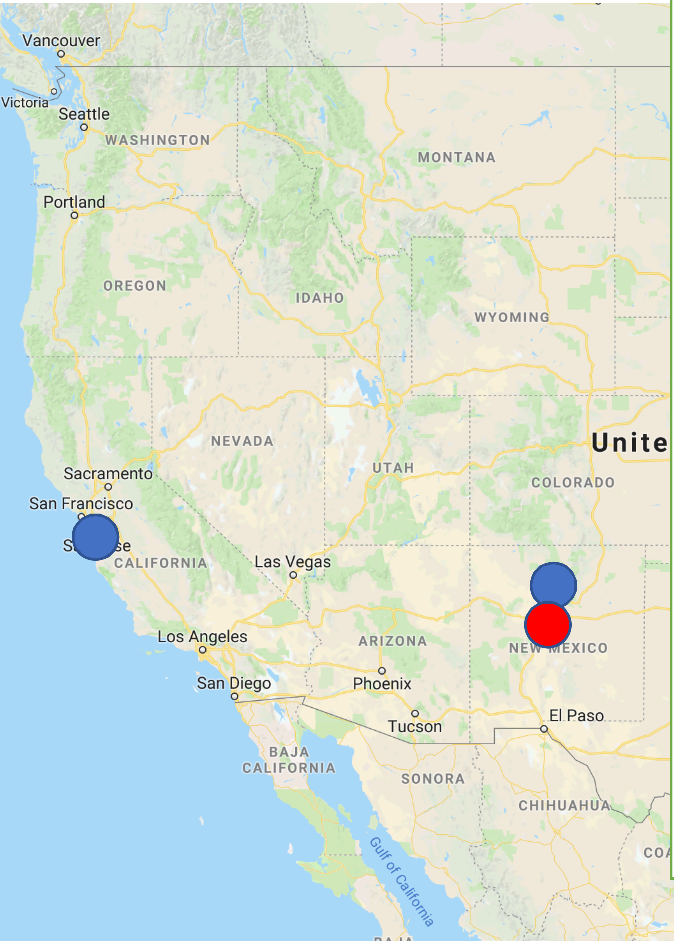
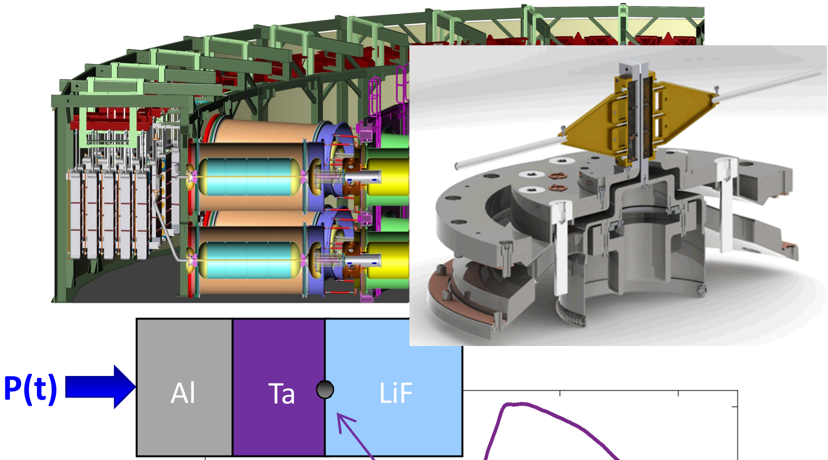
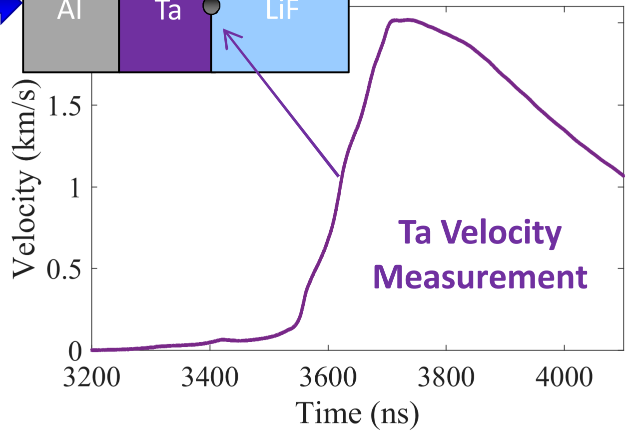
Z machine ramp-release (SNL)







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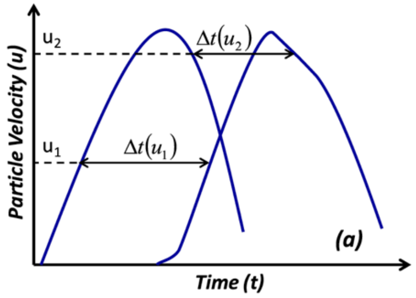
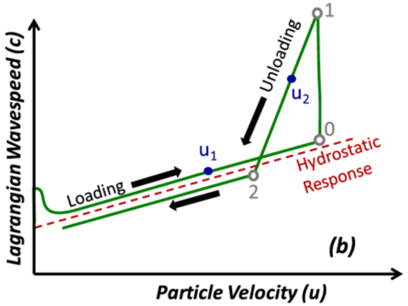
Peak pressure: ~50 to 380 GPa
Strain rate: 10^5 1/s

Experiment Description:
•Pulse-power driver 22 MA

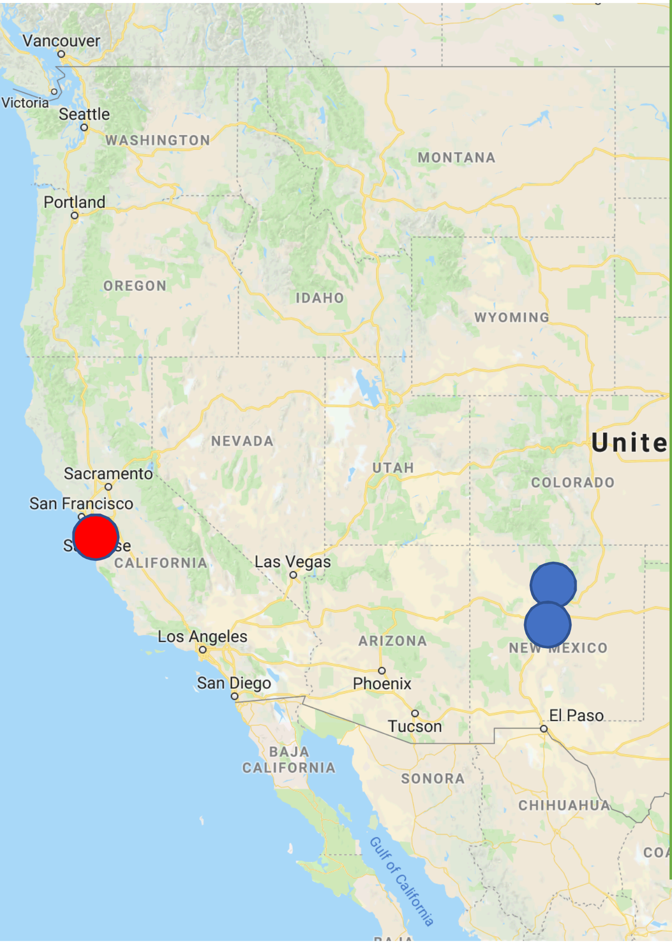
Measurement:
•The primary output is back surface time-resolved velocity profiles.

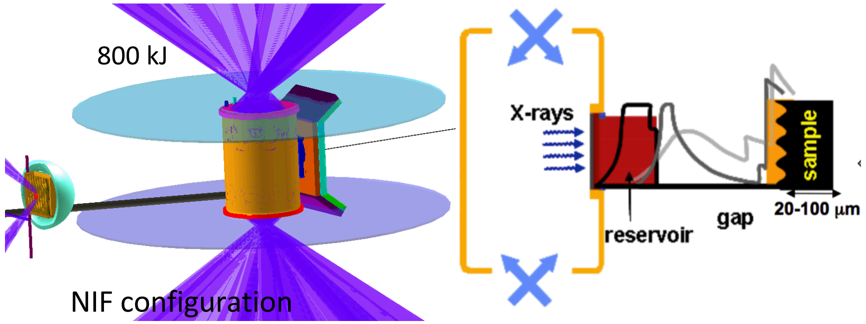
Strength Determination:
Strength model 1D wavespeed analysis to infer strength from the shear stress, τ



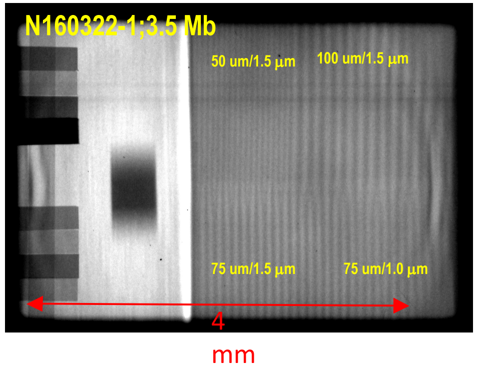


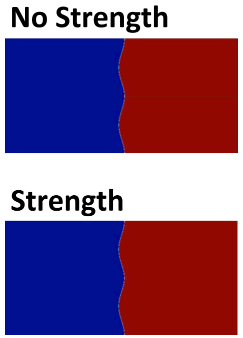
Rayleigh-Taylor (RT) instability growth (LLNL)





Strength will suppress RT growth





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:

