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Molecular modeling of high-pressure ramp waves in tantalum

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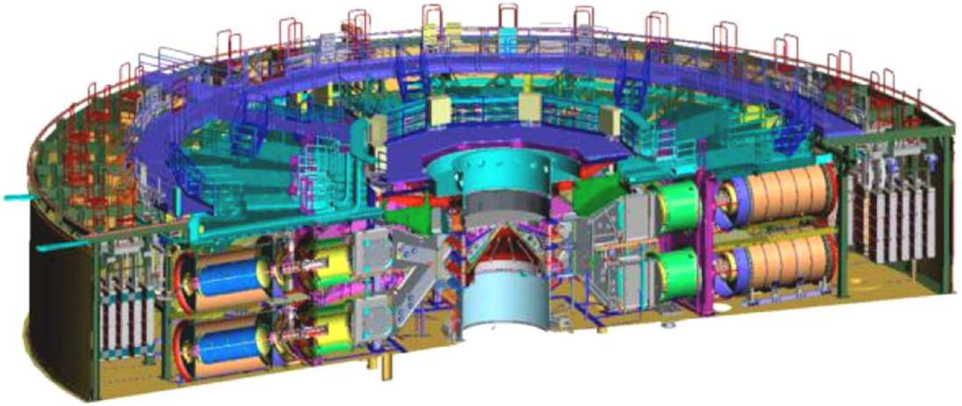
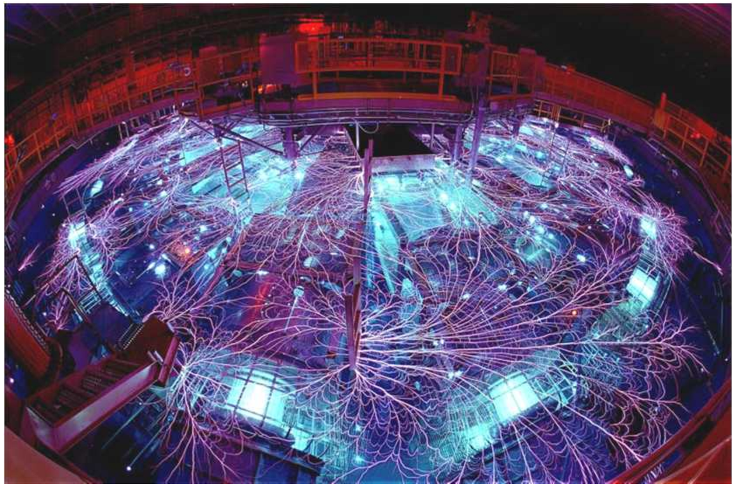
Z-machine and experiments in ramp waves



Z-machine at Sandia National Labs



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

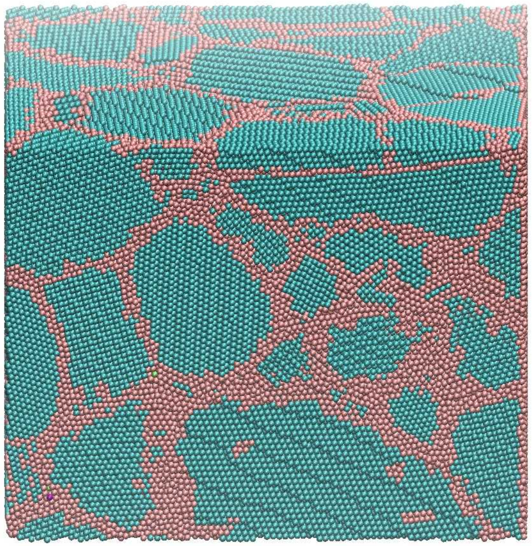
A brief tantalum overview

- **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)*

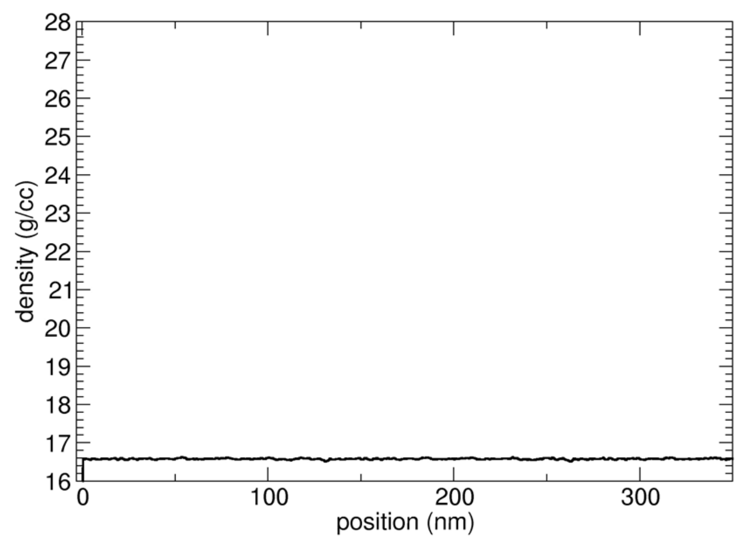
- **Significant variation in methodology and materials complicate:**
  - *Variation in drivers (laser ablation vs flyer)*
  - *Variation in strain rates (10^{10} to 10^5)*
  - *Variation in material microstructure and grain texture (characterized and uncharacterized)*
  - *Variation in strength extraction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

