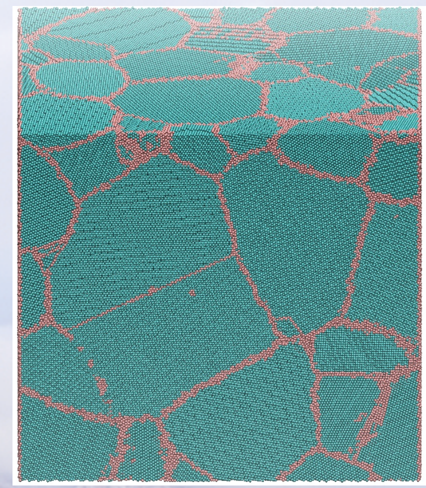
LAMMPS User Workshop
Albuquerque, NM
5 August 2015

Molecular modeling of high-pressure ramp waves in tantalum



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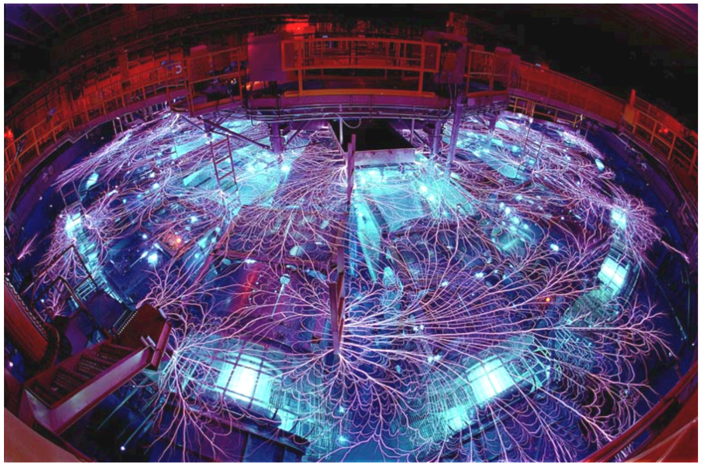
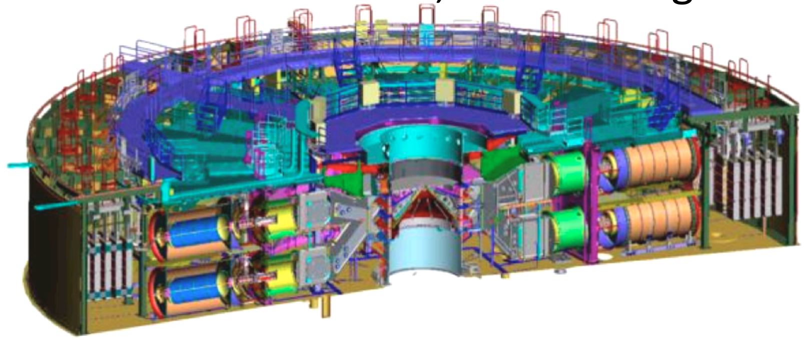
Motivation for ramp wave simulation

Z-machine at Sandia National Labs



33 m in diameter, 3 stories high



22 MJ stored energy

25 MA peak current

100-600 ns rise time

Z-machine is a pulsed power device which can drive mechanical waves in both shock and quasi-isentropic conditions

- Ramp waves to explore off-Hugoniot EOS
- Continuous data vs single shock points
- Study of material strength at extremely high pressures (>100s of GPa) and with control over strain rates.
- Complementary computational facilities incorporate quantum (DFT), classical (MD), and extensive continuum modeling to support experiments

25 MA is the max current load of 160,000 homes

Sandia National Laboratories

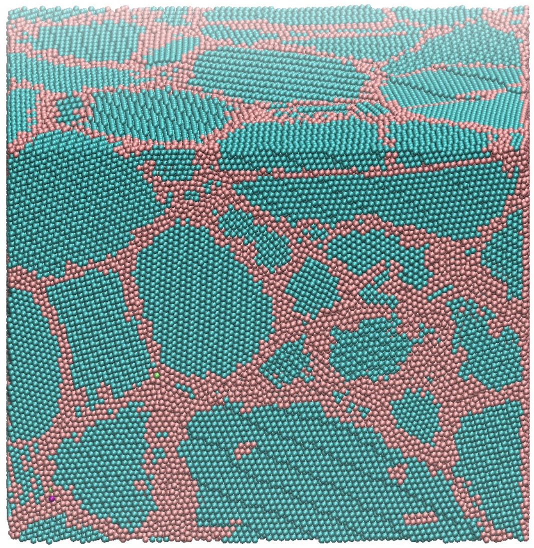
Tantalum's unexpected complexity

- **Tantalum, as a high-Z BCC metal with no high-pressure phase transitions, has potential use a standard for high-pressure studies. But, its properties depend on poorly understood elastic/plastic and dislocation dynamics.**

- **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)*

- **Significant variation in methodology and materials complicate:**
  - *Variation in drivers (laser ablation vs flyer)*
  - *Variation in strain rates (10^{10} to 10^5)*
  - *Variation in material microstructure and grain texture (characterized and uncharacterized)*
  - *Variation in strength extraction methods (Rayleigh-Taylor instability and ramp-release)*