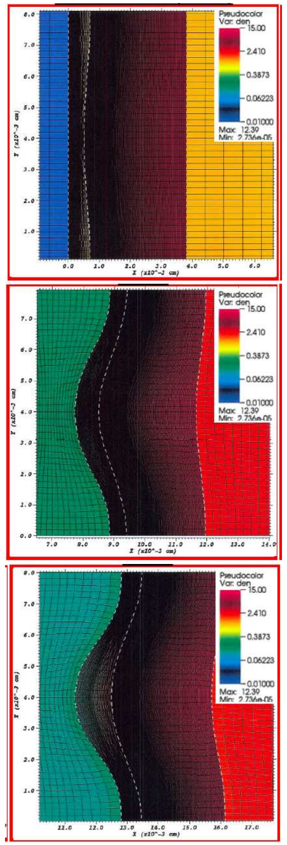
•800 kJ of laser energy focused to a small cylinder X-ray hohlraum

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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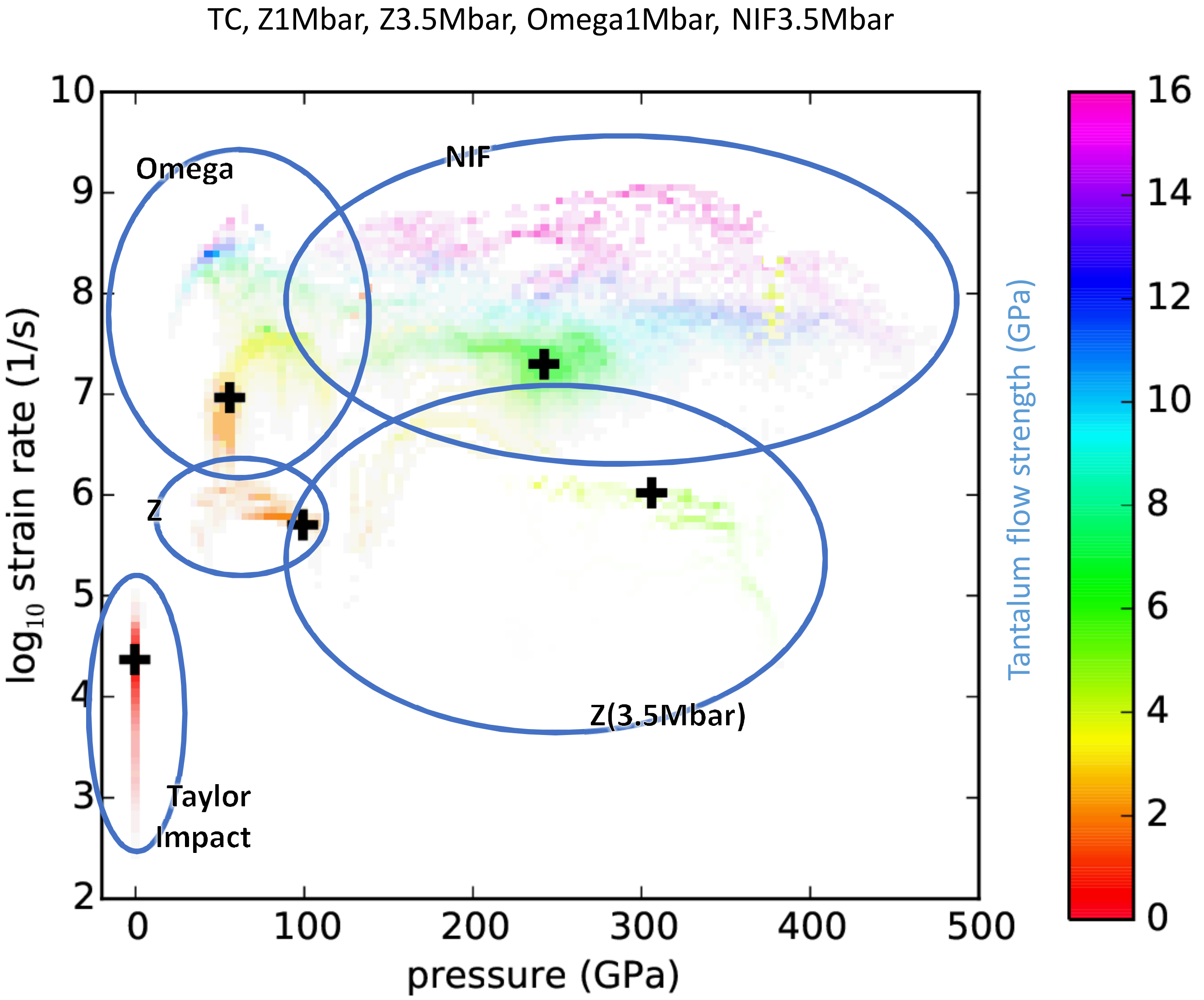
Cross-platform trends: pressure, strain rate

- Each experiment spans a range of parameters, and a range of strength states
- Shows dependence on other quantities – and path dependence
- Different models are being used in these simulations of the experiments!
- Atomistic and mesoscale simulations can help extend the range for each model



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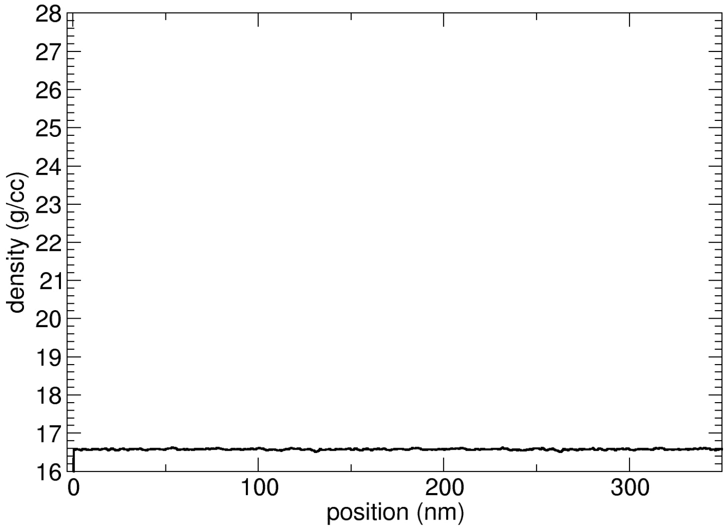
Molecular dynamics approach

- **Strengths of the MD methodology**
  - *Controlled material structures, i.e. grains, defects*
  - *Repeatable loading profiles at rates, from 10^{11} to 10^{8}*
  - *Full stress state throughout the sample*
  - *Strong dislocation and grain visualization tools in Ovito*

Several MD studies of shock, plasticity and dislocations

Ravelo, et al., PRB, 88 134101 (2013)
Tang, Bringa, Meyers, Mater. Sci. Eng. 580 414 (2013) &
Tramontina, et al., High Energy Density Phys, 10 (2014)

- **Classical molecular dynamics**
  - *Ta1 EAM potential by Ravelo was fit to isothermal EOS and verified against Hugoniot data*
    - does well with twinning and plastic flow in compression.
  - *Ramp wave modeled with accelerating infinite-mass piston with nonlinear profile $v_p = x/a + (x/a)^3$*
- **System size and grain structure**
  - *20 x 20 x 131 nm nanograin polycrystalline unit cell replicated in z to 20 μm and 350 million atoms*
  - *Two grain sizes of 5-10 nm and 8-20 nm*



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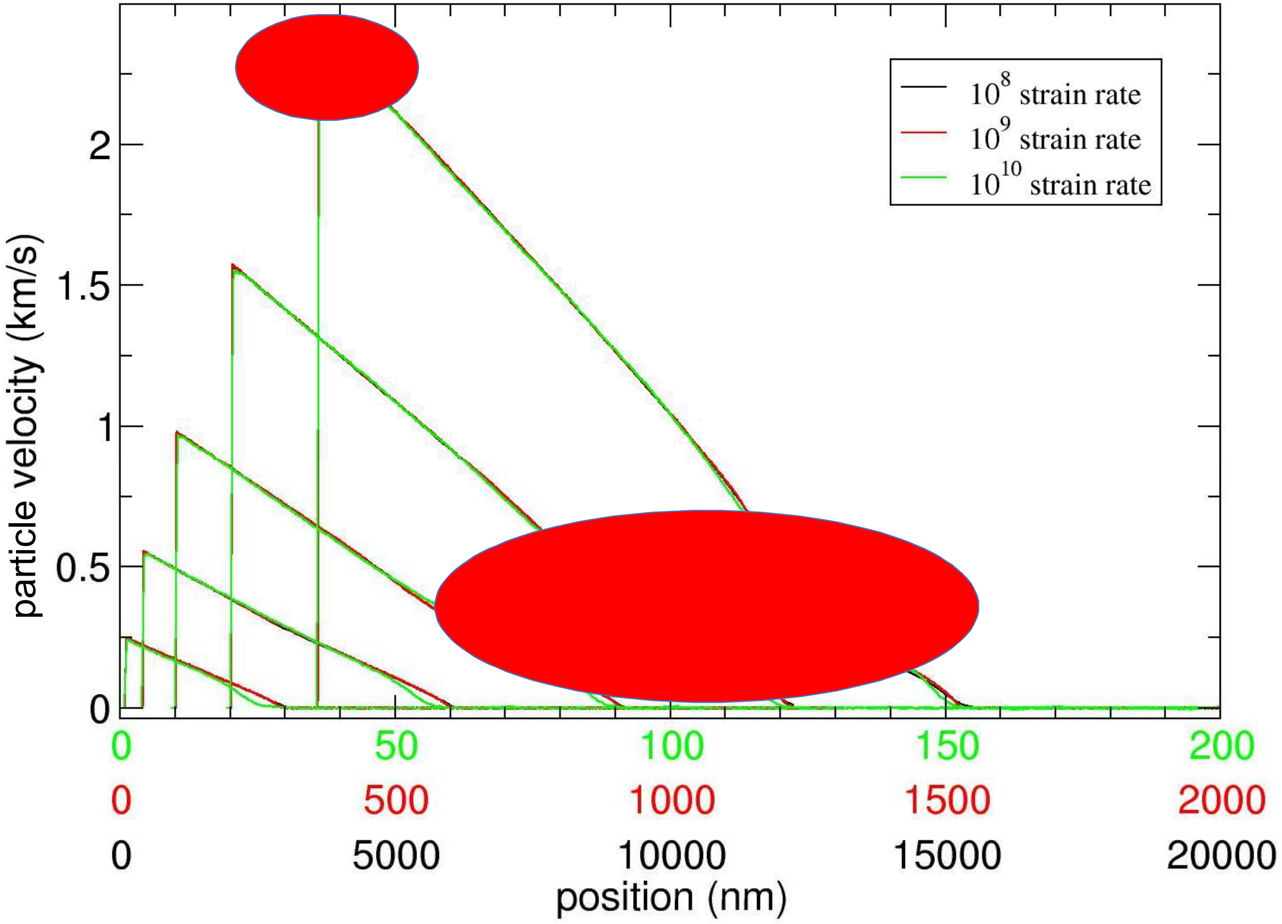
Scaled ramp profiles & strain-rate sensitivity