Molecular dynamics simulation methods



- **Classical molecular dynamics**
  - *Ta1 EAM style potential by Ravelo et al. PRB, 88 134101 (2013) was fit to isothermal EOS up to 300 GPa and verified against Hugoniot data - potential captures twinning and plastic flow.*
  - *Ramp wave modeled with accelerating infinite-mass piston with nonlinear profile $v_p = x/a + (x/a)^3$ to delay shock up.*
- **System size and grain structure**
  - *20 nm x 20 nm x 131 nm nanograin polycrystalline unit cell replicated in loading direction to 20 μm and 350 million atoms*
  - *Two grain sizes of 5-10 nm and 8-20 nm*
  - *Very controlled rates and structures*

- **Strengths of MD method**
  - *Full stress state throughout the sample*
  - *Very controlled material structures, i.e. grains initial defects, etc.*
  - *Very controlled and repeatable loading profiles at different rates, here ranging from 10^{11} to 10^8*
  - ***However**, we do not achieve overlap in strain rate, nor microstructure.*



Scaling and dynamic similarity theory

Scaling conditions for loading:

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

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

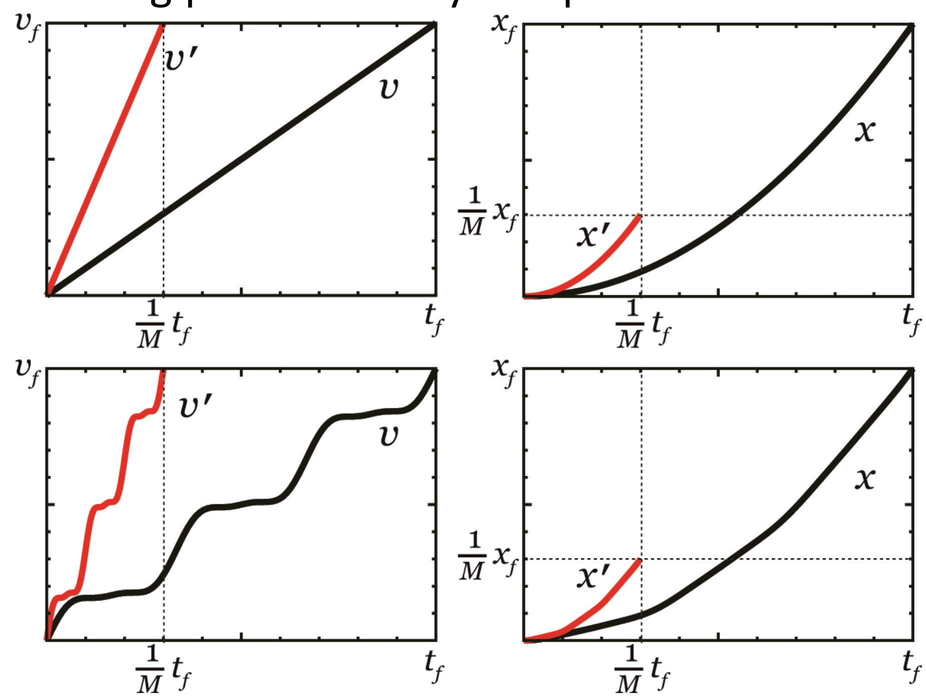
$$v'\left(\frac{1}{M}t\right) = v(t)$$

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:



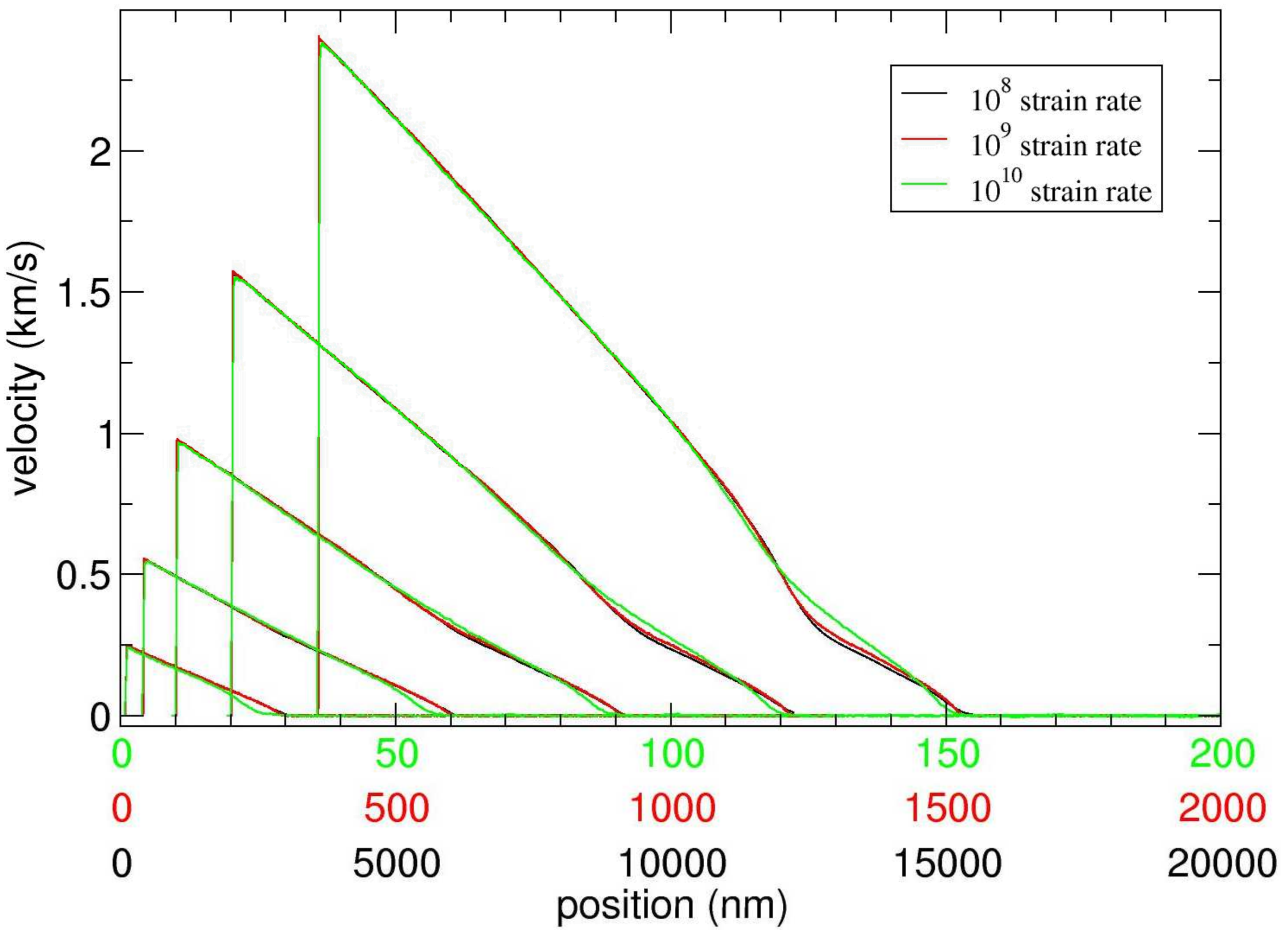
Invariant to scaling:

Velocity
Stress
Strain
Temperature*
Forces
Density

Not invariant:

Strain rates
Accelerations
Times and distances
any extensive variable…

Ramp profiles and shock up



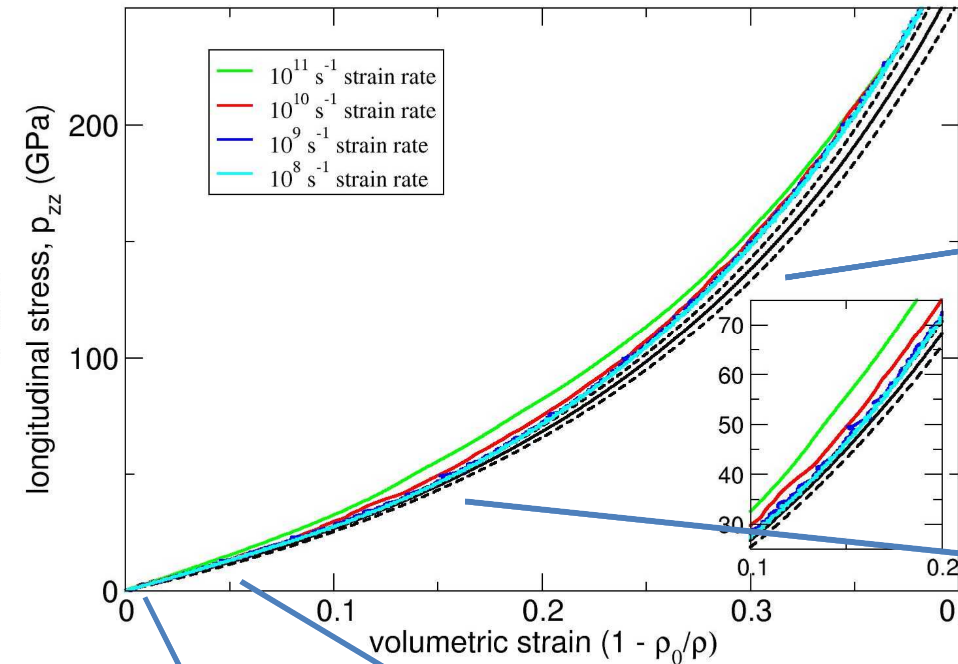
All ramp waves are driven nonlinearly from 0 to 2.4 km/s, giving peak pressures of 250 GPa.

