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Title: Modeling Thermo-mechanical behavior of PBX 9501

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Modeling Thermo-mechanical behavior of PBX 9501

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An engineering overview of constitutive modeling of the thermo-mechanical response of Plastic-Bonded eXplosives (PBXs), specifically PBX 9501 will be presented. A range of mechanical behavior is observed which includes small strain recoverable response in the form of viscoelasticity; change in stiffness and softening beyond peak strength due to damage in the form microcracks, debonding, and void formation; inelastic response in the form of plasticity as shown in cyclic tests, and viscoelastic creep combined with plastic response as demonstrated in creep and recovery tests. The main focus of the presentation is to step through the analysis of experimental data to obtain the parameters for a constitutive model which includes viscoelasticity and continuum damage to capturing a few of the above observed mechanisms. Examples of verification and validation as demonstrated against Brazilian disk and Iosipecu gemoetries will also be presented.

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Modeling Thermo-mechanical behavior of PBX 9501

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Talk Outline

Background
- Rationale, objective and goal of this study

PBX 9501
- What it is ? what are the issues ;

Mechanical Test Results
- Monotonic, Cyclic, Triaxial

Analysis of Experimental Data
- Statistical analysis, Viscoelastic properties, Damage Calibration

ViscoSCRAM model
- What it is, pros and cons

Verification and Validation Suite
- What are they, relevance to this study

Background

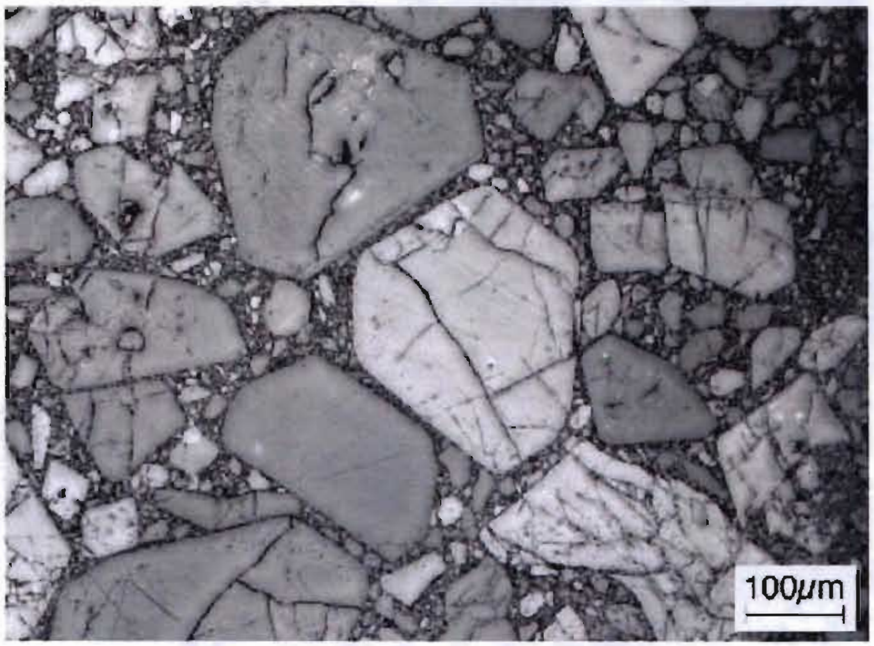
It is important to be able to accurately predict the behavior of high-explosive (HE) materials because,

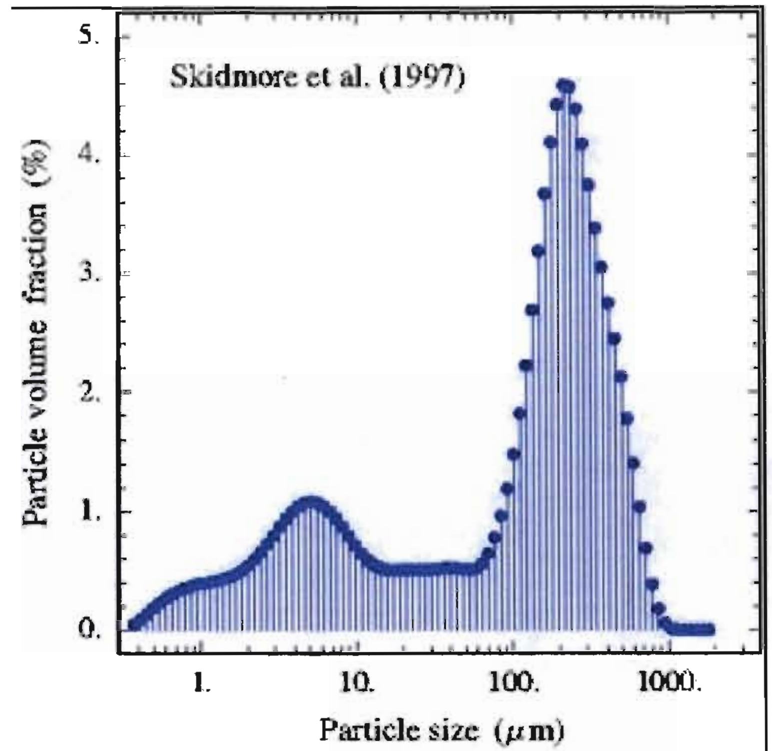
- extreme sensitivity with which they respond in the environment in which they are designed to perform, and
- to accidental mechanical shock, which might occur during handling.

Thus it is imperative that a capability exist to model the response of HE materials subjected to a variety of thermomechanical loading conditions, a response that is highly complex, requiring sophisticated material modeling to simulate.

What is PBX 9501 ?

Plastic Bonded Explosive





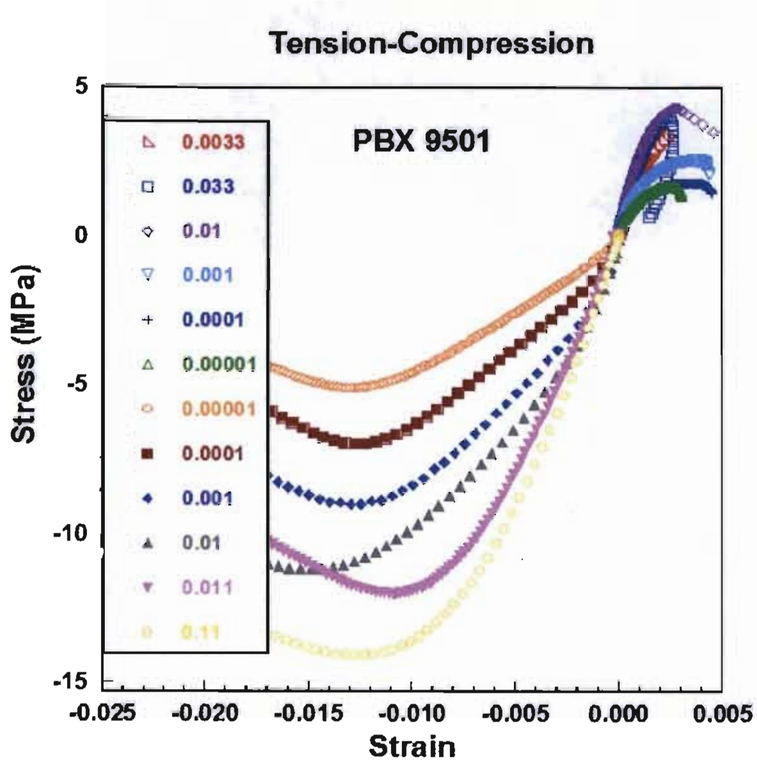
Composition of PBX 9501

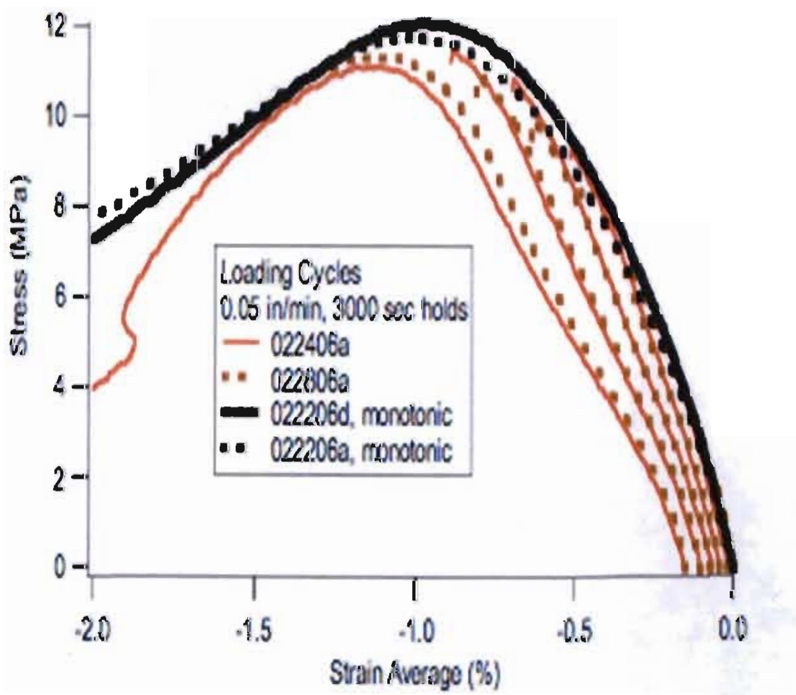
- 94.9% by wt. HMX (10 to 200 μm particles)
- 2.5% by wt. Estane 5703 (polymeric glue)
- 2.5% by wt. BDNPA/F nitroplasticizer (NP)
- 0.1% by wt. stabilizer. DPA or Irganox.