Using scaling arguments, we can compare strain rate response. ***Lane, Foiles, Lin, Brown, Phys. Rev. B, 94, 064301 (2016)***

All ramp waves driven nonlinearly from 0 to 2.4 km/s, giving peak pressures of 250 GPa.

10^{10} 1/s strain rate
Rises over 40 ps
150 nm & 2.5 million atoms

10^9 1/s strain rate
Rises over 400 ps
1.5 μm & 25 million atoms

10^8 1/s strain rate
Rises over 4 ns
15 μm & 350 million atoms

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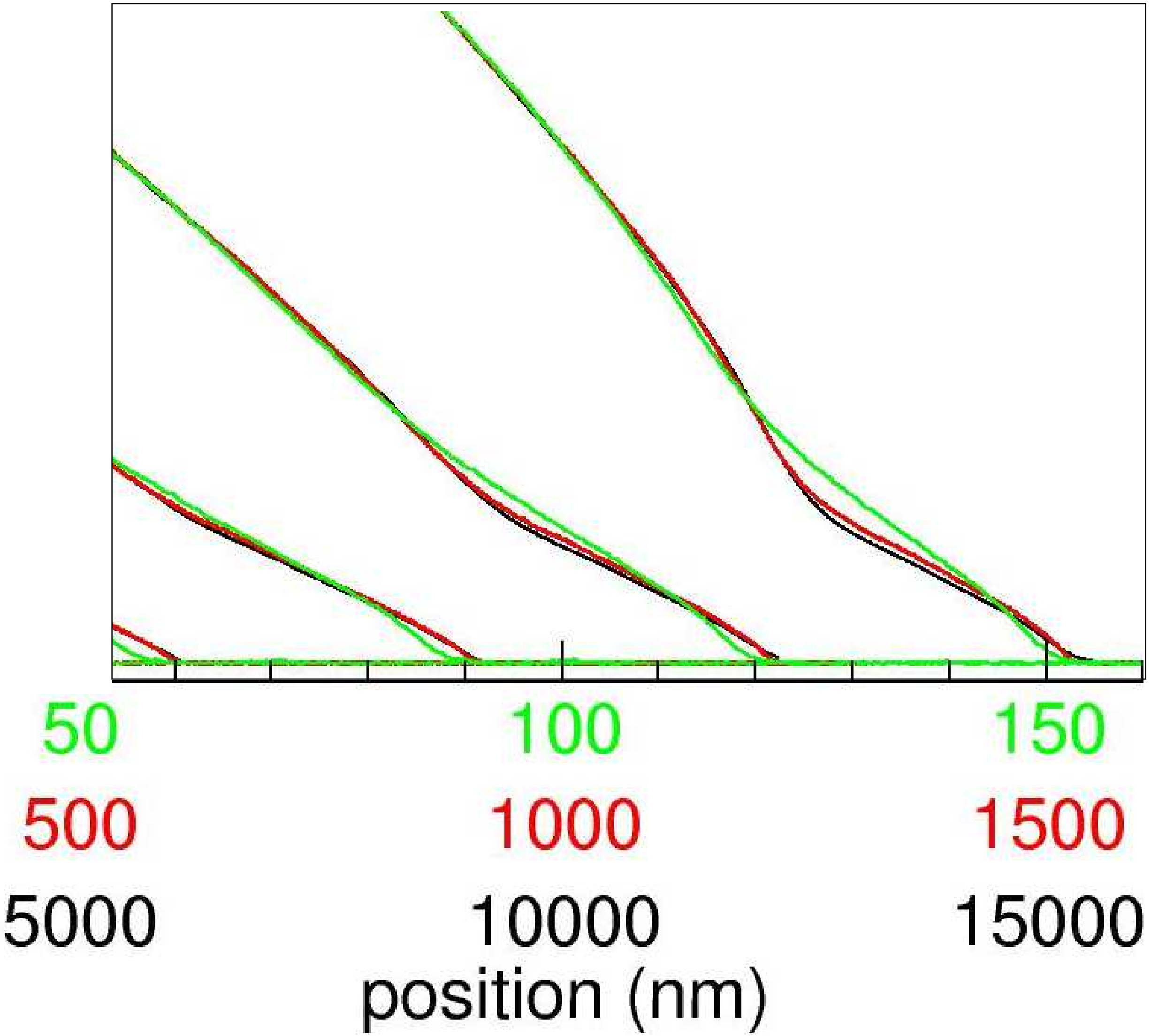
Precursor dependence on strain rate



Overlaying scaled profiles reveals where the wave profiles are dependent on strain-rate.

Elastic precursor and precursor decay depends significantly on strain rates.

High pressure portions of the waves are only weakly dependent on loading rate.

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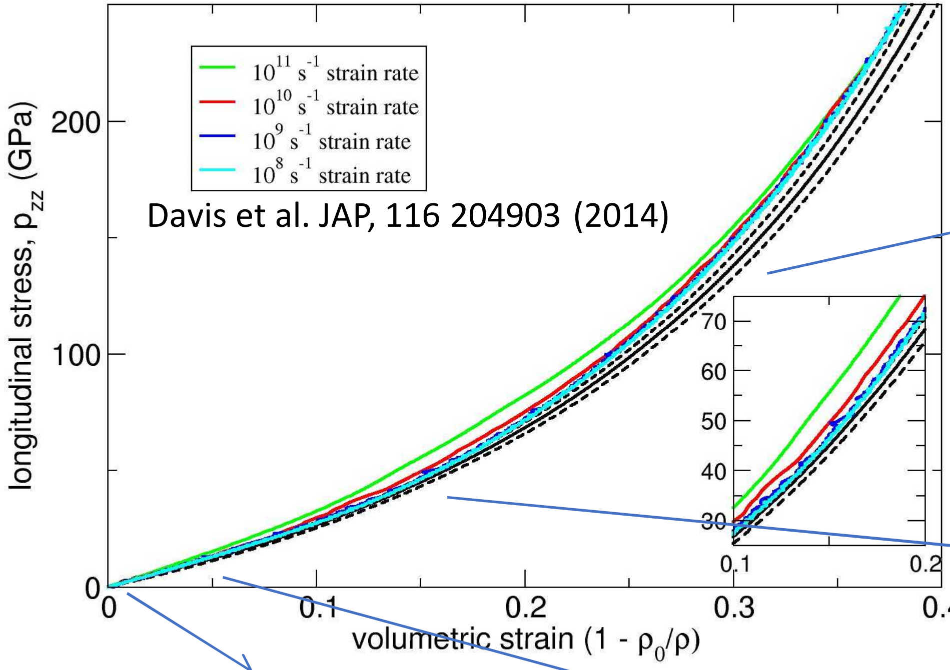
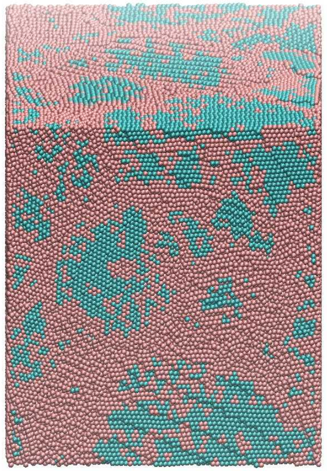
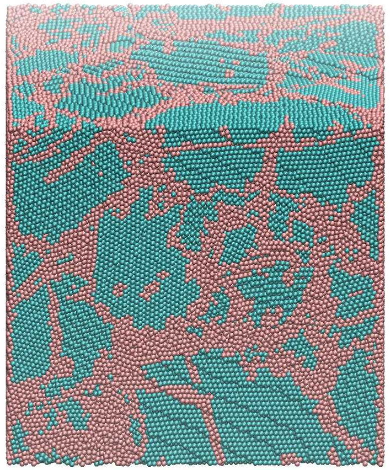
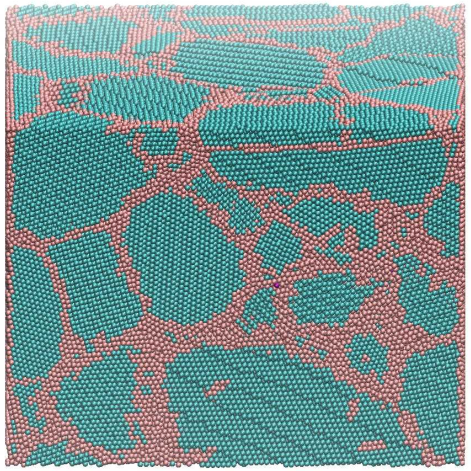
Comparison with experiment