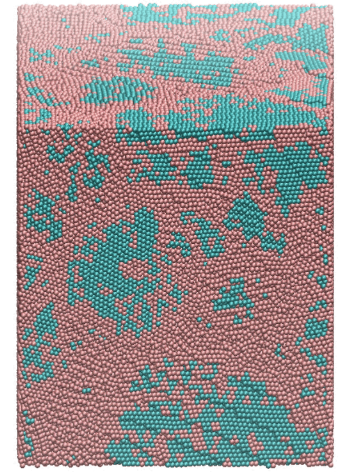
10^{10} 1/s strain rate
Rises over 40 ps
150 nm & 2.5 million atoms

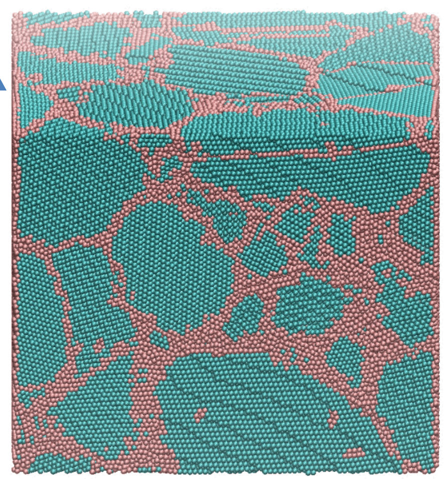
10^9 1/s strain rate
Rises over 400 ps
1.5 μm & 25 million atoms

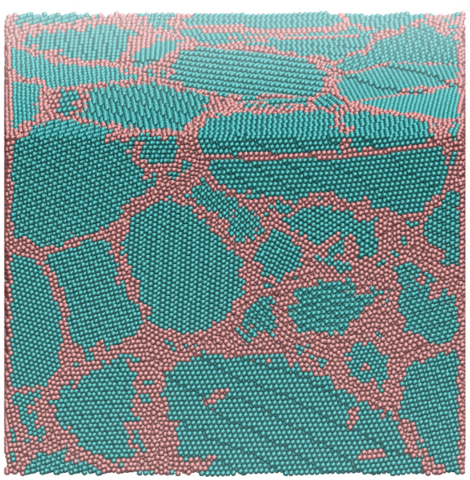
10^8 1/s strain rate
Rises over 4 ns
15 μm & 350 million atoms

