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Title: Energetic materials: mechanical phenomenology and modeling challenges

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Abstract

Engineered energetic materials are typically particulate composites. These materials usually exhibit a very small (or possibly nonexistent) range of linear mechanical response. They include large volume fractions (usually greater than 80%) of particulate phases, and may contain more than one particulate phase. The particulate phases and binder phases often have high contrast in their mechanical properties over relevant ranges of pressure, strain rate, and temperature.

Test data demonstrating a variety of mechanical behaviors of energetic materials will be presented. An overview and evaluation of constitutive modeling approaches used to describe these responses will be presented.

Energetic materials: mechanical phenomenology and modeling challenges

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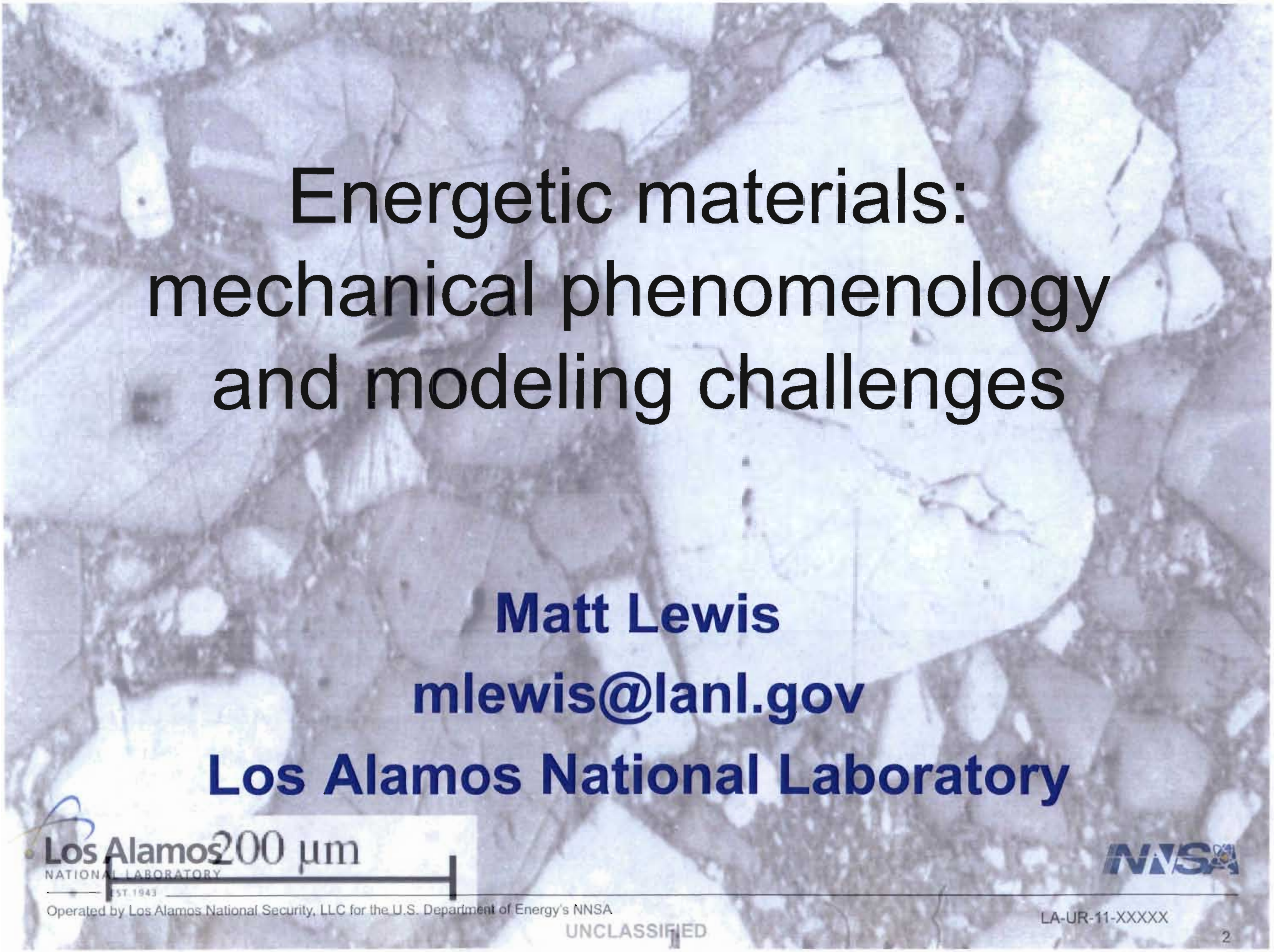


Thesis

Developing realistic mechanical constitutive models for practical energetic materials (solid propellants and explosives) is a significant challenge. These materials typically are particulate compositeswith large volume fractions (usually greater than 80%) of particulate phases. These materials usually exhibit a very small (or possibly nonexistent) range of linear mechanical response. These materials may contain more than one particulate phase. These phases often have high contrast in their mechanical properties over relevant ranges of pressure, strain rate, and temperature.

We can not afford the old style model development method of asserting mechanisms and then taking the minimum data necessary to fit these models. We need to be testing and micromechanically modeling to identify and characterize deformation mechanisms.

Overview

- Challenges
  - Material response
  - Testing
- Models
  - Models vs. Implementations
  - A quick mention of extant models and implementation status
- Types of tests
  - Monotonic uniaxial
  - Triaxial
  - DMA
  - Relaxation
  - Creep/recovery
  - Ratchet growth
  - Failure envelope and validation

Images and figures (and maybe even some ideas) have been stolen from at least the following people for this presentation:

Darla Graff Thompson

Philip Rae

Roberta Mulford

Ed Roemer

Bruce Cunningham

Mary Campbell

Paul Petersen

Cary Skidmore

Mike Kaneshige

Challenges in Modeling PBXs

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

200 μm

Challenges in Testing PBXs

- Testing limited to a few facilities
- Hard to test the intermediate strain rates (1-500/second)
- Machining and transporting samples = $$$
- Good mocks allow some workaround, at least elucidating mechanisms
  - The role of mocks COULD be greater if the challenge of developing good mocks was addressed
  - Ultimately, many characterization tests are still needed on the actual energetic materials

Models and Implementations

Definition:

A *material model* is a mathematical description developed to describe some aspect of material behavior (Cauchy stress as a function of displacement gradient history and temperature history, temperature as a function of internal energy, conductivity as a function of temperature gradient and density, *etc.*)

A model exists regardless of coding, and usually consists of one simple constitutive relation (like linear elasticity) and, possibly, state variable evolution equations (viscoelastic stresses, damage variables, plastic strain, back stress, *etc.*) typically as first order differential equations in "time."

Models and Implementations

Definition:

A material model *implementation* is a material model that has been algorithmized and coded in a programming language as a subroutine (typically) that a code (either a driver or a parent analysis code like ABAQUS/Explicit, ABAQUS/Standard, Adagio, ALE3D, or ParaDyn) can call to update the relevant state variables.

A model implementation depends on the calling code's arguments (variables), dimensionality, and kinematics (how are finite deformations and rotations handled?)

