Modeling and Experimental Investigation of Reactive Shear Bands in Energetic Solids Loaded in Torsion

by

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Support

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Research and Development Laboratories

Summer Faculty Research Program

Motivation

1. Development of insensitive explosives

   - Risk minimization in storage and handling

   - Weapon system development

2. Development of transient detonation models

   - steady detonation better characterized

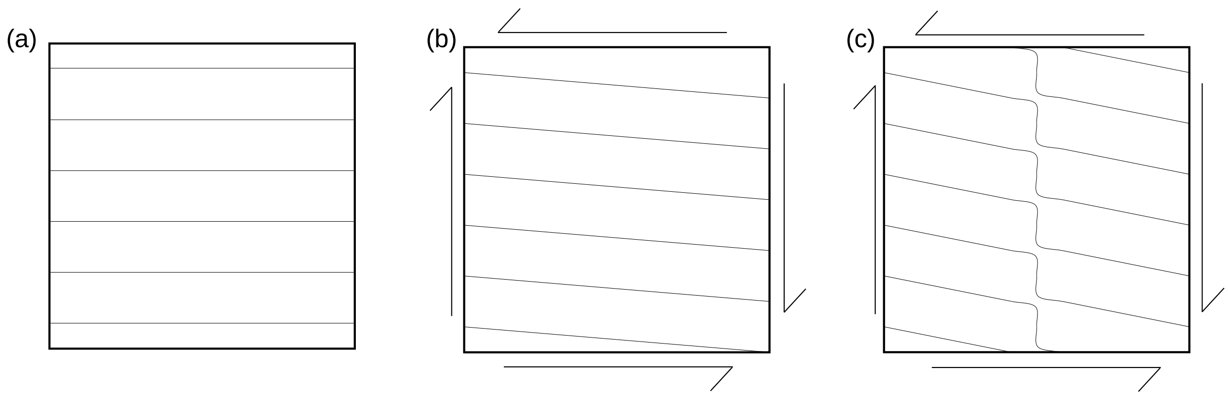
   - late-time hydrodynamics better characterized

   - early time ignition poorly understood

     - thermal stimuli

     - *mechanical stimuli, e.g. shear banding*

Shear Banding



Plastic work $\rightarrow$

- Strain hardening
- Strain rate hardening
- Thermal softening

$\rightarrow$ Shear localization

$\rightarrow$ Hot spot?

$\rightarrow$ Reaction?

Approach

1. Experiment

   - Obtain data for constitutive theory (via torsional split-Hopkinson bar)
   - Observe shear localization and other failure mechanisms (via ultra high speed photography)

2. Theory

   - Develop model
   - Implement numerical method-of-lines approach
   - Predict shear localization and ignition

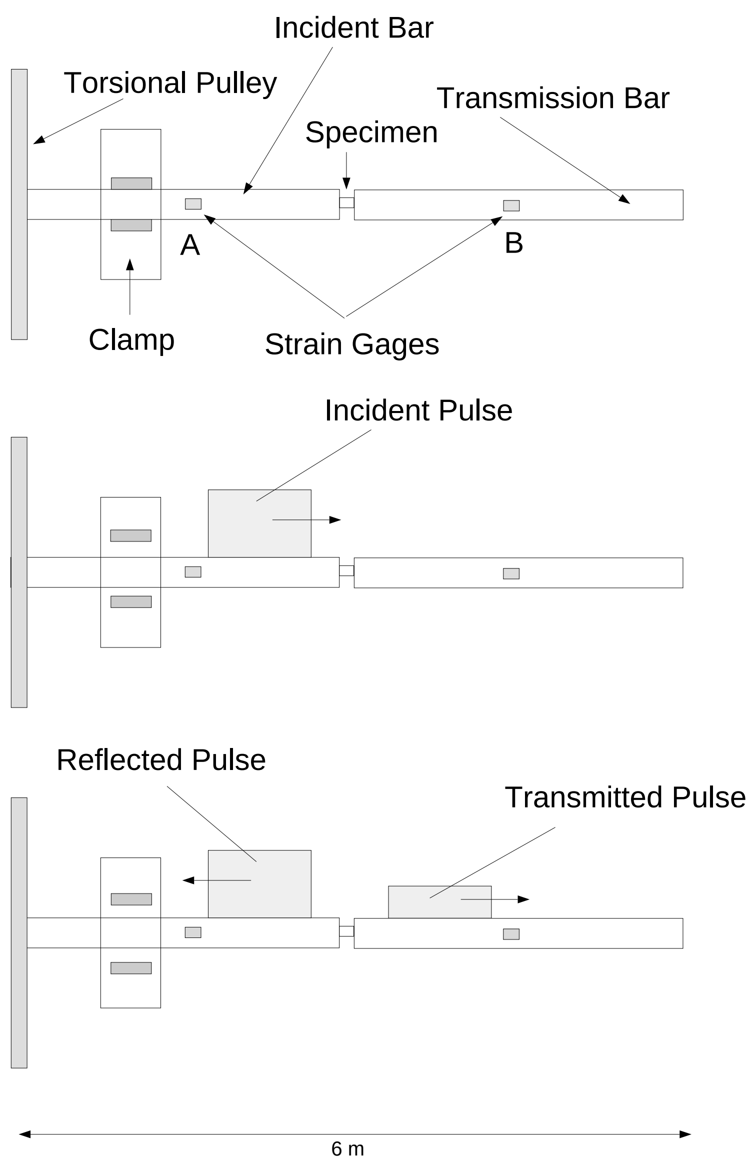
Novelty

1. Stress-strain-strain rate characterization of explosive simulant PBX 9501
   - $C_{1.47}H_{2.86}N_{2.6}O_{2.69}$
   - 95 % HMX; 2.5 % estane; 2.5 % BDNPA-F binder
   - rubbery material not well suited for shear localization studies!
2. Extension of Frey's (1981) analysis to include strain rate effects
3. Sensitivity analysis performed