Comparison with experiment & scaling



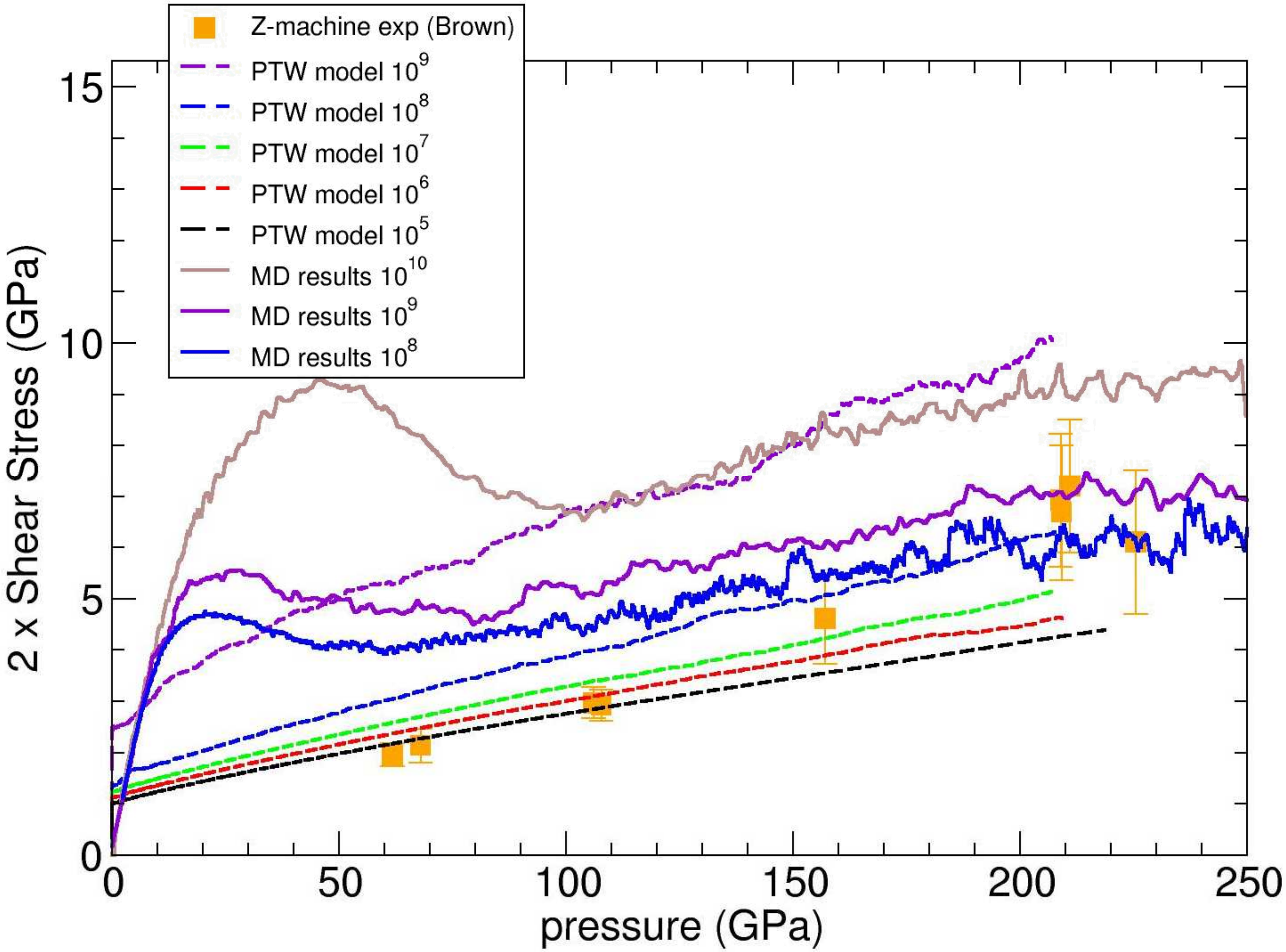






Inverse Hall-Petch response dominated by grain boundary sliding

Extraction of strength



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

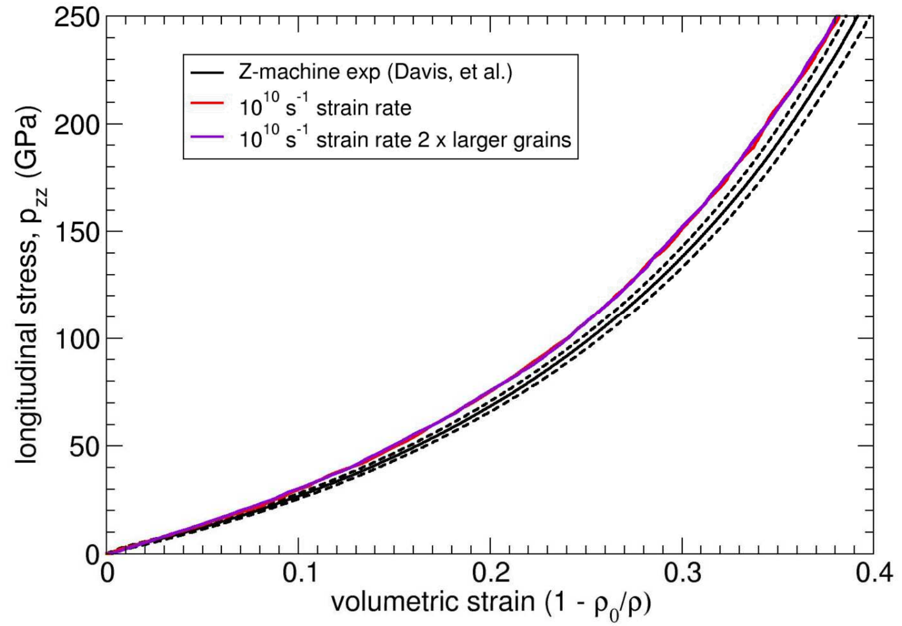
Relatively good agreement with PTW model above 100 GPa.

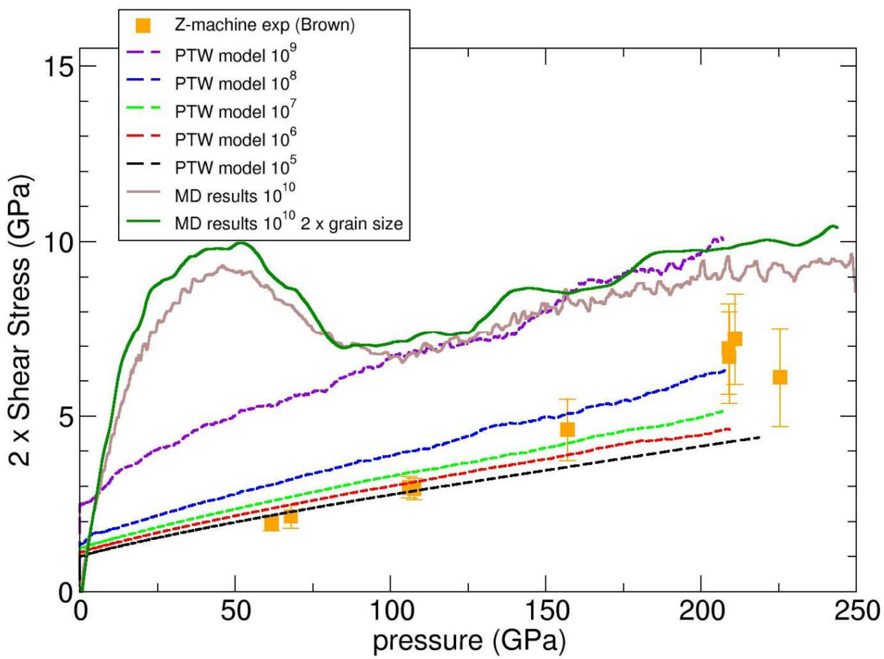
PTW model – Preston, Tonks, Wallace, JAP, 93 211 (2003)

