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Title: The Challenge and Promise of Developing Mechanical Constitutive Models for Energetic Materials

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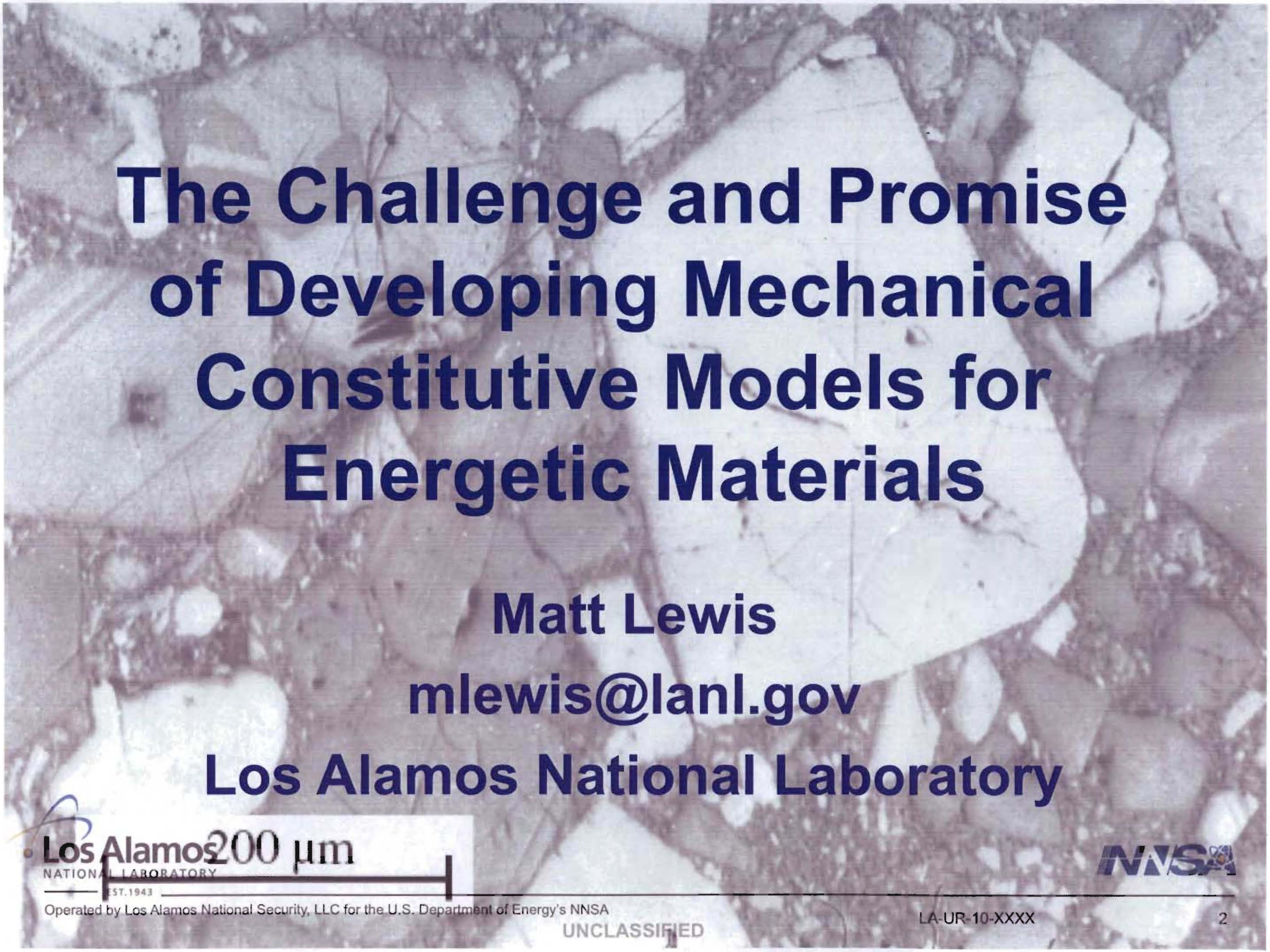
Abstract

Developing realistic mechanical constitutive models for practical energetic materials (solid propellants and explosives) is a significant challenge. These materials typically are particulate composites that 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. They 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.

The defense community has reached a point where not having validated, deformation mechanism-based models is affecting our ability to support important missions. Potential approaches for developing the next generation of mechanical constitutive models for these challenging materials through a combination of characterization and modeling will also be discussed.