Molecular dynamics approach

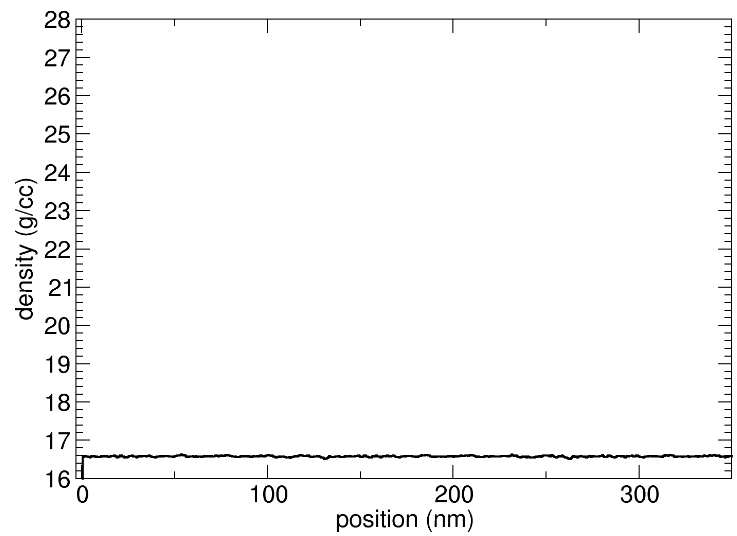


- **Strengths of MD method**
  - *Controlled material structures, i.e. grains, defects*
  - *Repeatable loading profiles at rates, from 10^{11} to 10^{8}*
  - *Full stress state throughout the sample*
  - ***However**, we do not achieve overlap in strain rate, nor microstructure.*

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*
    - captures twinning and plastic flow.
  - *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*



Using scaling to discern strain-rate dependence

Scaling conditions for loading:

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

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

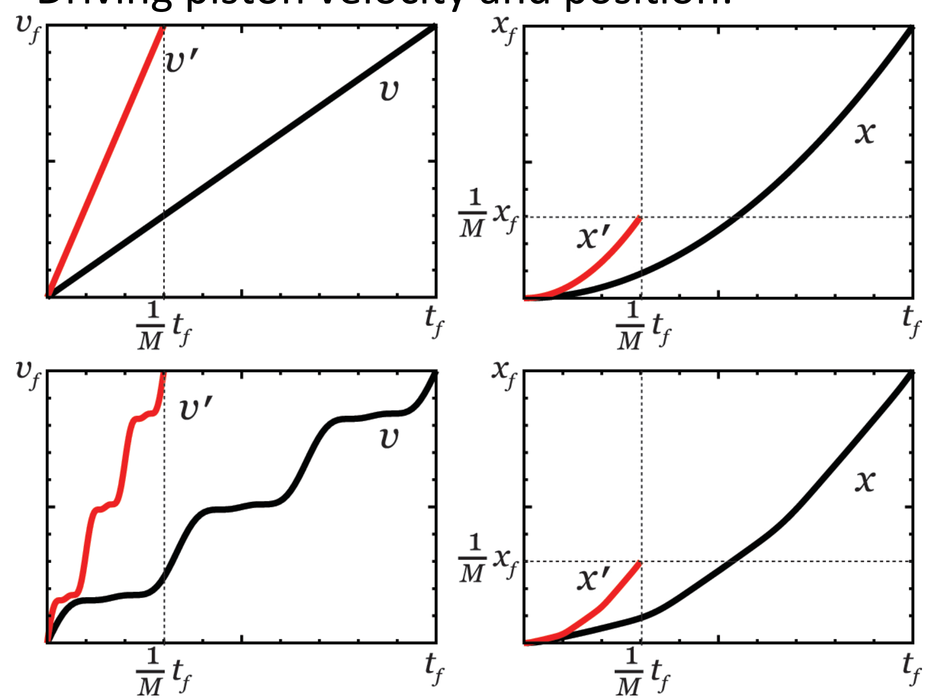
$$v'\left(\frac{1}{M}t\right) = v(t)$$

Dynamic similarity:

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

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

Driving piston velocity and position:



Invariant to scaling:

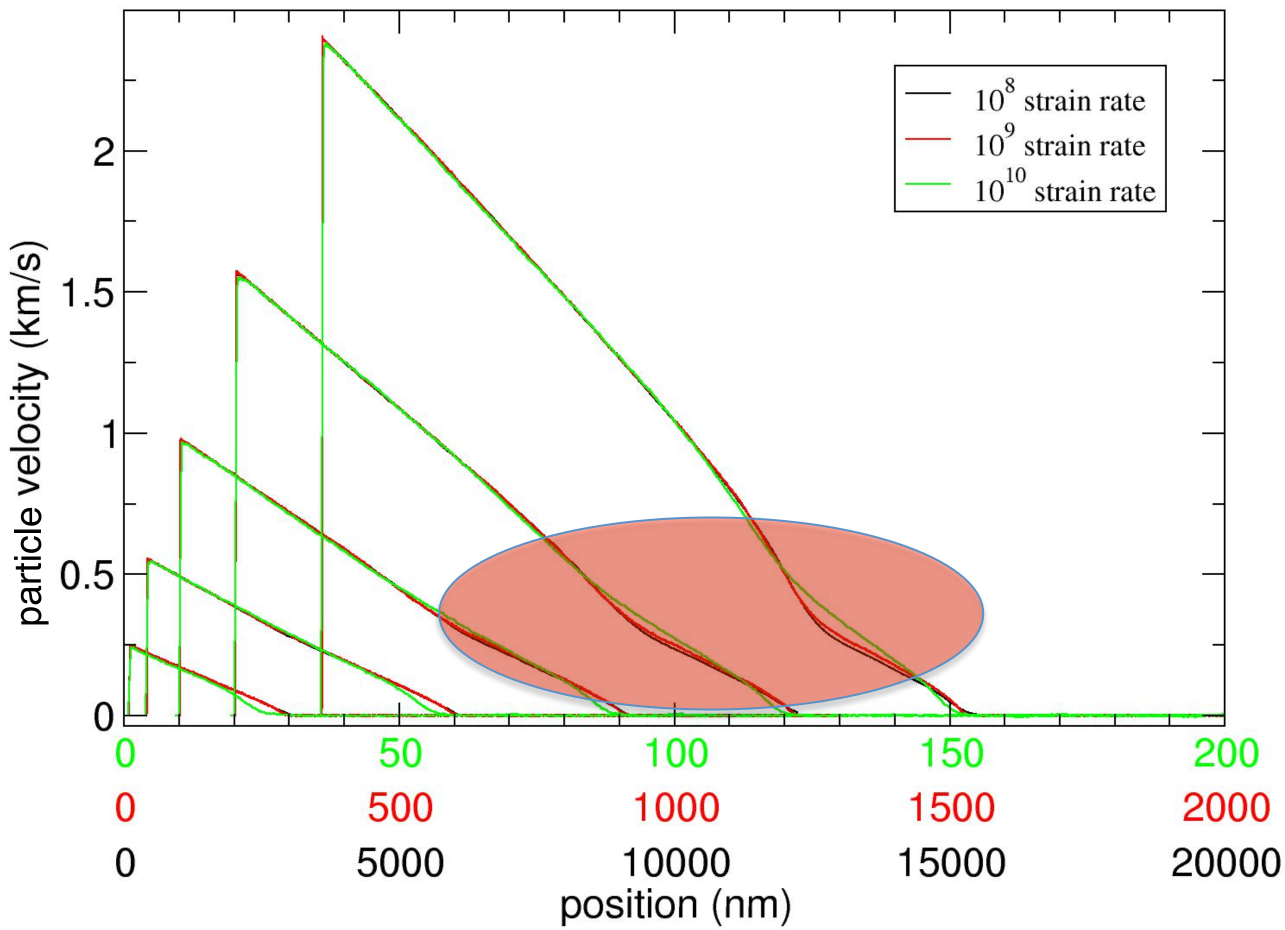
Velocity
Stress
Strain
Temperature*
Forces
Density