Models Appropriate for Codes

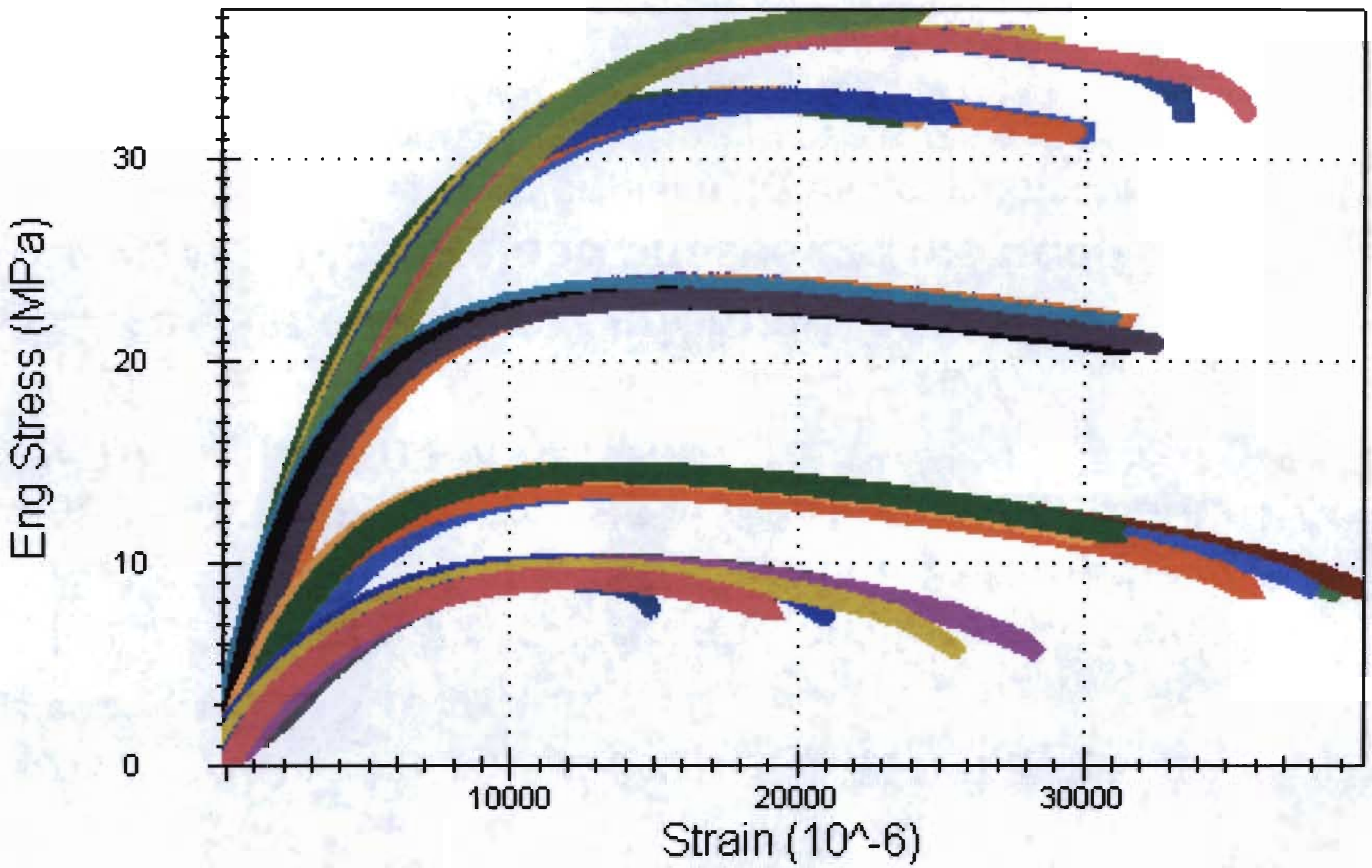
- Lagrangian vs. Eulerian or ALE
  - Eulerian requires advection of state variables, so the best models may become inaccurate in this framework (elastic-plastic may turn out to be best for this case, limit to monotonic loading cases)
  - Lagrangian best fidelity if mesh tangling can be avoided
  - ALE is promising, as our materials are typically rubble by the time we achieve enough deformation to require remapping

Existing Models

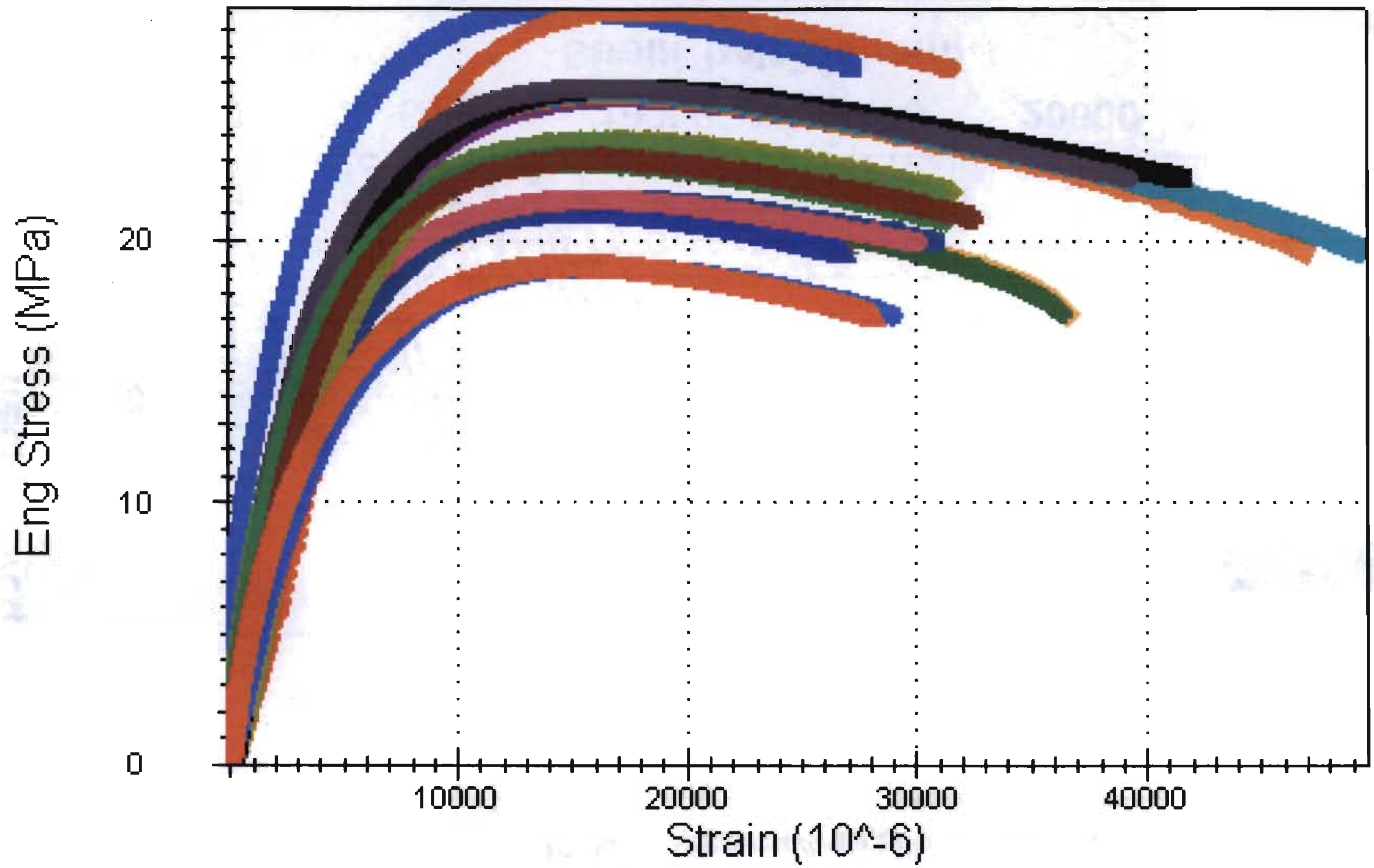
- Elastic-Plastic fits
  - May be okay at higher pressures
  - Available in most codes
  - Certainly an oversimplification for most energetics at moderate pressures (below a few MPa)
  - Will almost certainly produce bad unload-reload behavior
- ViscoSCraM
  - Based on statistical treatment of Linear Elastic Fracture Mechanics
  - Extended to include viscoelasticity
  - Not appropriate for more rubbery materials or materials that show substantial irrecoverable strains
- FRHE
  - New model
  - Based on viscoplastic theory with elastic damage---no viscoelastic recovery
  - Needs documentation, followed by implementation, verification, and validation
  - Only model of this list that produces observed dilatation under uniaxial compression

