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Title: Strength and Damage Modeling in FLAG (U)

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Strength and Damage Modeling
in FLAG (U)
LA-UR-XX-XXXXX

Abstract

Recent improvements to the FLAG code have included a modification of the Preston-Tonks-Wallace (PTW) strength model and a re-factoring the Tensile Elastic-Plastic (TEPla) damage model. The PTW strength model has been modified to enhance modeling through transitions from low strain-rate (thermal activation) regime to the high strain rate (over-driven shock) regime. The presentation discusses the implementation of the modified strength model and some of the computational issues.

Strength and Damage Modeling in FLAG (U)

LA-CP-XX-XXXXX

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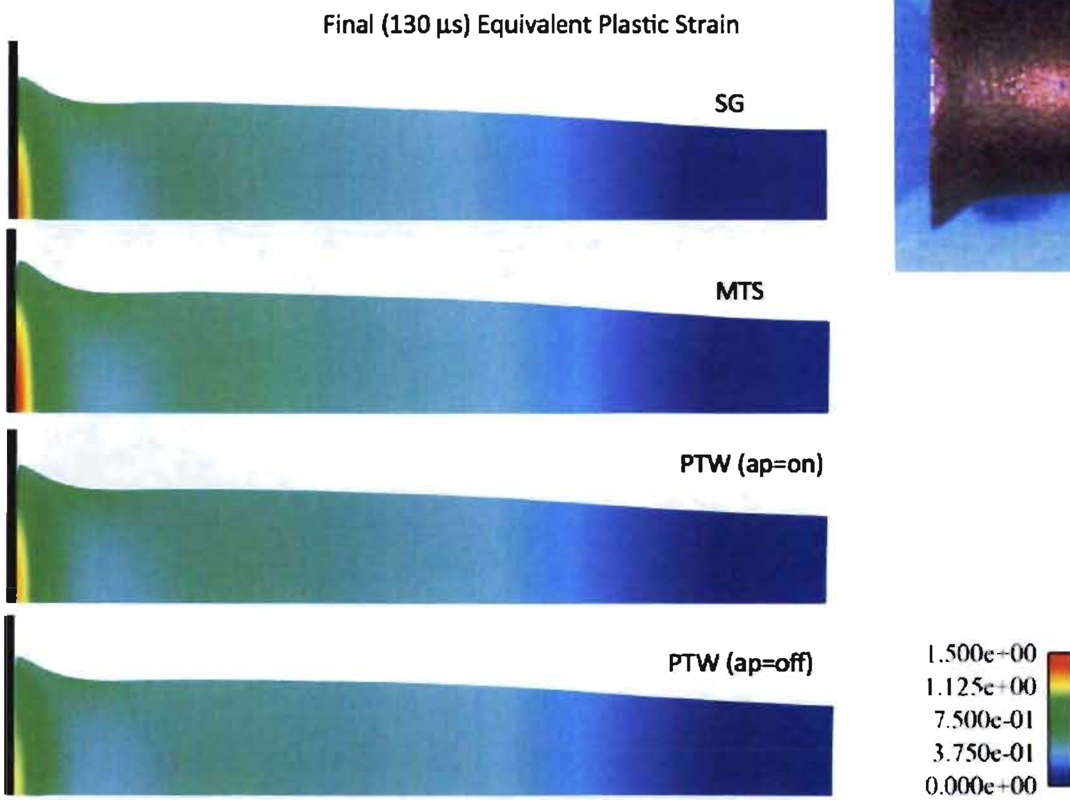
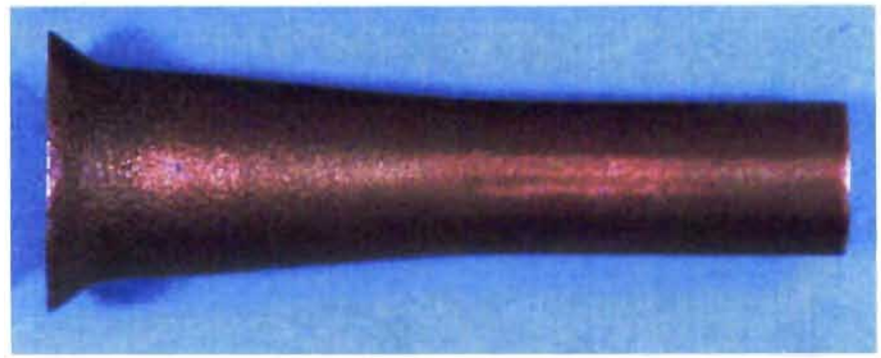
Strength and Damage Modeling
Outline

- Motivation
- PTW Strength Model Modifications
- Density Dependent Melt Temperature and Shear Modulus
- Damage and Failure Models – TEPla
- Discussion and Conclusions
- Future Directions

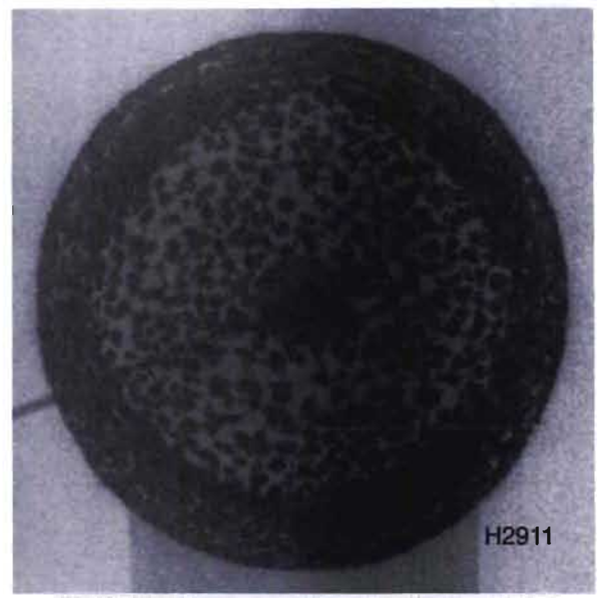
Strength and Damage Modeling Motivation



Annealed Cu Taylor Cylinder: Simulation



Cu ¾ Hardened Taylor Cylinder



Extended Ta-hemi in an extremely damaged state

Strength and Damage Modeling
Update PTW Model

- New Feature: Smooth interpolation of the saturation flow stress between the low strain-rate (thermal activation) and the high strain-rate regimes
- Fixed a few things
  - Rearranged the order of operations in the calculation of the dimensionless flow stress to insure proper initialization at all strain-rates.
  - Modified the Voce Hardening Law to remove a singularity.

Original PTW Strength Model

- Dimensionless Temperature: $$\hat{T} = \frac{T}{T_m(\rho)}$$
- Shear Modulus: $$G(\rho,\hat{T}) = G_0(\rho)\left[1-\alpha\hat{T}\right]$$
- Dimensionless Flow Stress Variable: $$\hat{\tau} = \frac{\tau}{G(\rho,\hat{T})}$$
- Critical Strain Rate: $$\dot{\varepsilon}_0 = \frac{\gamma}{2}\left(\frac{4\pi\rho}{3M}\right)^{\frac{1}{3}}\sqrt{\frac{G}{\rho}}$$

Original PTW Strength Model

- In the Thermal Activation Regime
  - Dimensionless Yield Stress:

$$\hat{\tau}_y^T = y_0 - (y_0 - y_\infty)\,\mathrm{erf}\left[-\kappa \hat{T} \ln\left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)\right]$$

  - Model for the gap and higher strain rates:

$$\hat{\tau}_y^g = y_1\left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)^{y_2}$$

  - Dimensionless Saturation Flow Stress:

$$\hat{\tau}_s^T = s_0 - (s_0 - s_\infty)\,\mathrm{erf}\left[-\kappa \hat{T} \ln\left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}\right)\right]$$

Original PTW Strength Model

- For strain rates above the threshold for Thermal Activation
  - Dimensionless Saturation Flow Stress:

$$\hat{\tau}_s^H = s_0 \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0} \right)^{\beta}$$

Original PTW Strength Model

- For all strain rates
  - Dimensionless Saturation Flow and Dimensionless Yield Stresses:

$$\hat{\tau}_s = \begin{cases} \hat{\tau}_s^T & \dot{\varepsilon} < \dot{\varepsilon}_0 \\ \hat{\tau}_s^H & \dot{\varepsilon} > \dot{\varepsilon}_0 \end{cases}$$

$$\hat{\tau}_y = \max\left[\hat{\tau}_y^T, \min\left[\hat{\tau}_y^g, \hat{\tau}_s\right]\right]$$

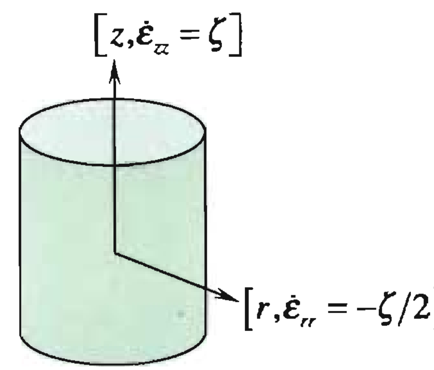
  - Modified Voce Hardening Law:

$$\frac{d\hat{\tau}}{d\varepsilon} = \theta \frac{\exp\left[p \frac{\hat{\tau}_s - \hat{\tau}}{s_0 - \hat{\tau}_y}\right] - 1}{\exp\left[p \frac{\hat{\tau}_s - \hat{\tau}_y}{s_0 - \hat{\tau}_y}\right] - 1}$$

*Singular when = 0

Original PTW Strength Model

- **Numerical experiment to study the model under isovolumetric and constant strain rate conditions**
  - Material DU
  - cylindrical pellet centered at the origin.
  - r and z velocities are specified on the surfaces of the 1 element test specimen.