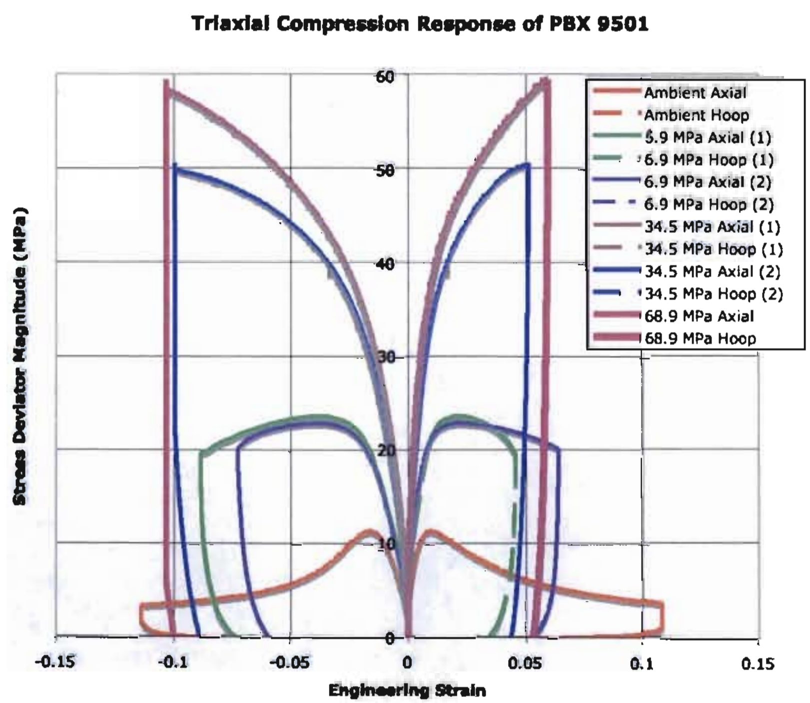
Energetic Materials Modeling

Challenges

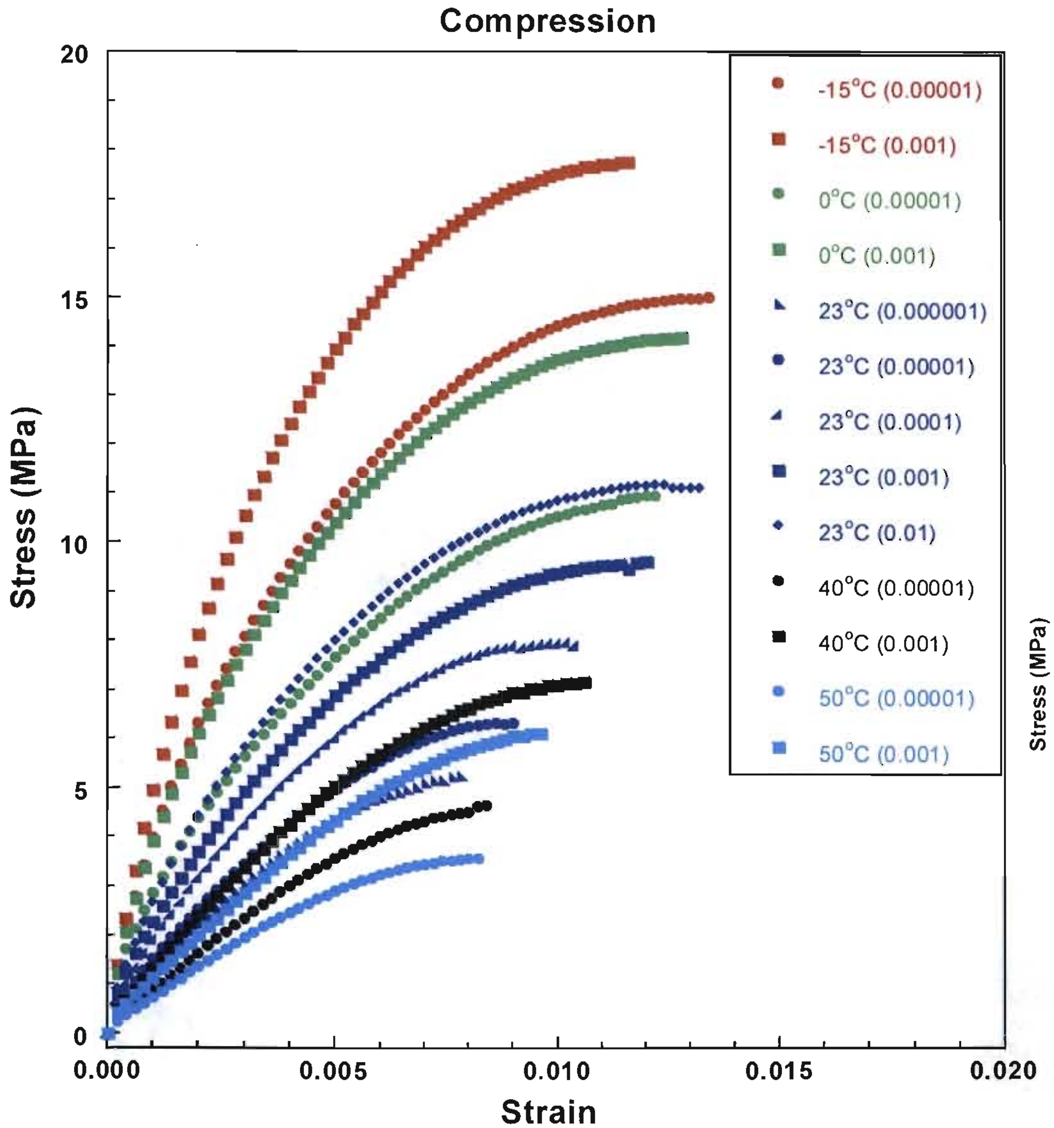
- Very heterogeneous materials
  - High volume fraction of discontinuous phase
  - High contrast in properties and behavior of phases
- Statistical variability
- Nonlinear response
  - Rate, temperature, density, and history dependence
- Multiple mechanisms of deformation
  - Viscoelasticity
  - Plasticity
  - Damage
    - Voids
    - Cracks

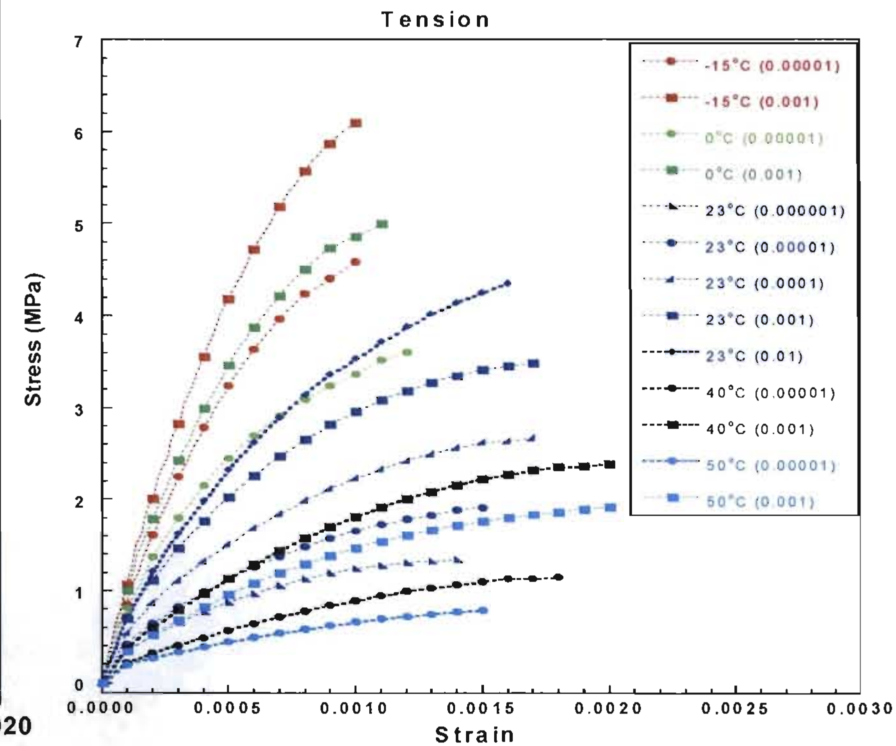

Tension-Compression
PBX 9501
0.0033
0.033
0.01
0.001
0.0001
0.00001
0.00001
0.0001
0.001
0.01
0.011
0.11
Stress (MPa)
5
0
-5
-10
-15
-0.025
-0.020
-0.015
-0.010
-0.005
0.000
0.005
Strain


Loading Cycles
0.05 in/min, 3000 sec holds
022406a
022806a
022206d, monotonic
022206a, monotonic
Stress (MPa)
12
10
8
6
4
2
0
-2.0
-1.5
-1.0
-0.5
0.0
Strain Average (%)


Triaxial Compression Response of PBX 9501
Ambient Axial
Ambient Hoop
6.9 MPa Axial (1)
6.9 MPa Hoop (1)
6.9 MPa Axial (2)
6.9 MPa Hoop (2)
34.5 MPa Axial (1)
34.5 MPa Hoop (1)
34.5 MPa Axial (2)
34.5 MPa Hoop (2)
68.9 MPa Axial
68.9 MPa Hoop
Stress Deviator Magnitude (MPa)
60
50
40
30
20
10
0
-0.15
-0.1
-0.05
0
0.05
0.1
0.15
Engineering Strain

Uniaxial Compression/Tension Mechanical Test Data

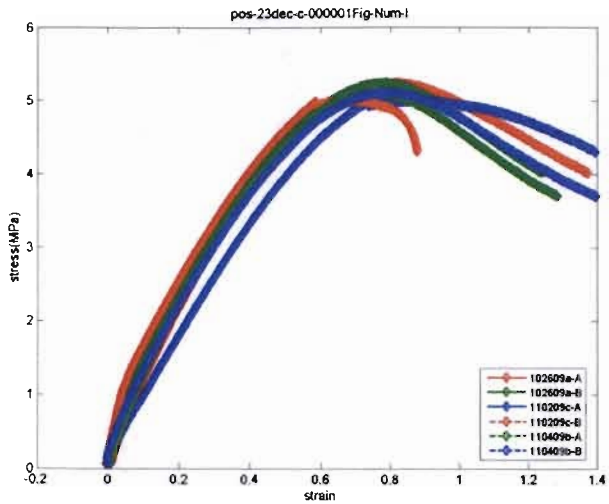




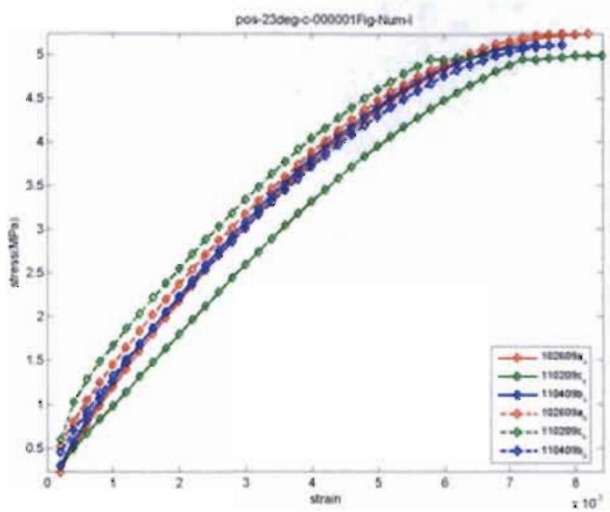
PBX Constitutive Modeling Needs for Engineering Analysis

- 3D (multiaxial stress states)
- Rate dependence
- Softening and failure
- Creep and relaxation
- Plasticity (permanent inelastic deformation)
- Damage (Modulus degradation)
- Temperature dependence of mechanical response
- Reliable ignition models
- Spatial heterogeneity
- Thermomechanical cyclic response (ratchet growth, damage accumulation, effect of confinement on these) PBX 9502

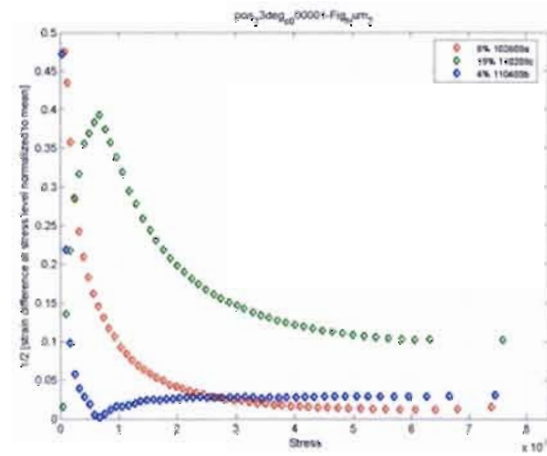
Statistical Analysis of Uniaxial Monotonic Stress Strain Data



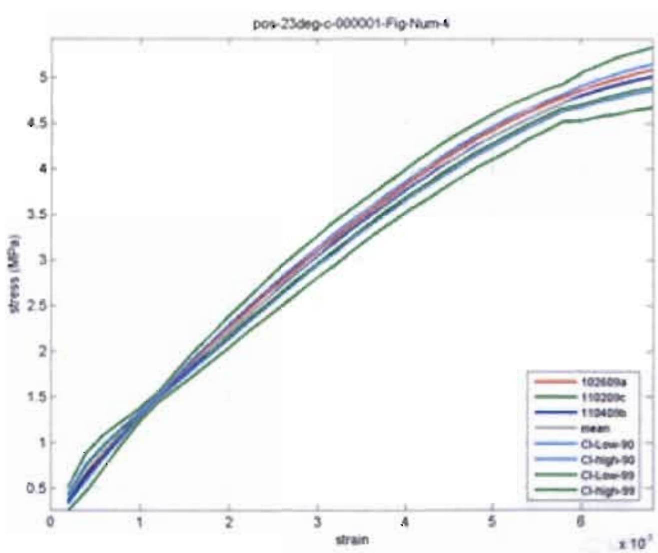
Compression Stress-Strain Curves for all test samples and extensometer outputs for test temperature off 23 deg C, and strain rate of 0.000001 (s^{-1}).