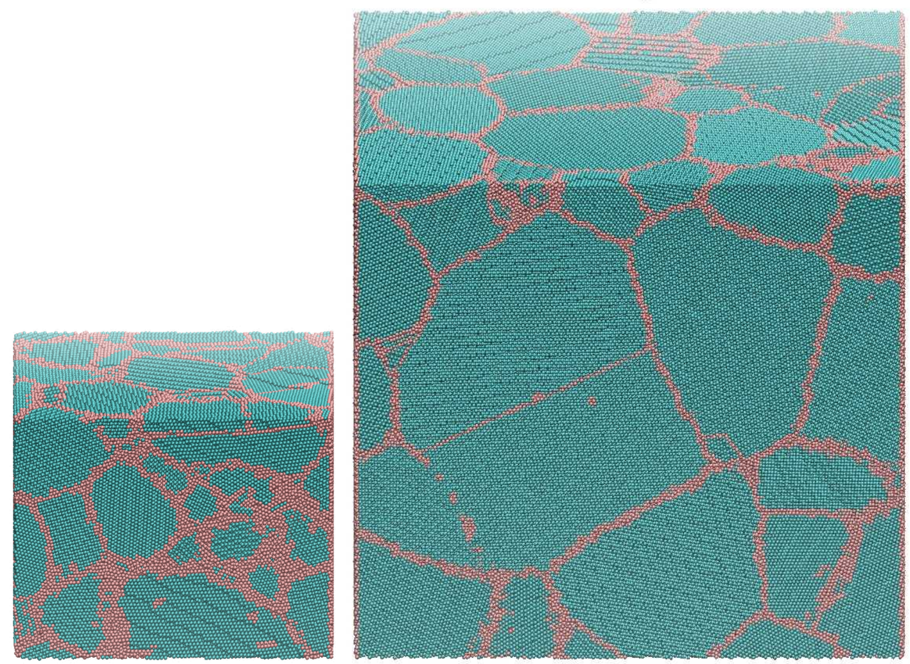
Increased grain size

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 strength model incorporating T, ε and P

Modified dislocation kink-pair theory:

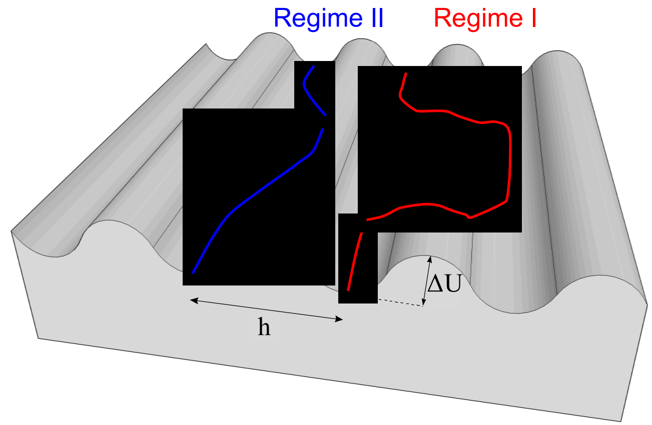
Temperature, strain rate & pressure dependence

$$\tau(T,\dot{\gamma}) = \tau^*(T,\dot{\gamma}) + \tau_{obs}$$

Thermal Athermal

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

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



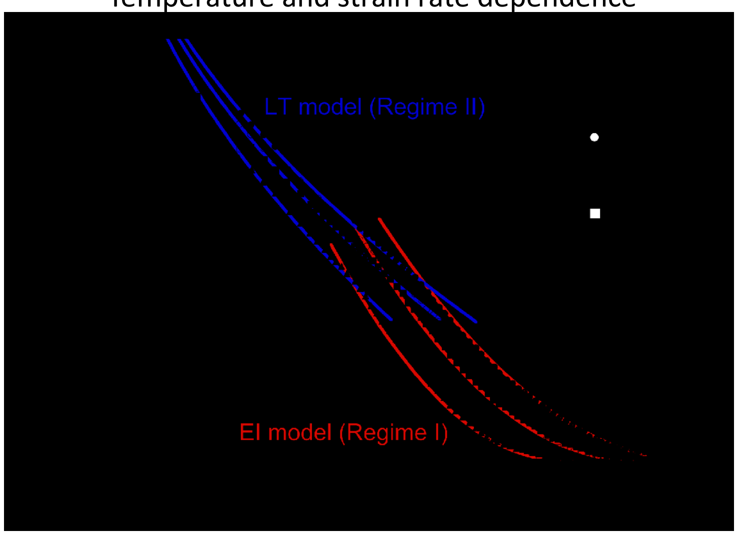
Elastic Interaction Model (Regime I)

$$\tau_{EI} = \frac{\mu}{\mu_0}\tau^0_{EI}\left[1 - \left(\frac{\mu_0}{\mu}\frac{T}{T_c^0(\dot{\gamma})}\right)\right]^2$$