  - Dimensionless Flow Stress at Constant Strain Rate:

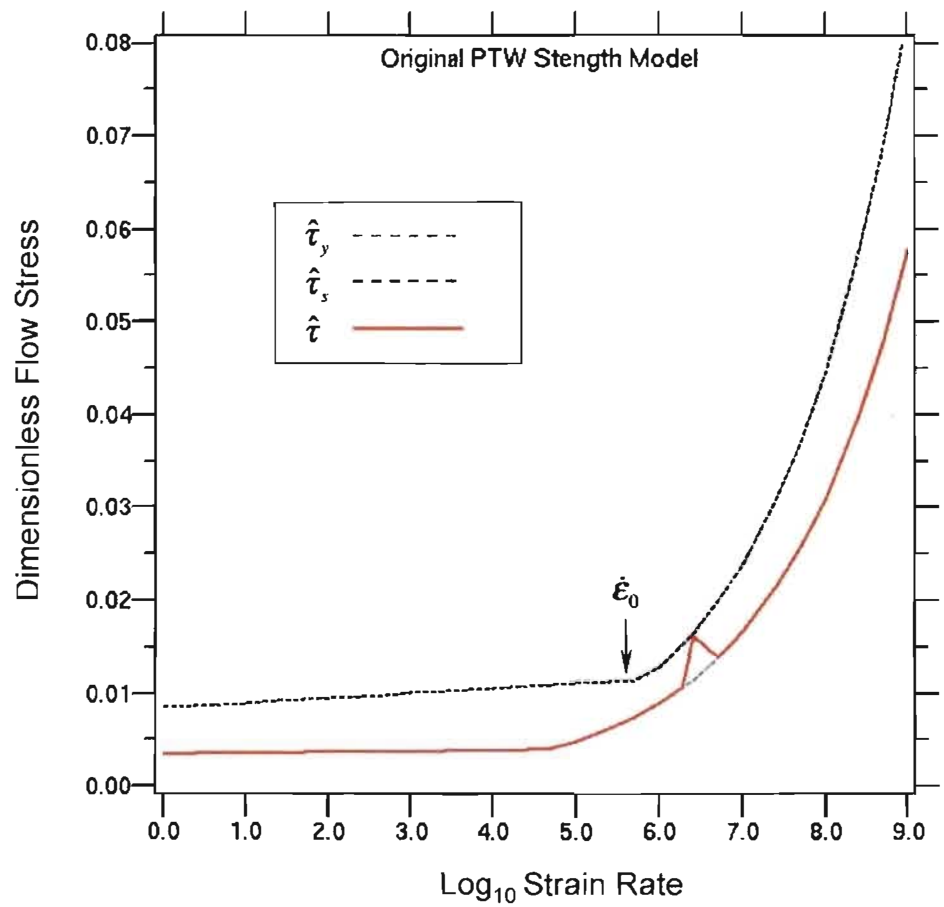
$$\hat{\tau} = \hat{\tau}_s + \frac{s_0 - \hat{\tau}_y}{p} \ln\left[1 - \left(1 - \exp\left\{-p\frac{\hat{\tau}_s - \hat{\tau}_y}{s_0 - \hat{\tau}_y}\right\}\right)\exp\left\{-\frac{p\theta\varepsilon}{(s_0 - \hat{\tau}_y)\exp\left\{p\frac{\hat{\tau}_s - \hat{\tau}_y}{s_0 - \hat{\tau}_y}\right\} - 1}\right\}\right]$$

DU PTW Parameters

PTW Parameter	*Nominal Value*
r	$0 \leq r \leq 4$
θ	0.088
p	3
s_0	0.0115
s_∞	0.0020
κ	0.1
γ	10^{-7}
y_0	0.004
y_∞	0.002
y_1	0.008
y_2	0.27
β	0.27
T_m	1405° K
G_0	1.078 Mbar
a_m	3.954×10^{-22} g/atom

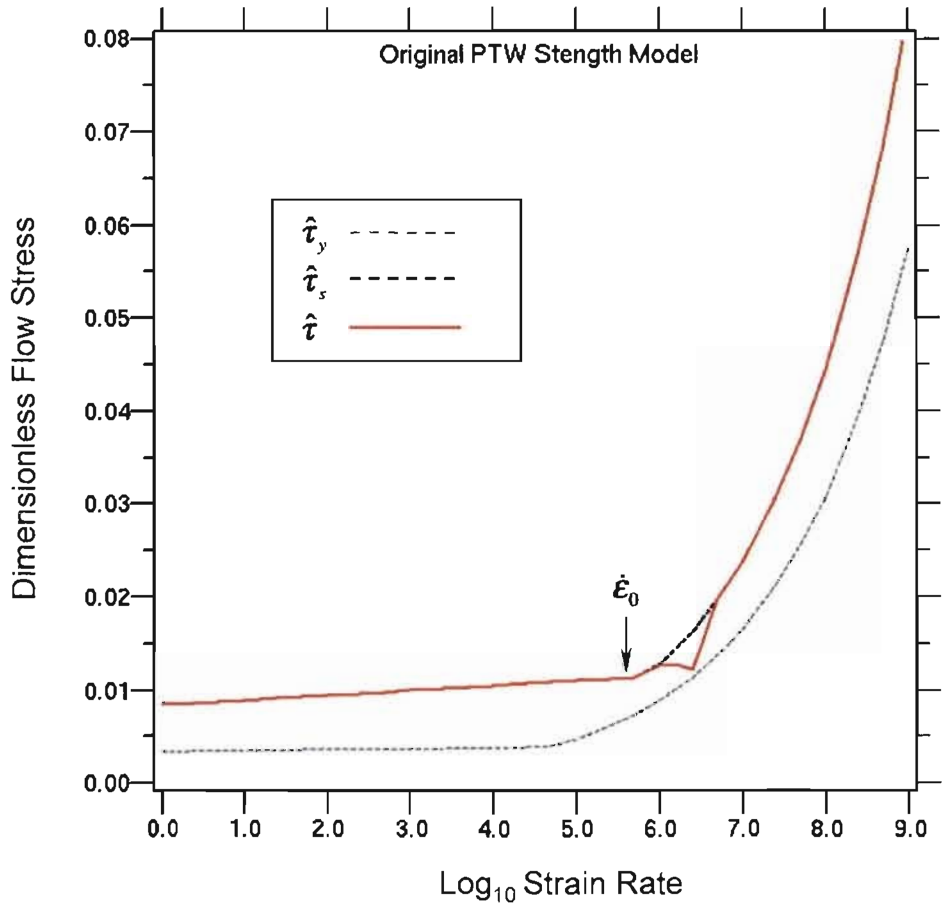
Original PTW Strength Model

Initial Condition ($\varepsilon^p=0$)



Original PTW Strength Model

Initial Condition ($\varepsilon^p=2$)



Modified PTW Strength Model

Change in the Hardening Rule:

- Subtle change in the VOCE Hardening Rule:

$$\frac{d\hat{\tau}}{d\varepsilon} = \theta \frac{\exp\left[p\dfrac{\hat{\tau}_s - \hat{\tau}}{\hat{\tau}_{s0} - \hat{\tau}_y}\right] - 1}{\exp\left[p\dfrac{\hat{\tau}_s - \hat{\tau}_y}{\hat{\tau}_{s0} - \hat{\tau}_y}\right] - 1}$$

where

$$\hat{\tau}_{s0} = \begin{cases} s_0 & \dot{\varepsilon} \le \dot{\varepsilon}_0 \\ \hat{\tau}_s & \dot{\varepsilon} > \dot{\varepsilon}_0 \end{cases}$$

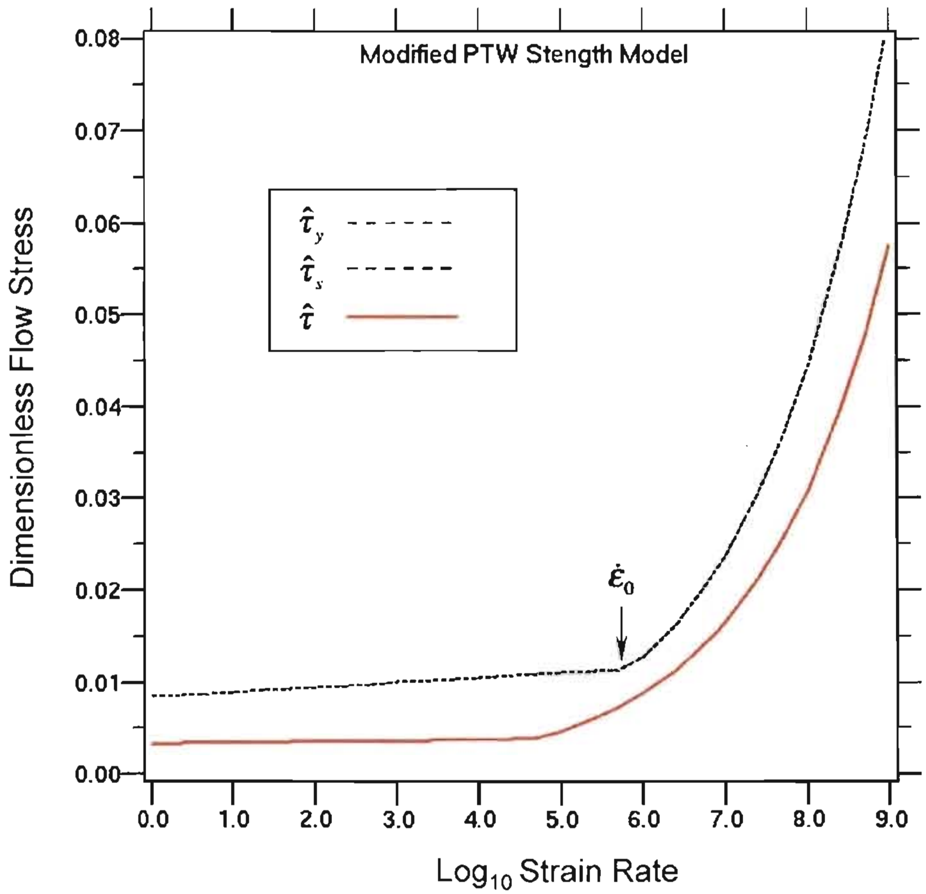
interpolating with respect to r :