Not invariant:

Strain rates
Accelerations
Times and distances
any extensive variable…

5

Scaled ramp profiles & strain-rate sensitivity



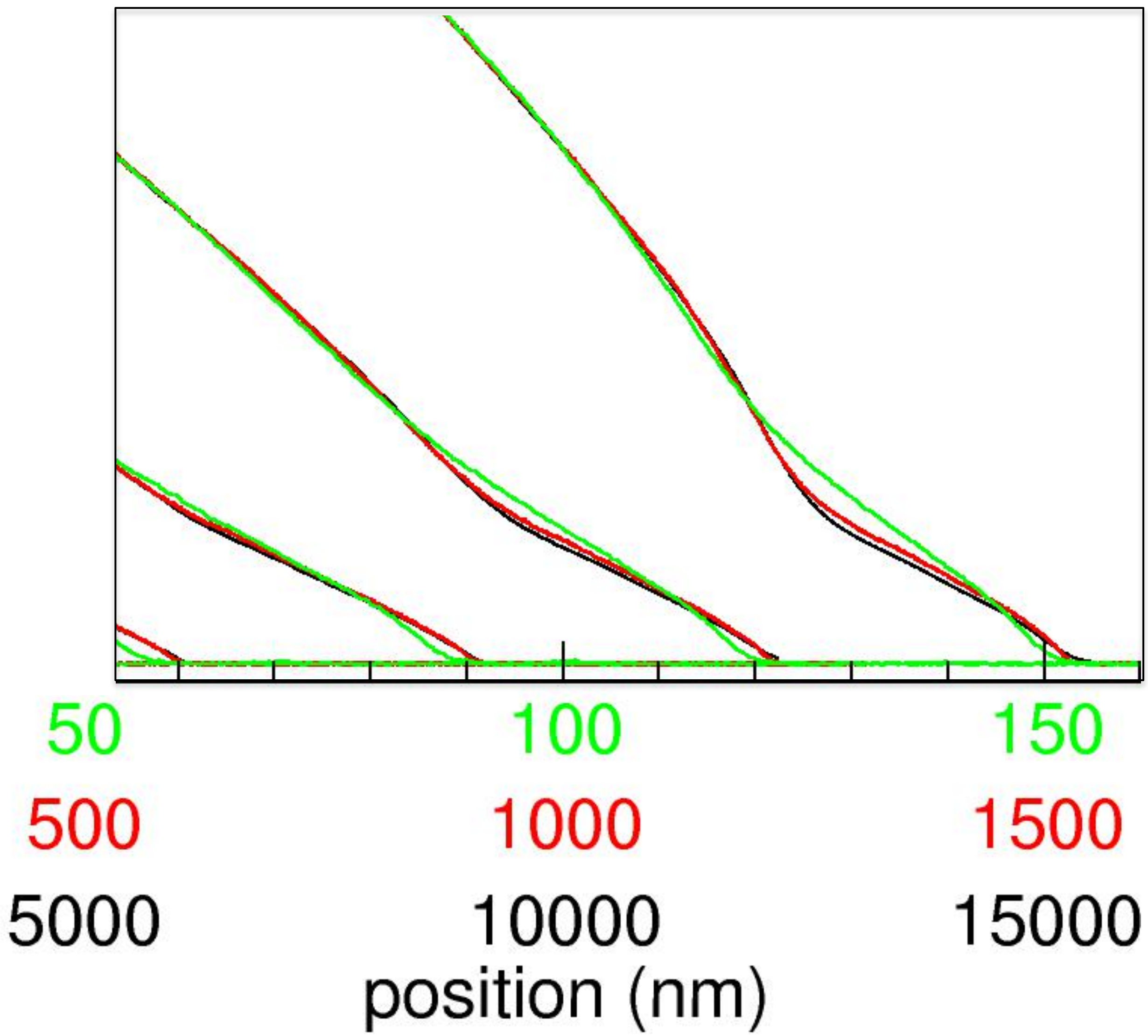
All ramp waves are driven nonlinearly from 0 to 2.4 km/s, giving peak pressures of 250 GPa.