The Challenge and Promise of Developing Mechanical Constitutive Models for Energetic Materials

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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

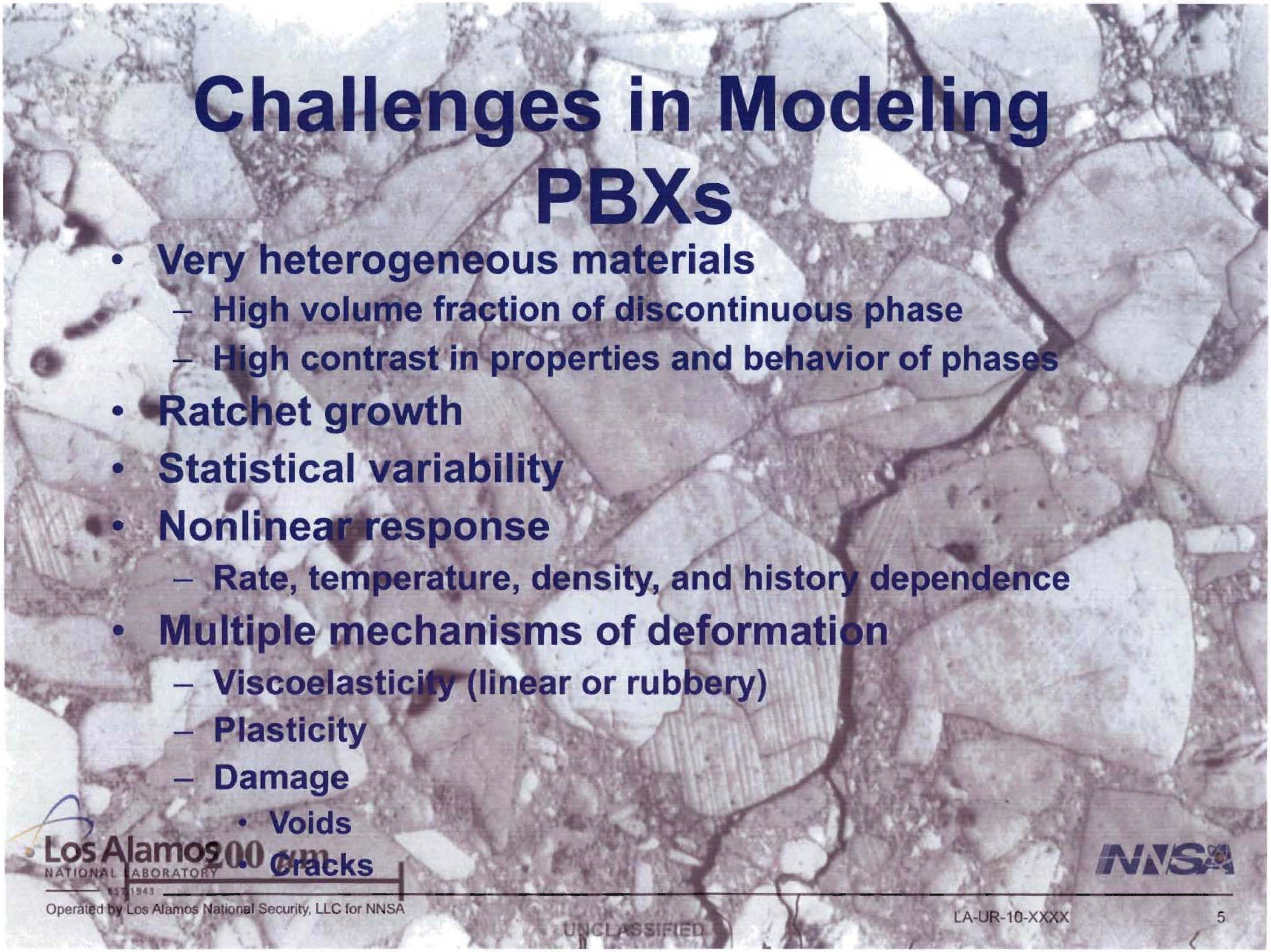
Paul Petersen

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



Challenges in Testing PBXs

- **Testing limited to a few facilities**
- **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**