Relevant Mechanical Characterization Tests

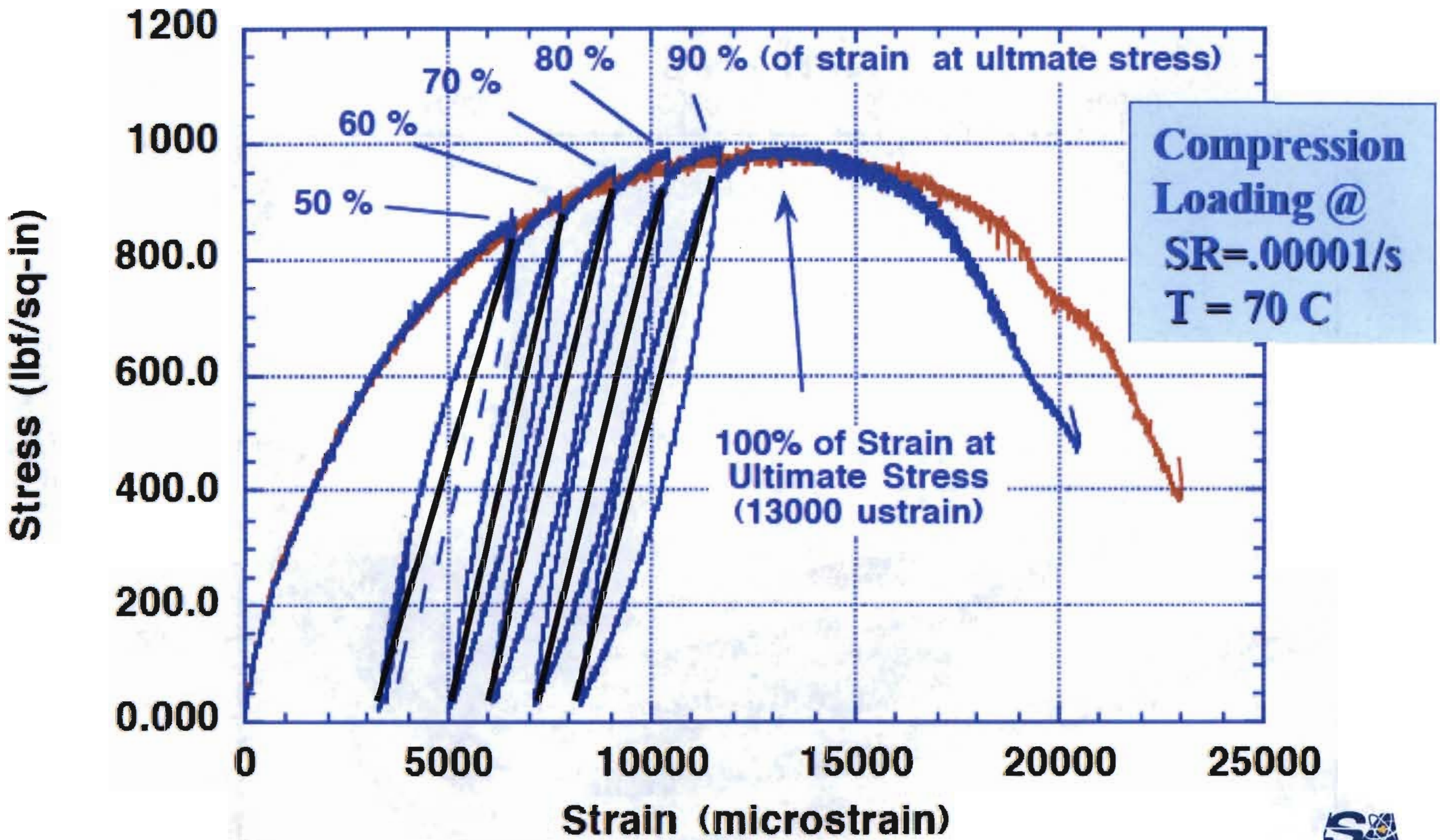
- **Monotonic Tension/Compression Tests** at constant strain rates
  - Provide uniaxial strength and strain measures at failure as functions of strain rate and temperature
  - Give an indication of stiffness dependence on strain rate and temperature
  - In the absence of nonlinearities, provide viscoelastic response information
  - Better if unload/reload phases are included
    - Identify damage and/or plasticity as active mechanisms
  - Rigid platens!