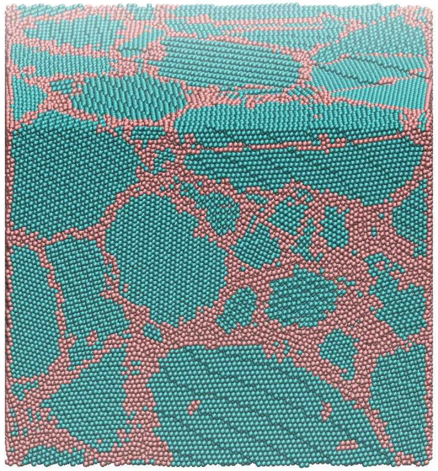


Davis et al. JAP, 116 204903 (2014)









Inverse Hall-Petch response dominated by grain boundary sliding -- Consistent with *Tang, Bringa, Meyers, Mater. Sci Eng. A,* ***580*** *(2013)*

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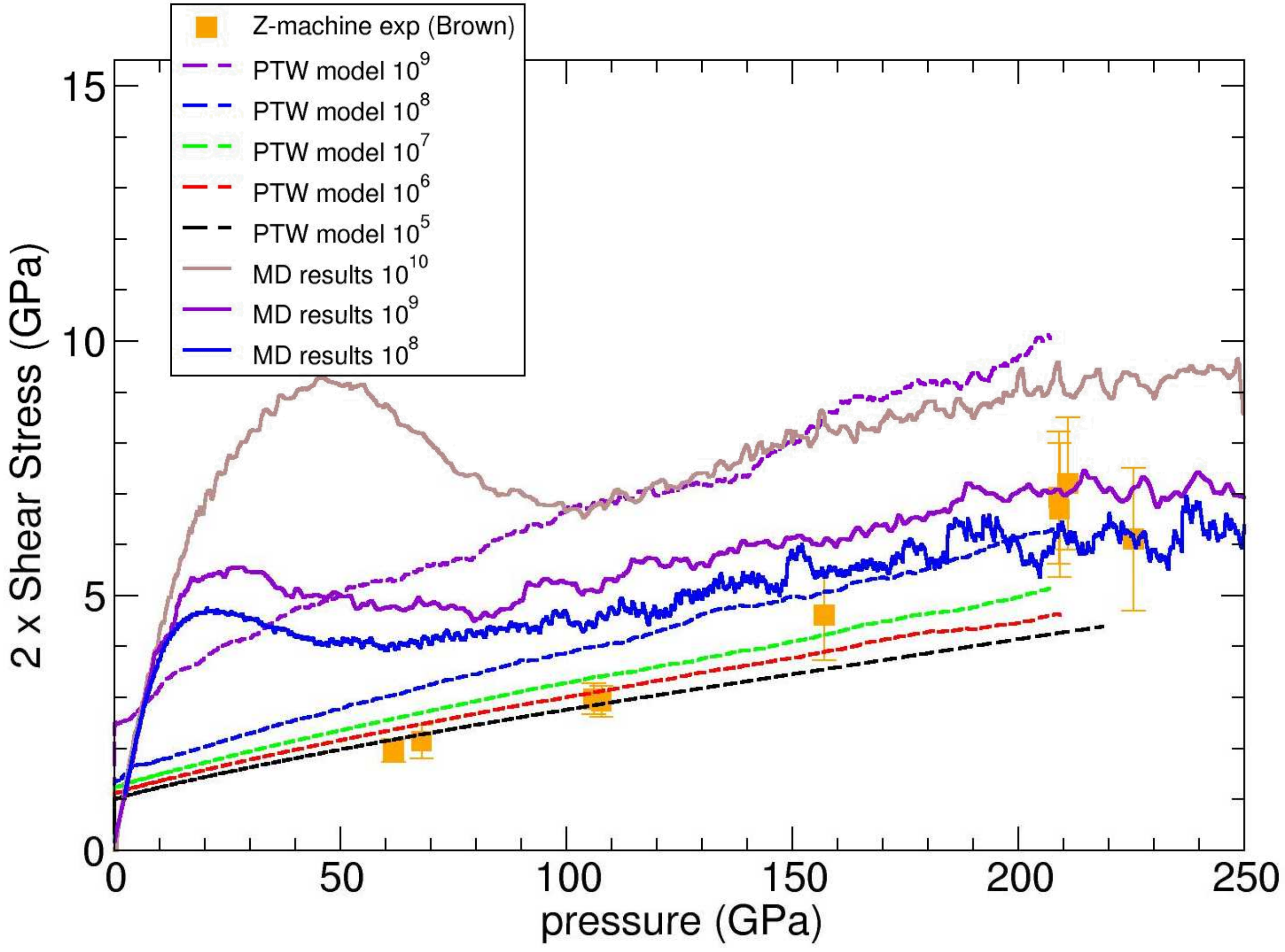
Extraction of strength



PTW model – Preston, Tonks, Wallace, JAP, 93 211 (2003)

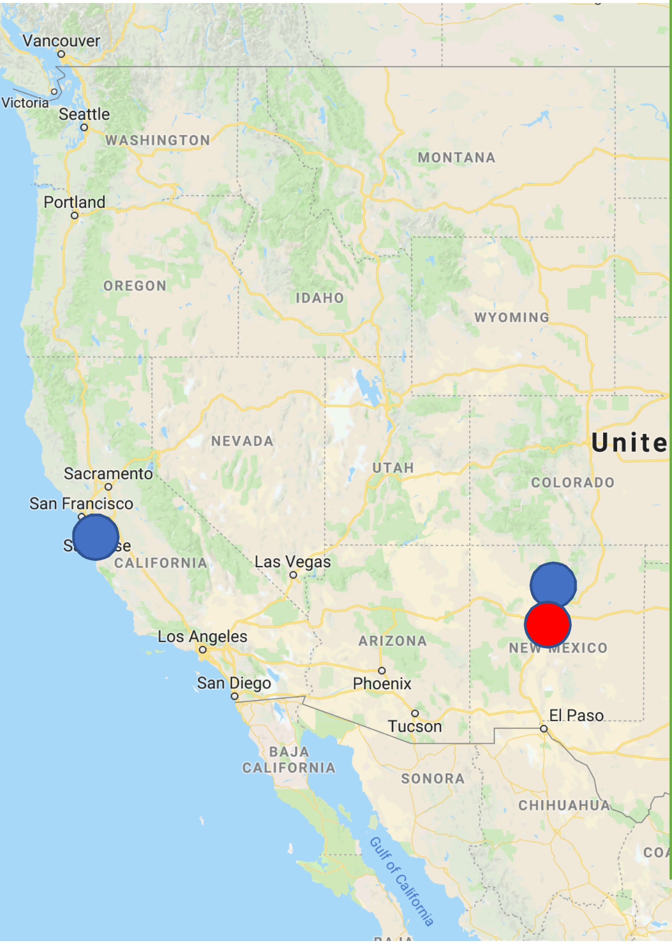
Exaggerated strength is seen below 100 GPa in the elastic precursor, especially at high strain rates. This is likely due to suppressed dislocation activity in nano size grains.

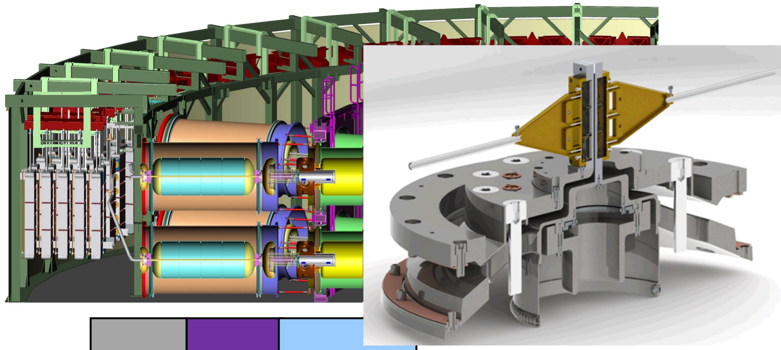
10^9 s^{-1} experiments have observed this high elastic strength

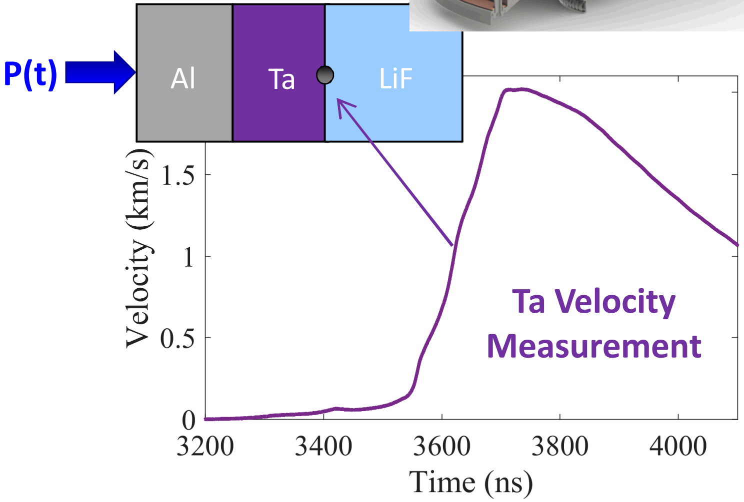
Crowhurst, Armstrong et al.,Appl. Phys. Lett. **109**, 094102 (2016)

Relatively good agreement with pressure dependence of the PTW model above 100 Gpa, especially at lower strain rates.