1um
5kV 25mm

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

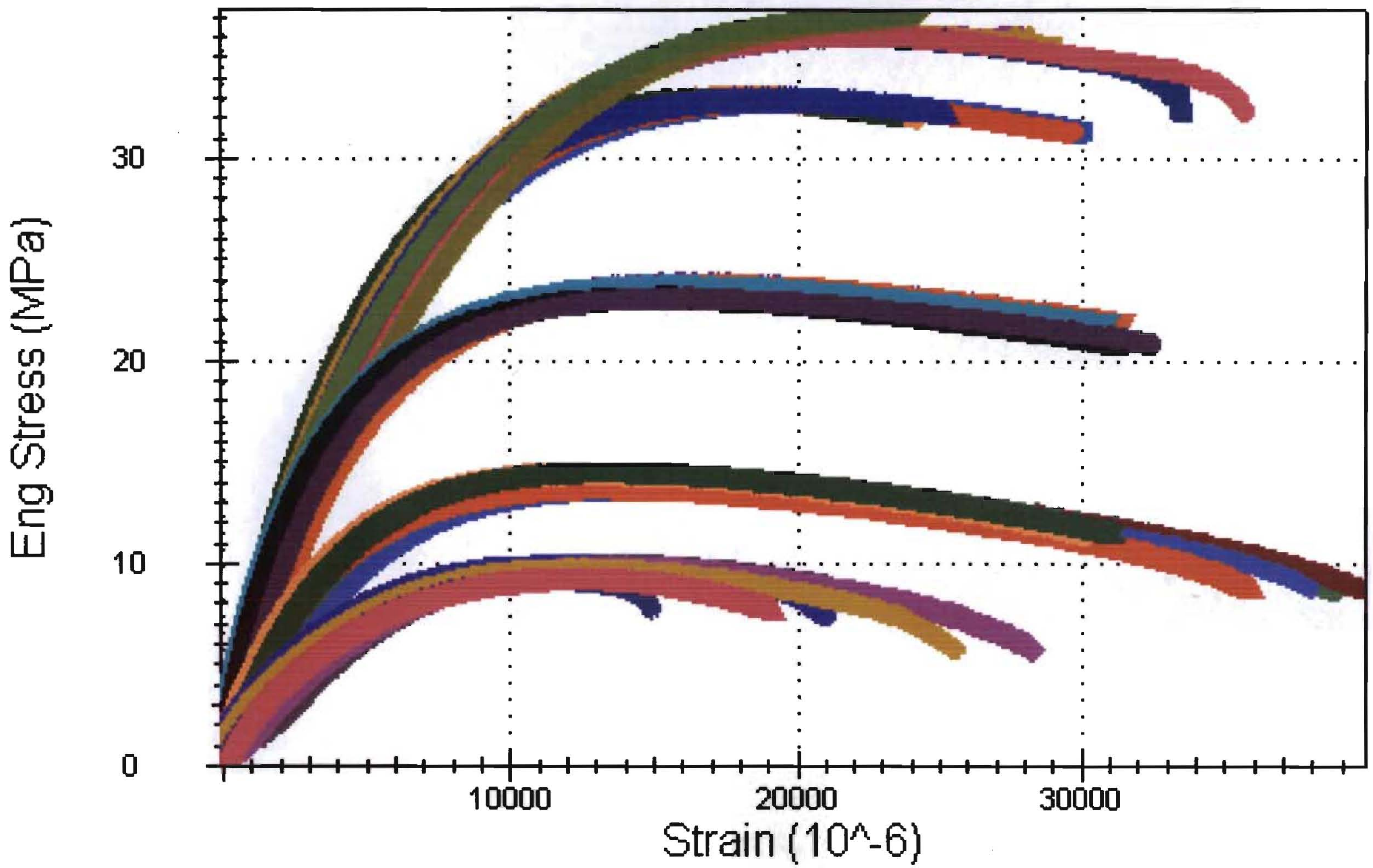
- Lagrangian vs. Eulerian or ALE
  - Eulerian requires advection of state variables, so the best models may become inaccurate in this framework (elastic-plastic may turn out to be best for this case, limit to monotonic loading cases)
  - Lagrangian best fidelity if mesh tangling can be avoided
  - ALE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