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

Precursor dependence on strain rate



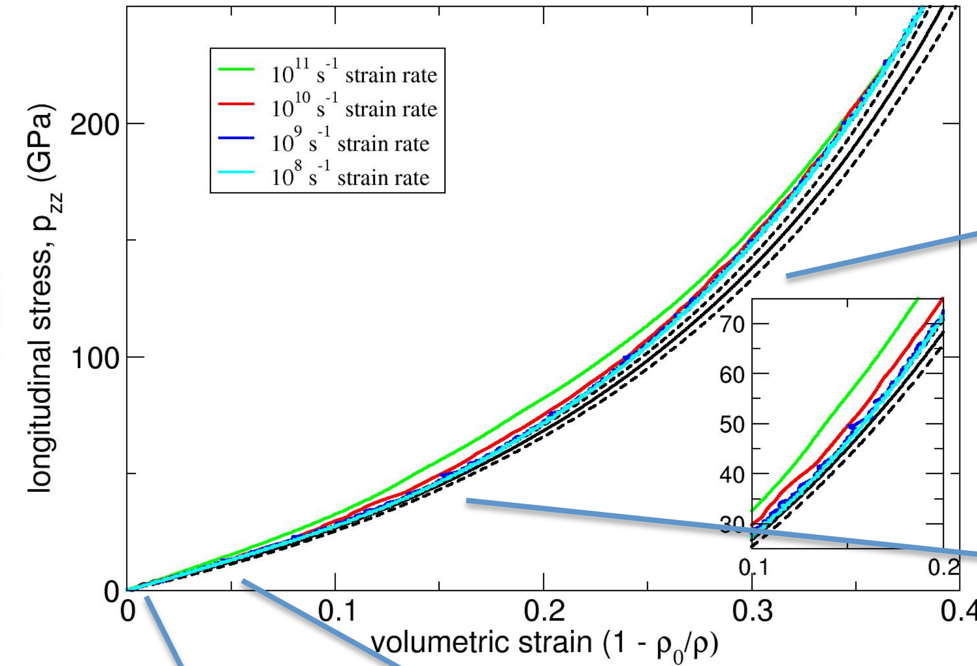
Overlaying scaled profiles reveals where the wave profiles are dependent on strain-rate.

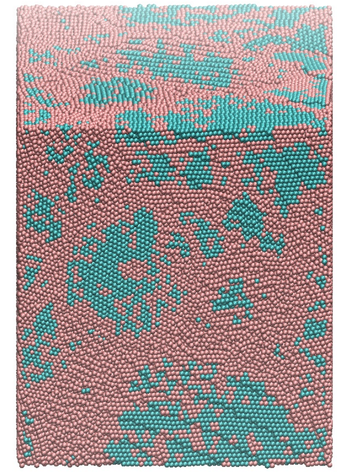
Elastic precursor and precursor decay depends significantly on strain rates.

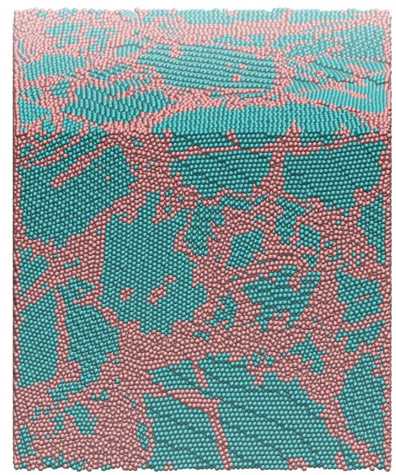
High pressure portions of the waves are only weakly dependent on loading rate.

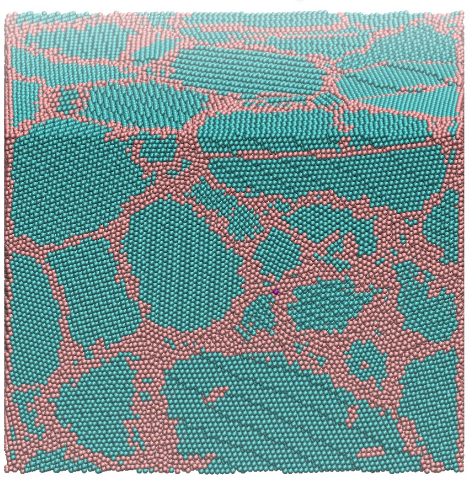
Comparison with experiment

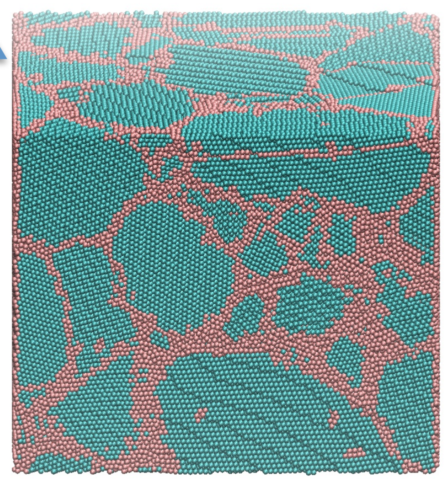
Davis et al. JAP, 116 204903 (2014)