$$\hat{\tau}_{s0} = s_0 10^{\frac{1}{4}\beta r\left(1+\frac{x}{r}\right)^2}$$

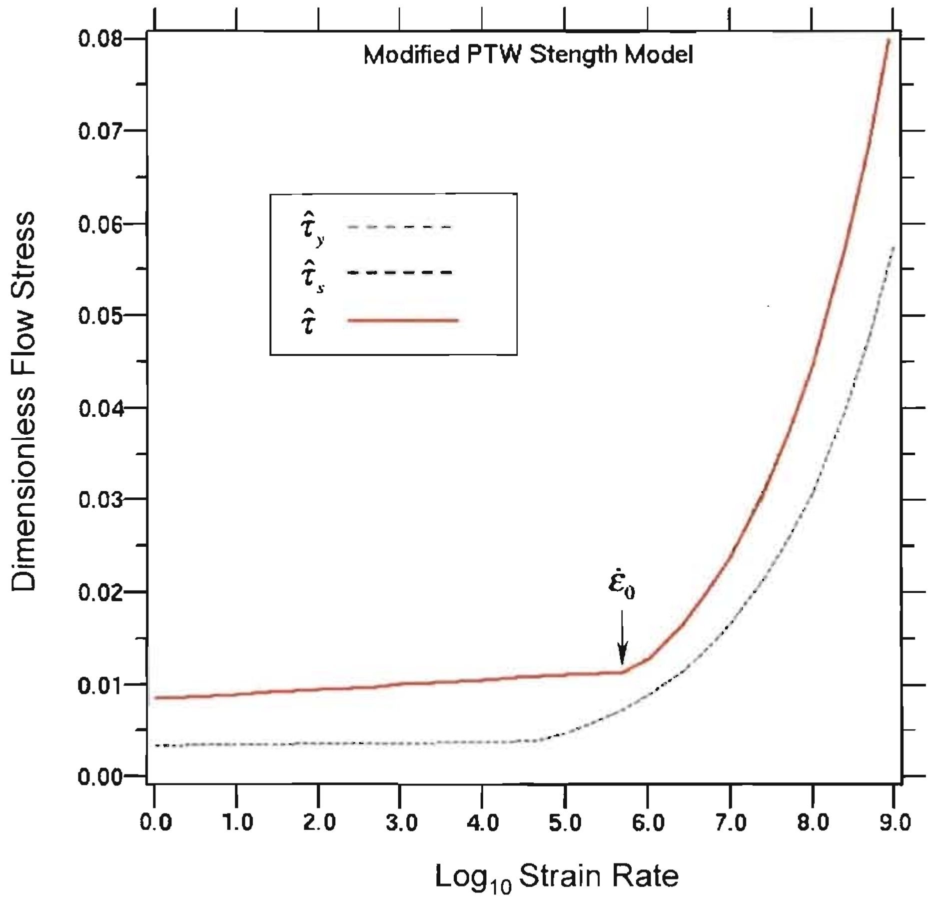
$$x = \log_{10}\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}$$

Modified PTW Strength Model

Change in the Hardening Rule - Initial Condition (ε^p=0)

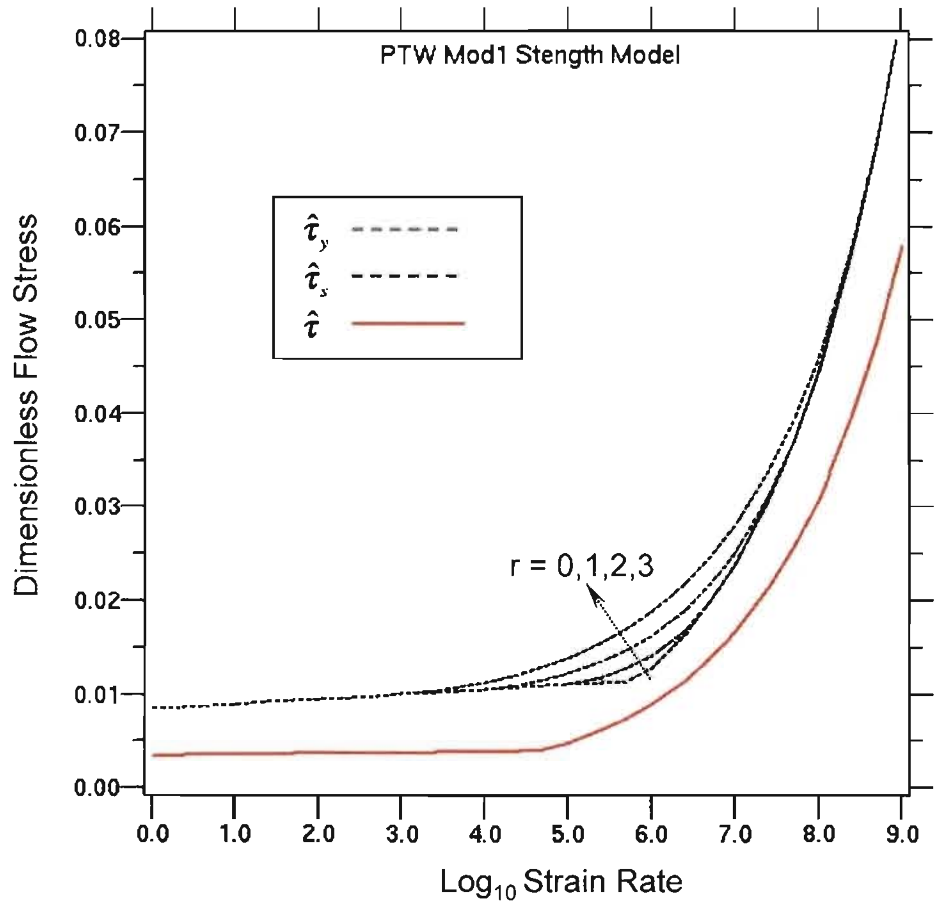


Modified PTW Strength Model
Change in the Hardening Rule - Initial Condition (ε^p=2)



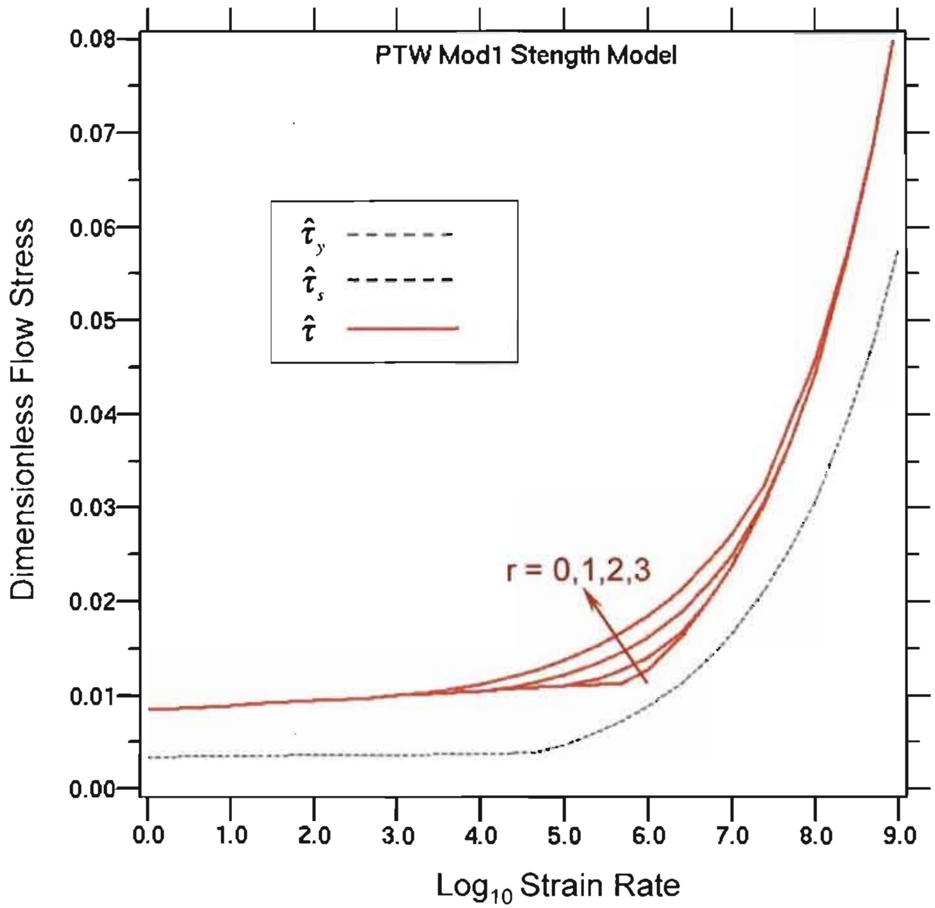
PTW Mod1 Strength Model

Change in the Hardening Rule - Initial Condition ($\varepsilon^p=0$)