Existing Models

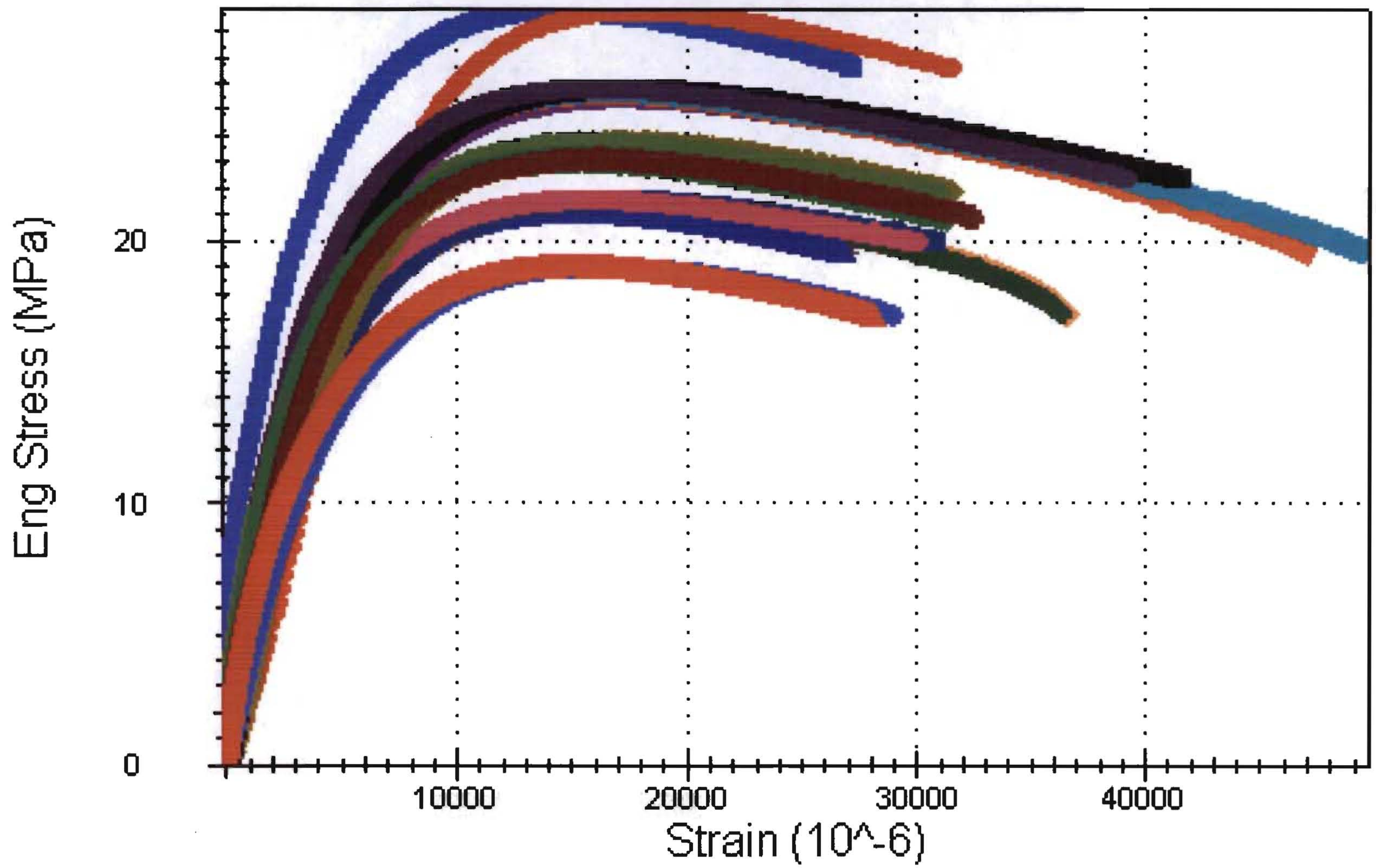
- Elastic-Plastic fits
  - May be okay at higher pressures
  - Available in most codes
  - Certainly an oversimplification for most energetics at moderate pressures (below a few MPa)
  - Will almost certainly produce bad unload-reload behavior
- ViscoSCraM
  - Based on statistical treatment of Linear 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

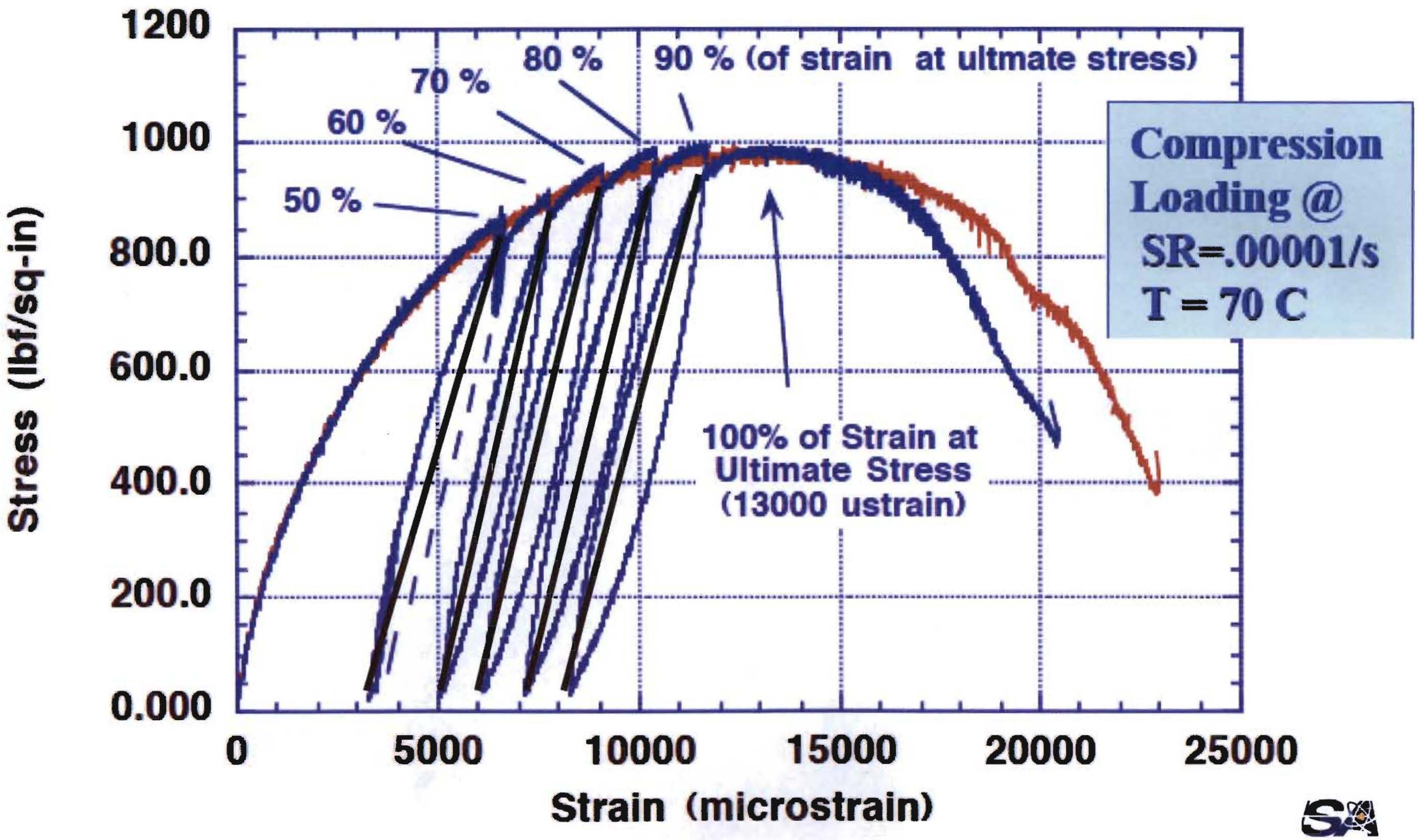
- Monotonic Tension/Compression Tests at constant strain rates
  - Provide uniaxial strength and strain measures at failure as functions of strain rate and temperature
  - Give an indication of stiffness dependence on strain rate and temperature
  - In the absence of nonlinearities, provide viscoelastic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