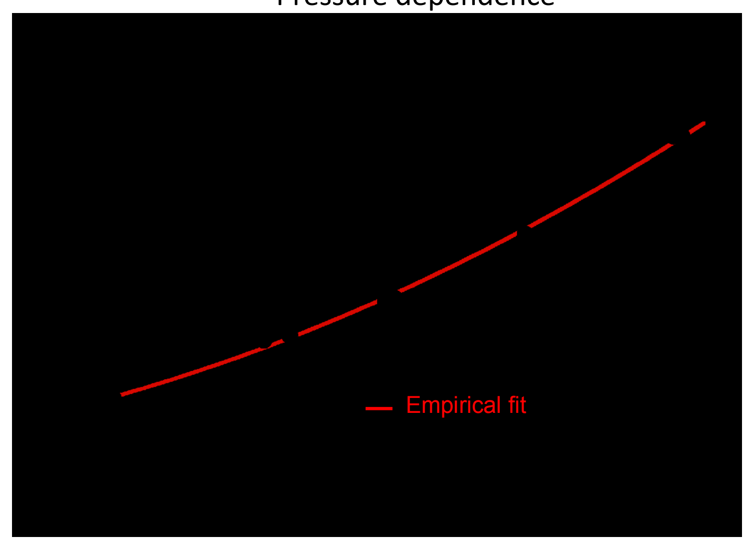
Line Tension Model (Regime II)

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

Temperature and strain rate dependence



Pressure dependence



Analytical model for polycrystalline Ta

Ta strength model incorporating temperature, strain rate and pressure

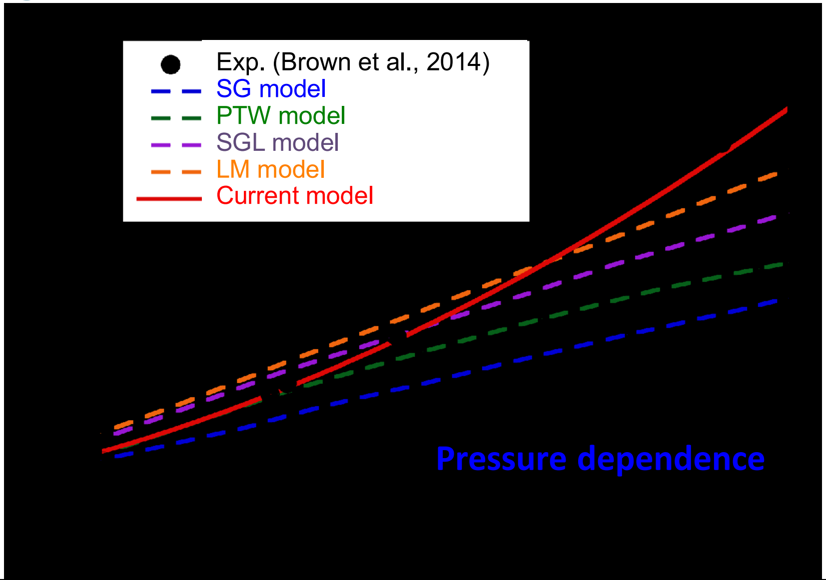
$$\tau = \min\left(\tau^*_{EI}, \tau^*_{LT}\right) + \tau_{obs}$$