Connecting atomistics to Z ramp-release







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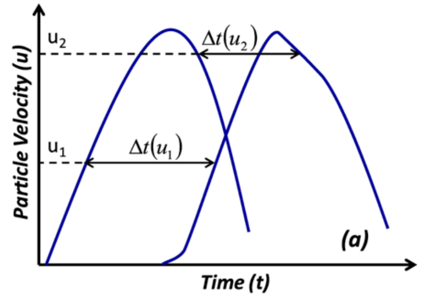
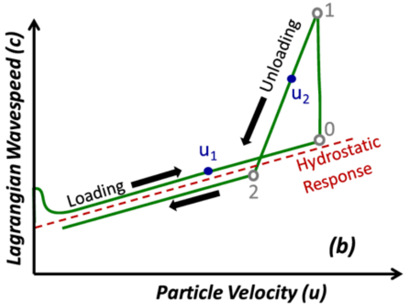
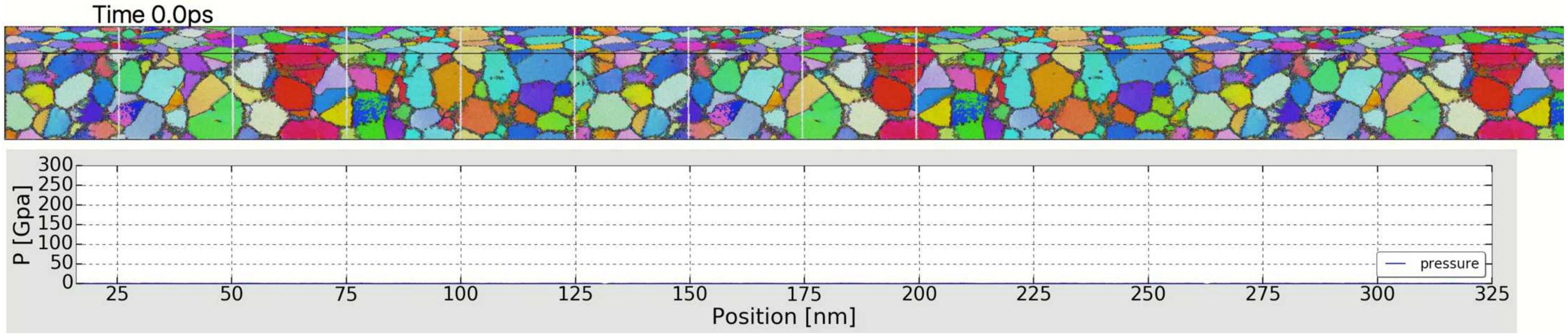




Atomistic simulations for microstructures



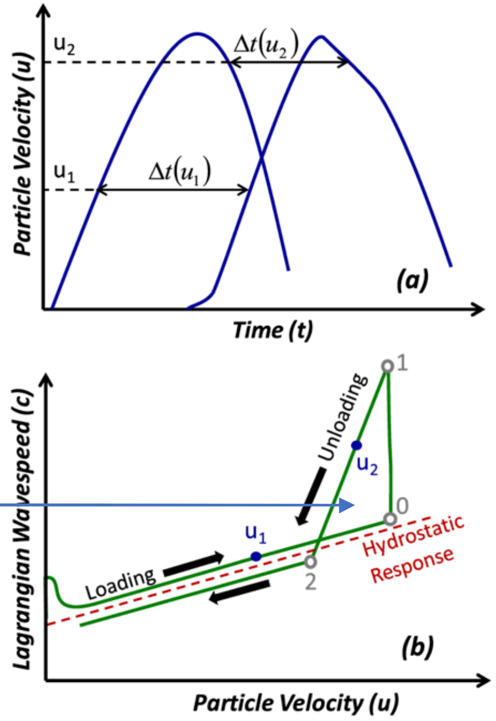
- For isentropic flow of simple waves, the Lagrangian wave speed can be calculated using the particle velocity histories at different locations.

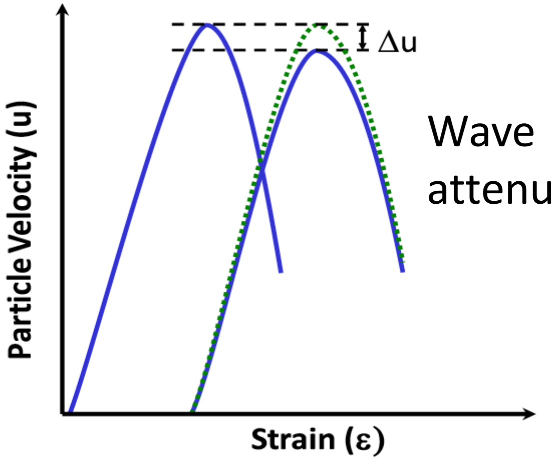
$$C_u = c_L(u_p) = (\partial X/\partial t)_u = \frac{\Delta X}{\Delta t}_u$$

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

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

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





Wave attenuation

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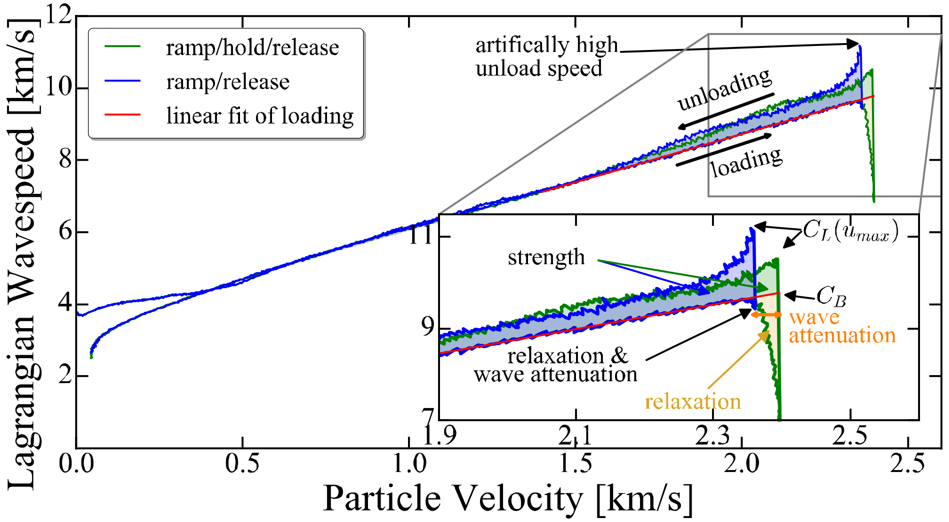
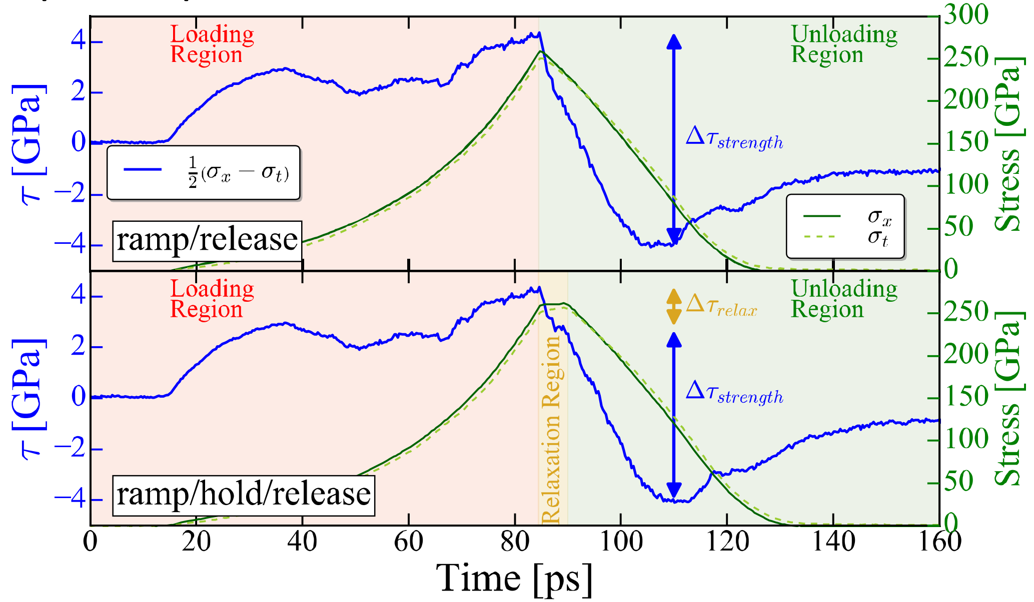
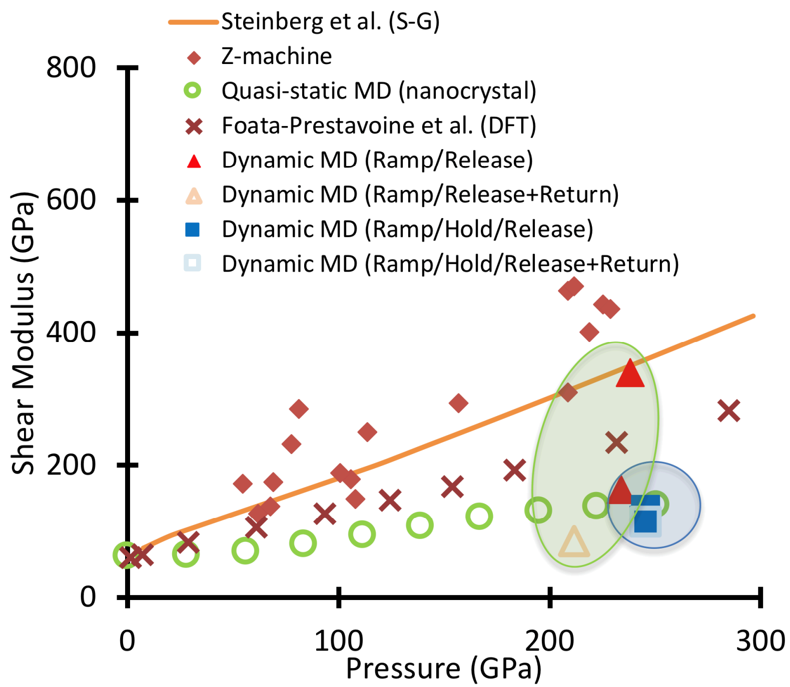
Atomistic for wave analysis improvements