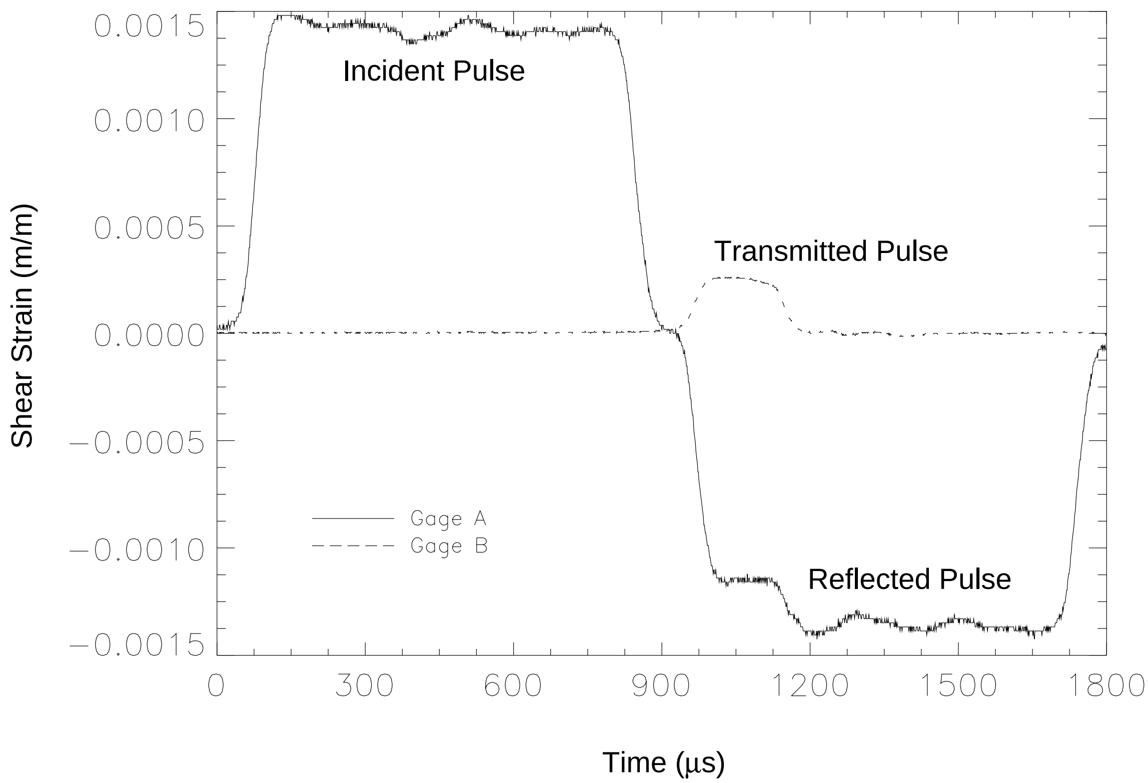
Experimental Method

Torsional Split-Hopkinson Bar

Notre Dame Solid Mechanics Laboratory



Data Analysis



Shear strain in the specimen:

$$\bar{\gamma}(t) = -\frac{2cd}{LD}\int_0^t \gamma_R(\tilde{t})\ d\tilde{t}$$

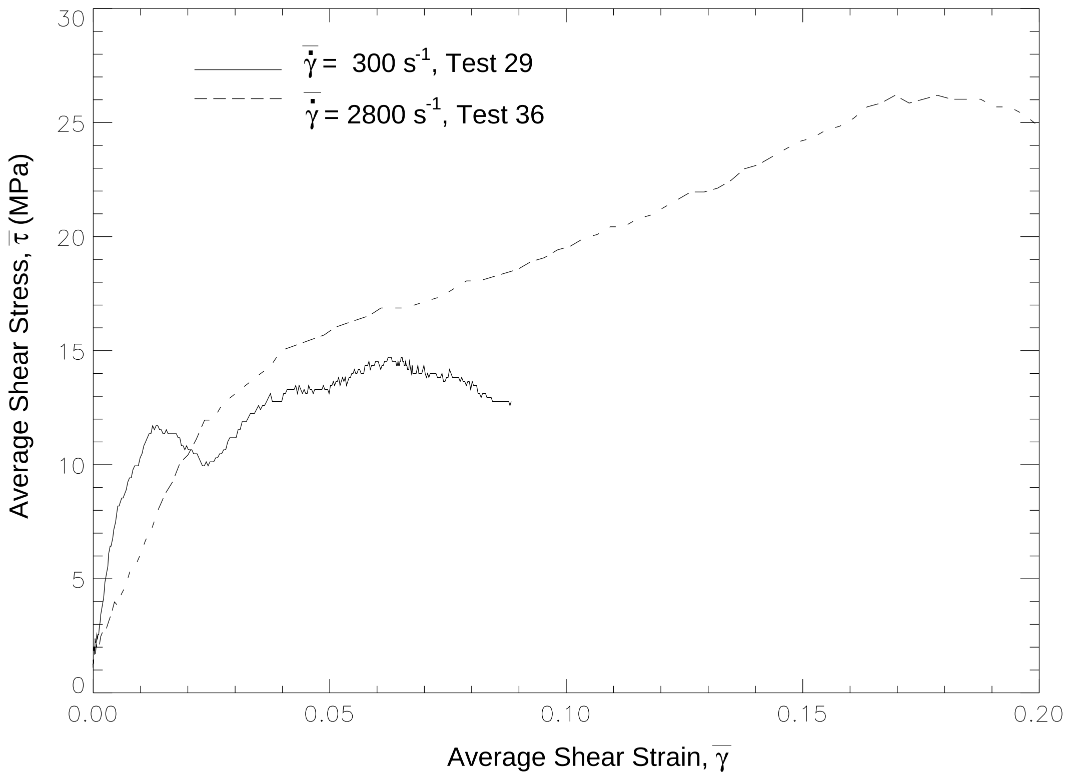
Shear stress in the specimen:

$$\bar{\tau}(t) = \frac{GD^3}{8d^2w}\gamma_T(t)$$

(Hartley, Duffy and Hawley, *Metals Handbook*, 1985)

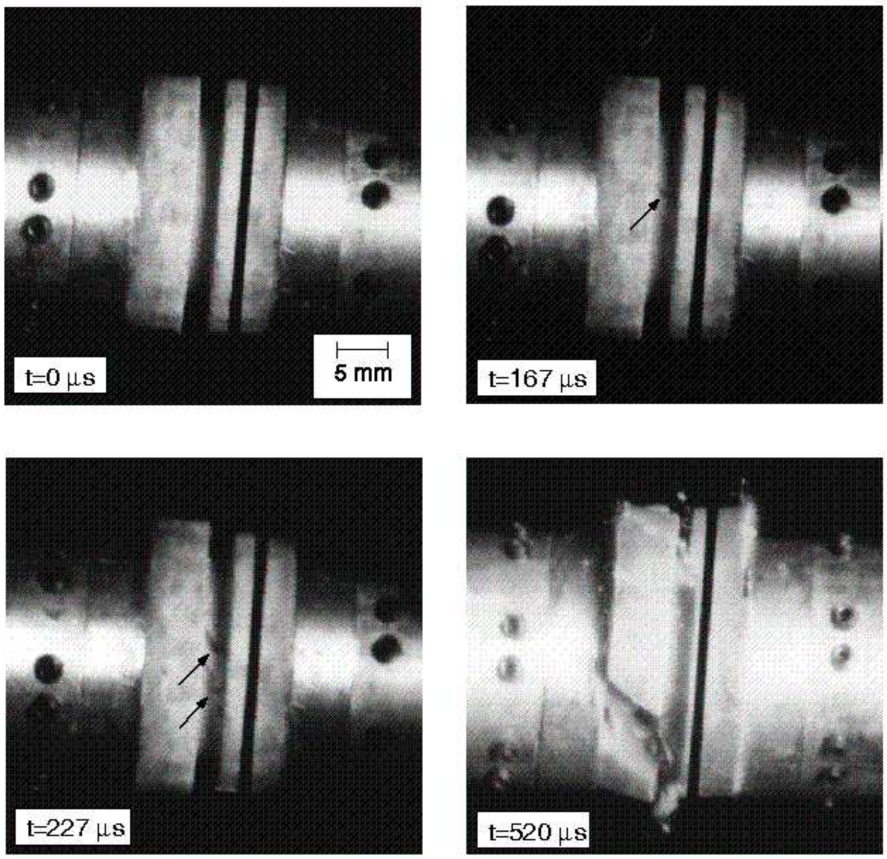
Experimental Results

Torsional Split Hopkinson Bar Tests of PBX 9501 Simulant



- Stress overshoot
- Lower strain rate failure $\rightarrow$ Void nucleation and growth
- Higher strain rate failure $\rightarrow$ Brittle fracture

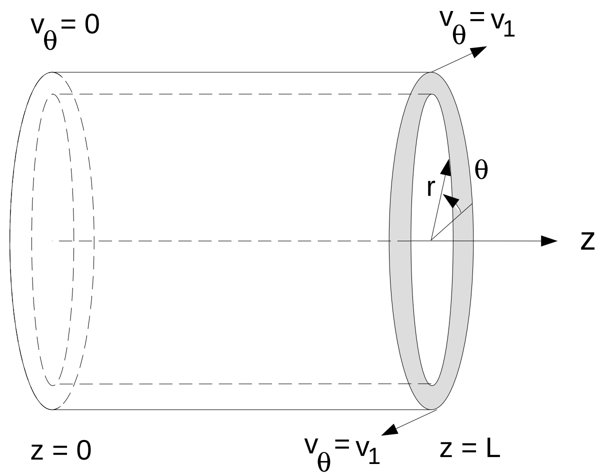
Ultra-High Photography of Failure



- photos with Notre Dame's Cordon 350 camera

- failure time correlates with strain gage results

Model



- Thin walled, cylindrical specimen
- Initially unreacted, unstressed, and at ambient temperature
- $v_r = v_z = u_r = u_z = 0$
- $\frac{\partial}{\partial \theta} = \frac{\partial}{\partial r} = 0$
- Plastic work completely converted to heat
- One-step Arrhenius chemistry