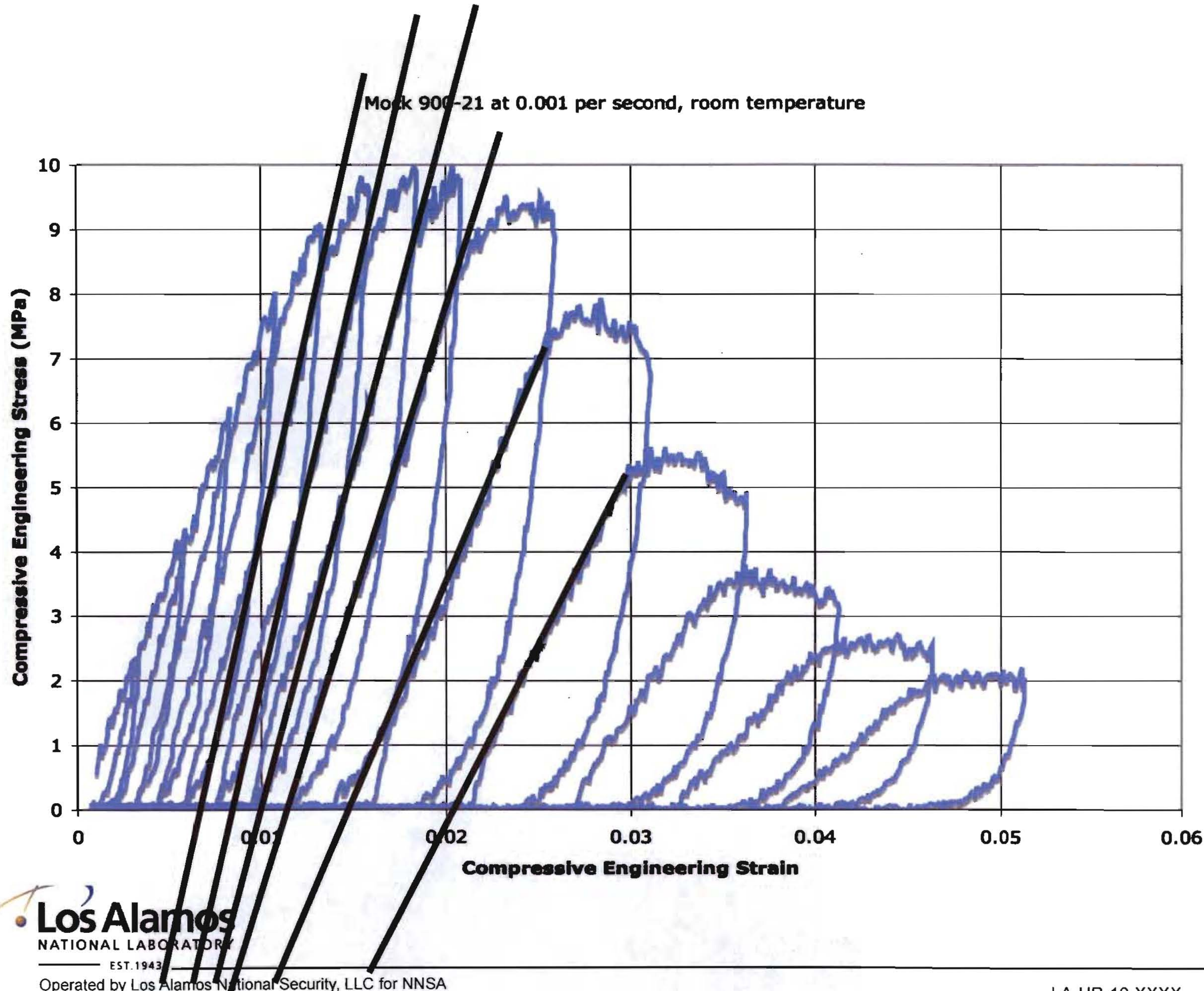
0.001/second Compression@ -52, -20, 20, 50, and 74°C