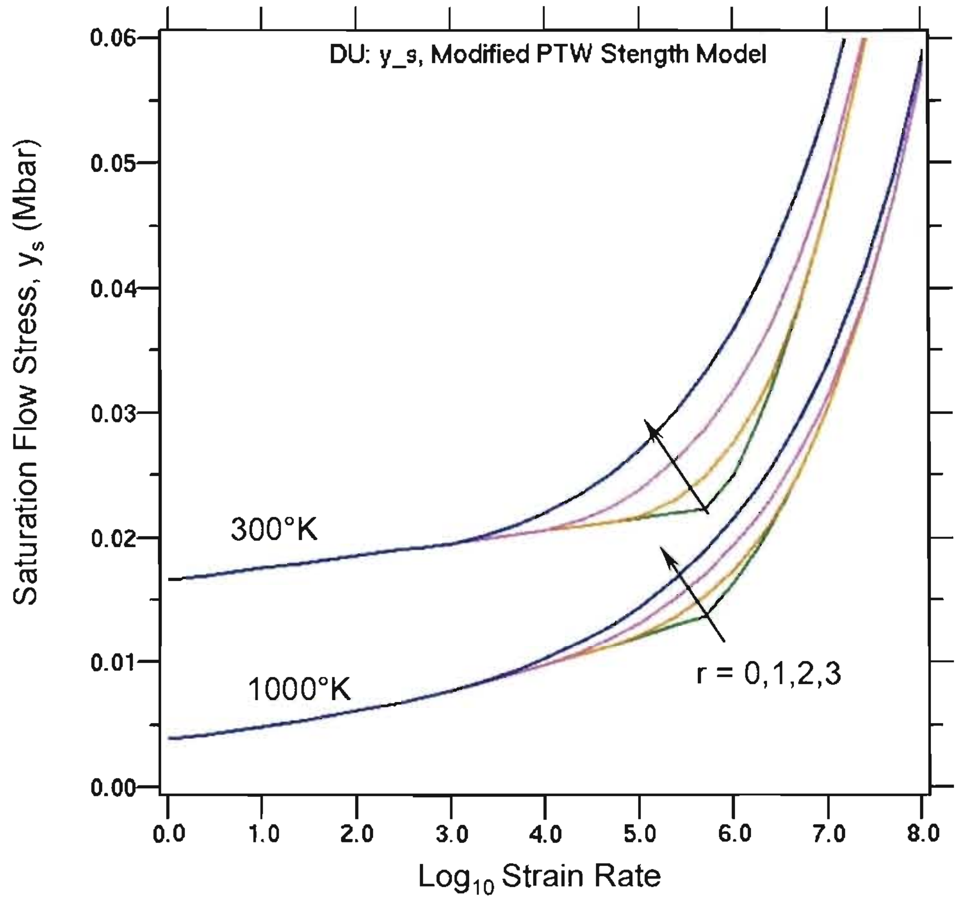
PTW Mod1 Strength Model

Change in the Hardening Rule - Initial Condition (ε^p=2)

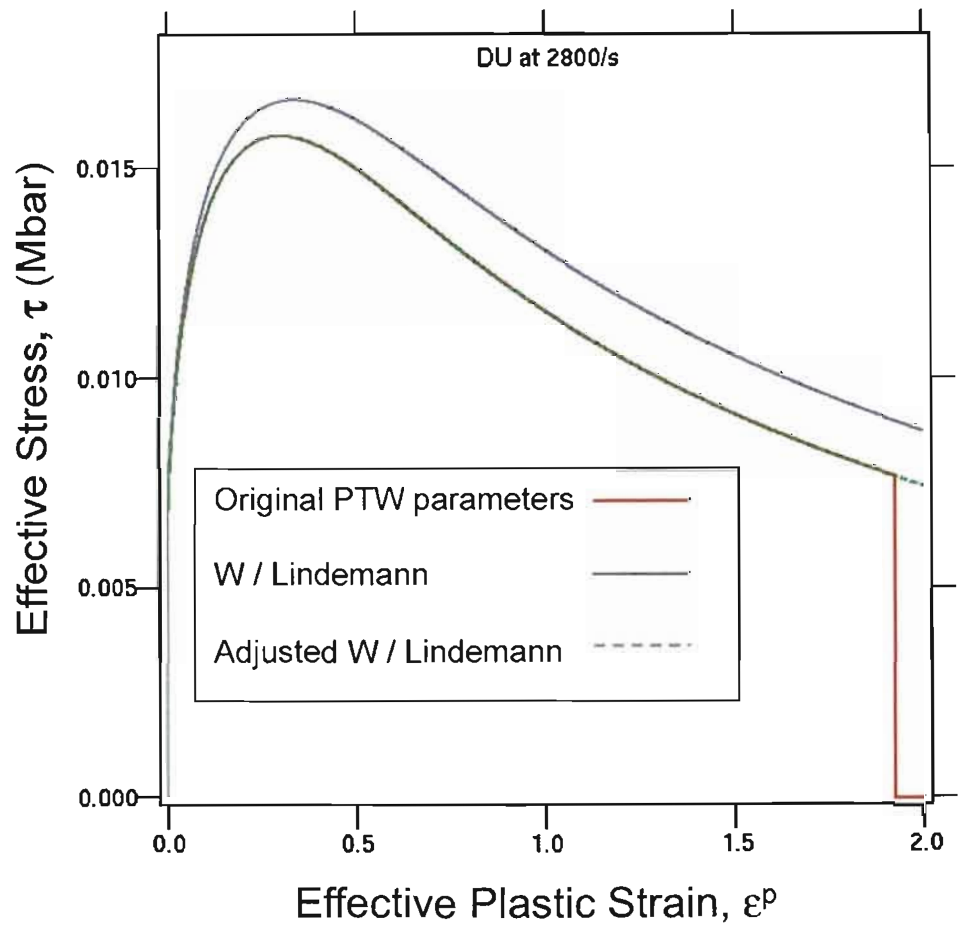


PTW Mod1 Strength Model

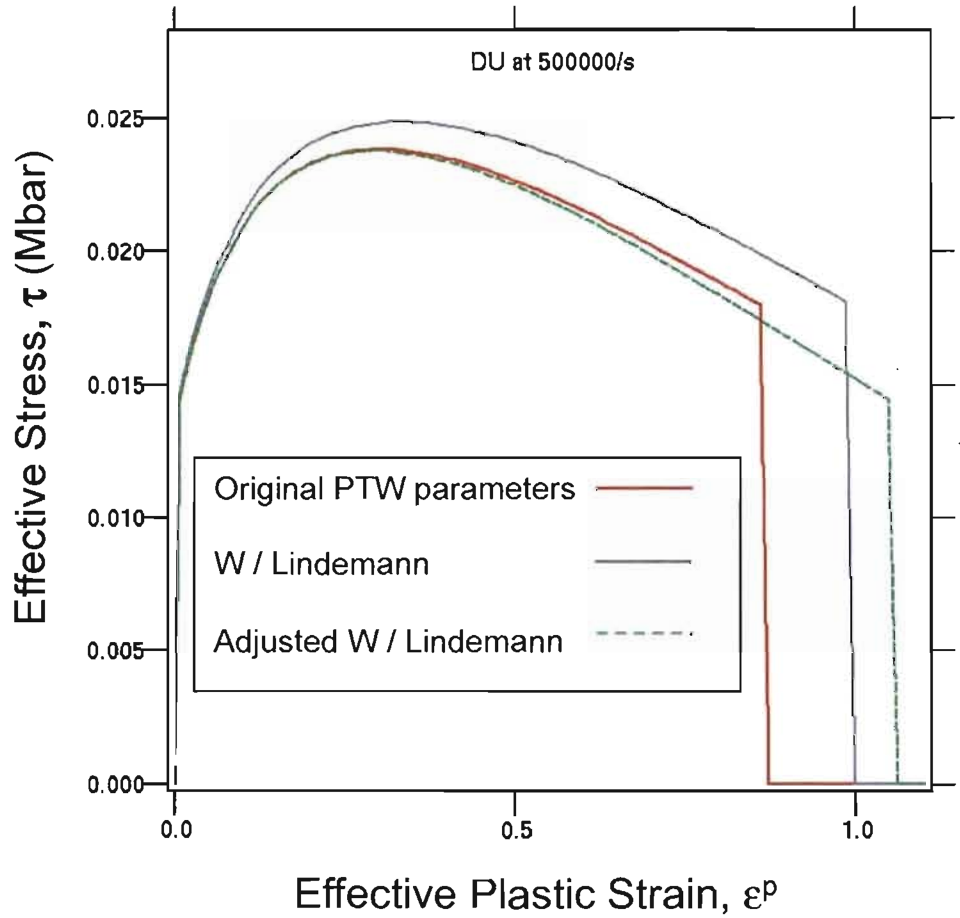
Change in the Hardening Rule - Initial Condition (ε^p=2)