Model Equations

$\rho w \dfrac{\partial v_\theta}{\partial t} = \dfrac{\partial}{\partial z}(w\tau)$	linear momentum
$\rho w \dfrac{\partial e}{\partial t} = w\tau \dfrac{\partial v_\theta}{\partial z} - \dfrac{\partial}{\partial z}(w q_z)$	energy conservation
$\dfrac{\partial \lambda}{\partial t} = Z(1-\lambda)\exp\left(-\dfrac{E}{RT}\right)$	reaction kinetics
$\gamma = \dfrac{\partial u_\theta}{\partial z}$	strain definition
$v_\theta = \dfrac{\partial u_\theta}{\partial t}$	velocity definition
$\tau = \alpha\ T^\nu\ \gamma^\eta\ \left\lvert\dfrac{\partial \gamma}{\partial t}\right\rvert^{\mu-1}\left(\dfrac{\partial \gamma}{\partial t}\right)$	stress relation
$q_z = -k\dfrac{\partial T}{\partial z}$	Fourier's Law
$e = Y_A e_A + Y_B e_B$	total internal energy
$e_A = c_A T + e_A^o$	reactant internal energy
$Y_A = 1 - \lambda$	reactant mass fraction
$e_B = c_B T + e_B^o$	product internal energy
$Y_B = \lambda$	product mass fraction
$w = w_0 - \dfrac{h_p}{2}\left[1 - \cos\left(\dfrac{2\pi z}{L_s}\right)\right]$	geometry

Reduced System

Parabolic Partial Differential Equation System

$$
\begin{aligned}
\frac{\partial v_\theta}{\partial t} &= \frac{1}{\rho w}\frac{\partial}{\partial z}\left[w\alpha\ T^\nu\ \left(\frac{\partial u_\theta}{\partial z}\right)^\eta\ \left|\frac{\partial v_\theta}{\partial z}\right|^{\mu-1}\frac{\partial v_\theta}{\partial z}\right] \\
\frac{\partial T}{\partial t} &= \frac{1}{\rho\left[c_A\left(1-\lambda\right)+c_B\lambda\right]}\left[\alpha T^\nu\ \left(\frac{\partial u_\theta}{\partial z}\right)^\eta\ \left|\frac{\partial v_\theta}{\partial z}\right|^{\mu+1}+\frac{k}{w}\frac{\partial}{\partial z}\left(w\frac{\partial T}{\partial z}\right)\right. \\
&+ \left. Z\ \rho\left[e_A^o-e_B^o+\left(c_A-c_B\right)T\right]\left(1-\lambda\right)\exp\left(-\frac{E}{RT}\right)\right] \\
\frac{\partial u_\theta}{\partial t} &= v_\theta \\
\frac{\partial \lambda}{\partial t} &= Z\left(1-\lambda\right)\exp\left(-\frac{E}{RT}\right)
\end{aligned}
$$

Boundary Conditions

$$
\begin{aligned}
v_\theta\left(t,0\right)=0\ ,\quad v_\theta\left(t,L\right)\ &= \begin{cases}\left(v_1-v_0\right)\frac{t}{t_1}+v_0 & t<t_1\\ v_1 & t\geq t_1\end{cases} \\
u_\theta\left(t,0\right)=0\ ,\quad u_\theta\left(t,L\right)\ &= \begin{cases}\left(v_1-v_0\right)\frac{t^2}{2t_1}+v_0 t & t<t_1\\ \left(v_1-v_0\right)\frac{t_1}{2}+v_0t_1+v_1\left(t-t_1\right) & t\geq t_1\end{cases} \\
\frac{\partial T}{\partial z}\left(t,0\right)=0\ ,\quad \frac{\partial T}{\partial z}\left(t,L\right)=0 & \qquad t\geq 0\ .
\end{aligned}
$$

Initial Conditions

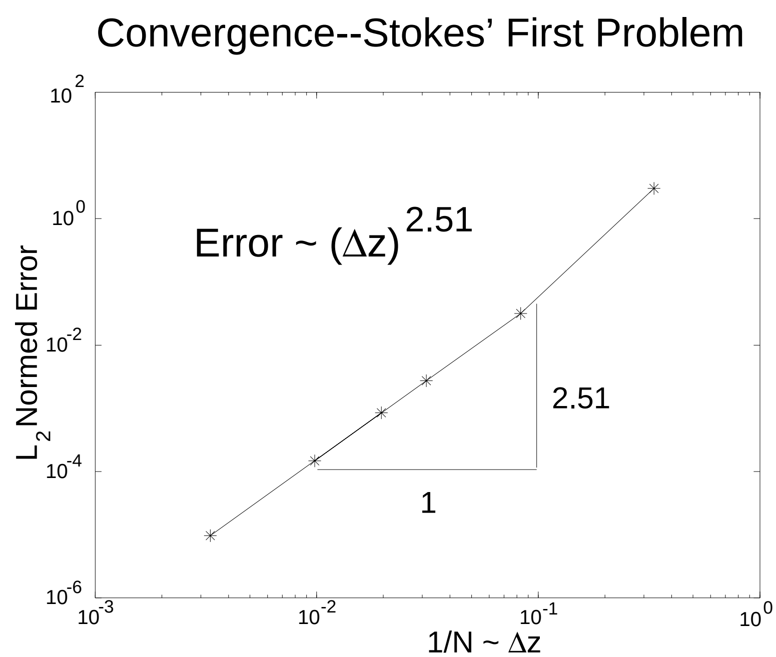
$$
v_\theta\left(0,z\right)=v_0\frac{z}{L}\ ,\qquad u_\theta\left(0,z\right)=0\ ,\qquad T\left(0,z\right)=T_0\ ,\qquad \lambda\left(0,z\right)=0.
$$