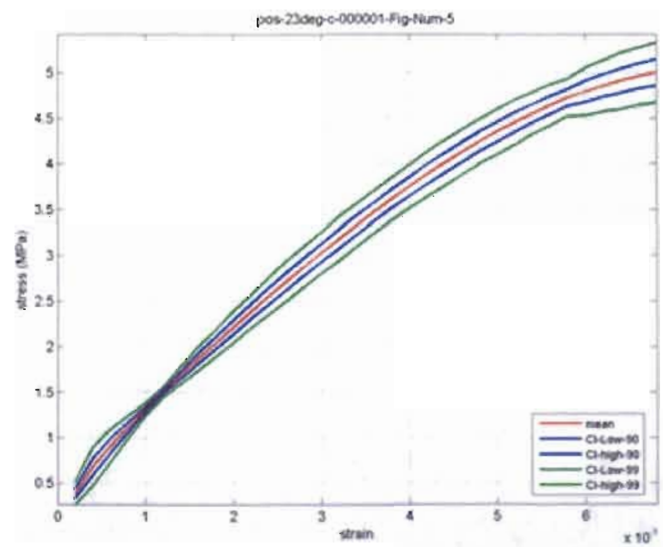
Stress-Strain Curves showing both extensometers



Plot of difference in strains between extensometers normalized with average of the strains and measured stress.



Selected average stress-stress curves with overall mean and confidence intervals

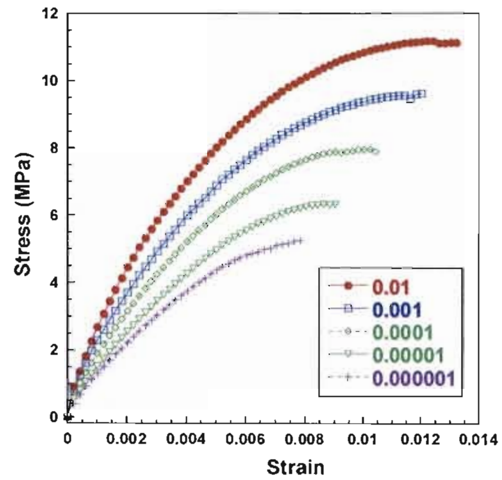


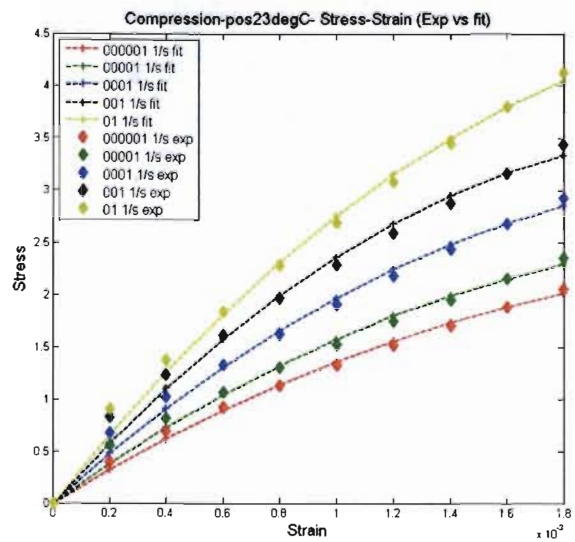
Overall mean stress-strain curve with confidence intervals

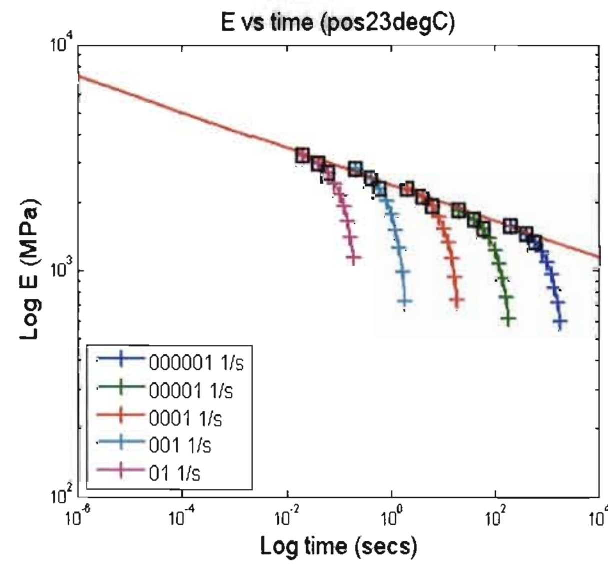
Table of failure strains with statistical confidence intervals

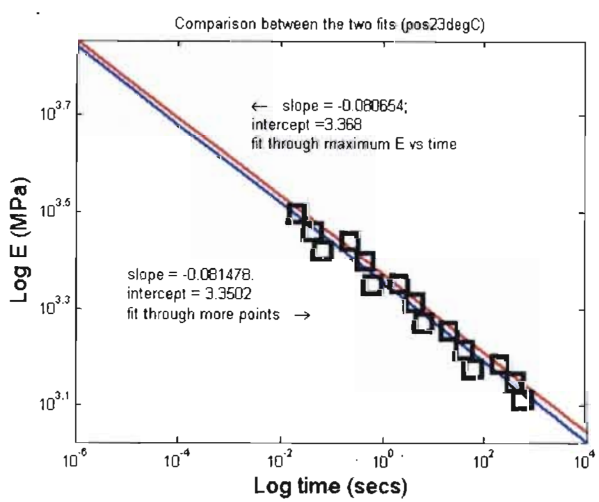
Compression Failure Strains												
Temp(deg C)	Strain Rate (1/s)	"@stress" MPa	Mean	Std_dev	N	DOF	CI_90_low	CI_90_high	CI_95_low	CI_95_high	CI_99_low	CI_99_high
-15	0.00001	14.80	0.0121	0.0004	6	5	0.0113	0.0128	0.0111	0.0130	0.0105	0.0136
-15	0.001	17.50	0.0105	0.0018	6	5	0.0068	0.0141	0.0058	0.0151	0.0032	0.0178
0	0.00001	10.60	0.0110	0.0010	6	5	0.0089	0.0130	0.0084	0.0135	0.0069	0.0150
0	0.001	14.10	0.0121	0.0013	6	5	0.0094	0.0147	0.0086	0.0155	0.0067	0.0174
23	0.000001	4.90	0.0069	0.0006	6	5	0.0056	0.0081	0.0053	0.0085	0.0044	0.0094
23	0.00001	6.20	0.0084	0.0005	6	5	0.0074	0.0094	0.0071	0.0097	0.0064	0.0104
23	0.0001	7.80	0.0092	0.0013	6	5	0.0066	0.0118	0.0059	0.0125	0.0040	0.0144
23	0.001	9.30	0.0101	0.0014	6	5	0.0073	0.0128	0.0065	0.0136	0.0045	0.0156
23	0.01	11.10	0.0116	0.0011	4	3	0.0091	0.0141	0.0082	0.0150	0.0054	0.0179
40	0.00001	4.30	0.0073	0.0007	6	5	0.0059	0.0087	0.0055	0.0091	0.0045	0.0101
40	0.001	7.00	0.0097	0.0018	4	3	0.0055	0.0140	0.0040	0.0155	-0.0008	0.0203
50	0.00001	3.20	0.0064	0.0011	6	5	0.0041	0.0086	0.0034	0.0093	0.0018	0.0109
50	0.001	6.10	0.0096	0.0012	4	3	0.0068	0.0124	0.0058	0.0134	0.0027	0.0166

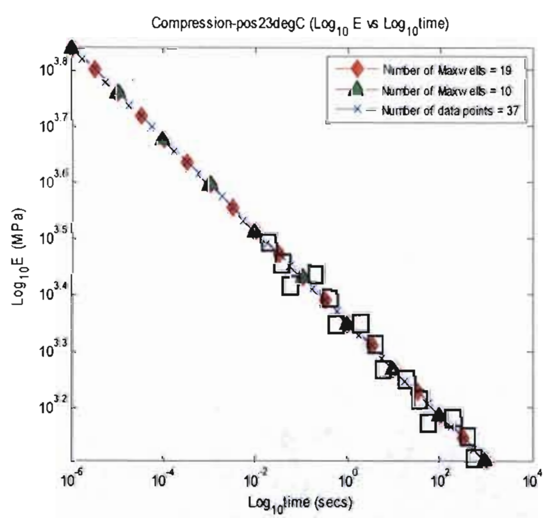
Obtaining Viscoelastic Properties from Uniaxial Stress Strain