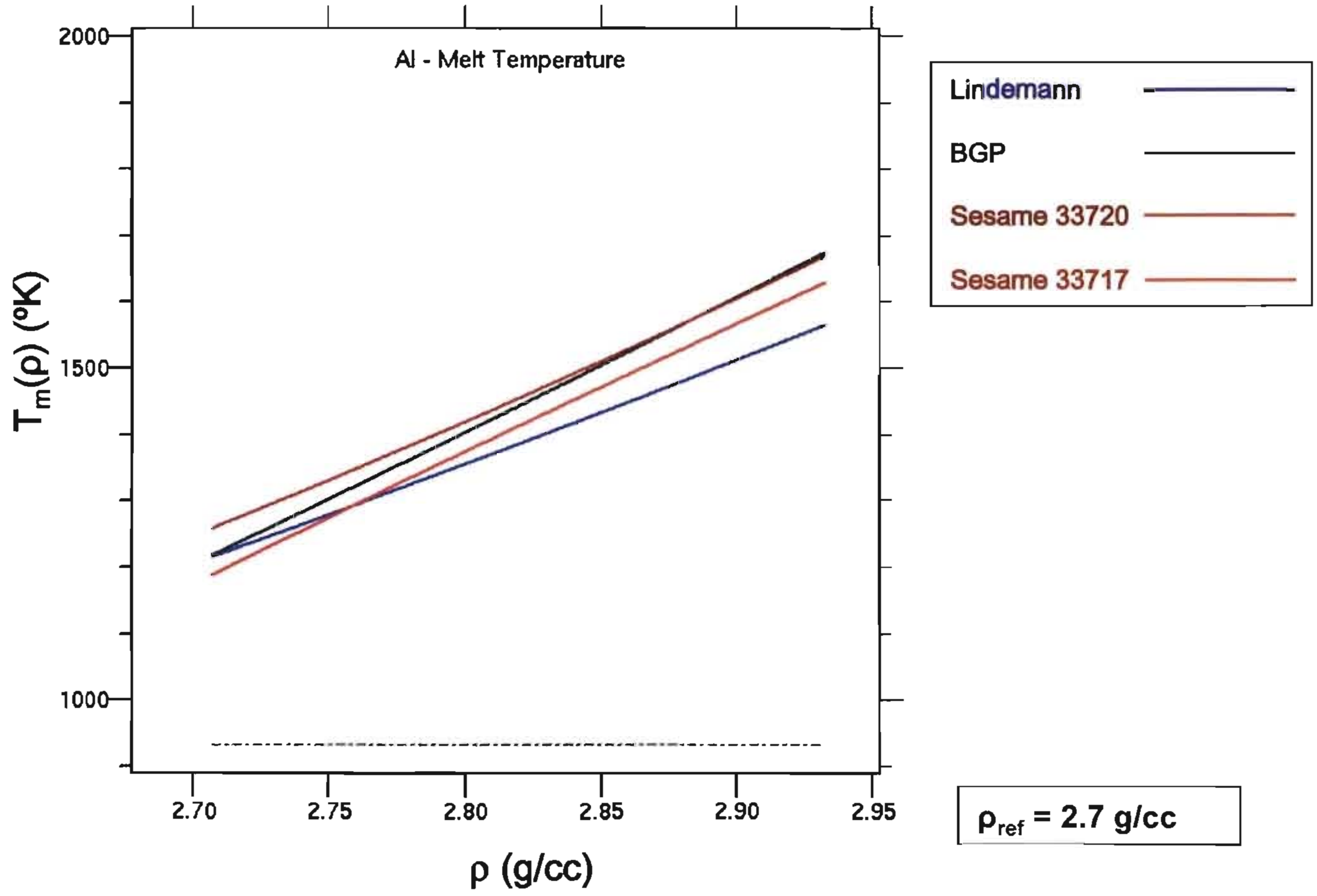
DU Stress-Strain Curve ($d\varepsilon^p/dt = 0.0028/\mu s$) with/without a density dependent Lindemann melt



DU Stress-Strain Curve ($d\varepsilon^p/dt = 0.5/\mu s$) with/without a density dependent Lindemann melt



Melt Temperatures for Aluminum

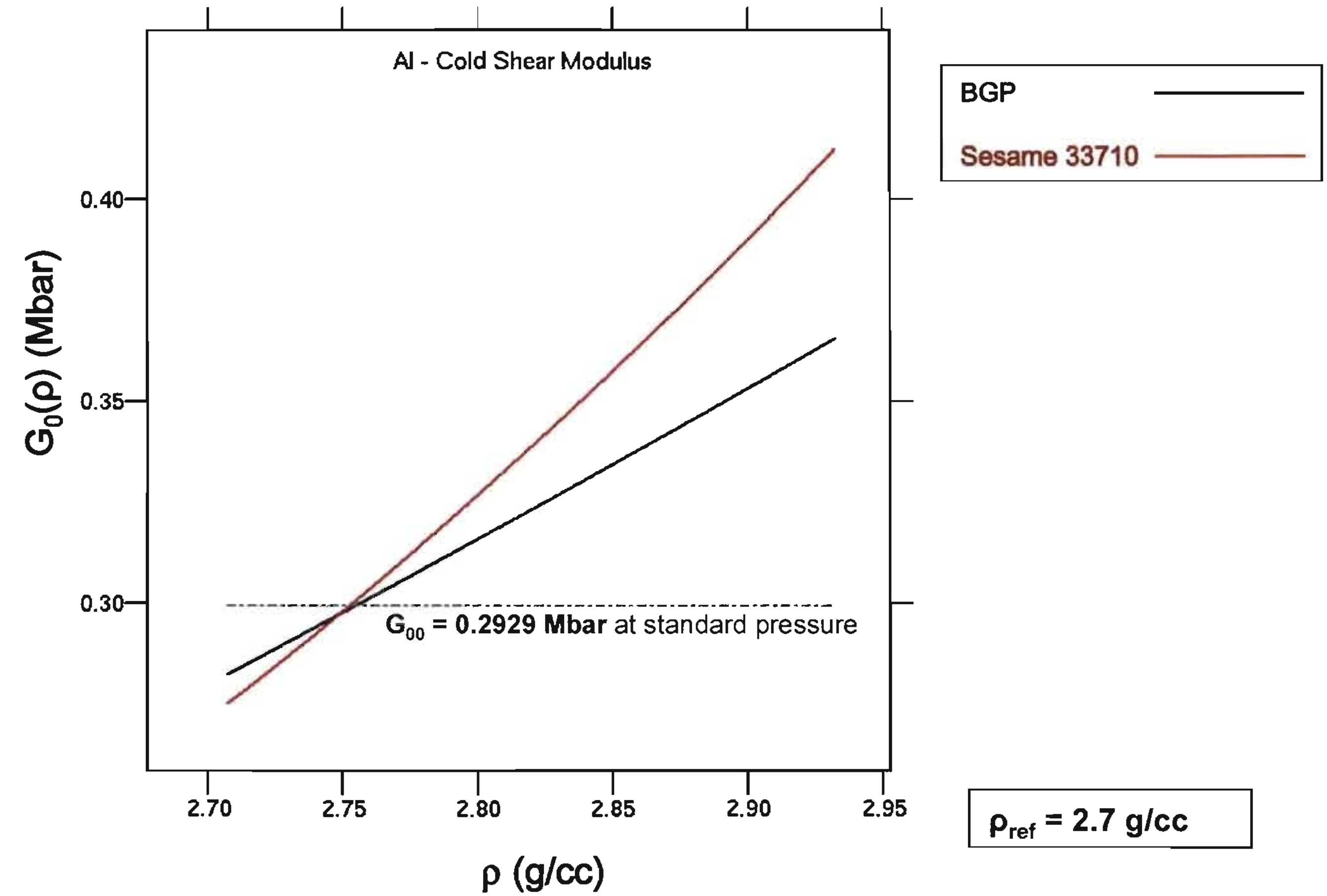


◎ 932° K

T_m at standard pressure

ρ_{ref} = 2.7 g/cc

Shear Moduli for Aluminum



PTW Adjustment
for density dependent Shear Modulus

Reasonable assumptions:

1) Density changes are small during MST experiments
2) Most experiments were performed at ambient temperature and pressure - (ρ_R, T_R)
3) Shear modulus of model should equal shear modulus MST parameter fit

$$G_{MST}(T_R) = G_{PTW}(\rho_R, T_R)$$

4) Compute adjusted parameters for the model

$$\alpha = \frac{T_m(\rho_R)}{T_R}\left[1 - \frac{G_{0a}}{G_0(\rho_R)}\left\{1 - \alpha' \frac{T_R}{T_{ma}}\right\}\right]$$

$$\kappa = \kappa' \frac{T_m(\rho_R)}{T_{ma}}$$

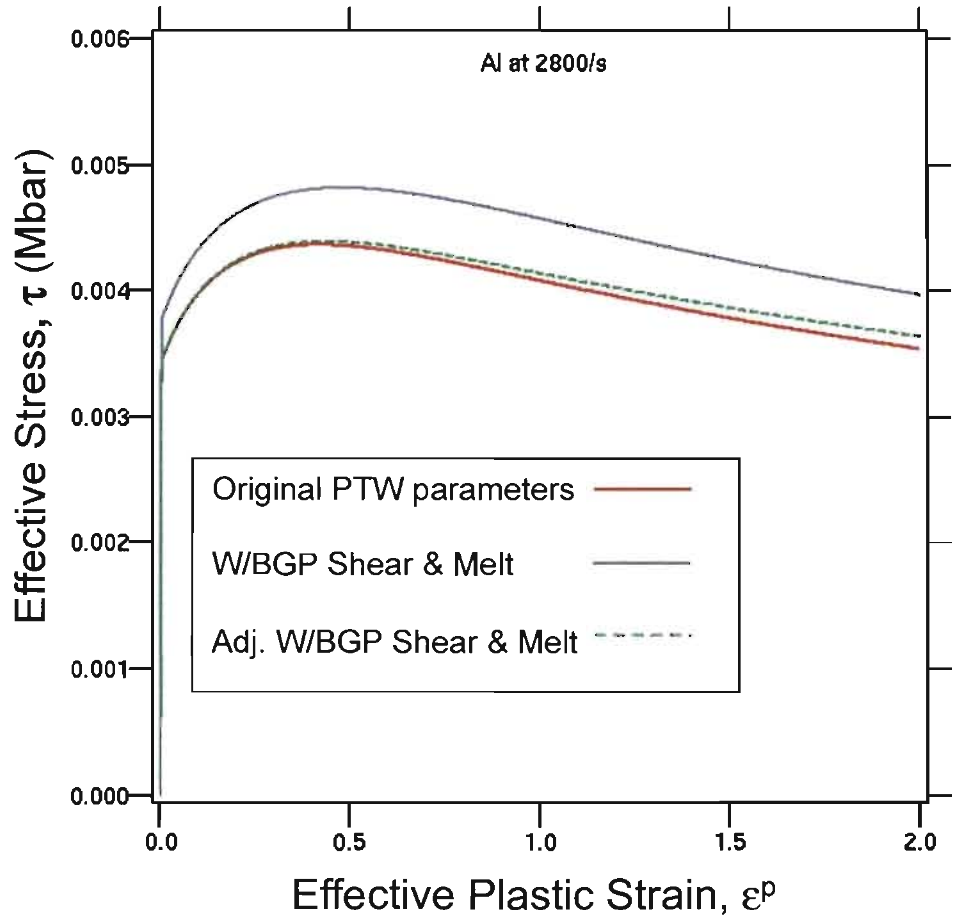
Al 6061-T6
Adjustment of PTW Parameters

Adjustment of the PTW parameters for ρ_0=2.703 g/cc at T_R=298°K

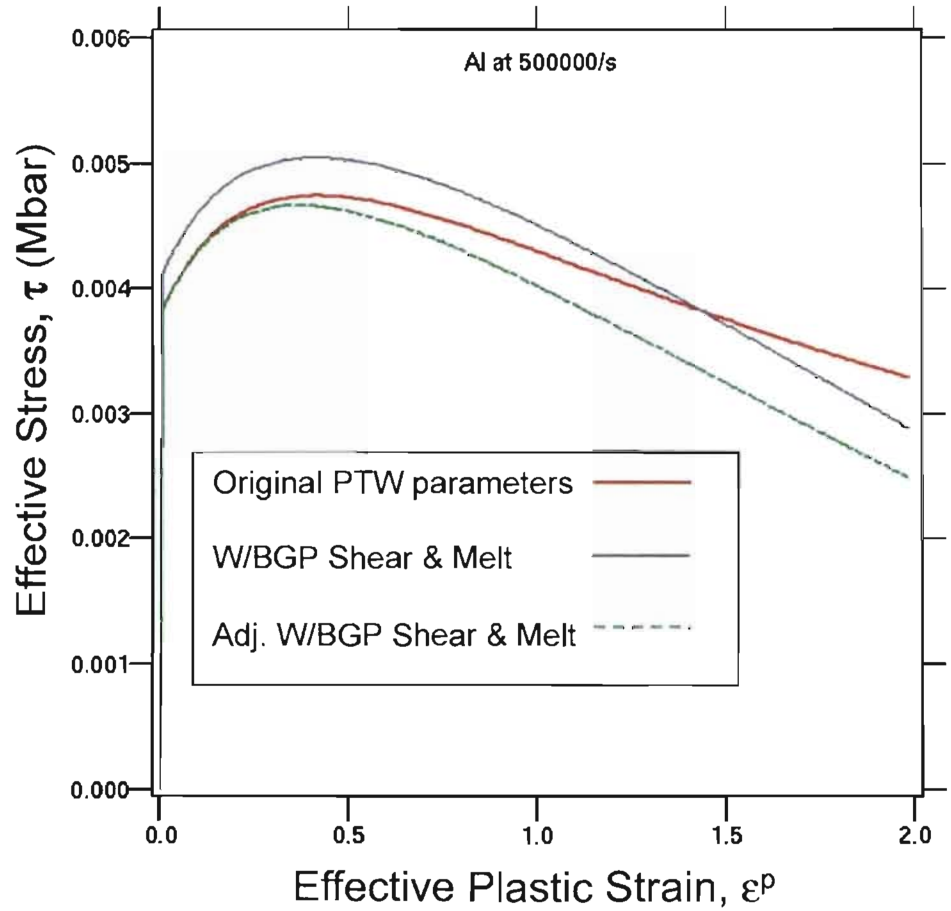
	α	κ	G_0 (Mbar)	T_m (°K)	G_R (Mbar)
Original Data Set	0.475	0.200	0.2992	932	0.254
for T_m only	0.651	0.274	0.2992	1277	0.254
for T_m and G_0	0.574	0.274	0.293	1277	0.254

* Steinberg has G = 0.276 Mbar

Al Stress-Strain Curve ($d\varepsilon^p/dt = 0.0028/\mu s$)



Al Stress-Strain Curve ($d\varepsilon^p/dt = 0.5/\mu s$)



Annealed Cu
Adjustment of PTW Parameters

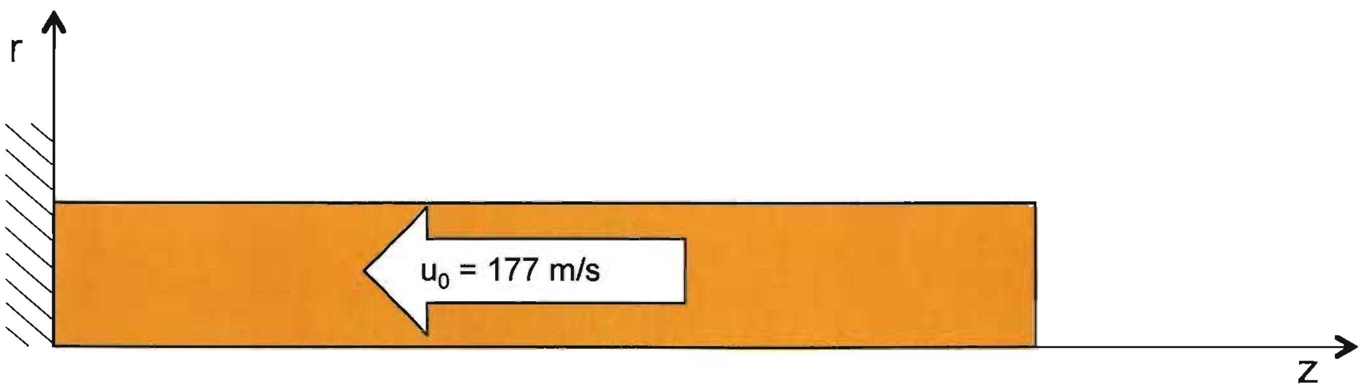
Adjustment of the PTW parameters for ρ_0=8.93 g/cc at T_R=298°K

	α	κ	G_0 (Mbar)	T_m (°K)	G_R (Mbar)
Original Data Set	0.447	0.170	0.525	1356	0.473
for T_m only	0.534	0.203	0.525	1620	0.473
for T_m and G_0	0.344	0.203	0.293	1620	0.473