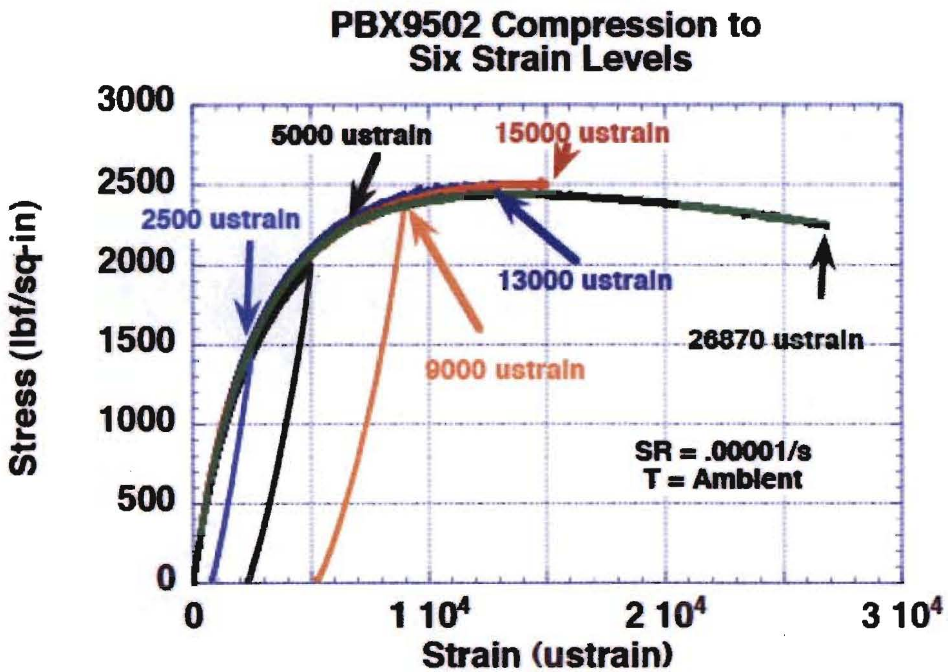


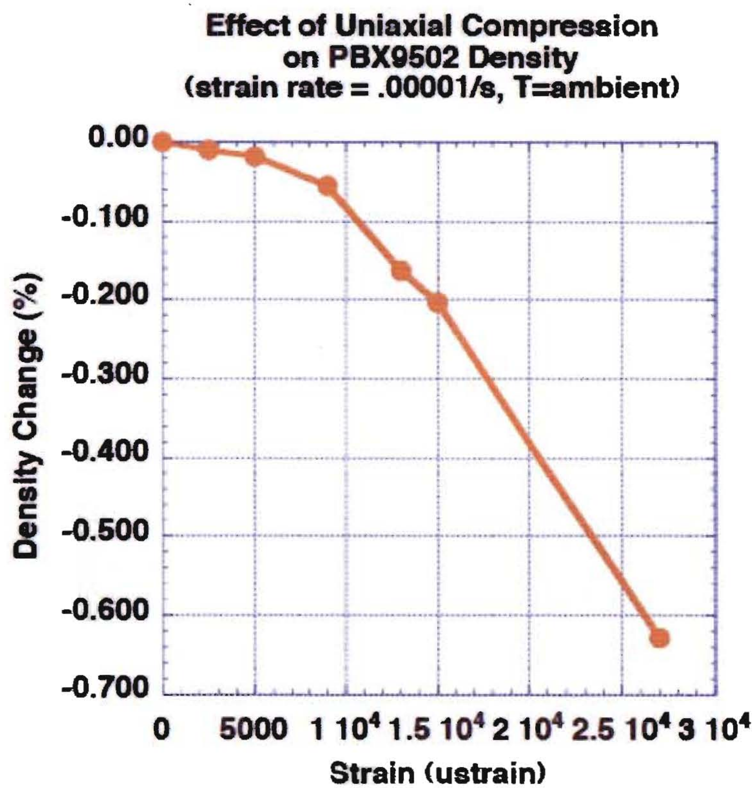
9502 Compression at 20°C, 0.00001/ second to 0.1/second