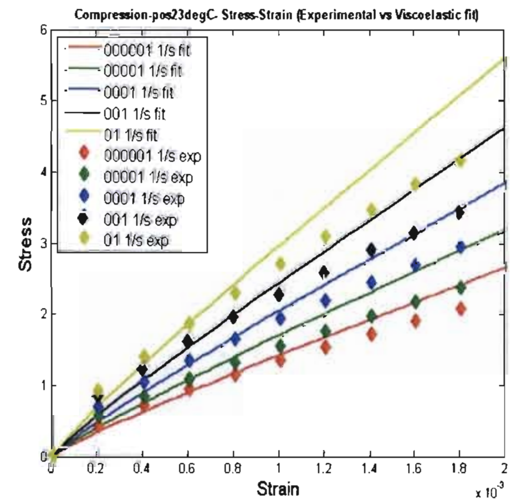




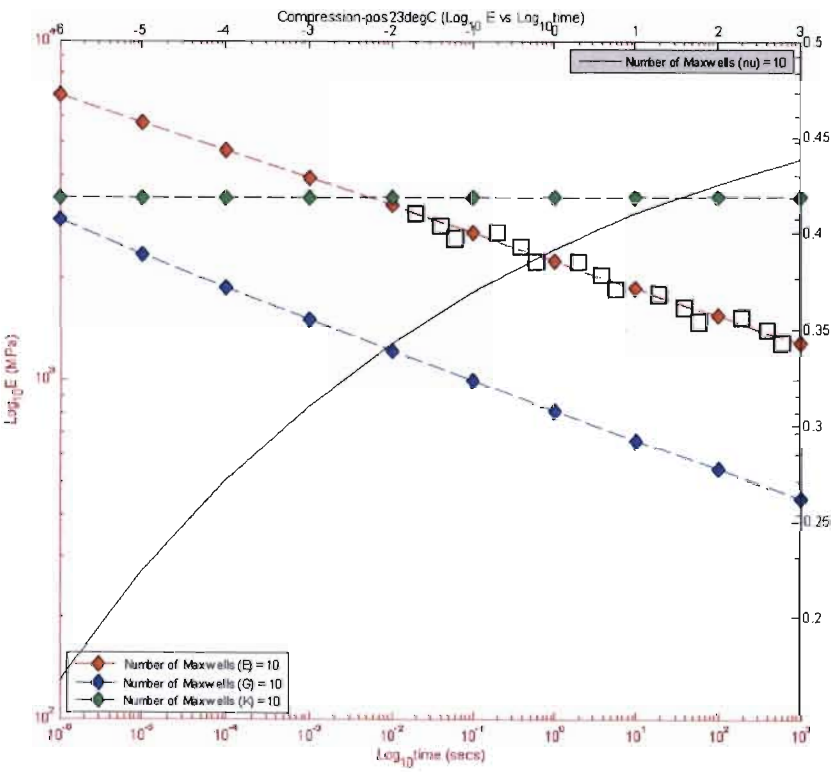




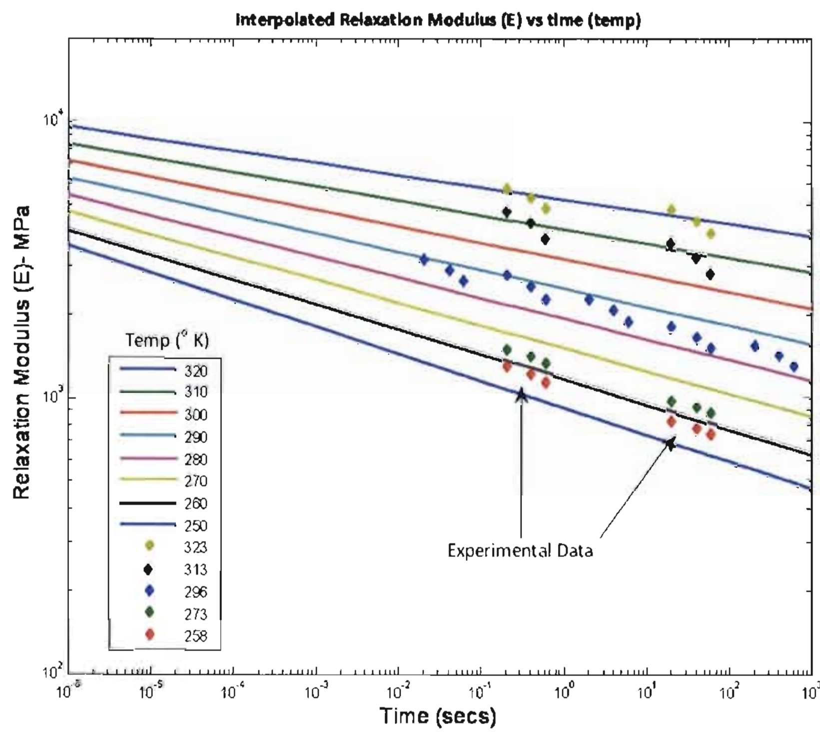


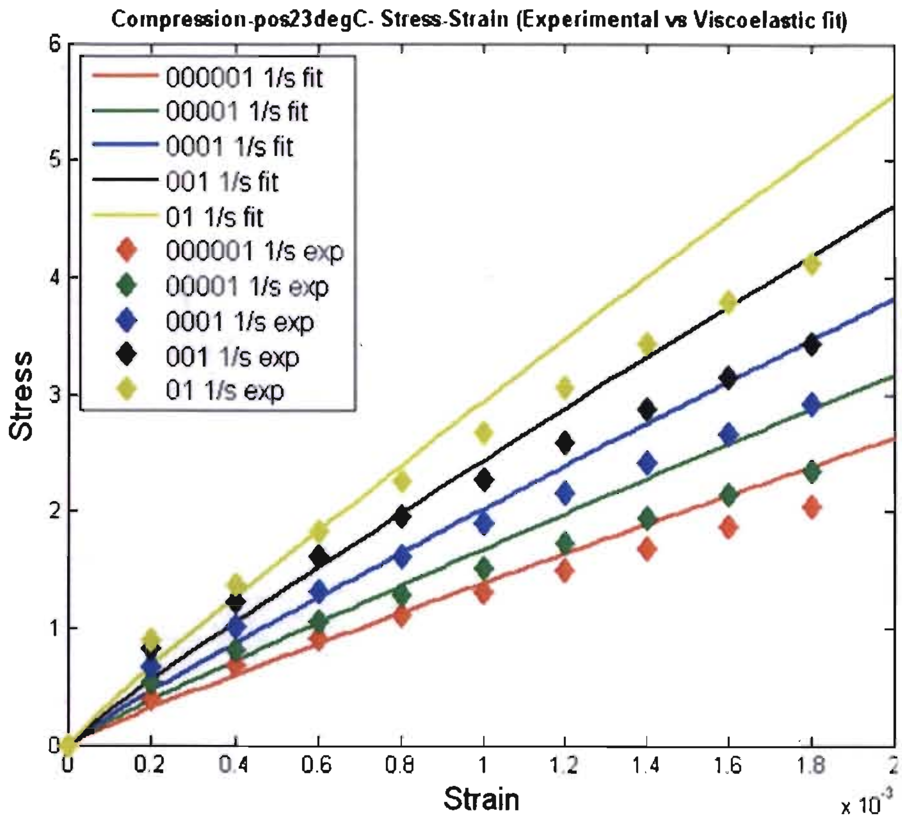


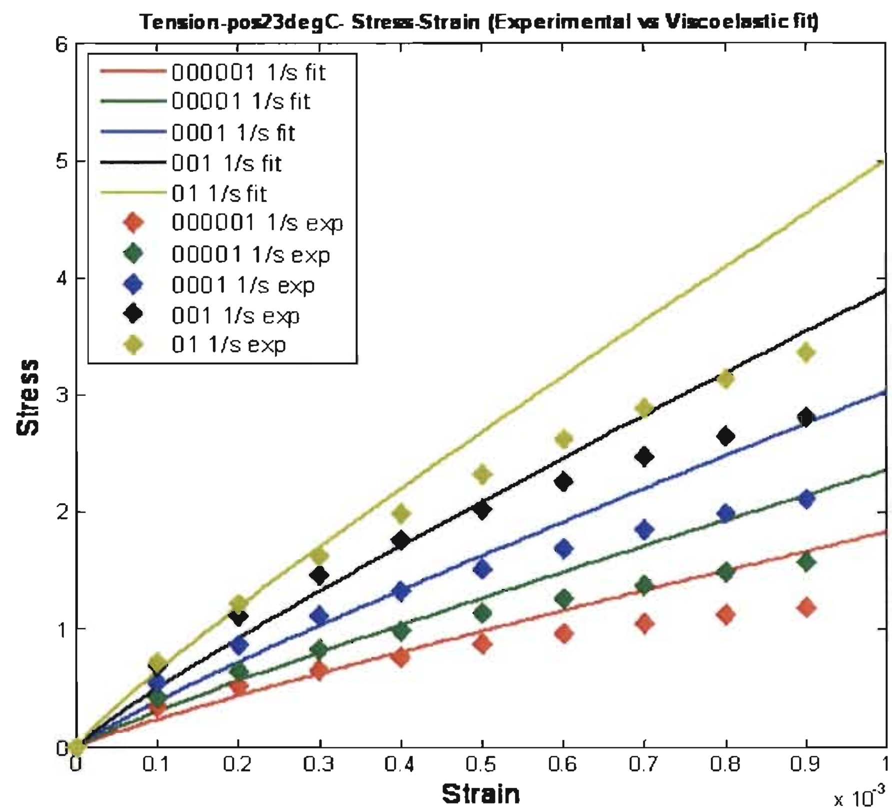
E, K, G, ν



E vs. Temp




Compression-pos23degC- Stress-Strain (Experimental vs Viscoelastic fit)
000001 1/s fit
00001 1/s fit
0001 1/s fit
001 1/s fit
01 1/s fit
000001 1/s exp
00001 1/s exp
0001 1/s exp
001 1/s exp
01 1/s exp
Stress
Strain
x 10^-3


Tension-pos23degC- Stress-Strain (Experimental vs Viscoelastic fit)
000001 1/s fit
00001 1/s fit
0001 1/s fit
001 1/s fit
01 1/s fit
000001 1/s exp
00001 1/s exp
0001 1/s exp
001 1/s exp
01 1/s exp
Stress
Strain
x 10^-3

What is ViscoSCRAM?

ViscoSCRAM was developed in the 1990s and early 2000s as an engineering constitutive model for Plastic-Bonded eXplosives (PBXs).

Model features include

- Linear viscoelastic shear response including Time Temperature Superposition
- Inelasticity initially only from microcracking (damage)
- Use only compressive part of damage surface
- Keep only shear crack strains
- Finite crack strain rate for any nonzero stress
- Stress dependent damage growth rate, *ad hoc* increased growth rate for mean tension
- No different moduli for tension vs. compression unless added *ad hoc*
- Crack friction
- Two initiation models for ignition modeling

Bennett et al, 1998, J. Mech. Phys. Solids. Vol. 46 (12)

ViscoSCRAM

$$\dot{\varepsilon}_{ij} = \frac{1}{3}\dot{\varepsilon}_{kk}\delta_{ij} + \dot{e}_{ij}$$

Strain rate decomposition

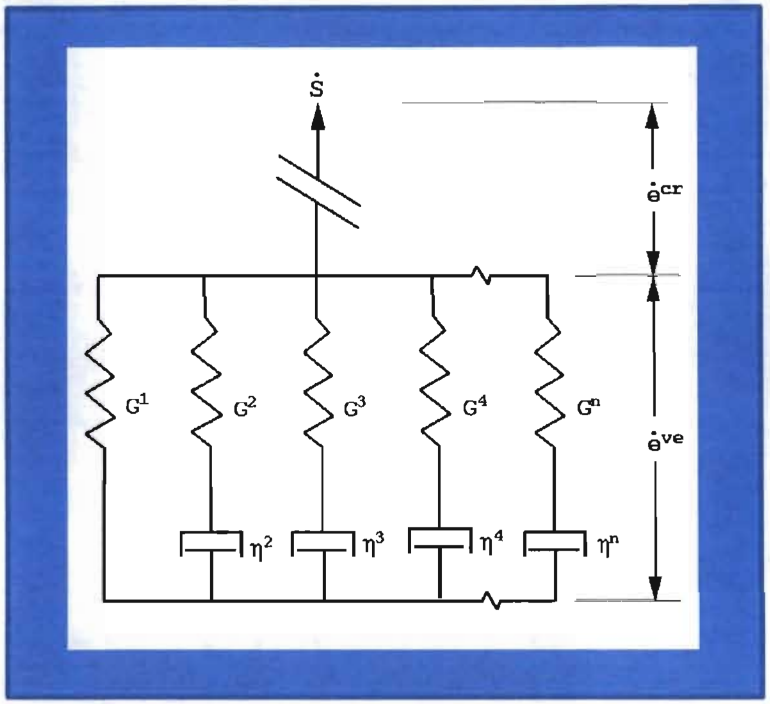
$$\dot{e}_{ij} = \dot{e}_{ij}^{ve} + \dot{e}_{ij}^{c}$$