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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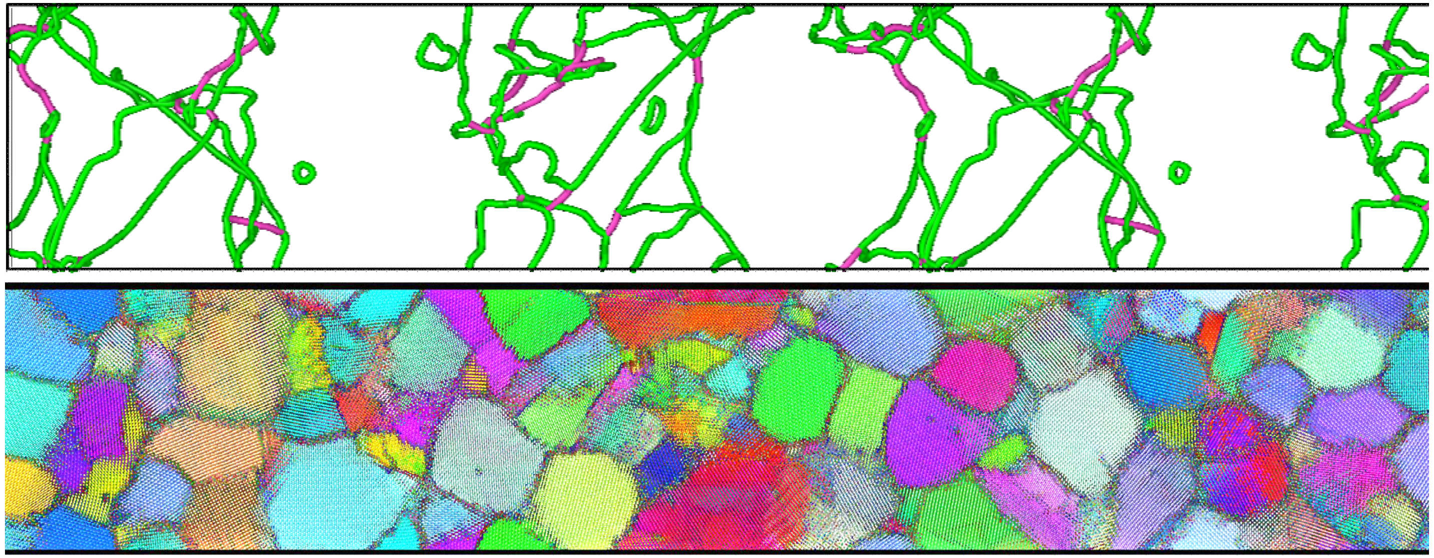
Exploring deformation mechanisms

- Dislocation and boundary dominated microstructures
  - Defective [100] Single Crystal Tantalum
  - Nanocrystalline Tantalum



Dislocation Type:
Green: screw
Magenta: edge
Dislocation density:
$2.35 \times 10^{16}\ m^{-2}$

6 nm average,
non-textured grains

- Dislocations were identified using Dislocation Extraction Algorithm (DXA).
- Twinning was visualized by examining changes in bcc crystal orientation, using the polyhedral template mapping (PTM) technique.

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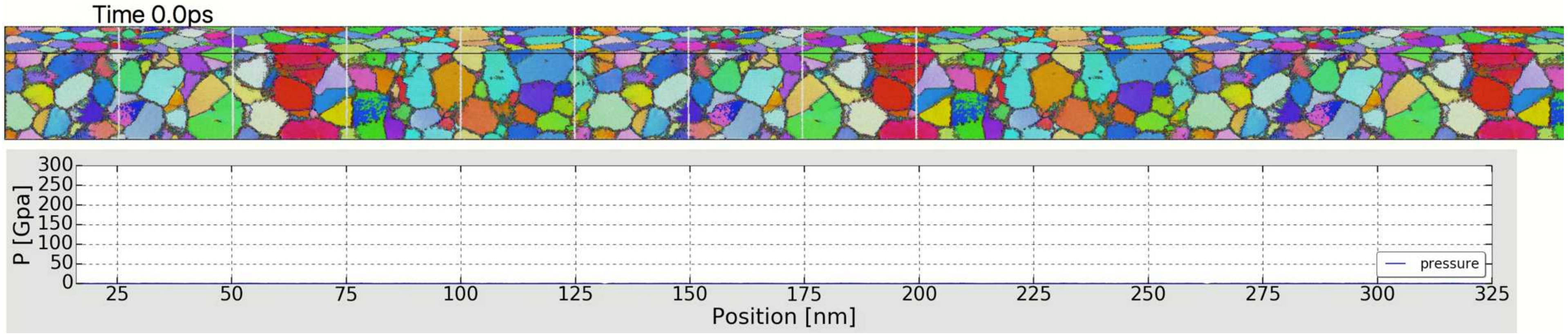
Atomistic simulations for microstructures

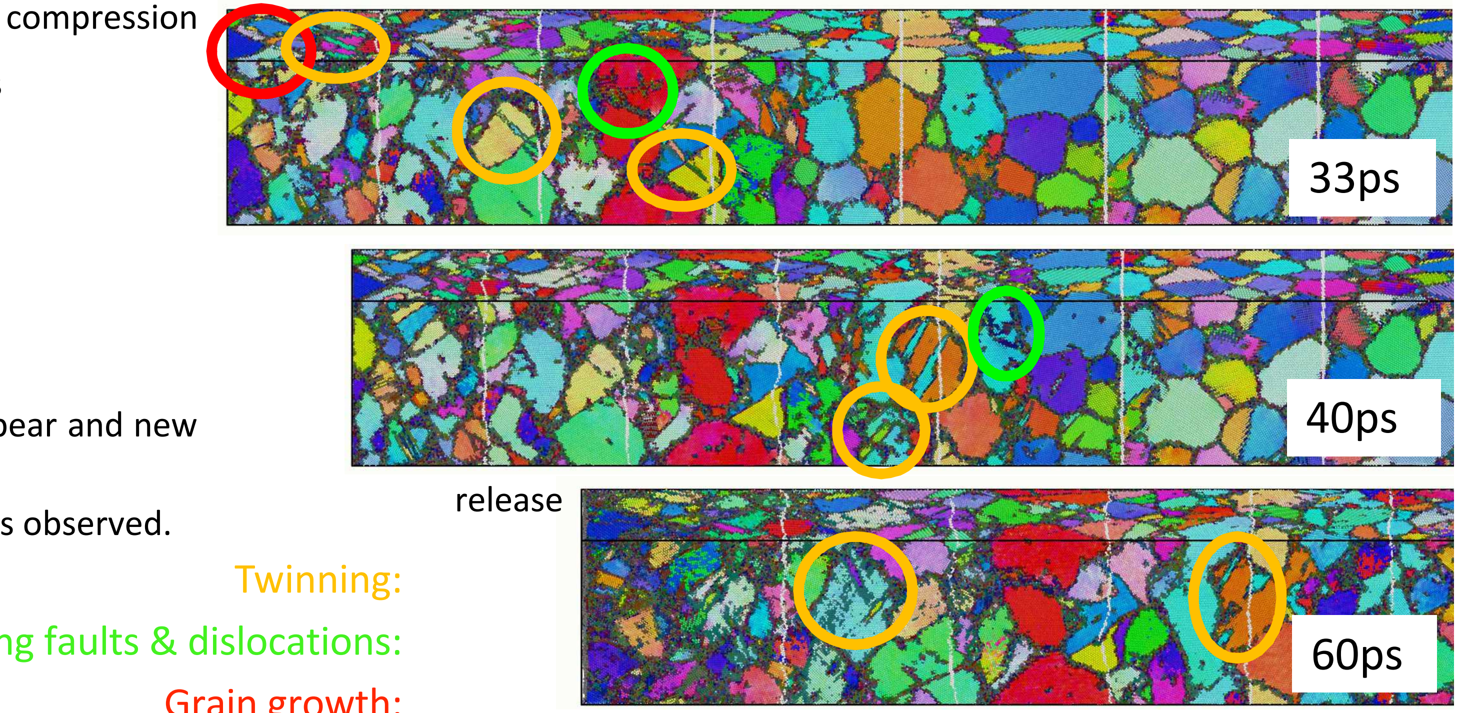


Compression:

- 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:

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NC Plasticity During Ramp Compression