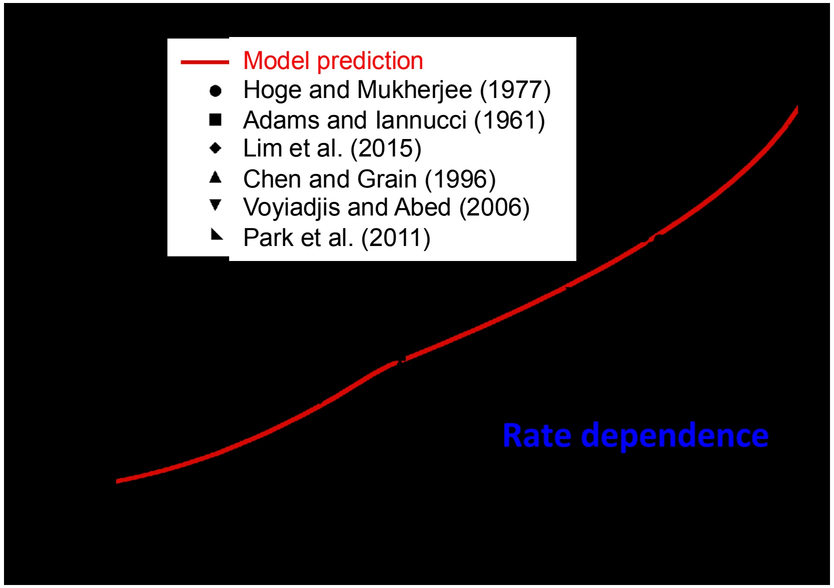
$$\sigma = M\tau$$

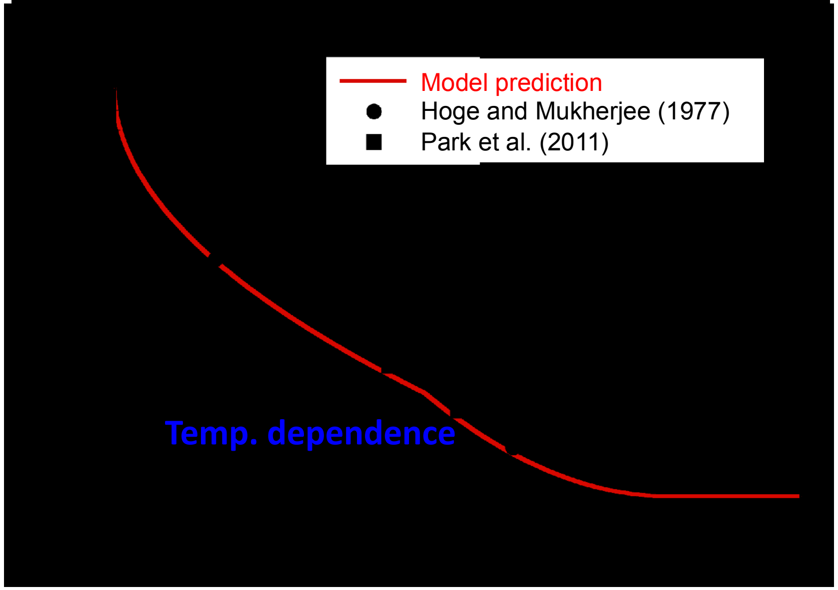
σ : Tensile stress of polycrystal

τ : Shear stress of single crystal

M : Taylor factor (~3.07 for BCC)

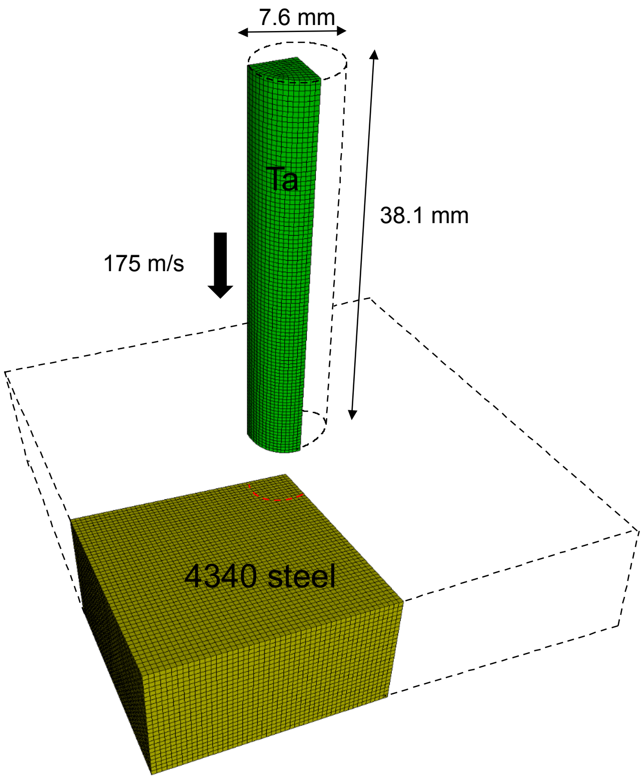




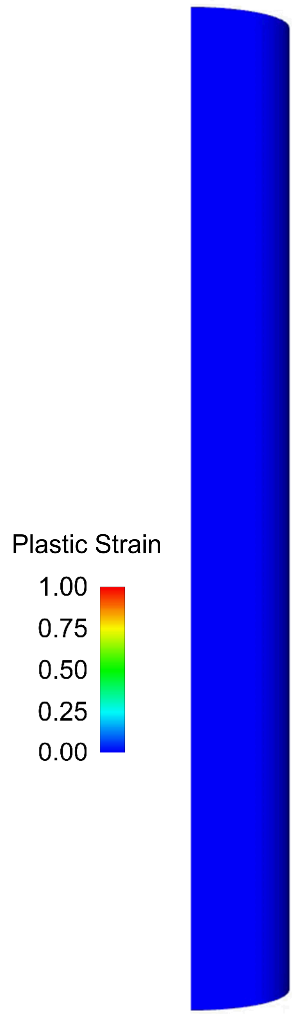


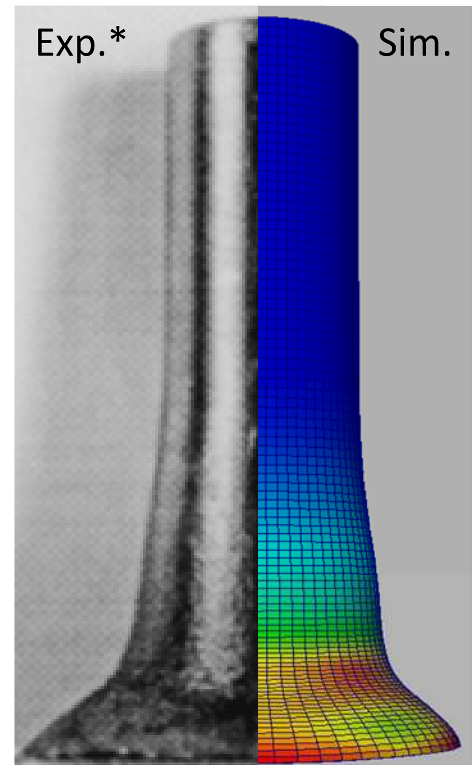
High-rate dynamic simulations

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)

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 low strain.
    - Over-represented elastic response produces a more robust precursor which drives 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.