Deviatoric strain rate decomposition

$$\dot{\sigma}_{ij} = \dot{S}_{ij} + \dot{\sigma}_m \delta_{ij}$$

$$\dot{\sigma}_m = K\dot{\varepsilon}_{ii}$$

Stress rate decomposition



$$\dot{S}_{ij} = \frac{2G\dot{e}_{ij} - \sum_{1}^{N}\frac{S_{ij}^{(n)}}{\tau^{(n)}} - 3\left(\frac{c}{a}\right)^2\frac{\dot{c}}{a}S_{ij}}{1+\left(\frac{c}{a}\right)^3}$$

$$S = \sum_{n=1}^{N} S^{(n)}$$

$$\tau = \frac{\eta}{G}$$

$$\dot{S}_{ij}^{(n)} = 2G^{(n)}\dot{e}_{ij} - \frac{S_{ij}^{(n)}}{\tau^{(n)}} - \frac{G^{(n)}}{G}\left[3\left(\frac{c}{a}\right)^2\frac{\dot{c}}{a}S_{ij} + \left(\frac{c}{a}\right)^3\dot{S}_{ij}\right]$$

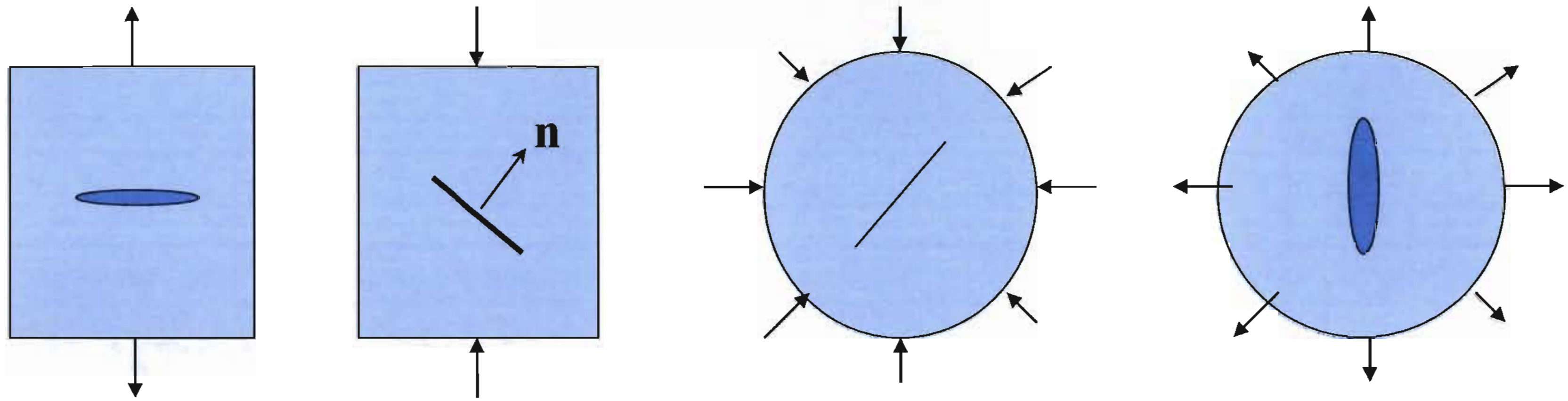
Linear ViscoElastic

Isotropic, Generalized Maxwell Model

Continuum Damage

Statistical Dist. of Randomly Oriented Micro Cracks

Crack Strains



$$\varepsilon_{ij}^{o} = \left[8\frac{(1-\nu)}{3VG} \right] n_i n_j n_k n_l c^3 \sigma_{kl}$$

open crack

$$\varepsilon_{ij}^{s} = \left[4\frac{(1-\nu)}{3VG(2-\nu)} \right] \left(\delta_{il} n_j n_k + \delta_{jl} n_i n_k + \delta_{ik} n_j n_l + \delta_{jk} n_i n_l - 4 n_i n_j n_k n_l \right) c^3 \sigma_{kl}$$

shear crack

Addessio, Johnson, J. Appl. Phys. 67 (7), 1990

Visco-elasticity and cracking

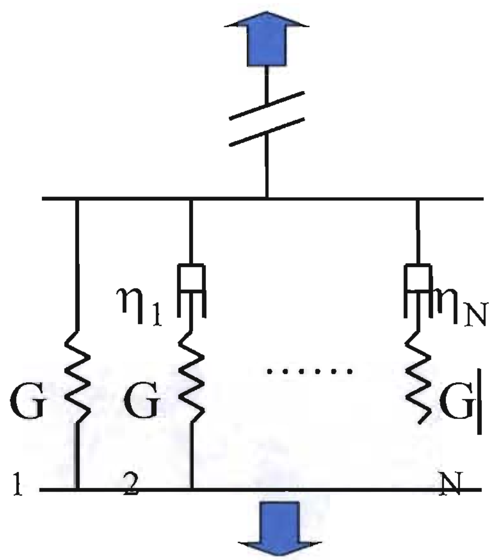
$$\dot{\varepsilon} = \dot{\varepsilon}^{ve} + \dot{\varepsilon}^{cr(s)}$$

$$\dot{\varepsilon} = \frac{1}{3K}\dot{\sigma}^{sp} + \frac{1}{2G}\left(\dot{\sigma}^{dev} + \sum_{n=1}^{N}\frac{s^{(n)}}{\tau^{(n)}}\right) + \frac{d}{dt}\left(\bar{c}^{3}\left(\beta^{e}N_{0}\frac{3}{1-\nu}\sigma^{dev} + N_{0}P^{+}\frac{64\pi 4\pi - \nu)}{15G}\left(P^{dev}\right)\sigma\right)\right)$$

$$\dot{\sigma}_{ij} = 3K\dot{\varepsilon}_{m}\delta_{ij} + \frac{2G}{1+\left(\frac{c}{a}\right)^{3}}\dot{e}_{ij} - \frac{\sum_{n=1}^{N}\frac{s^{(n)}}{\tau^{(n)}}}{1+\left(\frac{c}{a}\right)^{3}} - 3D(c)\left[\sigma_{ij} - 3K\varepsilon_{m}\right]$$