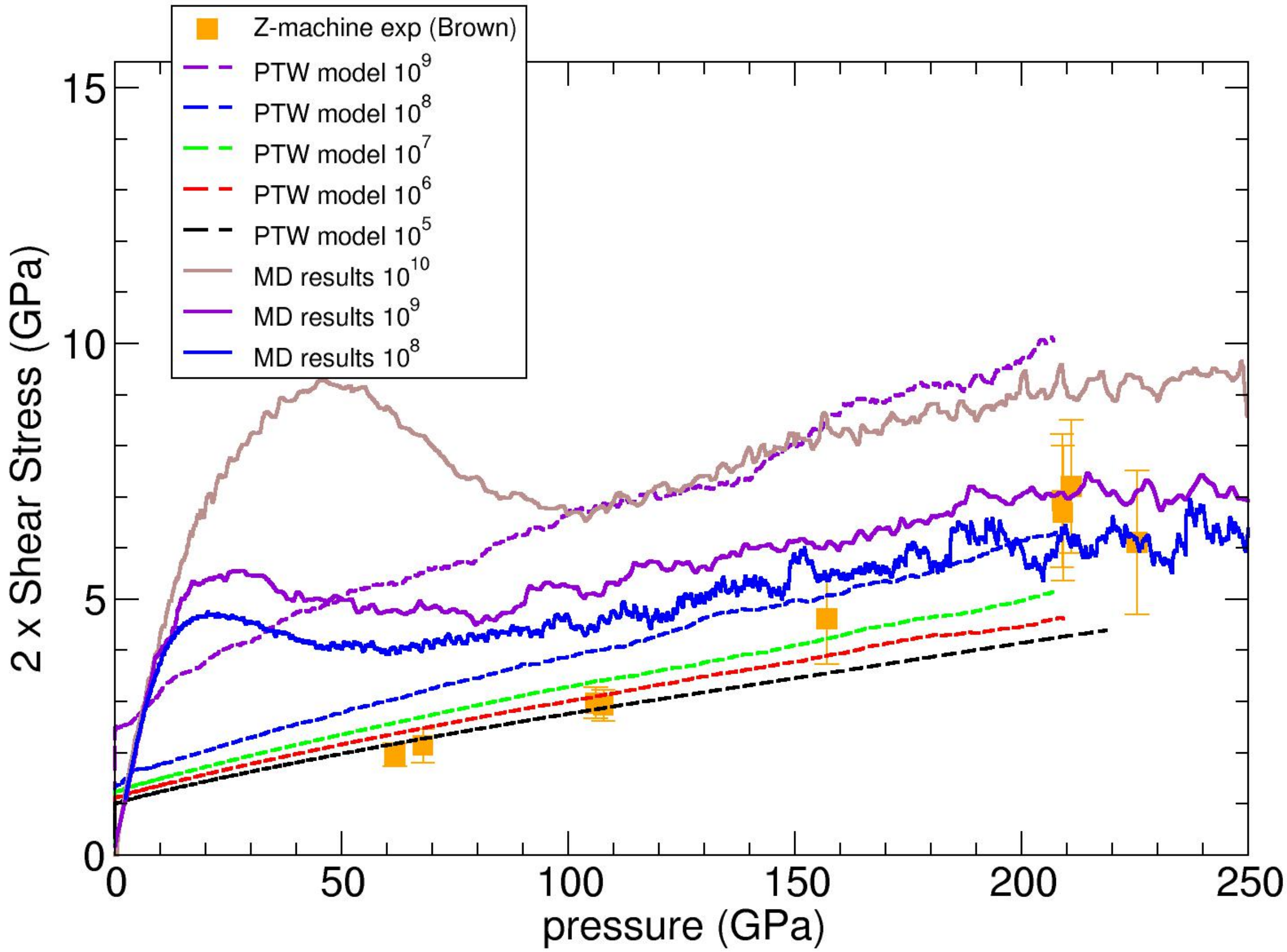




Inverse Hall-Petch response dominated by grain boundary sliding

Consistent with *Tang, Bringa, Meyers, Mater. Sci Eng. A,* ***580*** *(2013)*

Extraction of strength



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.

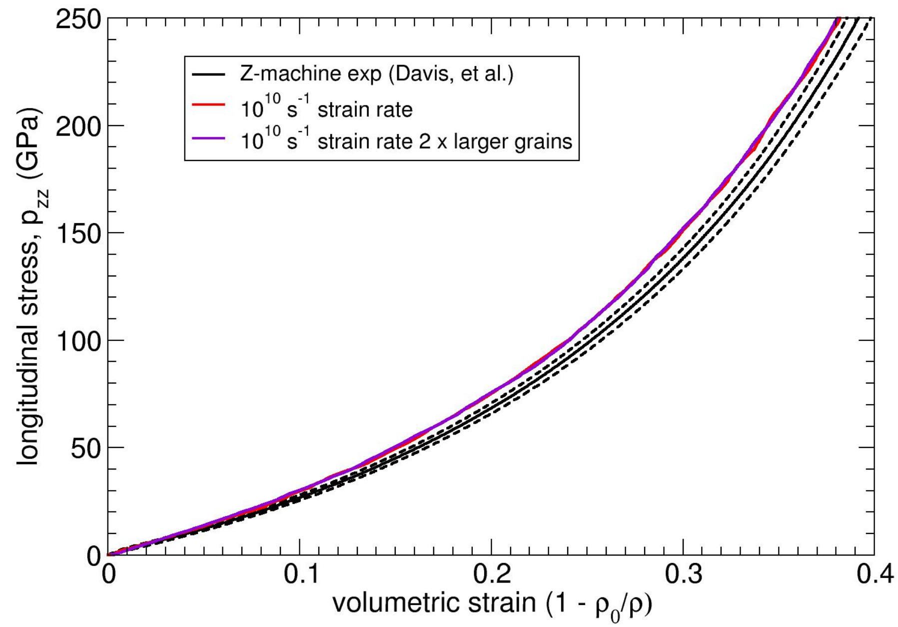
Relatively good agreement with pressure dependence of the PTW model above 100 Gpa, especially at lower strain rates.