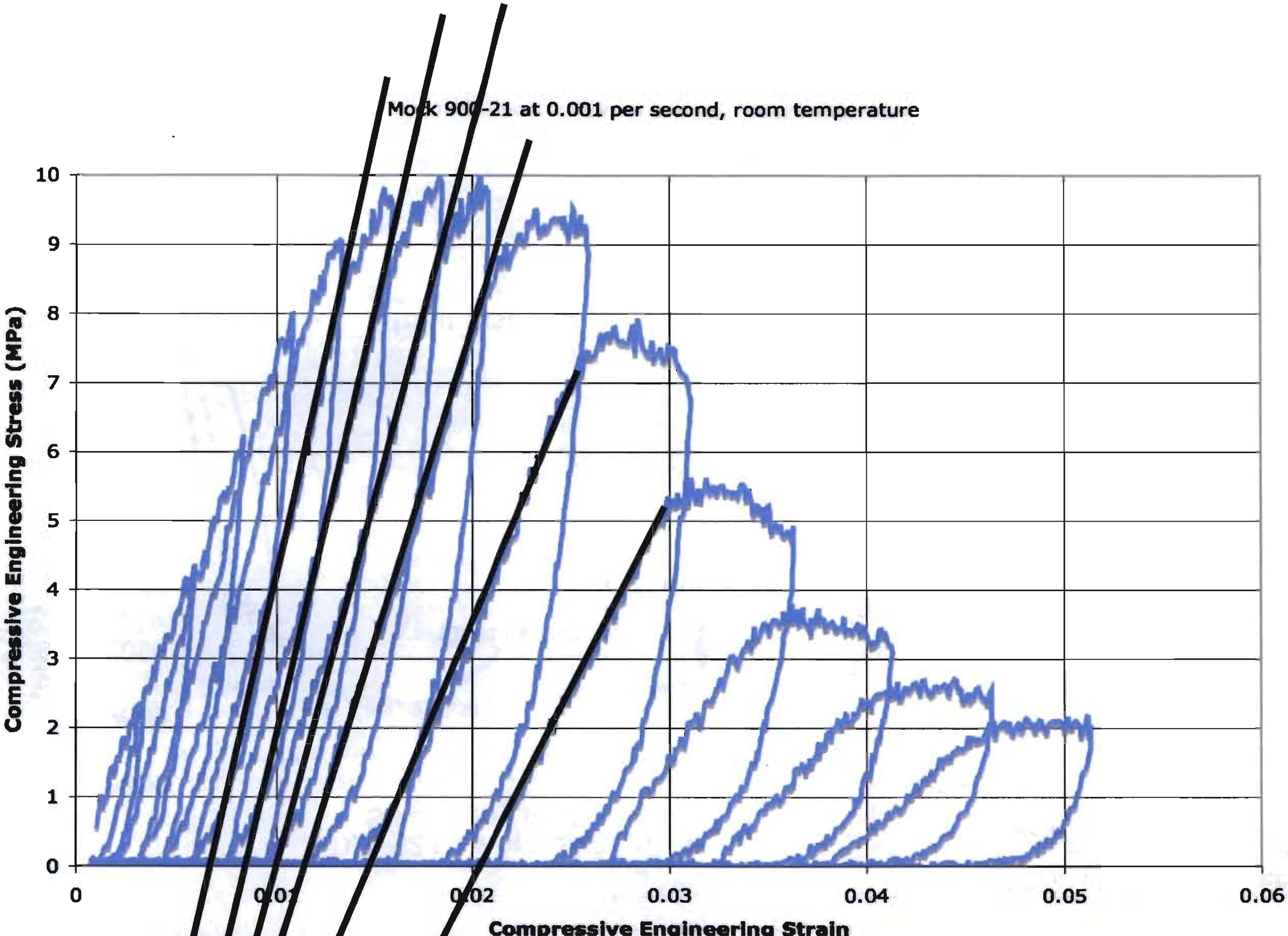


0.001/second Compression@ -52, -20, 20, 50, and 74°C



9502 Compression at 20°C, 0.00001/second to 0.1/second


1200
1000
800.0
600.0
400.0
200.0
0.000
Stress (lbf/sq-in)
0
5000
10000
15000
20000
25000
Strain (microstrain)
50 %
60 %
70 %
80 %
90 % (of strain at ultmate stress)
100% of Strain at
Ultimate Stress
(13000 ustrain)
Compression
Loading @
SR=.00001/s
T = 70 C



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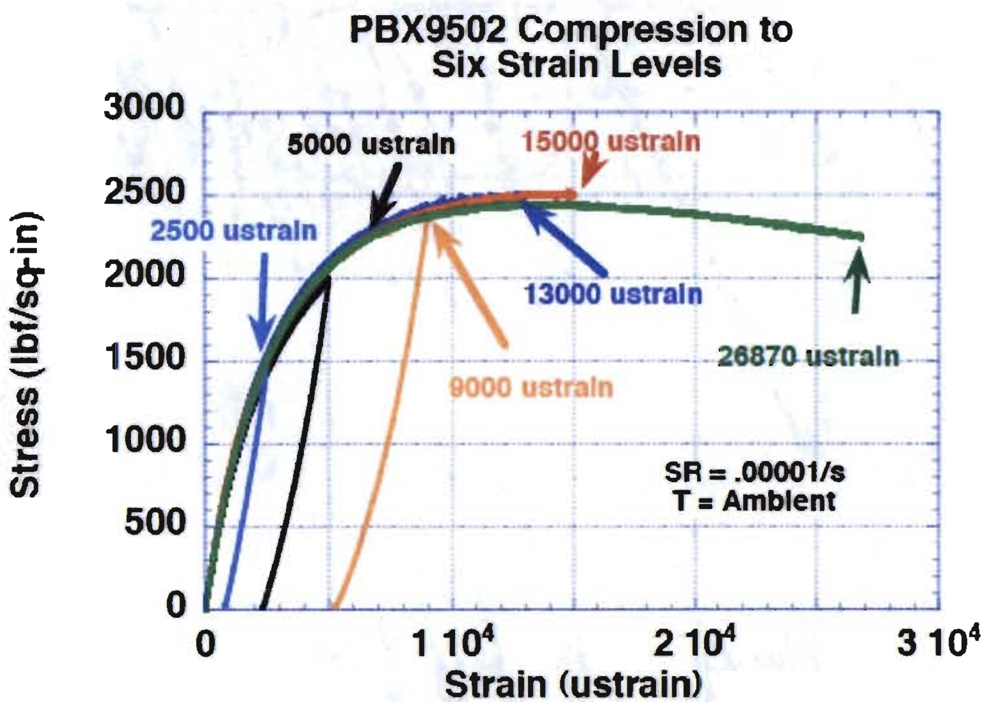
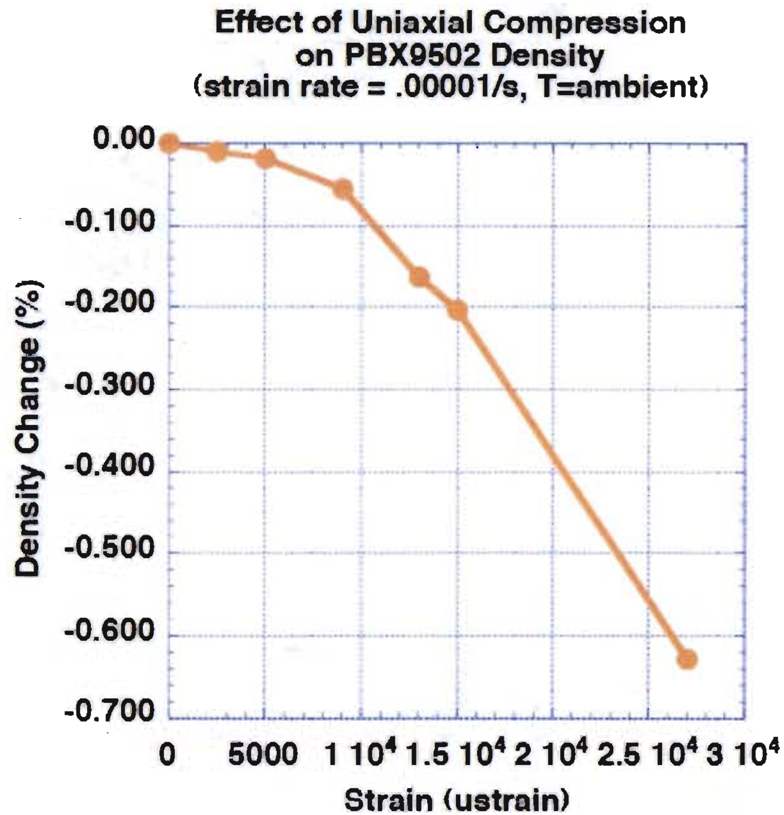
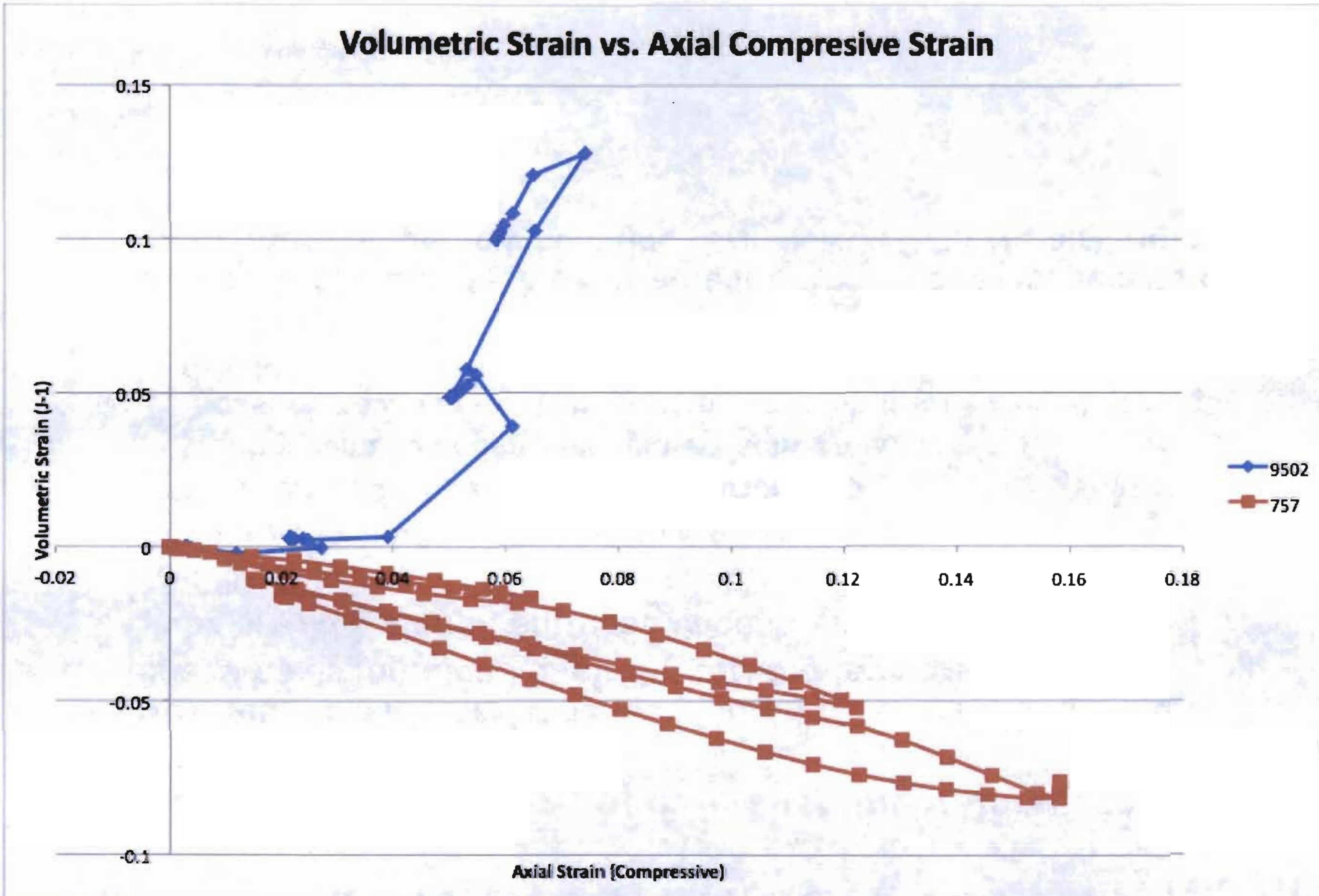