$$D(c) = \frac{(c/a)^{3}}{1+(c/a)^{3}}$$

Photomicrograph of PBX-9501

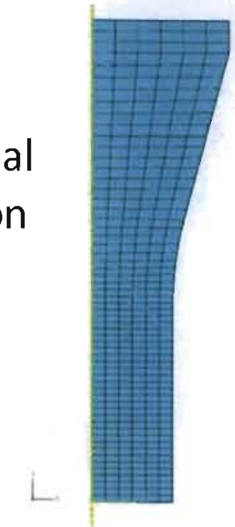


UMAT subroutine

Implicit FE code

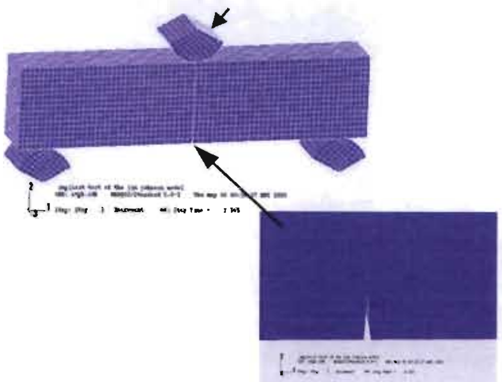
Validation tests for PBX 9501

Uniaxial Tension

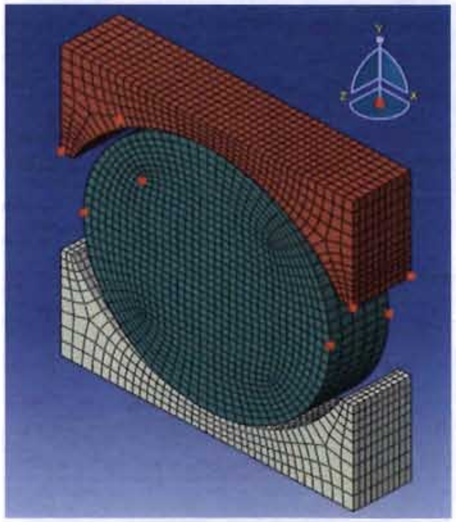


Uniaxial Compression

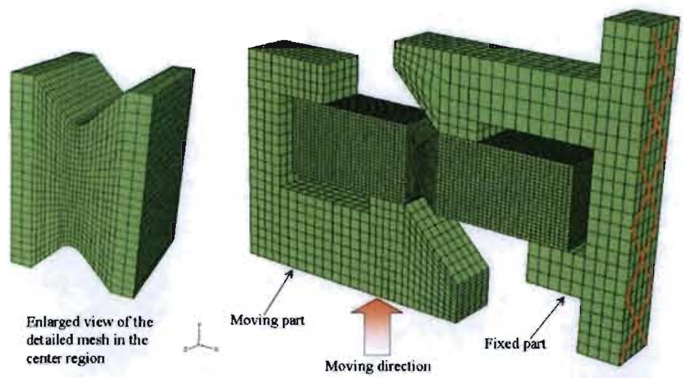
3 Point Bend

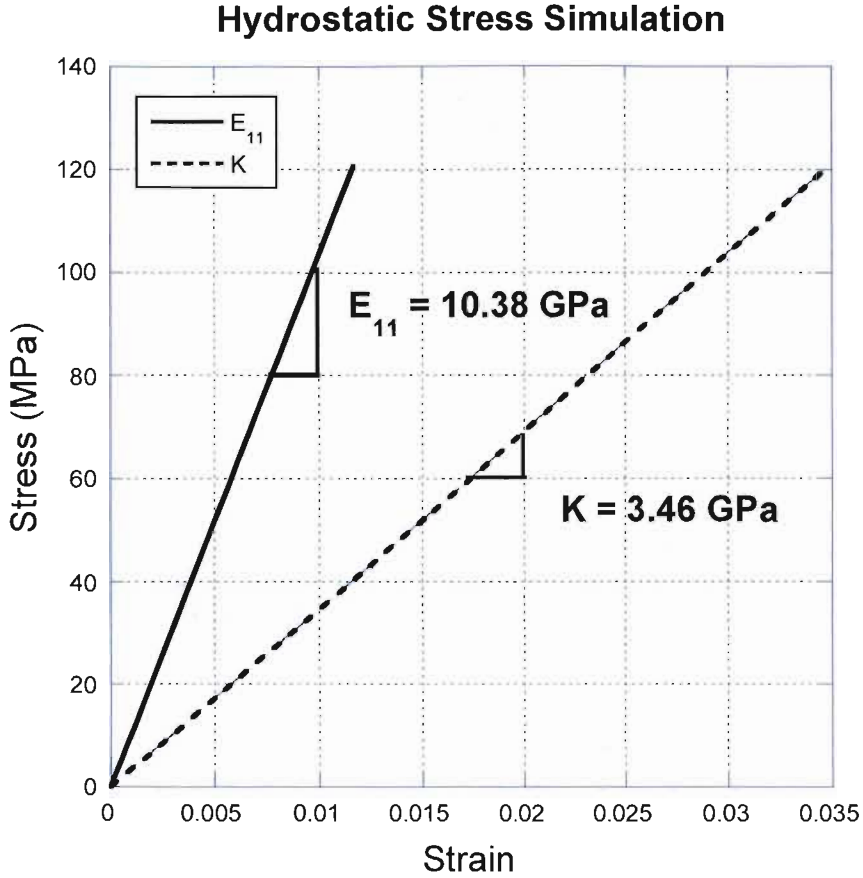


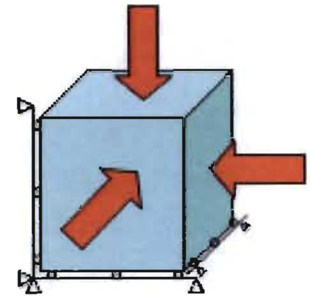
Brazil



Iosipescu



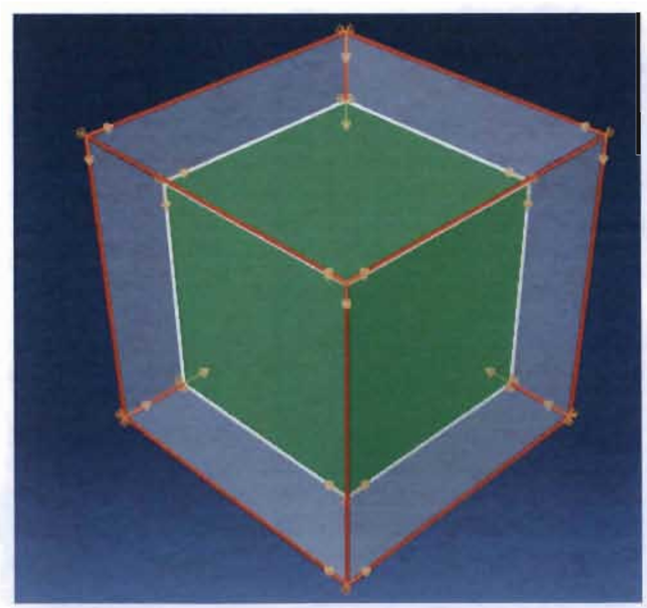




Purely elastic response

No deviatoric components of Stress/Strain

No Effects from Viscoelasticity and Damage

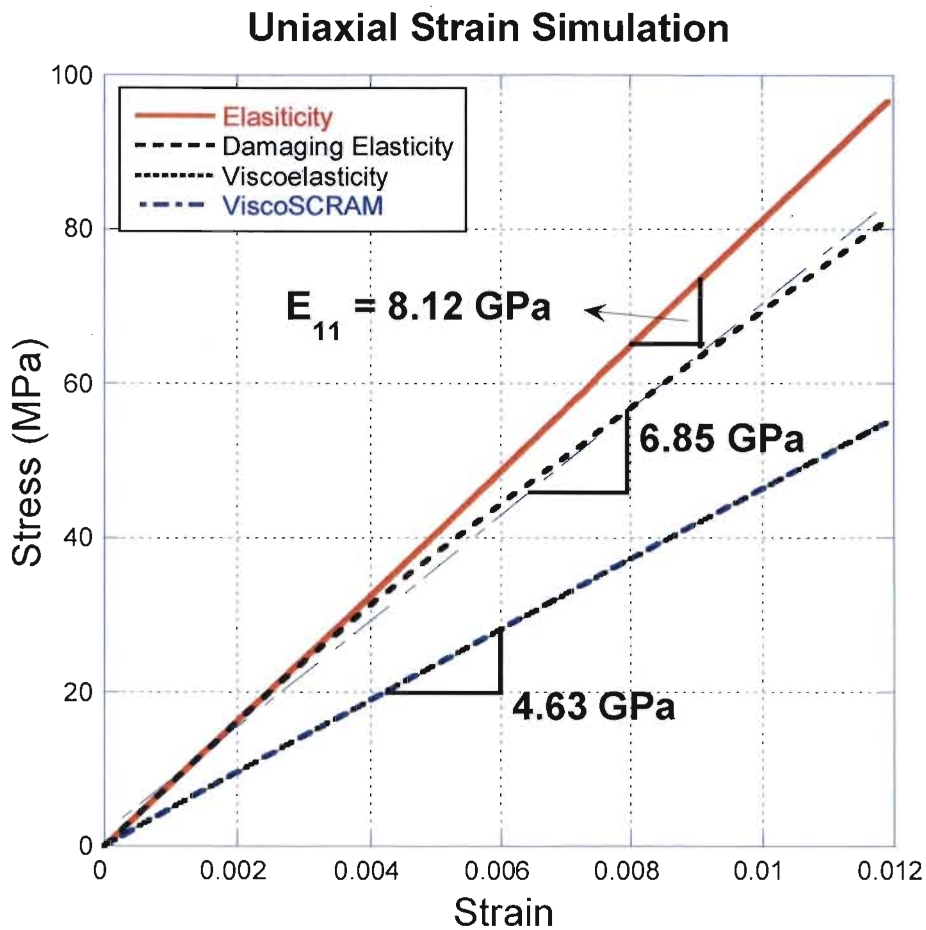


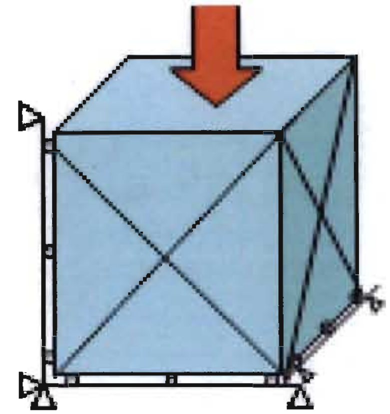
$K = 3.460$ GPa

$G = 3.492$ GPa

$\lambda = K - \frac{2}{3} G = 1.132$ Gpa

$E_{11} = 3\lambda + 2G = 10.38$ GPa





Effects of deviatoric stress on E_{11}

Lower: Damage only

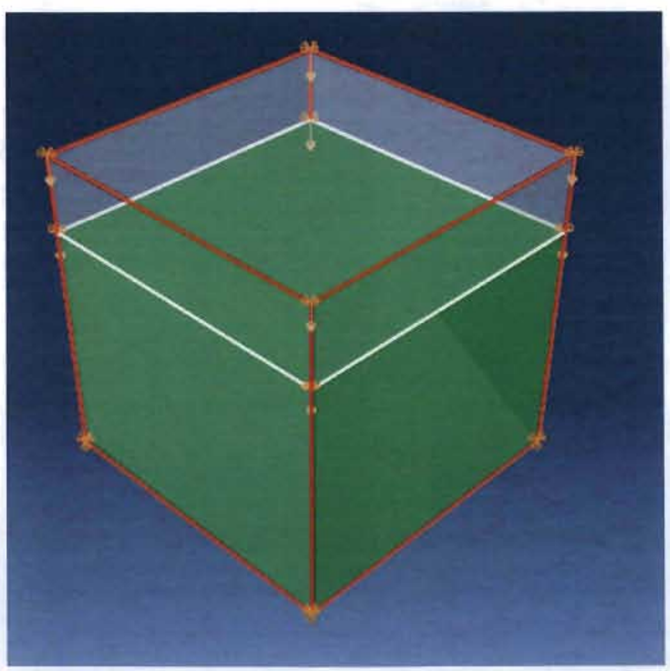
Higher: Viscoelasticity+ Damage

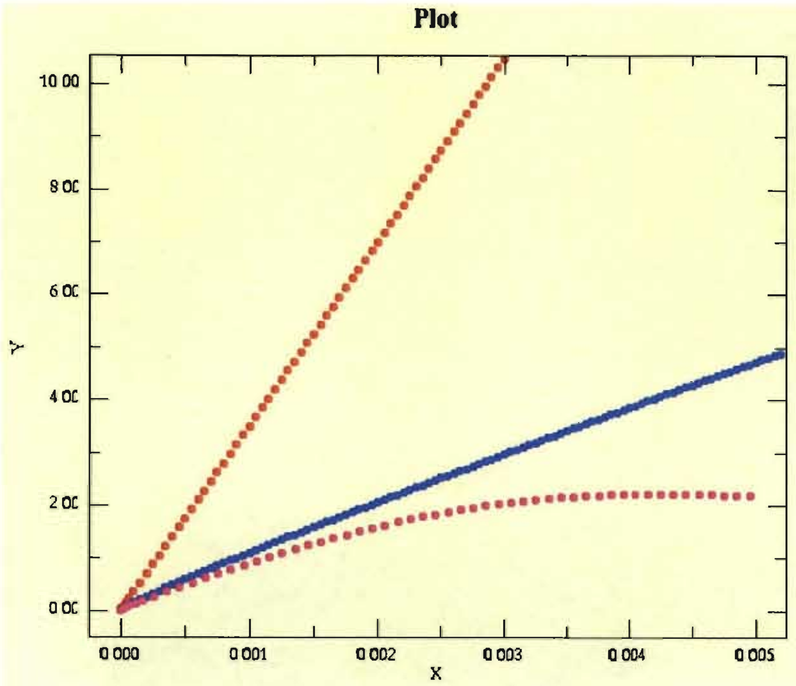
$K = 3.460$ GPa

$G = 3.492$ GPa

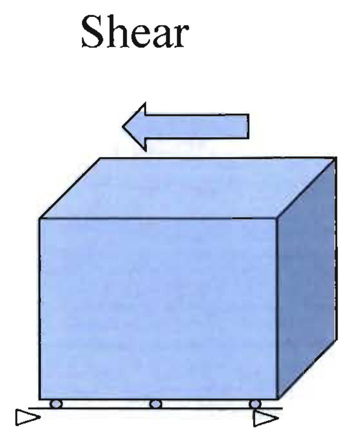
$\lambda = K - \frac{2}{3}G = 1.132$ Gpa