Numerical Method

- Parabolic system of PDE's–method of lines

- 2^{nd} order finite difference spatial discretization

- 4^{th} order implicit (LSODE) solution of ODE's in time



Localization Criteria

Adiabatic shear bands typically initiate at a point after a maximum stress is reached in the shear stress-shear strain relationship at that point (Zener and Hollomon, 1944):

$$\left.\frac{\partial \tau}{\partial \gamma}\right|_z \leq 0$$

With

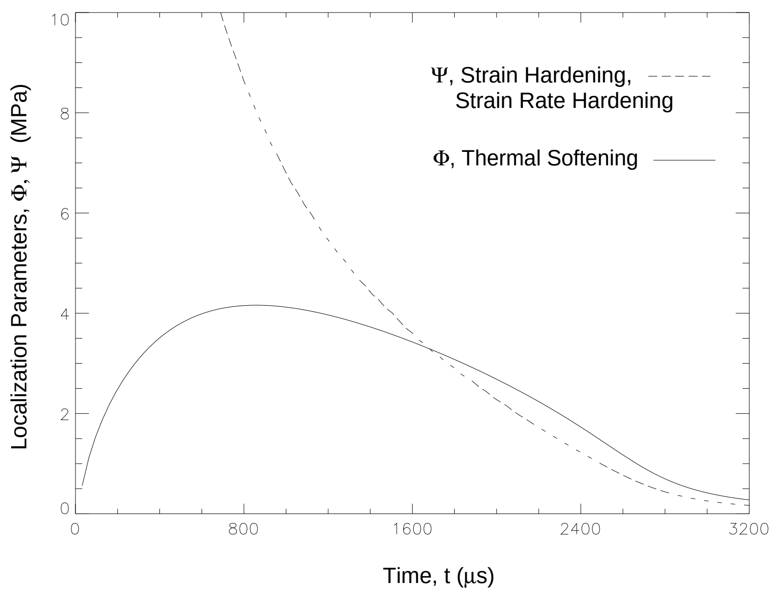
$$\tau = \tau\left(T, \gamma, \dot{\gamma}\right)$$

Localization criterion (Meyers, 1994):

$$\left.\frac{\partial \tau}{\partial \gamma}\right|_{T,\dot{\gamma}} + \left.\frac{\partial \tau}{\partial \dot{\gamma}}\right|_{T,\gamma} \frac{\partial \dot{\gamma}/\partial t|_z}{\partial \gamma/\partial t|_z} \leq -\frac{\tau}{\rho c_A} \left.\frac{\partial \tau}{\partial T}\right|_{\gamma,\dot{\gamma}}$$

Theoretical Results

1. PBX 9501 without reaction, $\dot{\gamma} = 2800\ s^{-1}$

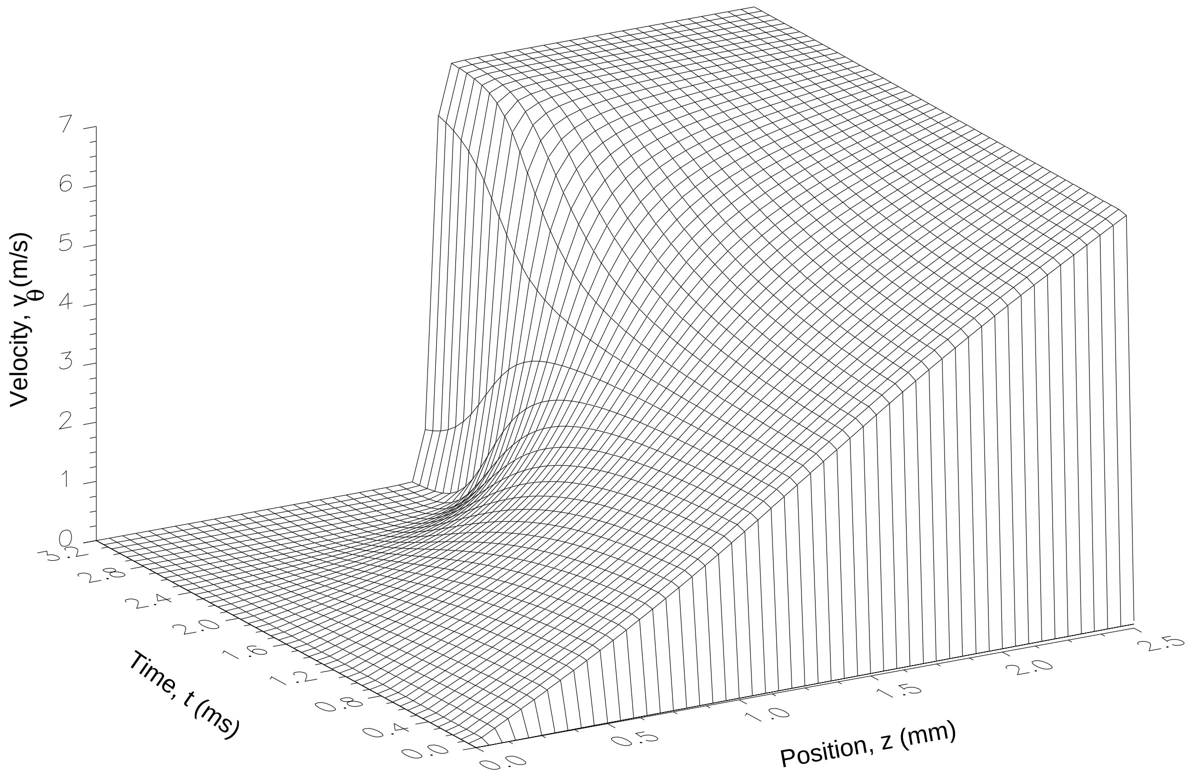


$$\left.\frac{\partial \tau}{\partial \gamma}\right|_{T,\dot{\gamma}} + \left.\frac{\partial \tau}{\partial \dot{\gamma}}\right|_{T,\gamma} \frac{\partial \dot{\gamma}/\partial t|_z}{\partial \gamma/\partial t|_z} \leq -\frac{\tau}{\rho c_A} \left.\frac{\partial \tau}{\partial T}\right|_{\gamma,\dot{\gamma}}$$

$$\Psi \leq \Phi$$

- Φ represents thermal softening
- Ψ represents strain and strain rate hardening
- Localization onset predicted after 1600 μs