PBX9502 Compression to
Six Strain Levels
Stress (lbf/sq-in)
Strain (ustrain)
5000 ustrain
15000 ustrain
2500 ustrain
13000 ustrain
26870 ustrain
9000 ustrain
SR = .00001/s
T = Ambient
3000
2500
2000
1500
1000
500
0
1 10^4
2 10^4
3 10^4



Effect of Uniaxial Compression
on PBX9502 Density
(strain rate = .00001/s, T=ambient)
Density Change (%)
Strain (ustrain)
0.00
-0.100
-0.200
-0.300
-0.400
-0.500
-0.600
-0.700
0
5000
1 10^4
1.5 10^4
2 10^4
2.5 10^4
3 10^4



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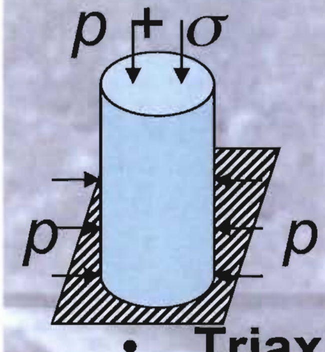
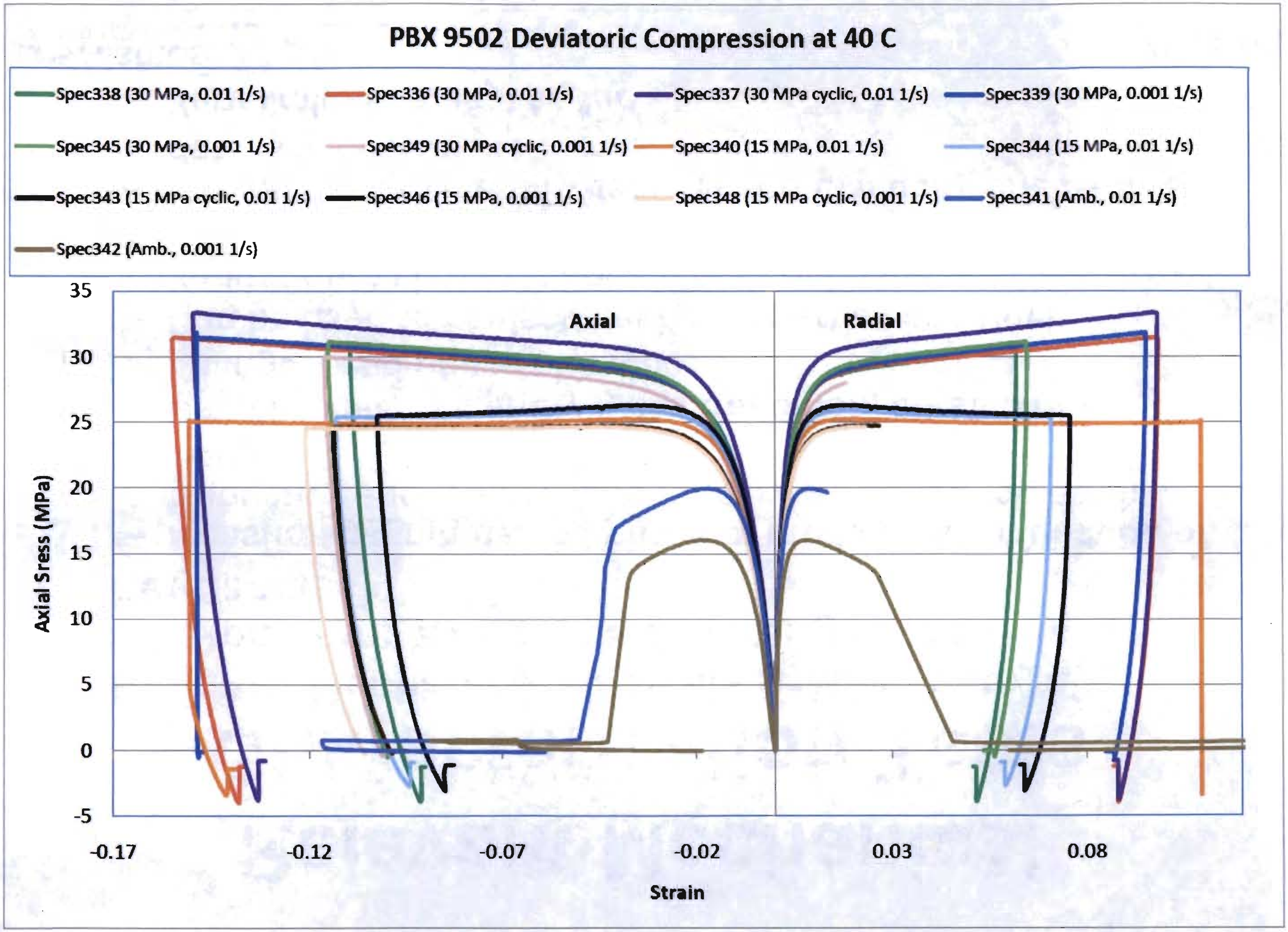