$E_{11} = \lambda + 2G = 8.12$ GPa





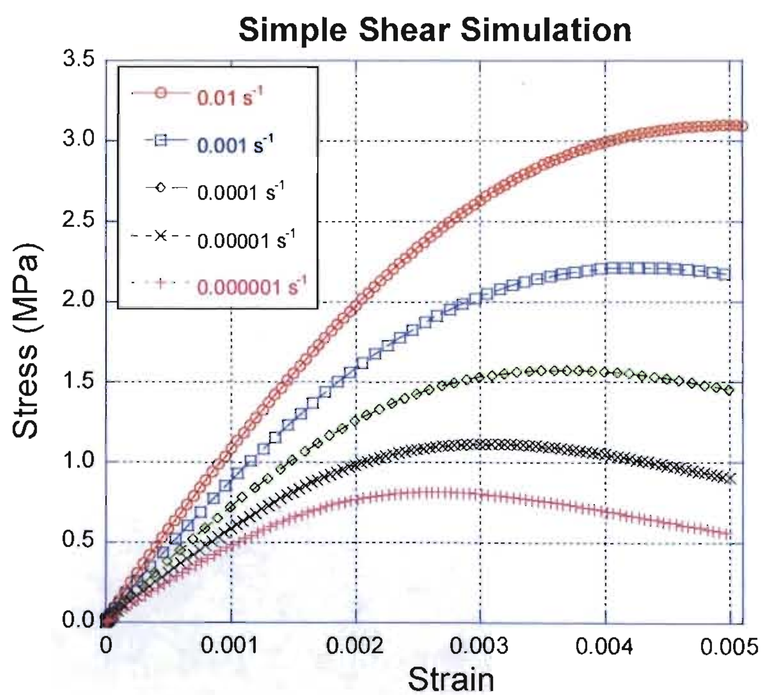
Deviatoric State of Stress Only

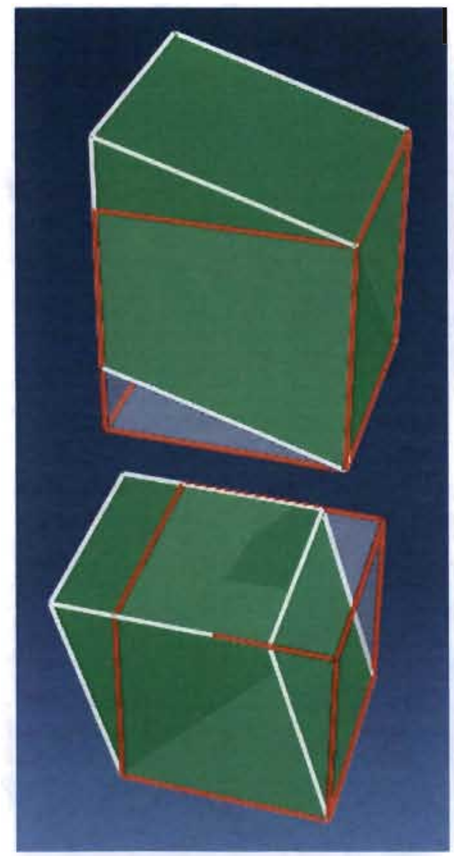


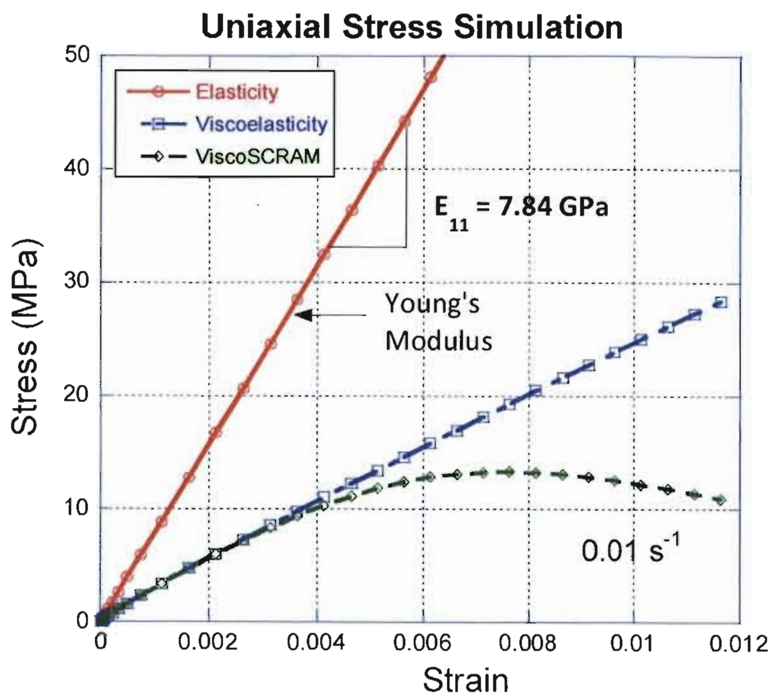
K = 3.460 GPa

G = 3.492 GPa

E_{11} = G = 3.492 GPa





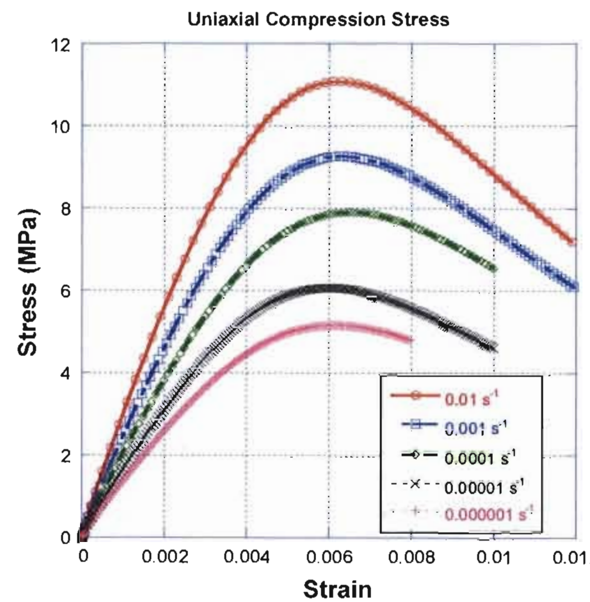


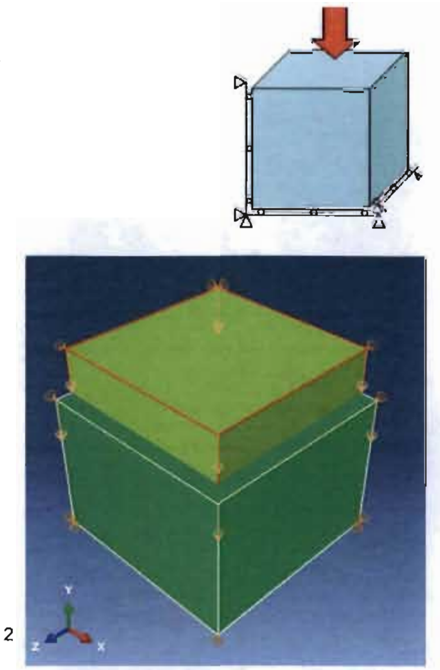
K = 3.460 GPa

G = 3.492 GPa

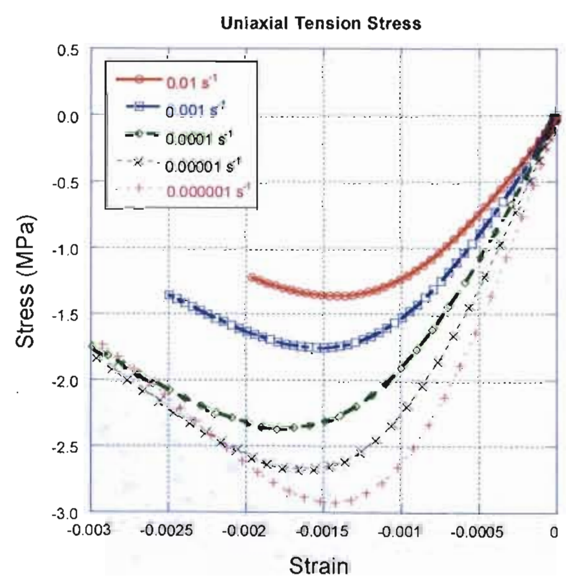
$$E_{11} = Y = \frac{9KG}{3K+G} = 7.84 \text{ GPa}$$

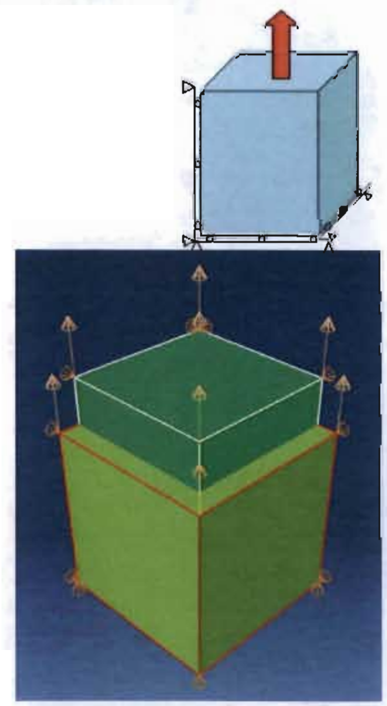
Compression



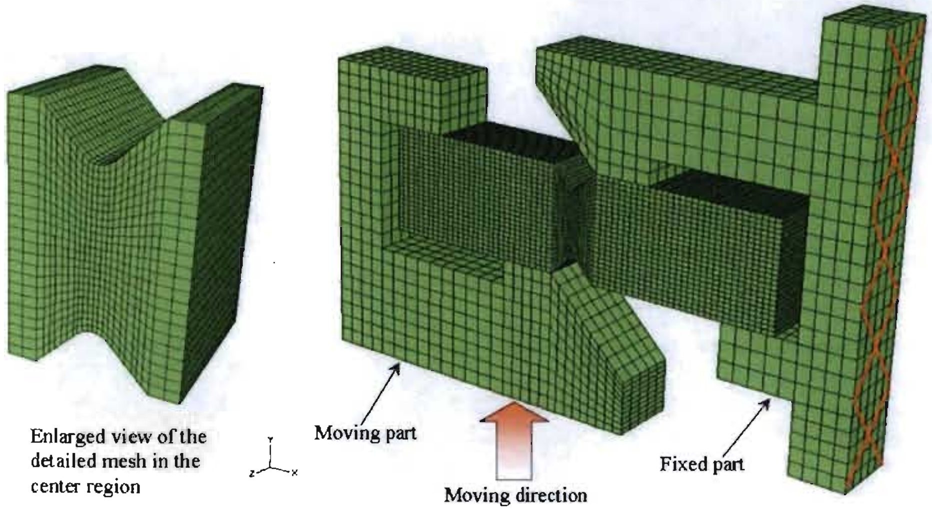


Tension





Validation of Iosipescu tests for Pristine PBX 9501



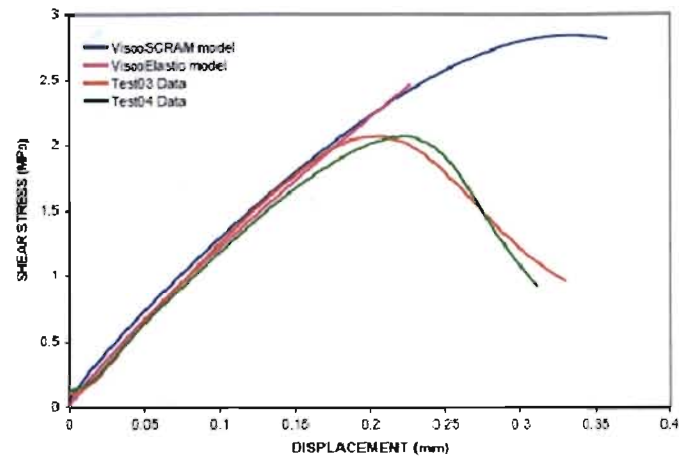
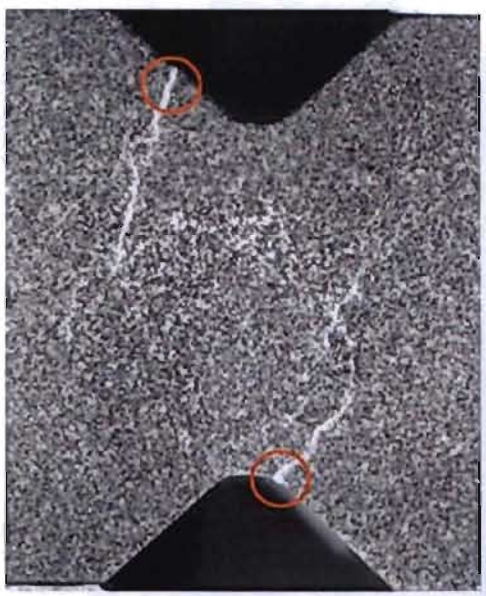
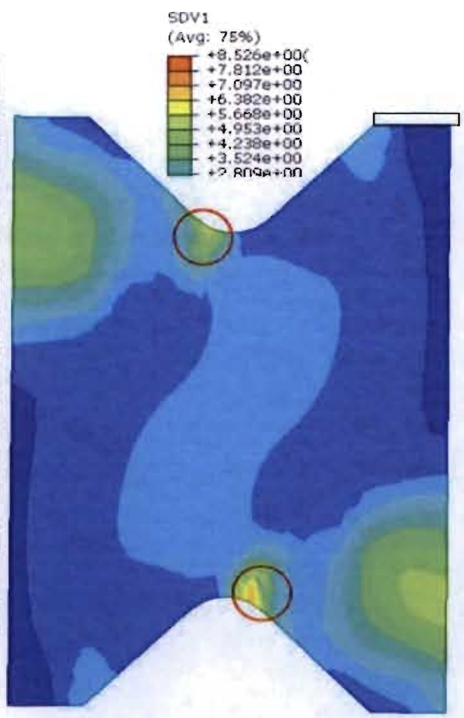
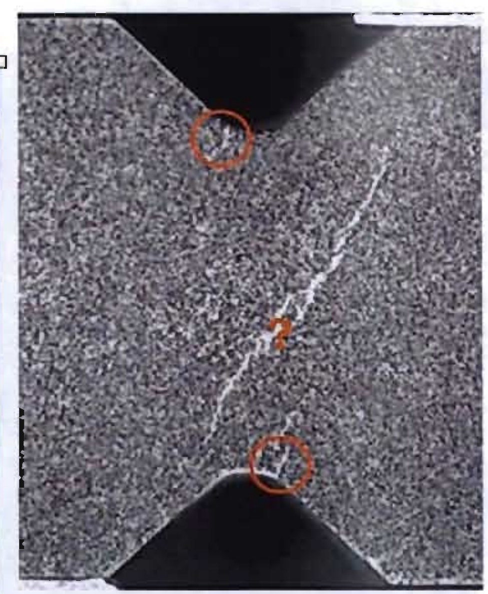