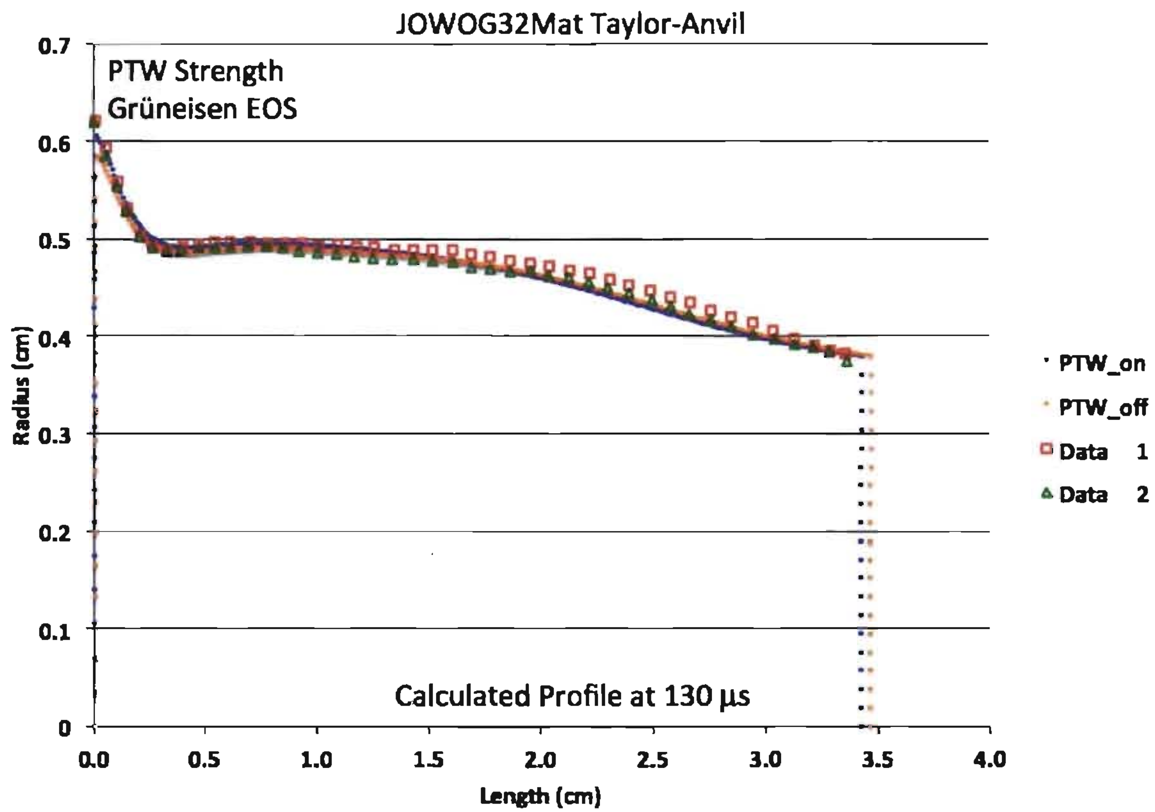
* Steinberg has G = 0.477 Mbar

Taylor Anvil Test Problem

- 2D Axisymmetric geometry.
- Initial dimensions: Z0=5.08cm, R0=0.381cm.
- Impact velocity 177m/s
- Mesh: Regular 200µm mesh. (254x20 cells)
- For simplicity, used a zero axial velocity boundary condition at the impact face.



Computed profiles for a Cu Taylor Rod
with PTW parameters adjusted for Lindemann $T_m(\rho)$ only.



TEPla (Tensile Elastic-Plastic Damage) Model

The stress bearing capability of a material is reduced by damage.

$$\bar{\sigma}_{ij} = (1-D)\sigma_{ij}$$

$$\bar{s}_{ij} = (1-D)s_{ij}$$

$$\bar{p} = (1-D)p$$

TEPla the damage parameter is the porosity

$$D = \phi = \frac{V_{void}}{V}$$

Refactored Tensile Elastic-Plastic Damage Model

TEPla Residual Equations:

$$\left(1+\frac{6G}{y_f}\frac{\Delta\lambda}{y_f}\right)\frac{\bar{\tau}}{y_f}-\frac{\bar{\tau}'}{y_f} = 0$$

$$\bar{\delta}-\bar{\delta}'+\frac{3q_2}{2}\frac{y_f}{y_s}\frac{\Delta\lambda}{y_f}\left[3q_1q_2\frac{\bar{\alpha}}{y_s}\phi\sinh\bar{\delta}+2\Gamma\left(\frac{\bar{\tau}}{y_f}\right)^2\right] = 0$$

$$\phi-\phi'-3q_1q_2\frac{y_f}{y_s}\frac{\Delta\lambda}{y_f}(1-\phi)\phi\sinh\bar{\delta} = 0$$

$$\left(\frac{\bar{\tau}}{y_f}\right)^2-\left[1+q_3\phi^2-2q_1\phi\cosh\bar{\delta}\right] = 0$$

where

$$\bar{\tau} = \sqrt{3/2\,\bar{s}_{ij}\bar{s}_{ij}}$$

$$\bar{\delta} = -3q_2\bar{p}/2y_s$$

$$\bar{\alpha} = \bar{B}-(1+\Gamma)\bar{p}$$

Failure Models

- **Modified Johnson-Cook ductile failure model (TEPla)**

$$F = \left(\frac{\phi}{\phi_f}\right)^2 + \left(\frac{\gamma}{\gamma_f}\right)^2 \geq 1$$

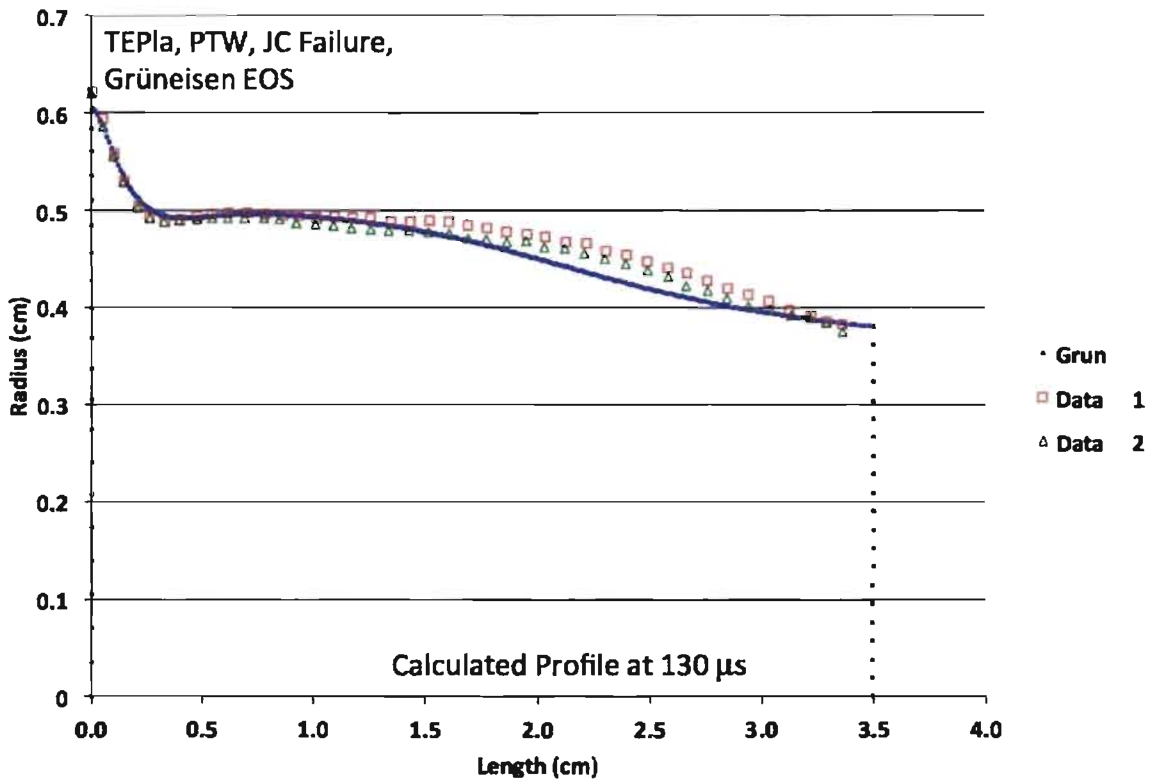
$$\gamma = \sqrt{\frac{2\varepsilon'_{ij}\varepsilon'_{ij}}{3}}$$

$$\gamma_f = \left[D_1 + D_2 e^{D_3 \sigma^{p}}\right]\left[1 + D_4 \ln\frac{\dot{\gamma}}{\dot{\gamma}_0}\right]\left[1 + D_5 \frac{T - T_{\mathrm{ref}}}{T_m - T_{\mathrm{ref}}}\right]$$

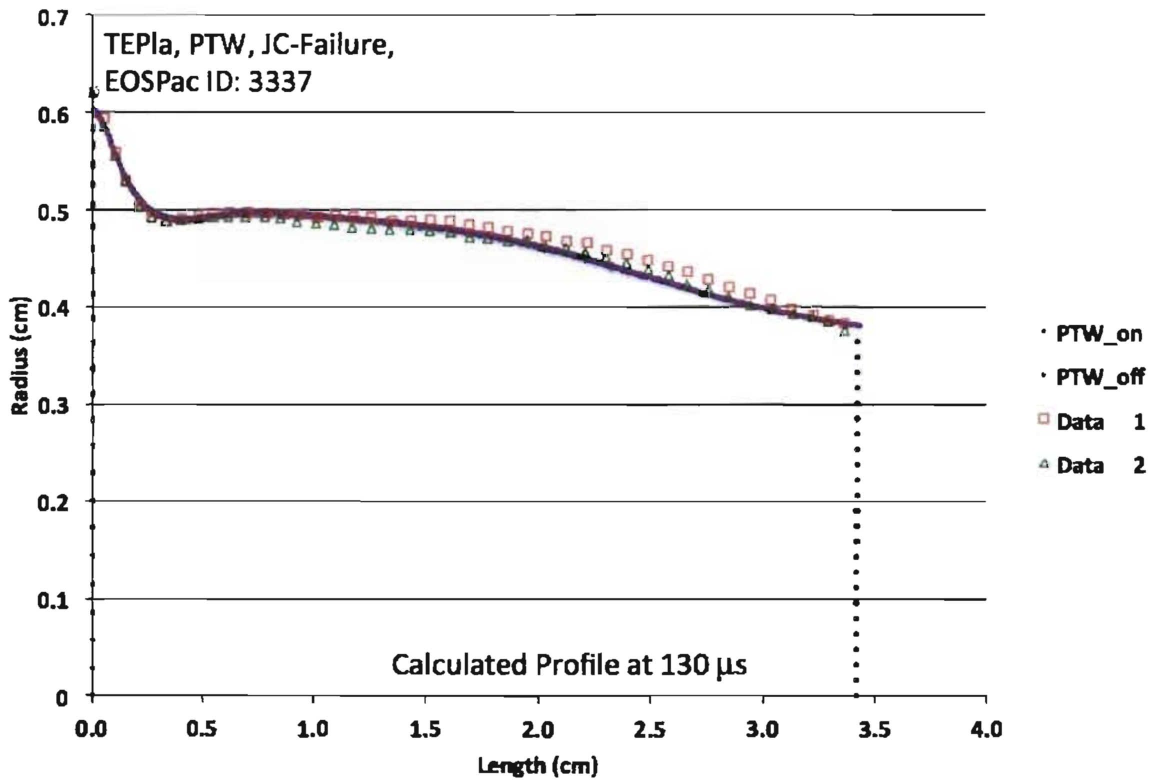
- **Maximum Tensile Stress**
- **P_{min} Spall**

Computed profile of a Taylor Rod

Modeled with Damage, JC Ductile Failure, T_m and G constant.