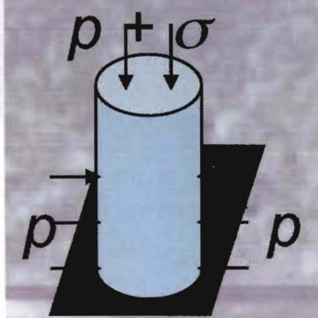


Compression
Loading @
SR=.00001/s
T = 70 C
1200
1000
800.0
600.0
400.0
200.0
0.000
Stress (lbf/sq-in)
0
5000
10000
15000
20000
25000
Strain (microstrain)
50 %
60 %
70 %
80 %
90 % (of strain at ultmate stress)
100% of Strain at
Ultimate Stress
(13000 ustrain)


Mock 900-21 at 0.001 per second, room temperature
Compressive Engineering Stress (MPa)
10
9
8
7
6
5
4
3
2
1
0
0
0.01
0.02
0.03
0.04
0.05
0.06
Compressive Engineering Strain

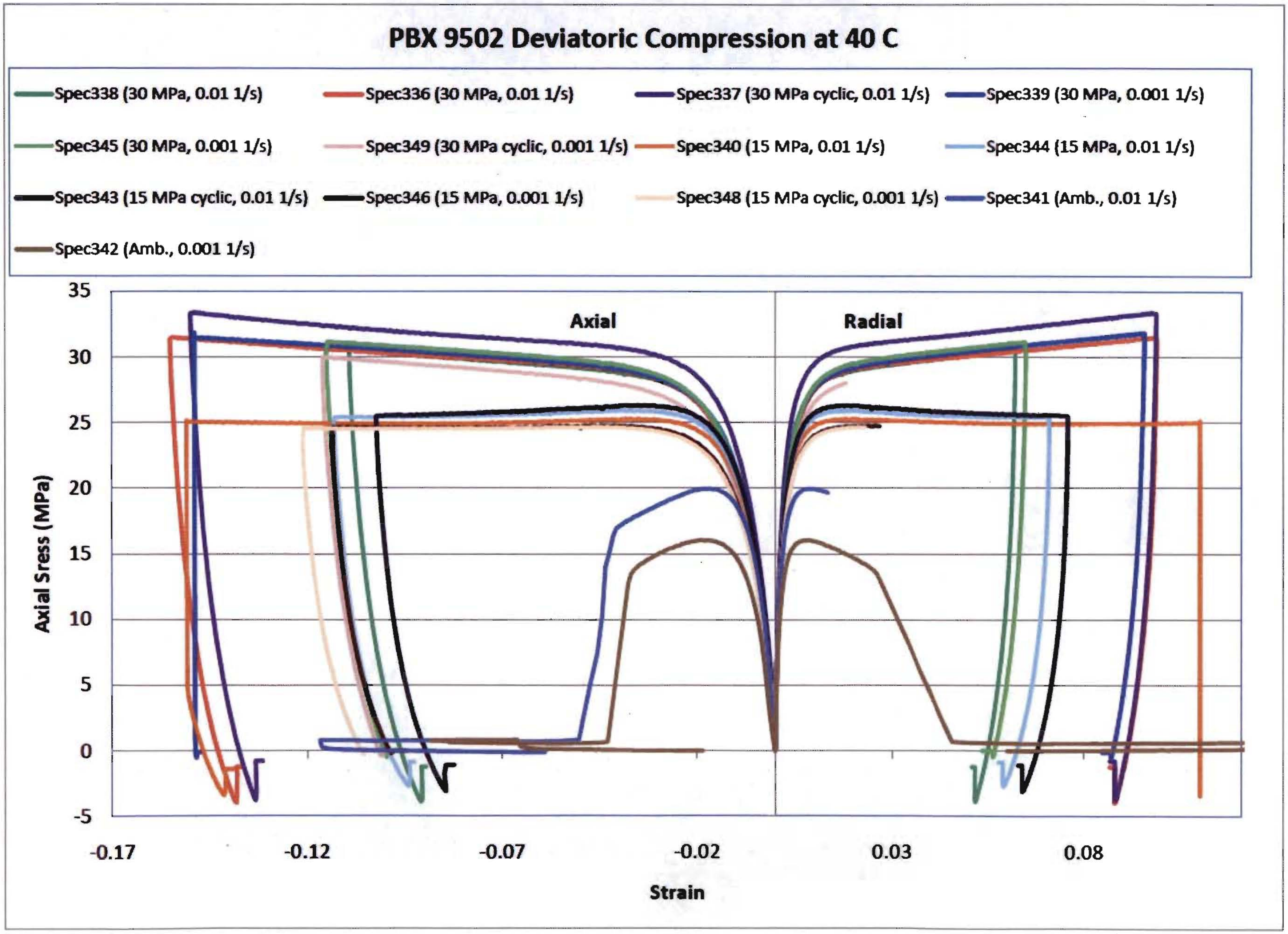

PBX9502 Compression to
Six Strain Levels
3000
2500
2000
1500
1000
500
0
Stress (lbf/sq-in)
5000 ustrain
15000 ustrain
2500 ustrain
13000 ustrain
26870 ustrain
9000 ustrain
SR = .00001/s
T = Ambient
0
1 10^4
2 10^4
3 10^4
Strain (ustrain)