Relevant Mechanical Characterization Tests

100 mm

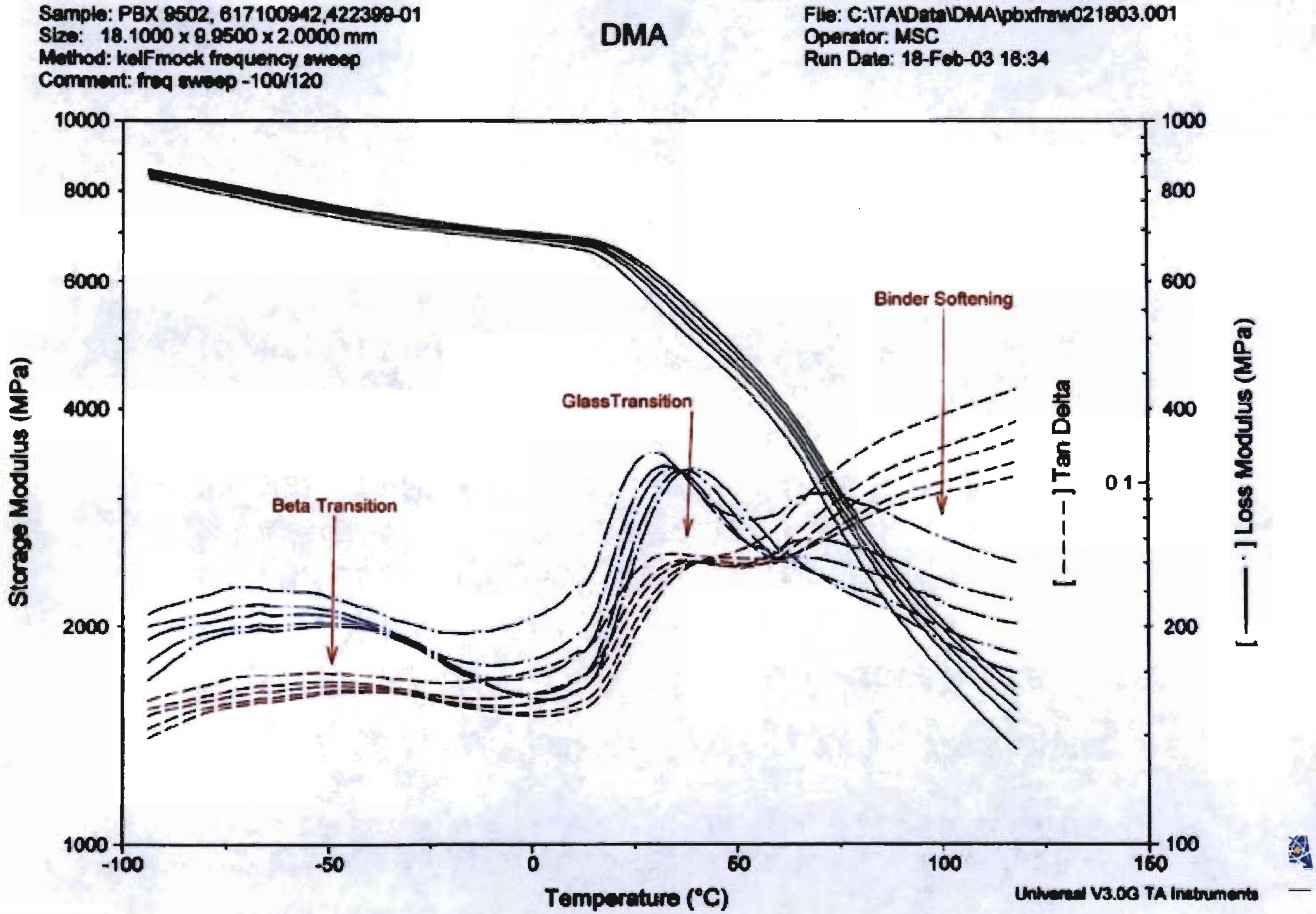
- **Triaxial Compression Tests** at different temperatures, rates, and pressures
  - Provides pressure dependence of strength and strain at failure measures as functions of strain rate and temperature
  - Gives an indication of stiffness dependence on strain rate and temperature
  - Can clarify plasticity dependence on pressure
  - Better if unload/reload phases are included
    - Identify damage and/or plasticity as active mechanisms
    - Pressure may prevent damage from accruing (pores closed as they develop), allowing better characterization of plasticity
    - May help to clarify pressure effects on viscoelastic response
  - Issues: Sleeve effects, measurement of lateral strains, accessible temperature range, few facilities (SNL, ARDEC, LLNL-air), rigid platens!


PBX 9502 Deviatoric Compression at 40 C
Spec338 (30 MPa, 0.01 1/s)
Spec336 (30 MPa, 0.01 1/s)
Spec337 (30 MPa cyclic, 0.01 1/s)
Spec339 (30 MPa, 0.001 1/s)
Spec345 (30 MPa, 0.001 1/s)
Spec349 (30 MPa cyclic, 0.001 1/s)
Spec340 (15 MPa, 0.01 1/s)
Spec344 (15 MPa, 0.01 1/s)
Spec343 (15 MPa cyclic, 0.01 1/s)
Spec346 (15 MPa, 0.001 1/s)
Spec348 (15 MPa cyclic, 0.001 1/s)
Spec341 (Amb., 0.01 1/s)
Spec342 (Amb., 0.001 1/s)
Axial
Radial
Axial Sress (MPa)
35
30
25
20
15
10
5
0
-5
-0.17
-0.12
-0.07
-0.02
0.03
0.08
Strain

Relevant Mechanical Characterization Tests

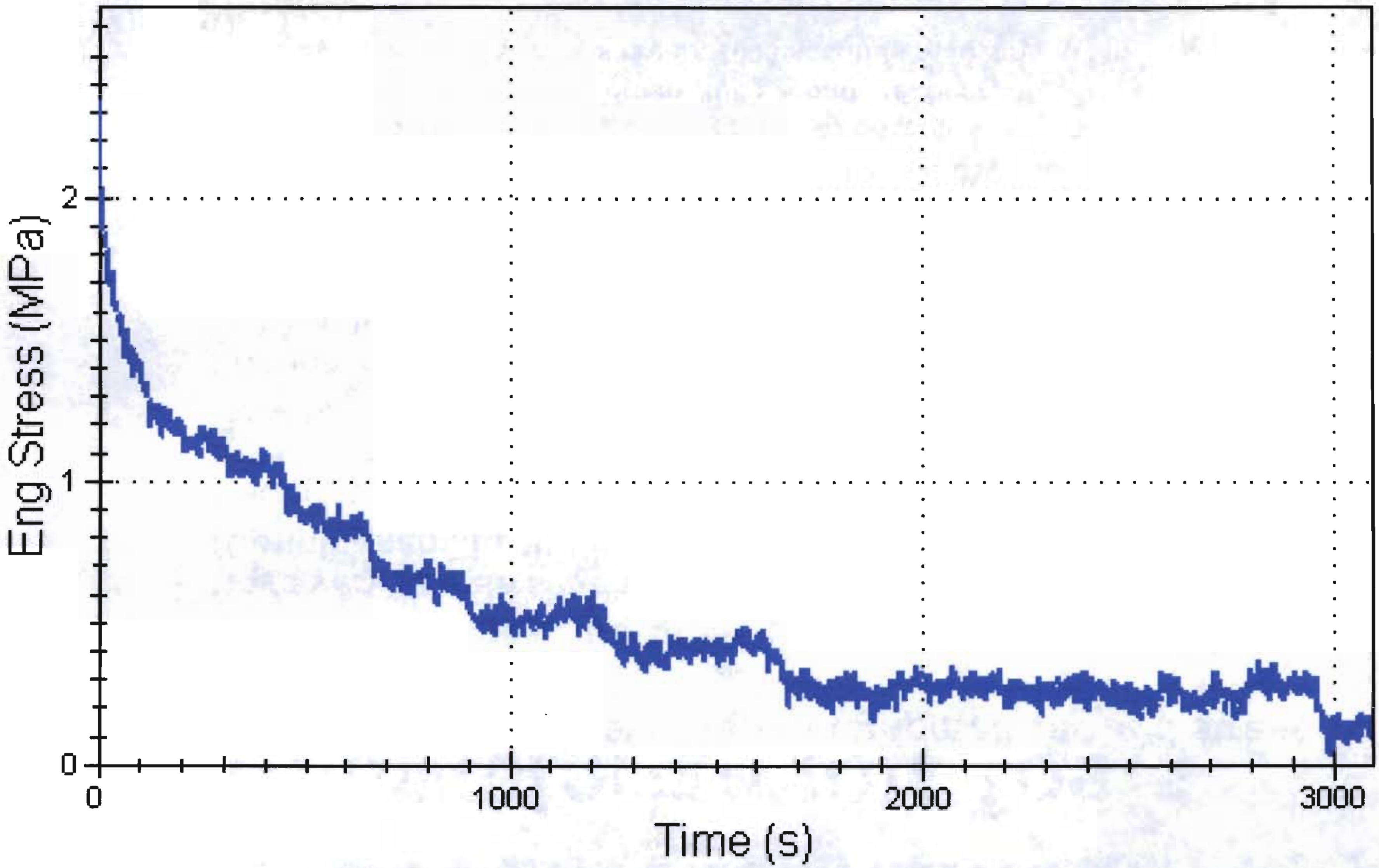
- **Dynamic Mechanical Analysis (DMA) Tests** at different temperatures, strain ranges, and frequencies:
  - Measure magnitude and phase of modulus as a function of frequency and temperature (and, when asked for, strain range)
  - Usually used to identify glass transition, crystallinity changes, and phase changes
  - Can be used to fit viscoelastic properties and time-temperature shift functions if material behaves linearly over strain range tested
  - Can be used to identify damage and plasticity effects if raw data is accessible
  - Very limited dataset so far