Figure 6: Comparison of Iosipescu test data and analysis results for displacement versus shear stress at the gauge section



Test03 at 78sec, the last recorded image

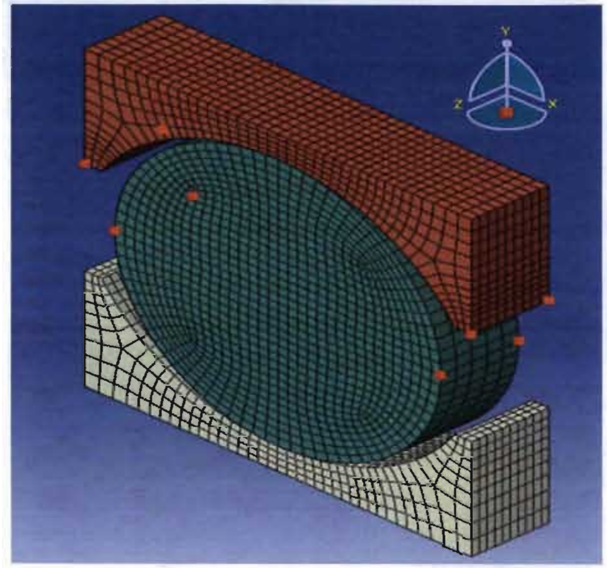


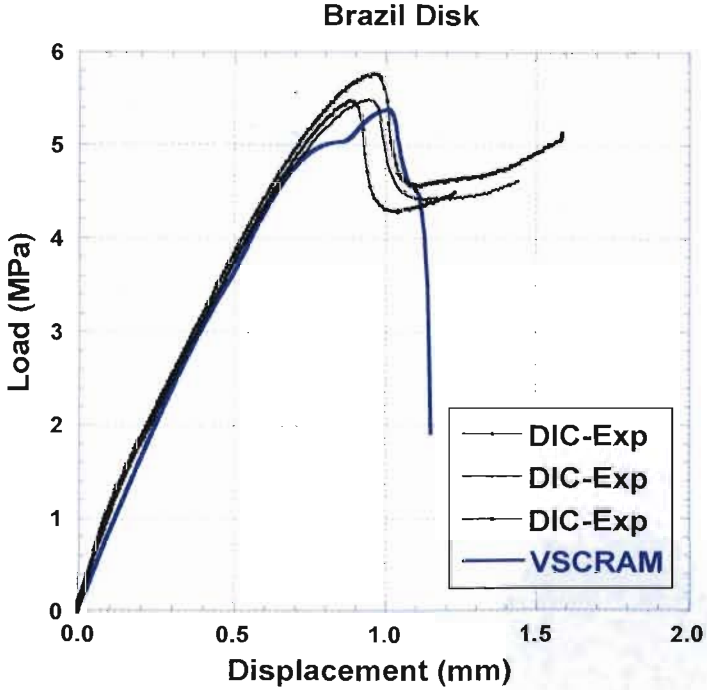


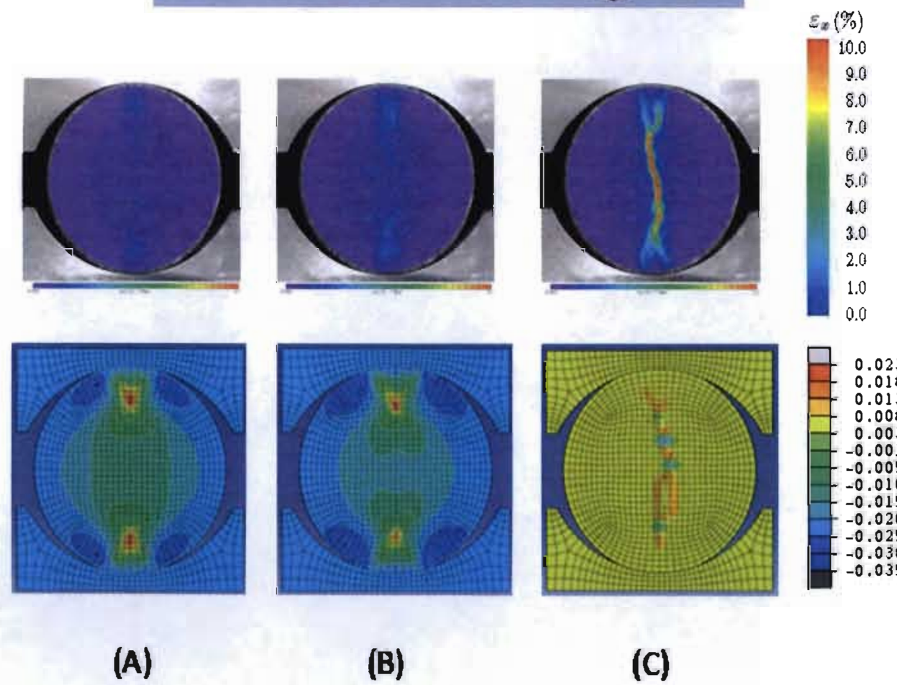
Test04 at 73.6 sec, the last recorded image

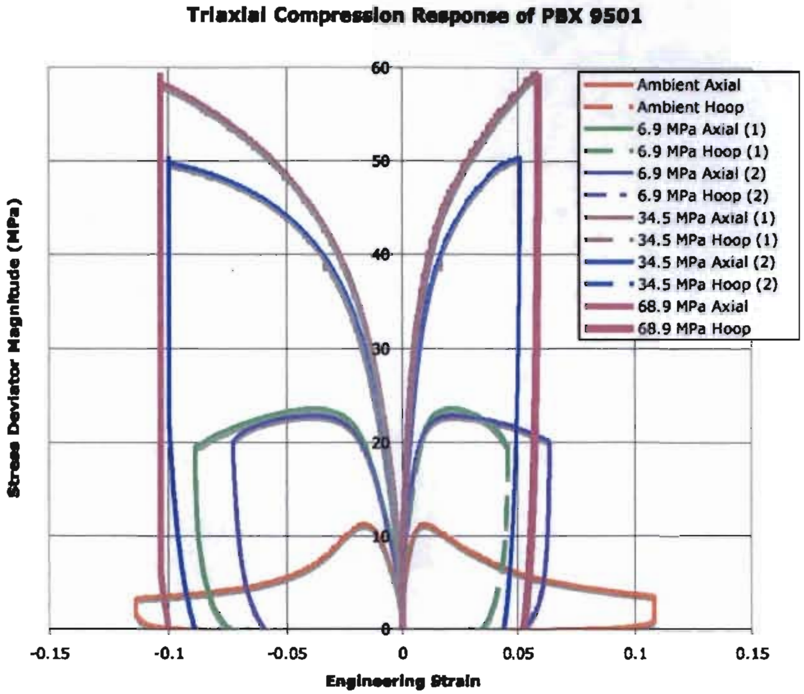
Crack size at the last recorded moment – FEA result at 85second

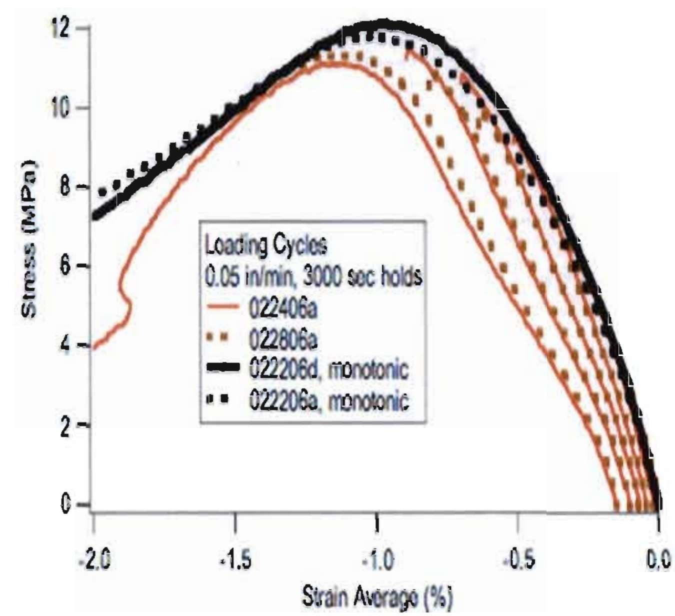
Validation of Brazil Disk Test
Deformation and Failure of PBX 9501 High Explosive








Triaxial Compression Response of PBX 9501
Ambient Axial
Ambient Hoop
6.9 MPa Axial (1)
6.9 MPa Hoop (1)
6.9 MPa Axial (2)
6.9 MPa Hoop (2)
34.5 MPa Axial (1)
34.5 MPa Hoop (1)
34.5 MPa Axial (2)
34.5 MPa Hoop (2)
68.9 MPa Axial
68.9 MPa Hoop
Stress Deviator Magnitude (MPa)
Engineering Strain


Loading Cycles
0.05 in/min, 3000 sec holds
022406a
022806a
022206d, monotonic
022206a, monotonic
Stress (MPa)
Strain Average (%)

Future Modeling

Pursue Current Best Modeling Options

- ViscoDCA
  - Damaging linear viscoelasticity
  - Rate and temperature dependence
  - Implemented in ABAQUS/Standard and EPIC
    - Plans for /Explicit, ParaDyn
- FRHE
  - Viscoplastic with volumetric plastic component
  - Rate and temperature dependence
  - Directional damaging elasticity based on plastic strain accumulation
  - Implemented in ABAQUS/Explicit and Epic