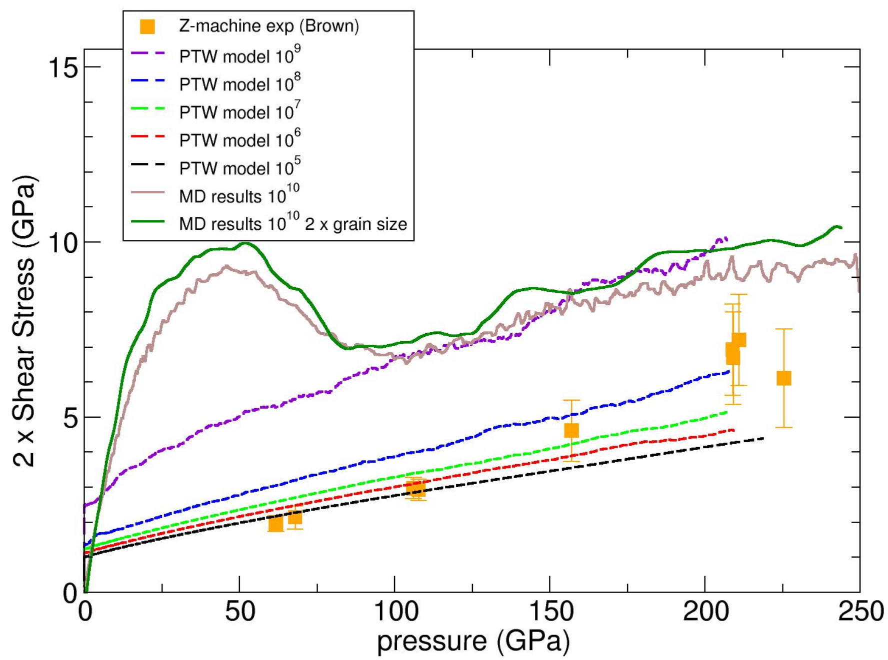
PTW model – Preston, Tonks, Wallace, JAP, 93 211 (2003)

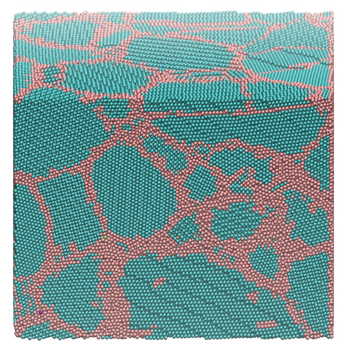
Increased grain size

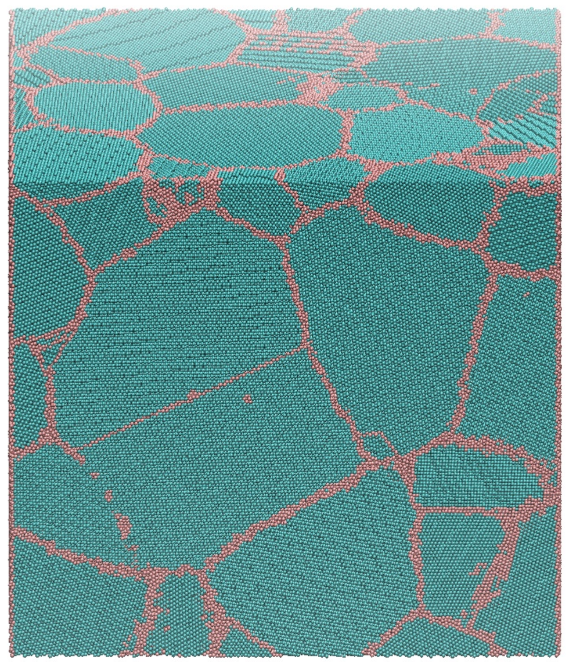
Increasing grain size by a factor of two, to 8-20 nm confirms an inverse Hall-Petch response

At high strain rates the stress-strain relations are not impacted by grain size, while strength is marginally increased.









Ta crystal plasticity for low-rate strength model

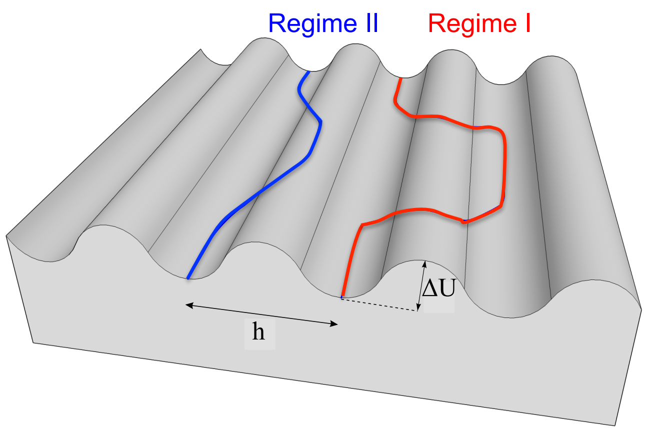
Modified dislocation kink-pair theory:
Temperature, strain rate & pressure dependence

Hojun Lim

$$\tau(T,\dot{\gamma}) = \underbrace{\tau^{*}(T,\dot{\gamma})}_{\text{Thermal}} + \underbrace{\tau_{obs}}_{\text{Athermal}}$$

In FCC metals, $\tau^{*} \approx 0$

In BCC metals, $\tau^{*} >> 0 \qquad (T << T_c)$



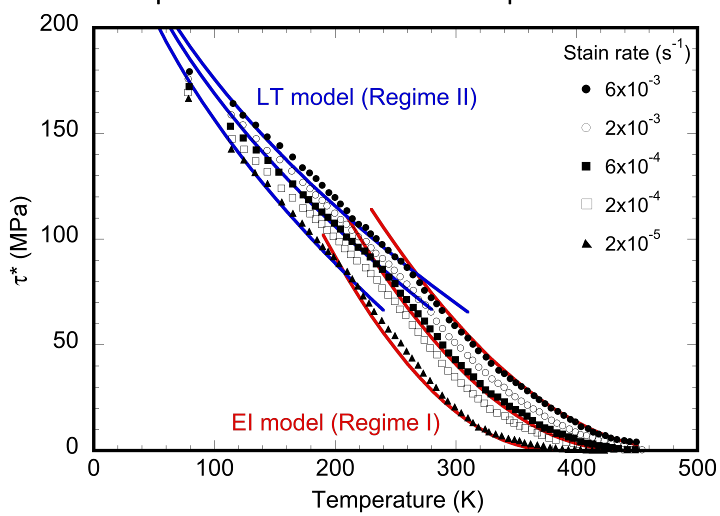
Elastic Interaction Model (Regime I)

$$\tau^{*}_{EI} = \frac{\mu}{\mu_0}\tau^{0}_{EI}\left(1 - \frac{\mu_0}{\mu}\frac{T}{T^{0}_{c}(\dot{\gamma})}\right)^{2}$$