200 µm


Sample: PBX 9502, 617100942,422399-01
Size: 18.1000 x 9.9500 x 2.0000 mm
Method: kelFmock frequency sweep
Comment: freq sweep -100/120
DMA
File: C:\TA\Data\DMA\pbxfraw021803.001
Operator: MSC
Run Date: 18-Feb-03 16:34
Binder Softening
GlassTransition
Beta Transition
Storage Modulus (MPa)
Tan Delta
Loss Modulus (MPa)
10000
8000
6000
4000
2000
1000
1000
800
600
400
0.1
200
100
-100
-50
0
50
100
150
Temperature (°C)
Universal V3.0G TA Instruments

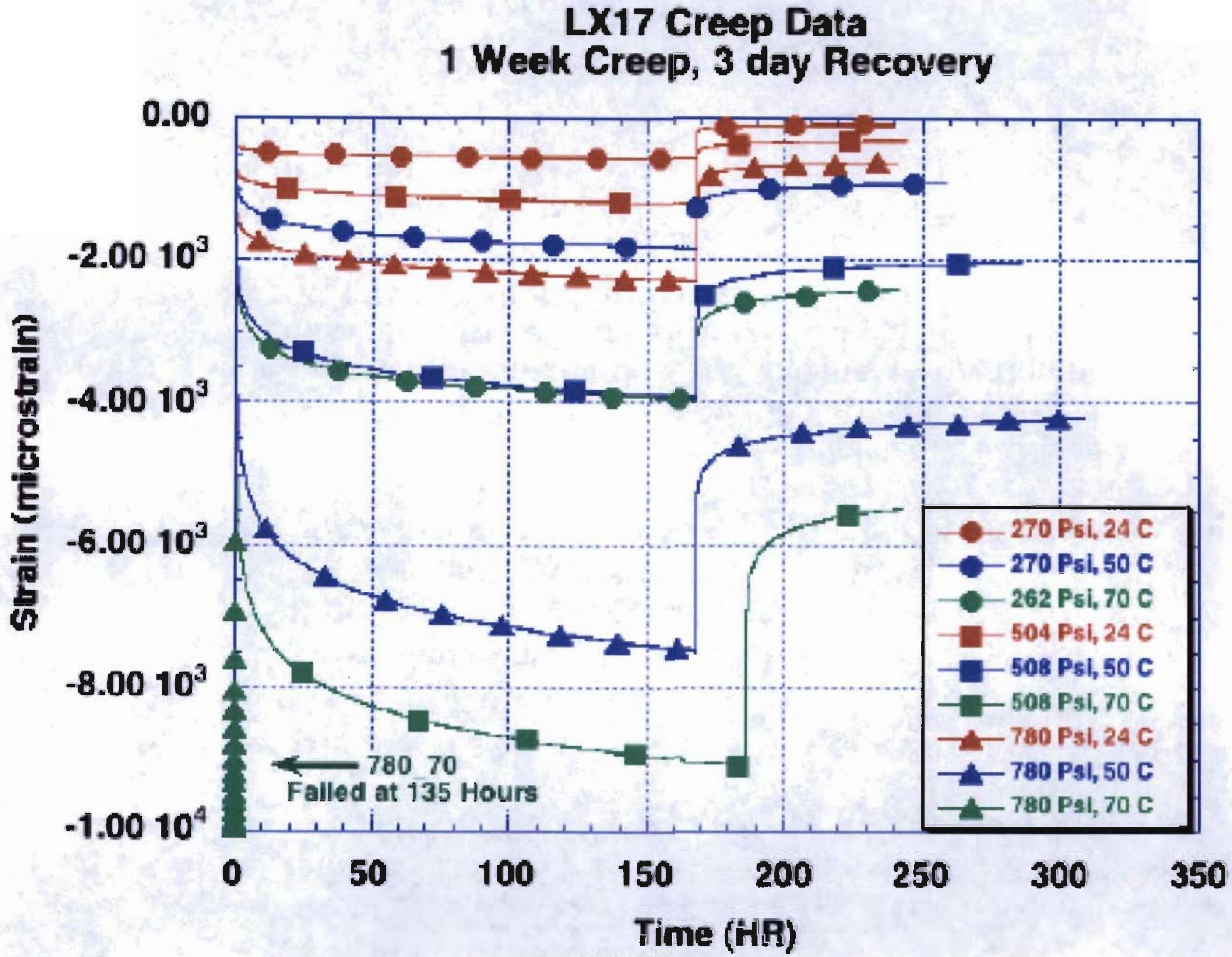
Relevant Mechanical Characterization Tests

- **Relaxation Tests** at different temperatures, strain levels, and loading :
  - Can be used to fit viscoelastic properties if material behaves linearly over strain range tested
  - No data on PBXs yet, but limited data from Mocks
  - Requires good temperature control and reliable load measurement over long periods
  - Rigid platens!