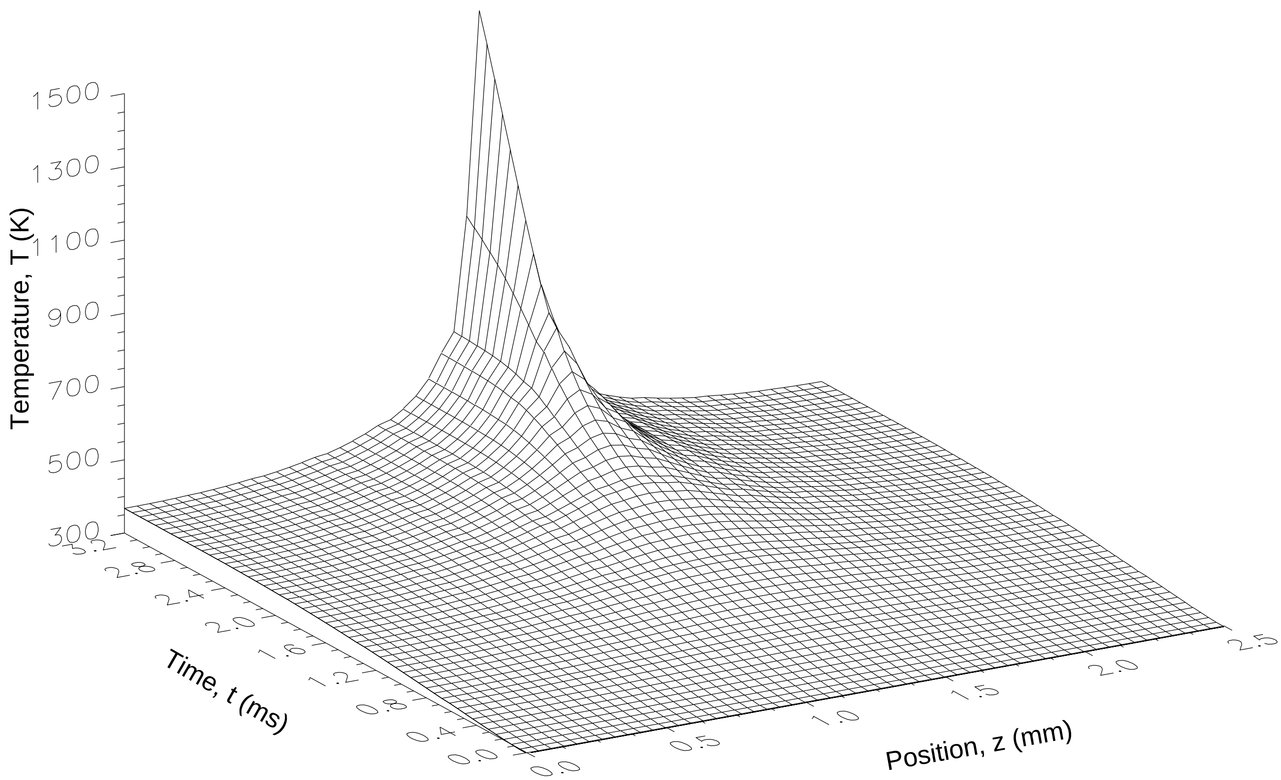
PBX 9501 without reaction, Cont.



Three stage localization process (Marchand and Duffy, 1988):

- Stage I: Homogeneous deformation
- Stage II: Inhomogeneous deformation
- Stage III: Shear band or shear localization

PBX 9501 without reaction, Cont.