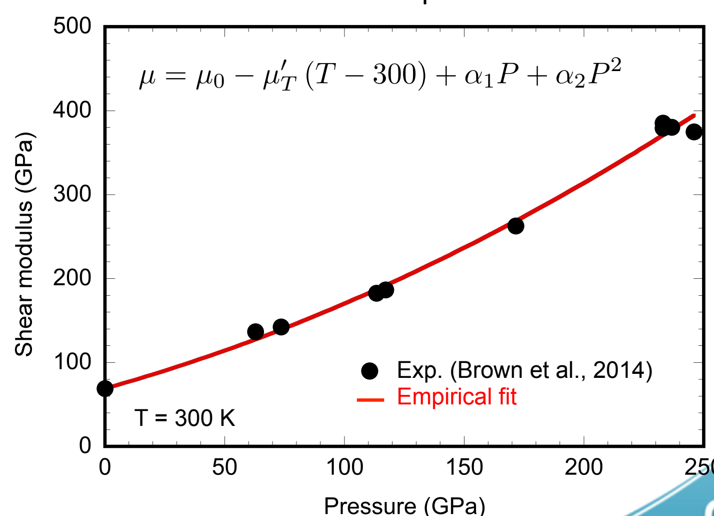
Line Tension Model (Regime II)

$$\tau^{*}_{LT} = \frac{\mu}{\mu_0}\tau^{0}_{LT}\left(1 - \left(\frac{\mu_0}{\mu}\frac{T}{T^{0}_{c}(\dot{\gamma})}\right)^{1/2}\right)$$

Temperature and strain rate dependence



Pressure dependence



Analytical model for polycrystalline Ta

Ta strength model incorporating temperature, strain rate and pressure

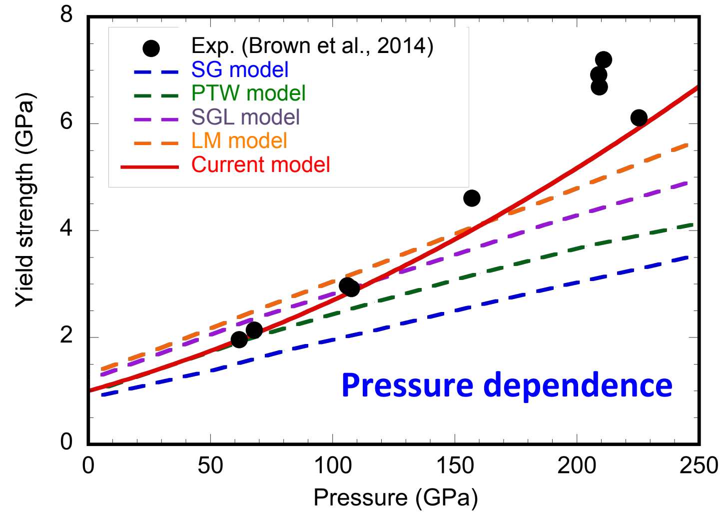
$$\tau = \min\left(\tau^*_{EI}, \tau^*_{LT}\right) + \tau_{obs}$$