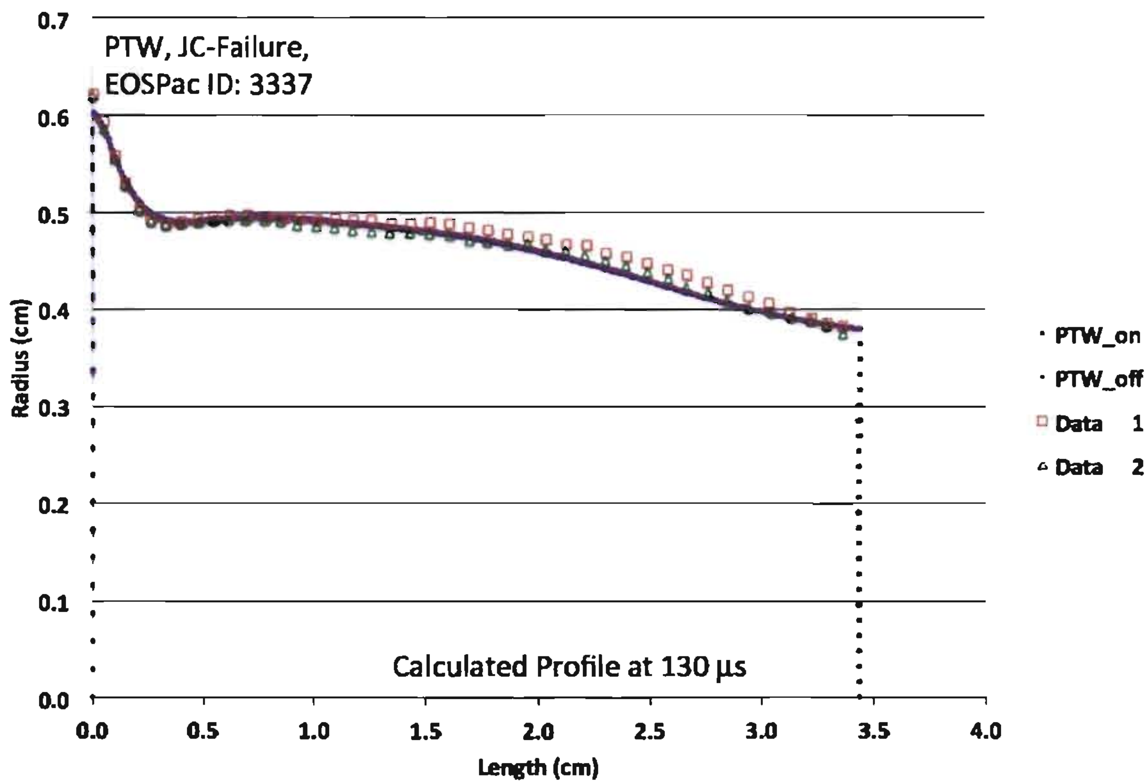


Computed profile of a Taylor Rod
Modeled with Damage PTW Mod 1 and JC Ductile Failure.

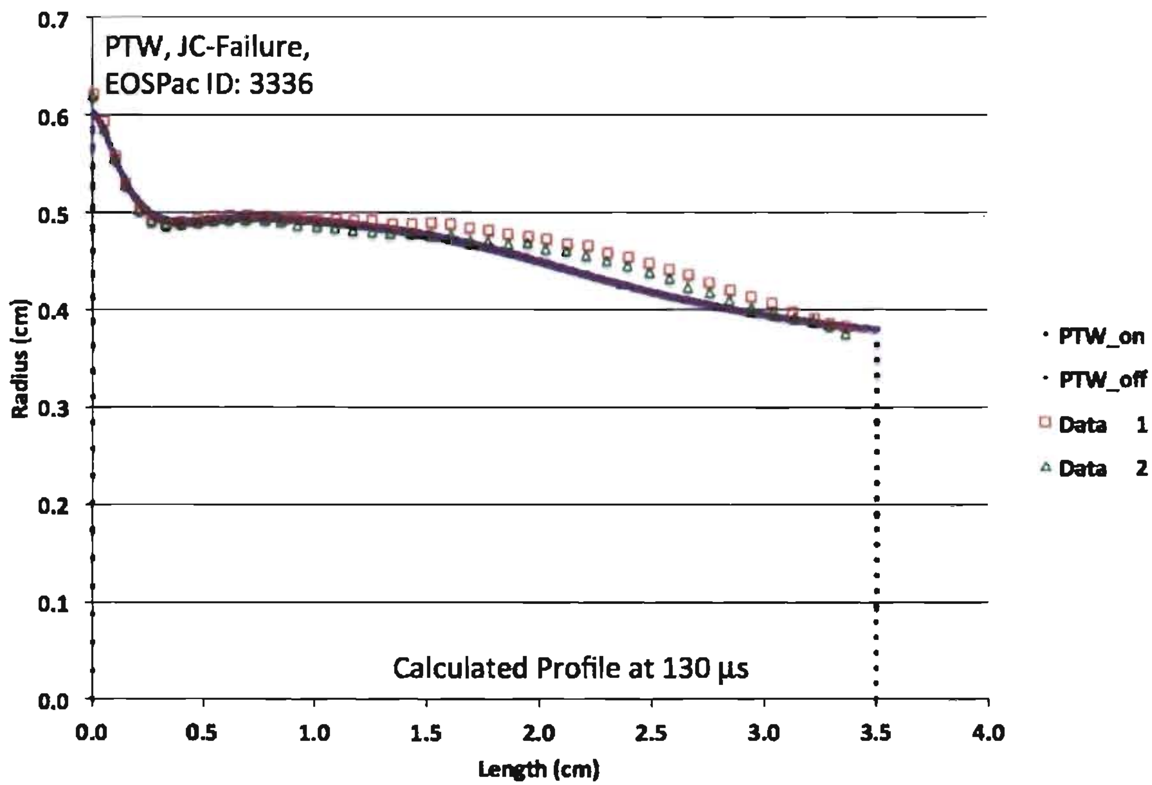


Computed profile of a Taylor Rod

Modeled with PTW Mod 1 and J-C Ductile Failure.



Computed profile of a Taylor Rod
Modeled with PTW Mod 1 and J-C Ductile Failure,



Discussion and Conclusion

- **Updated PTW Model**
  - It is a more robust implementation of the original model.
  - Tested over an extended strain-rate regime.
  - Data fits cover a limited range of interest.
  - Extension to overdriven stress/high strain-rate regime needs to be re-visited.
  - Auto-adjust feature
    - Self correcting
    - Detected compatibility issues with some of the data fits (Stainless-Steel)
- **TEPla Refactor**
  - Modularity has allowed us to implement alternative solvers (Zou-Rice).
  - Used in the Taylor Anvil studies.

Future Directions

- **PTW**
  - Need to characterize the high strain-rate behavior of the model
    - Revisit overdriven shock experiments
    - DFT Simulations
- **Modeling of Anisotropic Elastic-Plastic Solids**
  - B-basis solver
  - Need to consider coupling between the pressure and deviator components of stress and strain.
- **TEPla**
  - Continue work on more robust solvers.
  - Anisotropic Damage
  - Multiphase Damage

References

1. Leonid Burakovsky, Carl W. Greeff and Dean L. Preston, An Analytic Model of Shear Modulus at all Temperatures and Densities, LA-UR-02-3291, LANL, November 2002.
2. Dean L. Preston, Davis L. Tonks and Duane C. Wallace, "Model of plastic deformation for extreme loading conditions", J Appl. Physics, V93, N1, 211-220, 2003.
3. Shuh-Rong Chen and G. T. (Rusty) Gray III, Summary of the PTW Model Parameters, LA-CP-04-0920, LANL, December 2004.
4. Shuh-Rong Chen and G. T. (Rusty) Gray III, Mechanical Properties and Constitutive Modeling of Metals, LU-UR-09-07780, LANL, 2009.
5. Dean L. Preston, PTW Mod 1, LA-UR-10-06436, LANL, 2010.
6. Q. H. Zou and Jeremy R. Rice, "An explicit algorithm for a rate-dependent ductile failure model", J. Appl. Physics, V104, 104-112, 2008.