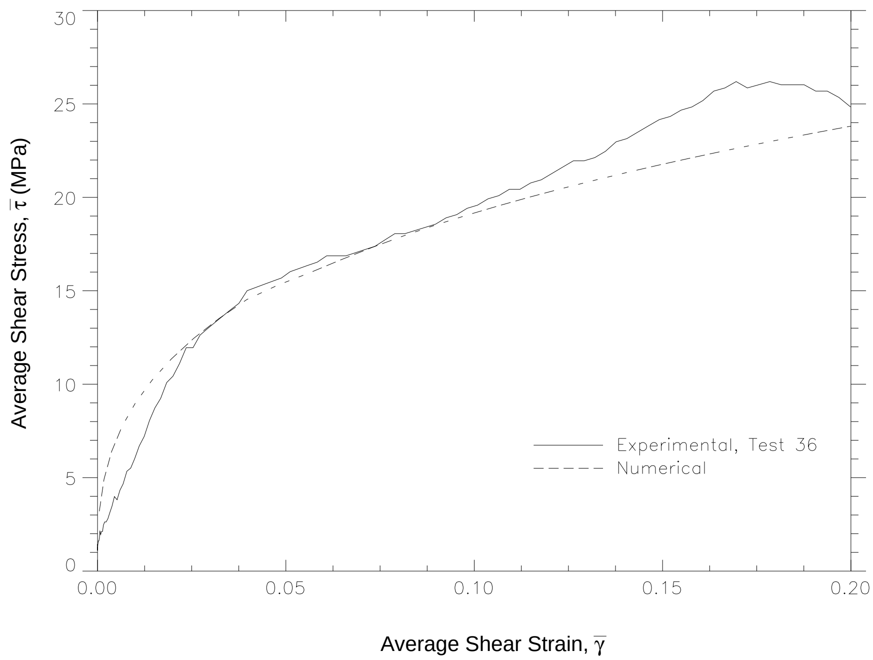
Key Issues

(a) Formation of spike following onset of localization

- After 1.67 ms, $T_{max} = 458\ K$
- After 3.2 ms, $T_{max} = 1590\ K$

(b) Initiation temperature is only 513 K

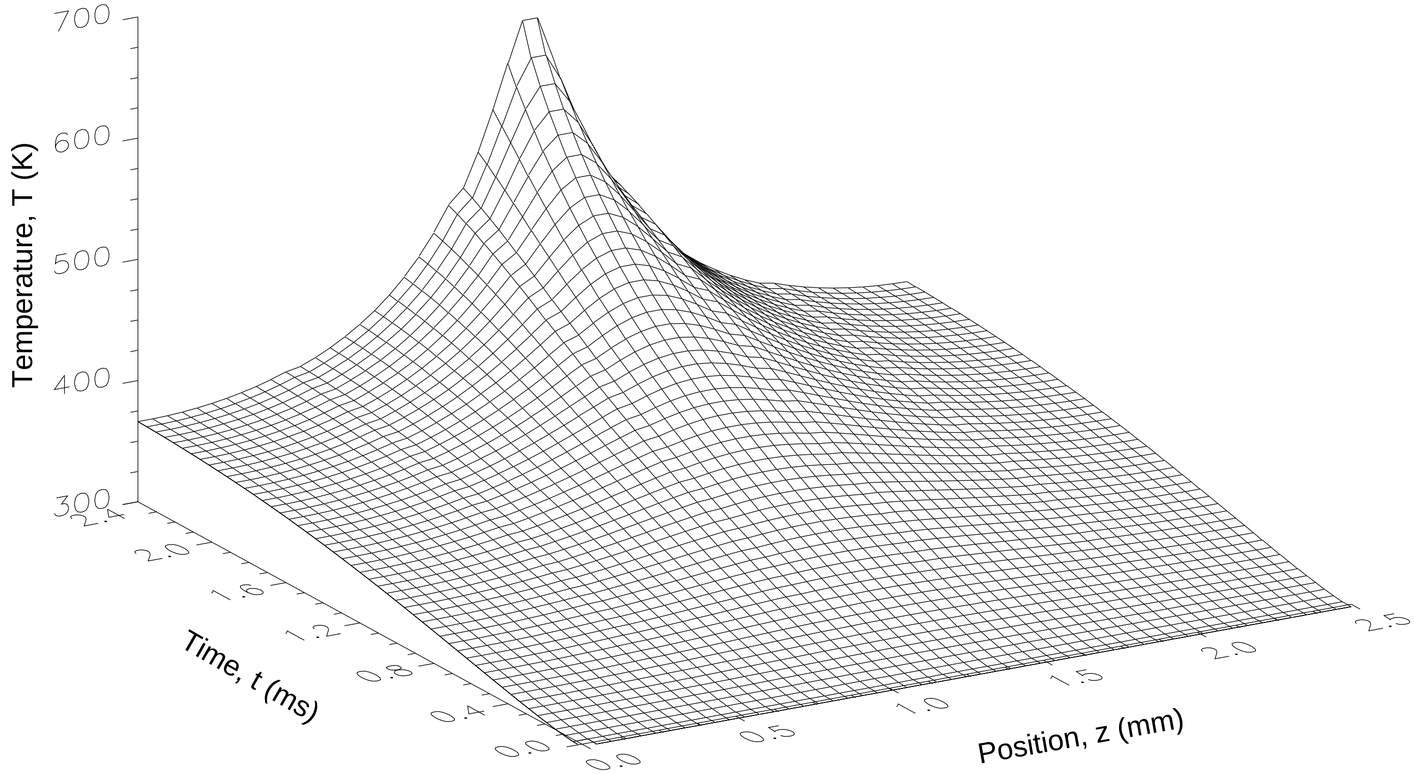
PBX 9501 without reaction, Cont.