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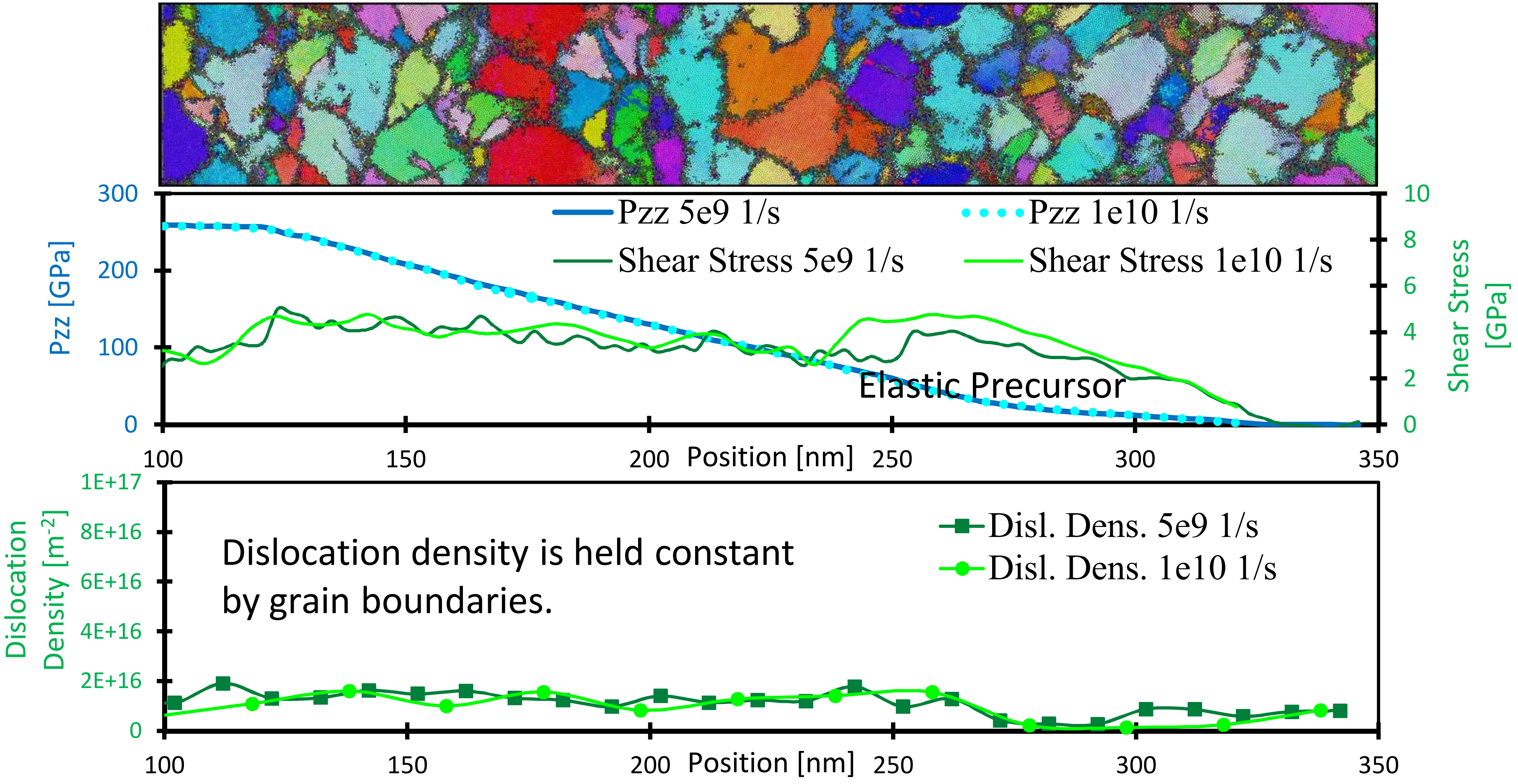

- Grain boundaries are seen to help stabilize twins.

- Experimental observations of elastic precursor:
- Armstrong, R. W., and Zerilli, F. J., *JAP* 43.49 (2010): 49200
- Smith, R. F., et al. *PRB* 86.24 (2012): 245204.

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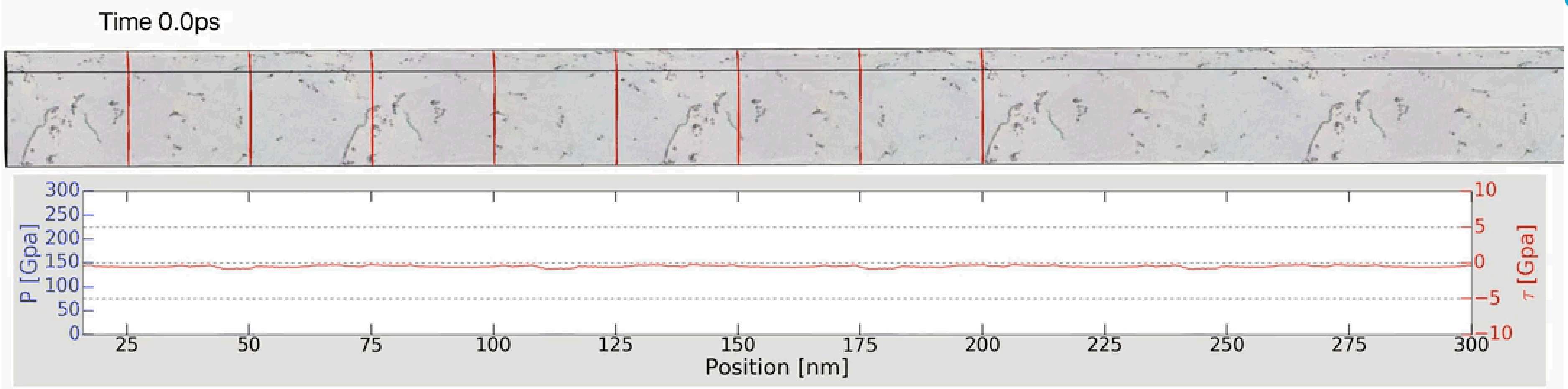
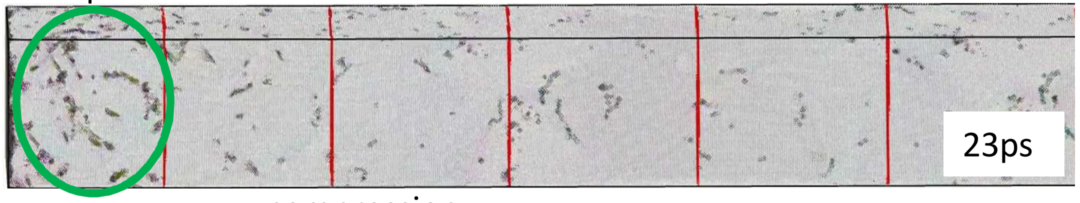
Defective [100] Single Crystal (SC)



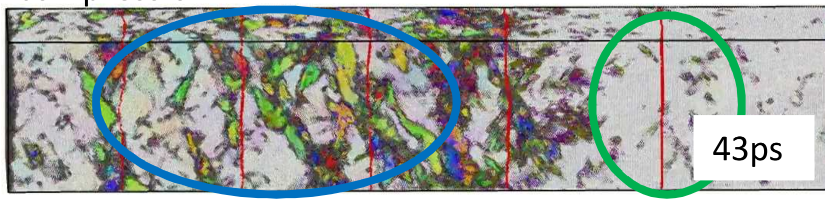
Observed plasticity mechanisms:

- Dislocation motion and multiplication/annihilation
- Twinning/De-twinning

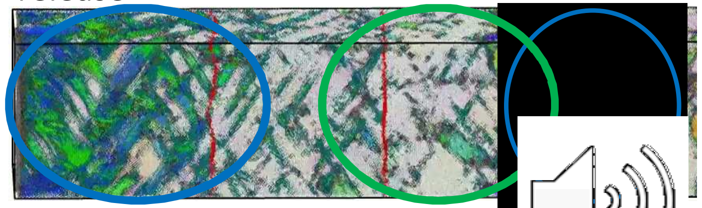
compression



compression



release



- Dislocation multiplication and annihilation evolves from dislocation interactions.
- Stacking faults nucleate from dissociating ½<111> bcc screw dislocations, which then grow forming twins.

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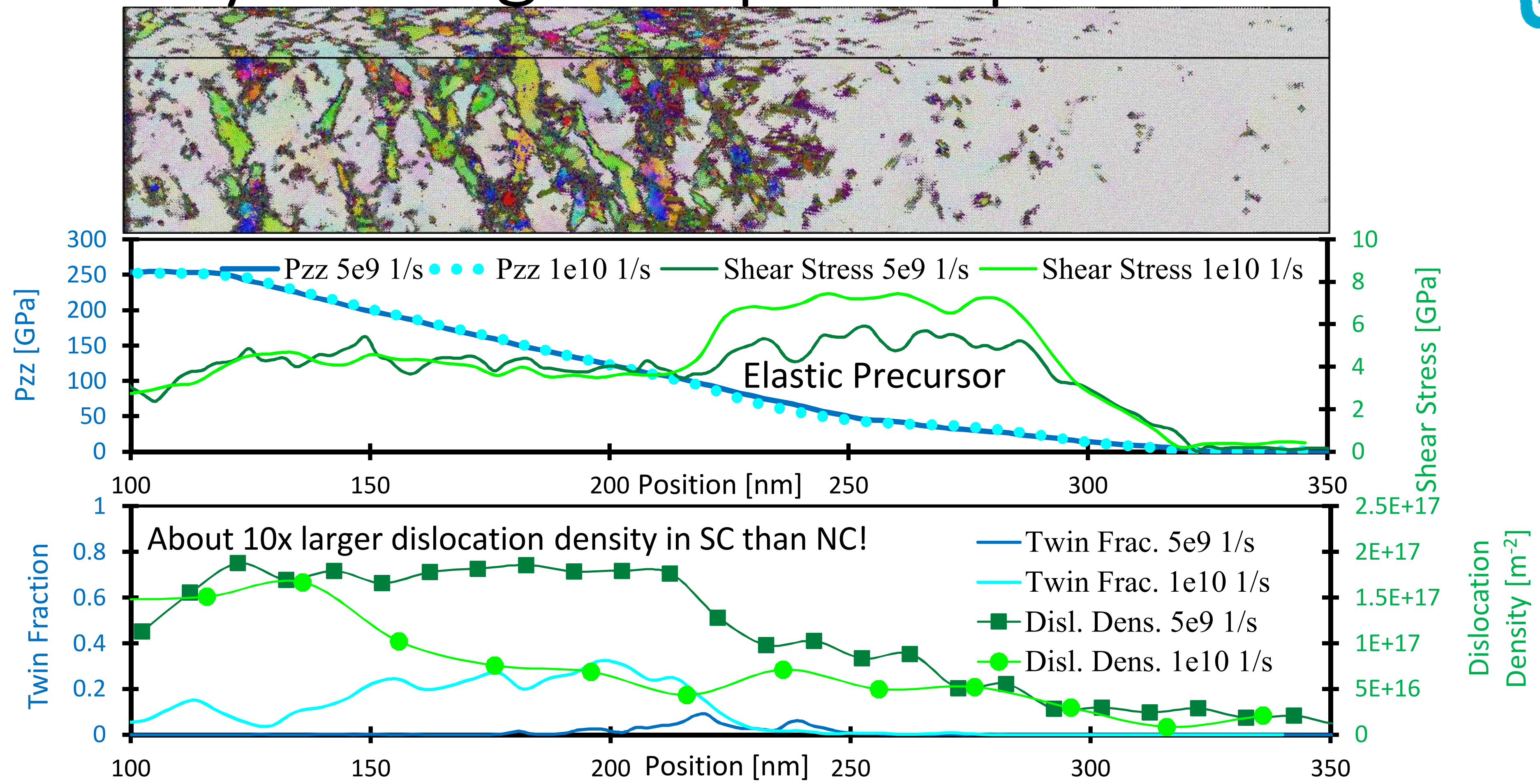
SC Plasticity During Ramp Compression