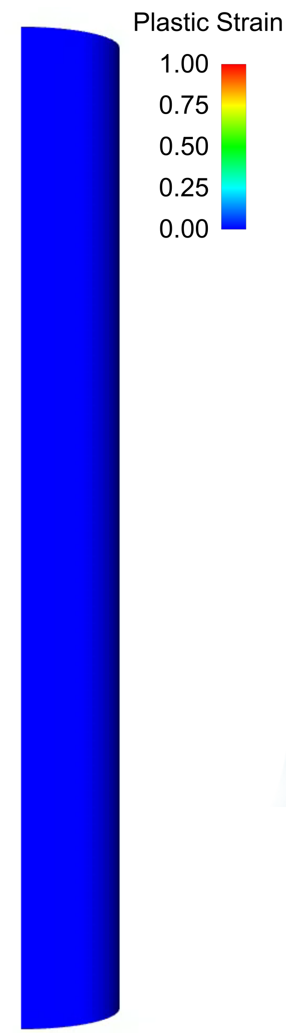
$$\sigma = \bar{M}\tau$$

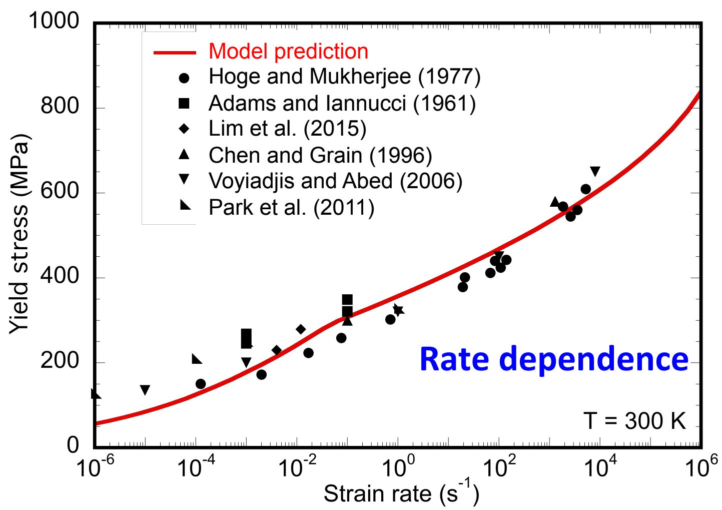
σ : Tensile stress of polycrystal

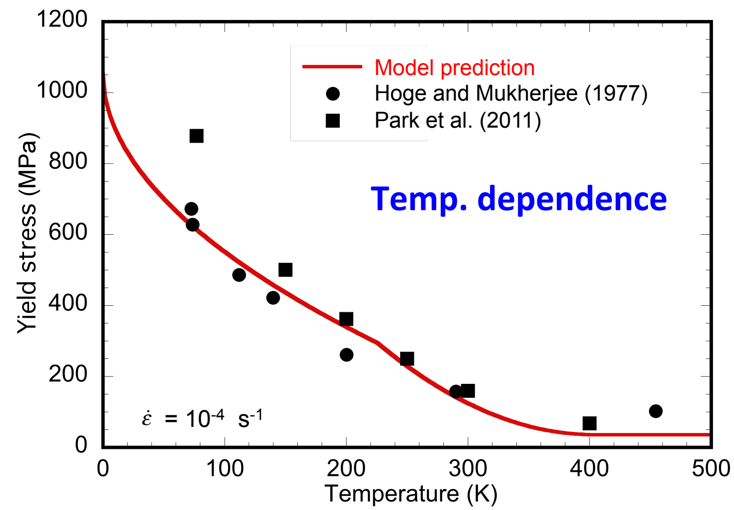
τ : Shear stress of single crystal

$\bar{M}$: Taylor factor (~3.07 for BCC)









Summary and conclusions

- We've studied dynamic ramp wave response in nanograin polycrystal tantalum at 10^{11} to 10^{8} 1/s strain rates with molecular dynamics and ramp profile scaling analysis.

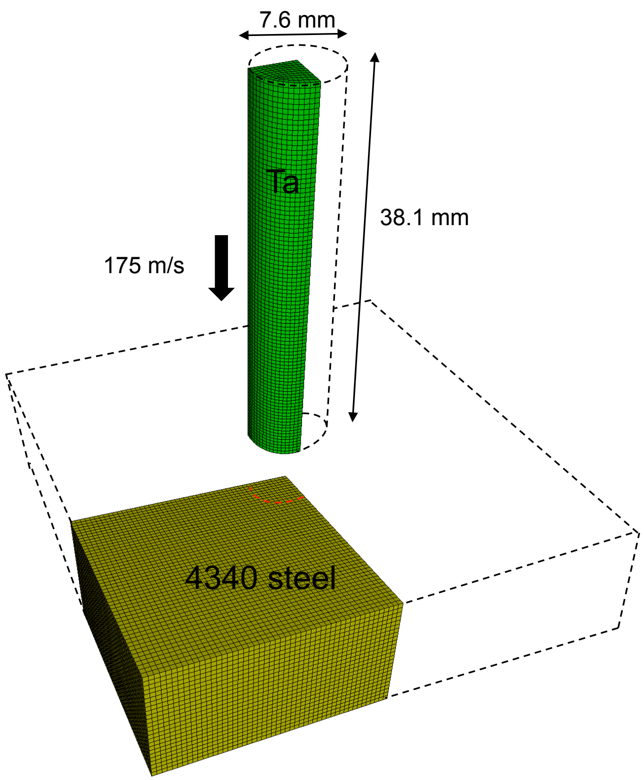
- Reasonable agreement in stress-strain response with lower-rate experiments (Davis, et al.)
    - Lower strain rate brings better comparison, especially at strain below 0.2
    - Over-represented elastic response produces a more robust precursor which may drive up longitudinal stress at high strains.

- At pressures below 100 GPa high strength is observed due to nanograin suppression of dislocations (inverse Hall-Petch).

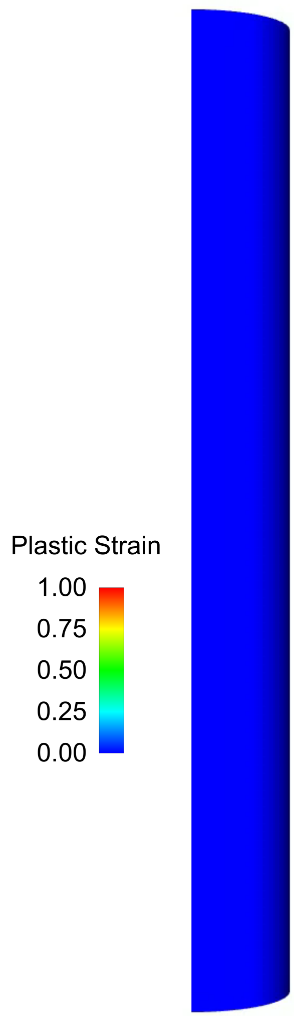
- Above 100 GPa we show good agreement with high-pressure and high strain-rate trends in the PTW model.

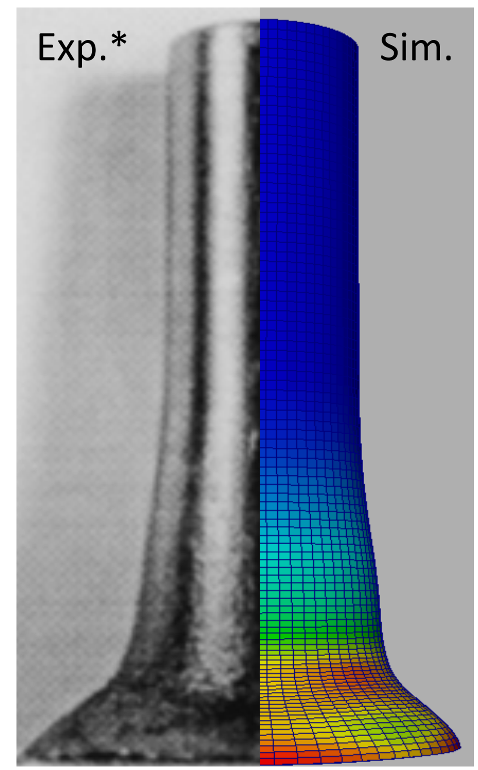
High-rate dynamic simulations

Taylor cylinder impact test



- ALEGRA solid dynamics code (Sandia)
- Kerley Mie-Grüneisen equation of state
- Strength models:
  - Kink-pair (KP) model
  - Johnson-Cook (JC) model
  - Zerilli-Armstrong (ZA) model





Deformed geometry

* Maudline et al., IJP (1999)