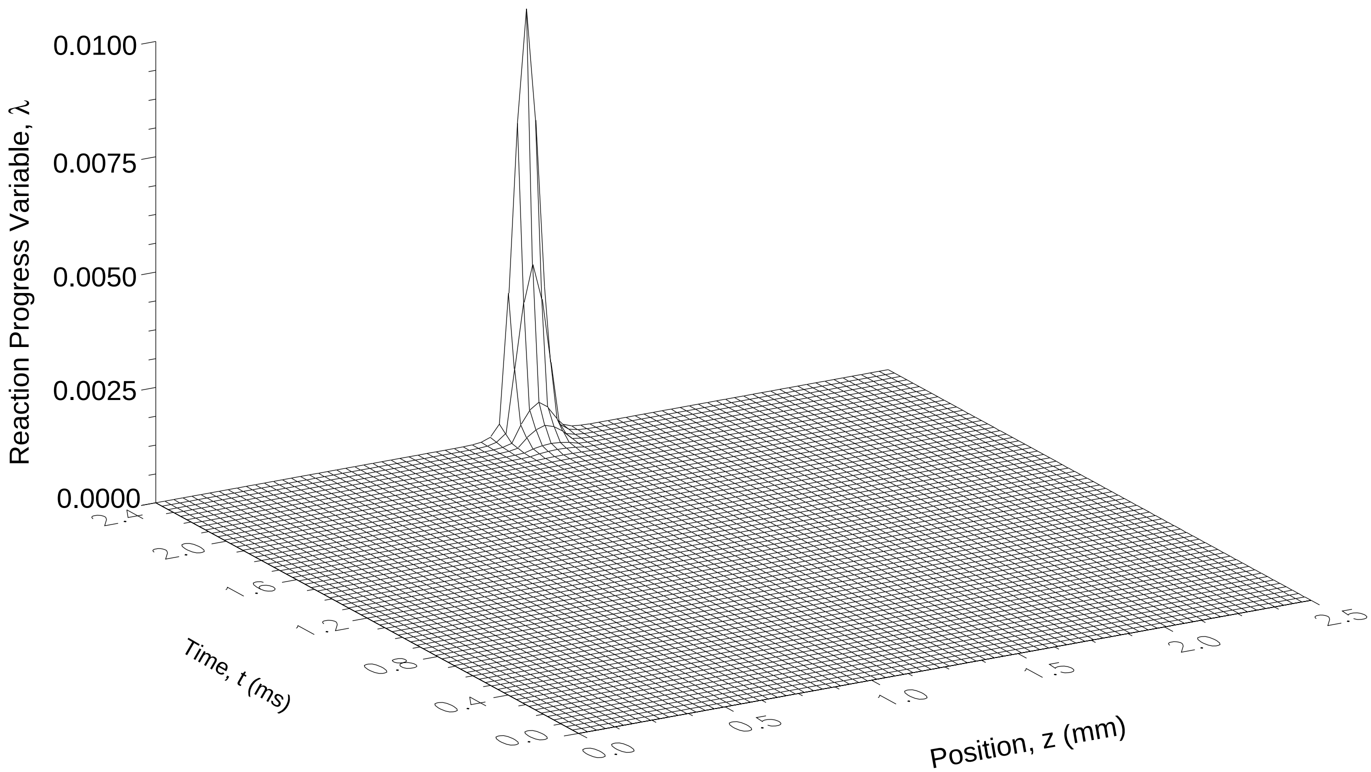
- Predictions accurate for $\bar{\gamma} \leq 0.2$
- Experimental failure at $\bar{\gamma} \approx 0.2$
- Predicted localization at $\bar{\gamma} \approx 3.5$
- Predicted failure at $\bar{\gamma} \approx 8.0$
- Failure occurs due to mechanisms other than shear localization

Theoretical Results, Cont.

2. PBX 9501 with reaction



PBX 9501 with Reaction, Cont.



- Reaction occurred before development of temperature spike
- Initiation extremely sensitive to temperature
  - No significant reaction prior to localization
  - Reaction proceeds quickly once reaction temperature reached
  - Reaction occurs at localized hot spot
- Strain at reaction is 6.4, (but experimental failure at $\bar{\gamma} = 0.2$)

Sensitivity Analysis

Parameter	Definition	Description	Value	$\hat{t}_{loc} = \frac{v_1 t_{loc}}{L}$
$\hat{\alpha}$	$\frac{\alpha T_o^{\nu} v_1^{\mu-2}}{\rho L^{\mu}}$	Stress Constant	47.019 **470.19** 4701.9	4.707 **4.710** 4.713
$\hat{\alpha}\ Ec$	$\frac{\alpha T_o^{\nu-1} v_1^{\mu}}{\rho c_A L^{\mu}}$	*(Stress Constant)(Eckert Number)*	0.0068 **0.068** 0.68	26.703 **4.710** 0.857
Pe	$\frac{\rho c_A v_1 L}{k}$	Peclet Number	8.01×10^2 $\mathbf{8.01 \times 10^4}$ 8.01×10^8	4.791 **4.710** 4.707
$\hat{Q}$	$\frac{e_A^o - a_B^o}{c_A T_o}$	Scaled Heat Release	8.64 **17.49** 34.56	4.701 **4.710** 4.713
$\hat{Z}$	$\frac{ZL}{v_1}$	Scaled Kinetic Rate Constant	1.79×10^6 1.79×10^{11} $\mathbf{1.79 \times 10^{16}}$	4.712 4.712 **4.710**
$\hat{E}$	$\frac{E}{RT_o}$	*Scaled Activation Energy*	44.52 **89.04**	Reaction **4.710**
$\hat{c}$	$\frac{c_B}{c_A}$	Ratio of Specific Heats	0.5 **1.0** 2.0	4.715 **4.710** 4.705
η		*Strain Hardening Parameter*	0.032 0.16 **0.320** 0.640	1.311 4.056 **4.710** Reaction
μ		*Strain Rate Hardening Parameter*	0.02 **0.080** 0.32	2.954 **4.710** Reaction
ν		*Thermal Softening Parameter*	-0.345 **-1.28**	Reaction **4.710**

Conclusions

- Numerical modeling indicates that if shear banding occurs, it can lead to reaction initiation
- Experiments consistently revealed failure due to mechanisms other than shear localization
  - ductile mechanisms at low strain rate, 300 s^{-1}
  - brittle mechanisms at high strain rate, 2800 s^{-1}
- Decreasing the strain and/or strain rate effects and increasing the thermal softening effect increases the susceptibility to localization

Future

- Study explosives which are more susceptible to shear banding
- Use ultra-high speed photography to observe failure ignition
- Apply hydrostatic pressure to suppress brittle failure mechanisms
- Extend models to account for material heterogeneity
- Extension to multi-dimensionality