- Initiation of twinning drastically drops the shear stress.
- Drastic transition from twinning to dislocation generation when doubling loading rate.
- Larger elastic precursor than NC.
- End of elastic precursor associated with change in twinning or dislocation density.

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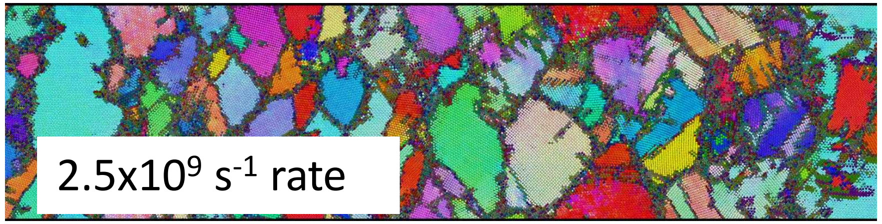
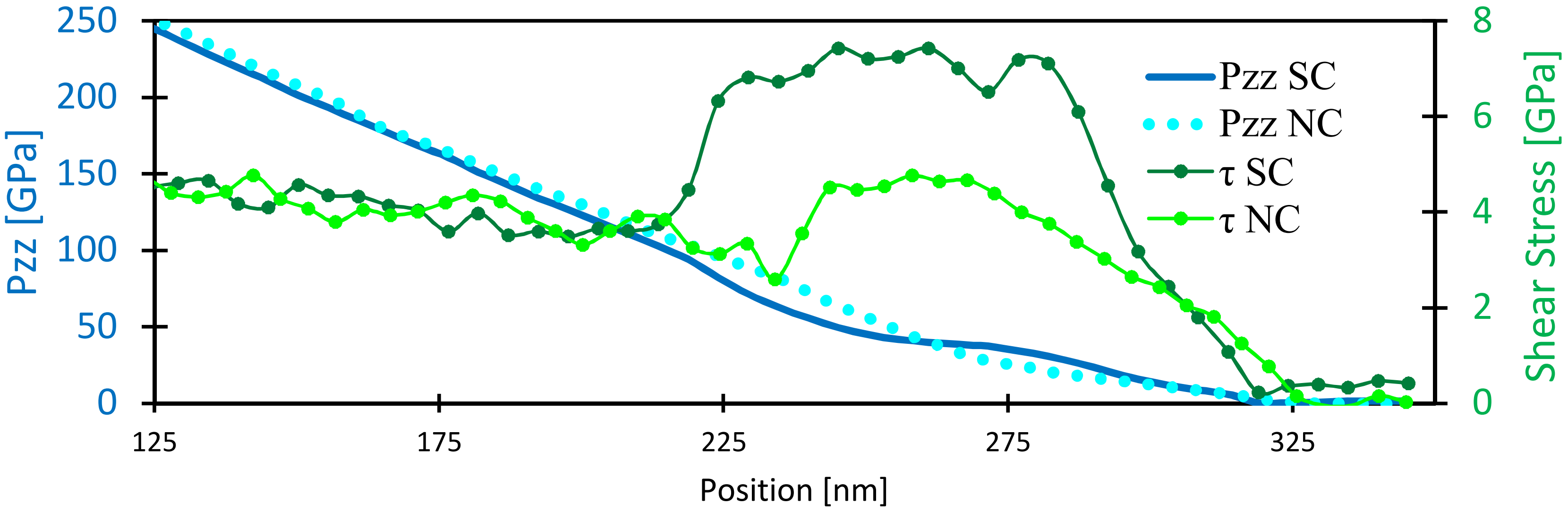
Single vs Nano Crystal Strength & Plasticity

- It can be seen that twinning is still present in NC simulations at a loading rate at which SC simulations no longer observed compression twinning.





- Elastic precursor region: Is greatly affected by the plastic mechanisms.
- Fully plastic region: Even though there are significant differences in the observed SC and NC plastic mechanisms, the shear stresses are similar.

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Atomistic progress review

- We've studied **dynamic ramp wave response in tantalum at 10^{10} to 10^{8} 1/s** strain rates with molecular dynamics and ramp profile scaling analysis.
- **Agreement in stress-strain response** with lower-rate Z experiments
    - Lower strain rate brings better comparison, especially at strain below 0.2
    - High rates produce a more robust elastic precursor as seen in laser experiments
- Using MD we have **validated the self-consistent Lagrangian analysis** and identifies the need for improved experiments to improve reliability.
- More **recently we've attempted to tie specific mechanisms to strength** measurements.
    - We find that **grain boundaries and interfaces play a large role** in mediating dislocation density.
    - We observed **twins that nucleate from grain boundaries versus dissociated dislocations** are more likely at slower strain rates.
    - Dislocation density and twinning appear to play a large role in the elastic precursor region, but surprisingly did not in the fully plastic region.

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Scaling to discern strain-rate dependence

Scaling conditions for loading:

$$v(t) = v'(t') \qquad \& \qquad t' = \frac{1}{M}t$$

$$x'\left(\frac{1}{M}t\right) = \frac{1}{M}x(t)$$

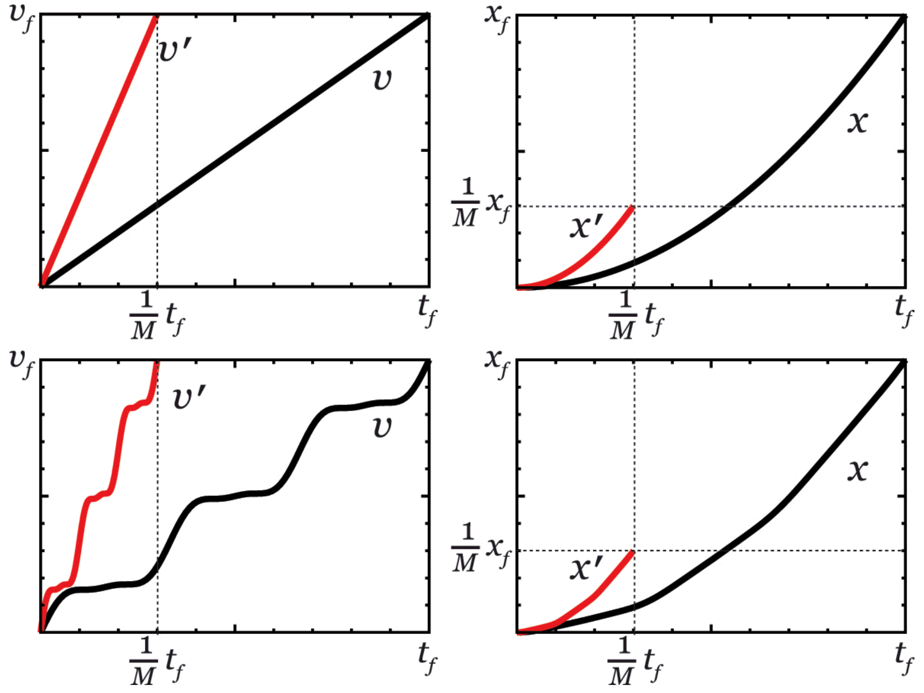
$$v'\left(\frac{1}{M}t\right) = v(t)$$

Dynamic similarity:

$$\frac{F_{\text{model}}}{F_{\text{actual}}} = \frac{M_{\text{m}}\frac{L_{\text{m}}}{T_{\text{m}}^2}}{M_{\text{a}}\frac{L_{\text{a}}}{T_{\text{a}}^2}} = \frac{\rho_{\text{m}} A \frac{L_{\text{m}}^2}{T_{\text{m}}^2}}{\rho_{\text{a}} A \frac{L_{\text{a}}^2}{T_{\text{a}}^2}}$$

$$= \lambda_\rho \left(\frac{\lambda_L}{\lambda_T}\right)^2 = 1$$

Driving piston velocity and position:



Invariant to scaling:

Velocity
Stress
Strain
Temperature*
Forces
Density

Not invariant:

Strain rates
Accelerations
Times and distances
any extensive variable…

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