Eng Stress (MPa)
2
1
0
0
1000
2000
3000
Time (s)

Relevant Mechanical Characterization Tests

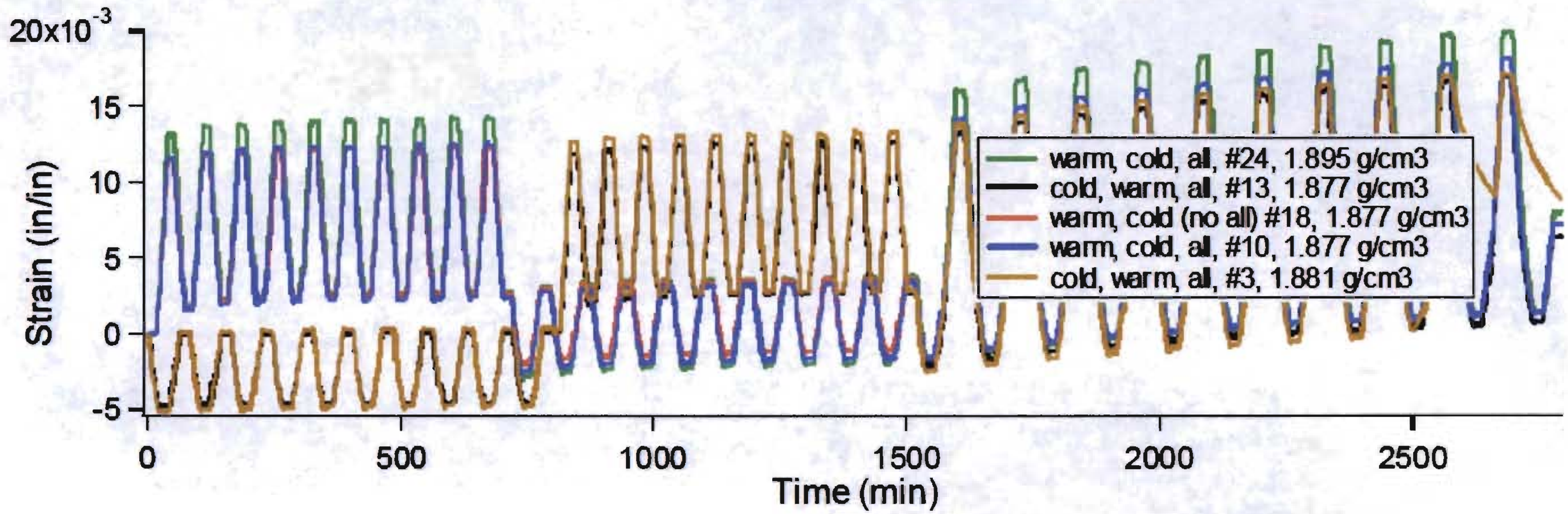
- **Creep/Recovery Tests** at different temperatures and stress levels:
  - Constant load, measure strain vs. time
  - Have *very sparse* set data set for 9501, slightly better for 9502 (Cunningham, LLNL)
  - Requires good temperature control and reliable strain measurement over very long periods and tying up valuable floor space! Verification of applied load is important.
  - We need to change our way of doing this test
    - Just like monotonic tests, without doing recovery mechanisms are indistinct---how much is recoverable? Is there damage? Plasticity?
    - Recovery is important to identify recoverable part of creep strain which has everything to do with measured contours!
      - Suggestion: Creep and recovery by decades
        - » 100 seconds creep, 100 seconds recovery
        - » 1000 seconds creep, 1000 seconds recovery
        - » Etc.



UNCLASSIFIED

Relevant Mechanical Characterization Tests

- **Ratchet Growth Tests** over different temperature ranges with different confinement:
  - What is the mechanism for ratchet growth?
    - Lots of handwaving, little real materials science
      - Hypothesize, test, repeat!
  - Quantifies ratchet growth possible at a given pressure (not just axial stress!)
    - Very little of this testing has been completed at LANL and LLNL, except for ambient pressure conditions and a few axial loads
  - Measurement of axial and lateral strains + final density measurements to validate strain measurement (given temperature variations during tests)
  - Characterization post-testing of instrumented ratchet growth test specimens can be used to measure effects on other mechanisms:
    - Plasticity
    - Damage
    - Viscoelastic properties
    - Overall uniaxial and triaxial response
  - Darla (GT) and Bruce (C.) have started to look at this



20x10^-3
15
10
5
0
-5
Strain (in/in)
0
500
1000
1500
2000
2500
Time (min)
warm, cold, all, #24, 1.895 g/cm3
cold, warm, all, #13, 1.877 g/cm3
warm, cold (no all) #18, 1.877 g/cm3
warm, cold, all, #10, 1.877 g/cm3
cold, warm, all, #3, 1.881 g/cm3

Failure Envelope and Validation Tests

- Controlled state tests for failure envelope determination
  - Combined torsion and compression/tension
  - Others?
- Not much done on validation, but are we ready yet?
  - Validation
    - Brazil disk
    - Surveillance data
    - Iosipescu
    - HATCH
    - 3- or 4-point bend
    - Others?

Issues

- **There are a wide variety of issues that need to be addressed in model development**
  - Extreme differences in material properties
  - Anistropic phase properties
  - Complex rate and temperature dependent constituent behaviors
  - Damage (cracking) in constituents
  - Debonding at the interfaces and associated frictional sliding
  - Computational issues (numerical schemes/implementation)
  - Stochastic microstructures (arrangements, sizes, orientations, etc)
  - Coupled (thermo-mechanical-diffusional) field effects
  - Aging effects
  - Phase transformations

Issues

- Nonshock initiation
  - Thermal localization
  - Chemical kinetics
  - Uncertainty quantification
    - Model parameters
  - Experimental data
    - Suitability of the experimental data for characterization
    - Tomography and the translation into model input
    - Non-uniqueness of unidirectional testing
  - Unified multiscale modeling capable of coupling different modeling approaches effectively
    - Micro-modeling of phases
    - DNS
    - Various homogenization models
  - Applicable to a variety of different types of HEs

Differences in the Approaches

- Micromechanically based models
  - Directly account for microphysics
  - More computationally demanding
- Continuum level models
  - Don't directly account for microphysics
  - Computationally very efficient. More easily implemented into large analysis codes
- Ideal : Use micromechanical models in large analyses when possible and/or use micromechanical modeling to develop more accurate and predictive continuum level models

Thermomechanical Tests with Best "Bang for the Buck"

- Uniaxial compression and tension with enough instrumentation to get lateral response, too
  - Relevant rates and temperatures
  - Cyclic for highest information content
- Triaxial compression at relevant pressures
  - Relevant rates and temperatures (can we go faster and colder?)
  - Cyclic for highest information content
- DMA for viscoelasticity properties
  - Relevant temperatures, determine if TTS can expand time scale of response
- Uniaxial Creep
- Others?
- What are the most useful ways to measure strain?

Minisymposium

11th U.S. National Congress on Computational Mechanics
Minisymposium Proposal Submission

Title Mechanical Constitutive Modeling of Energetic Materials

Description

Developing realistic mechanical constitutive models for practical energetic materials (solid propellants and explosives) is a significant challenge. These materials typically are particulate composites. They also include large volume fractions (usually greater than 80%) of particulate phases. These materials usually exhibit a very small (or possibly nonexistent) range of linear mechanical response. These materials may contain more than one particulate phase. These phases often have high contrast in their mechanical properties over relevant ranges of pressure, strain rate, and temperature. This minisymposium will be focused on these materials and computational and theoretical methods for developing mechanical constitutive models for them. Papers that incorporate mechanisms characterized experimentally either on a composite system or a particular constituent are of particular interest. Modeling approaches that address the multiple length scales seen in energetic materials are also desired.

Targeted themes

- Composites Modeling
- Energetic Materials
- Mechanical Constitutive Theories
- Integration with Characterization Testing
- Multiple Length Scales

Organizers:

Summary

This is a hard problem, which is why it has not yet been solved. One model will not work for all energetic materials.

Developing good mechanical mocks may allow more to work on the right set of tests and micromechanical modeling synthesis to produce better models for these materials.

Ultimately, the "best" tests will need to be conducted on the actual materials of interest.