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



Relevant Mechanical Characterization Tests

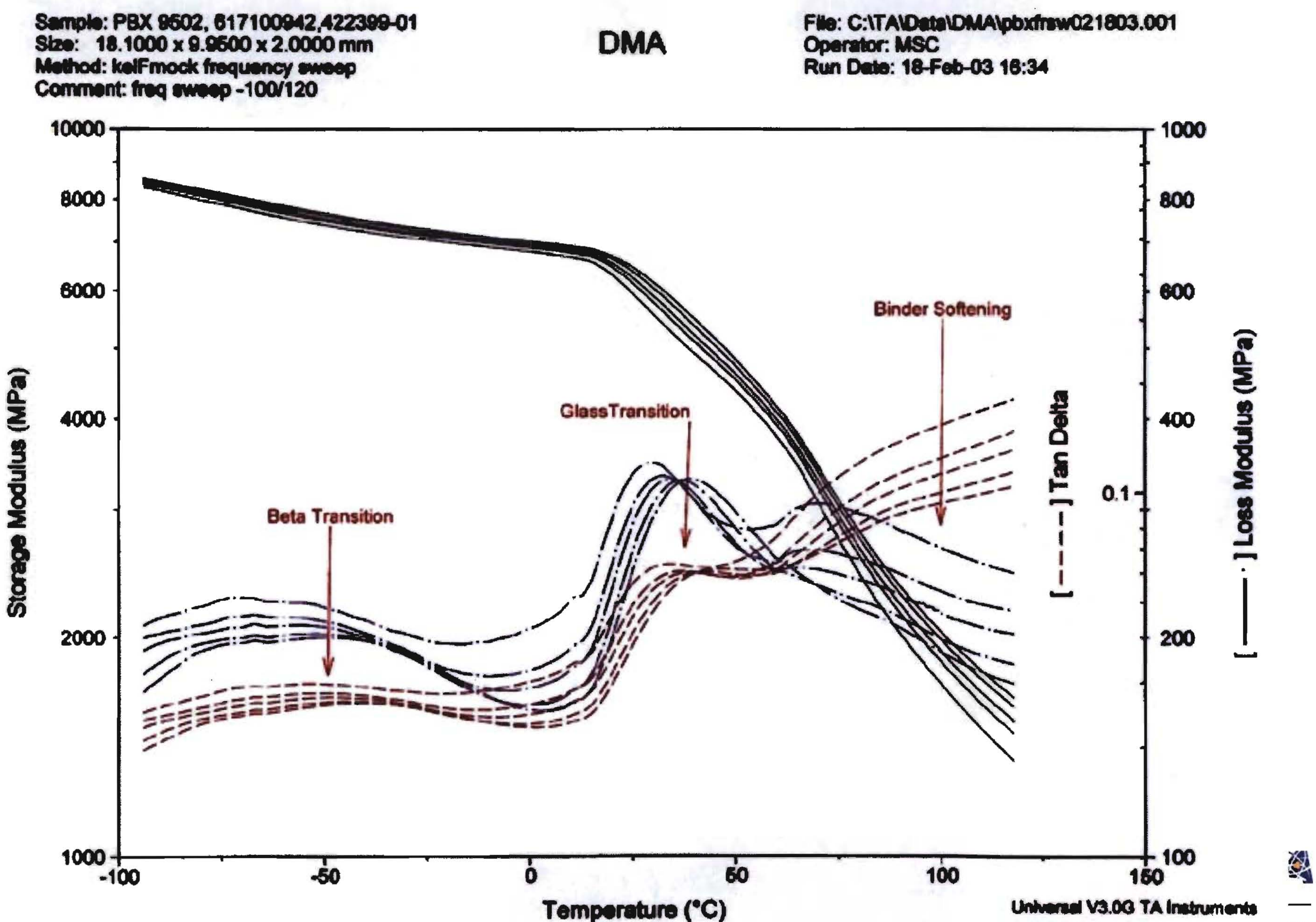
- **Triaxial Compression Tests at different temperatures, rates, and pressures**
  - **Provides pressure dependence of strength and strain at failure measures as functions of strain rate and temperature**
  - **Gives an indication of stiffness dependence on strain rate and temperature**
  - **Can clarify 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

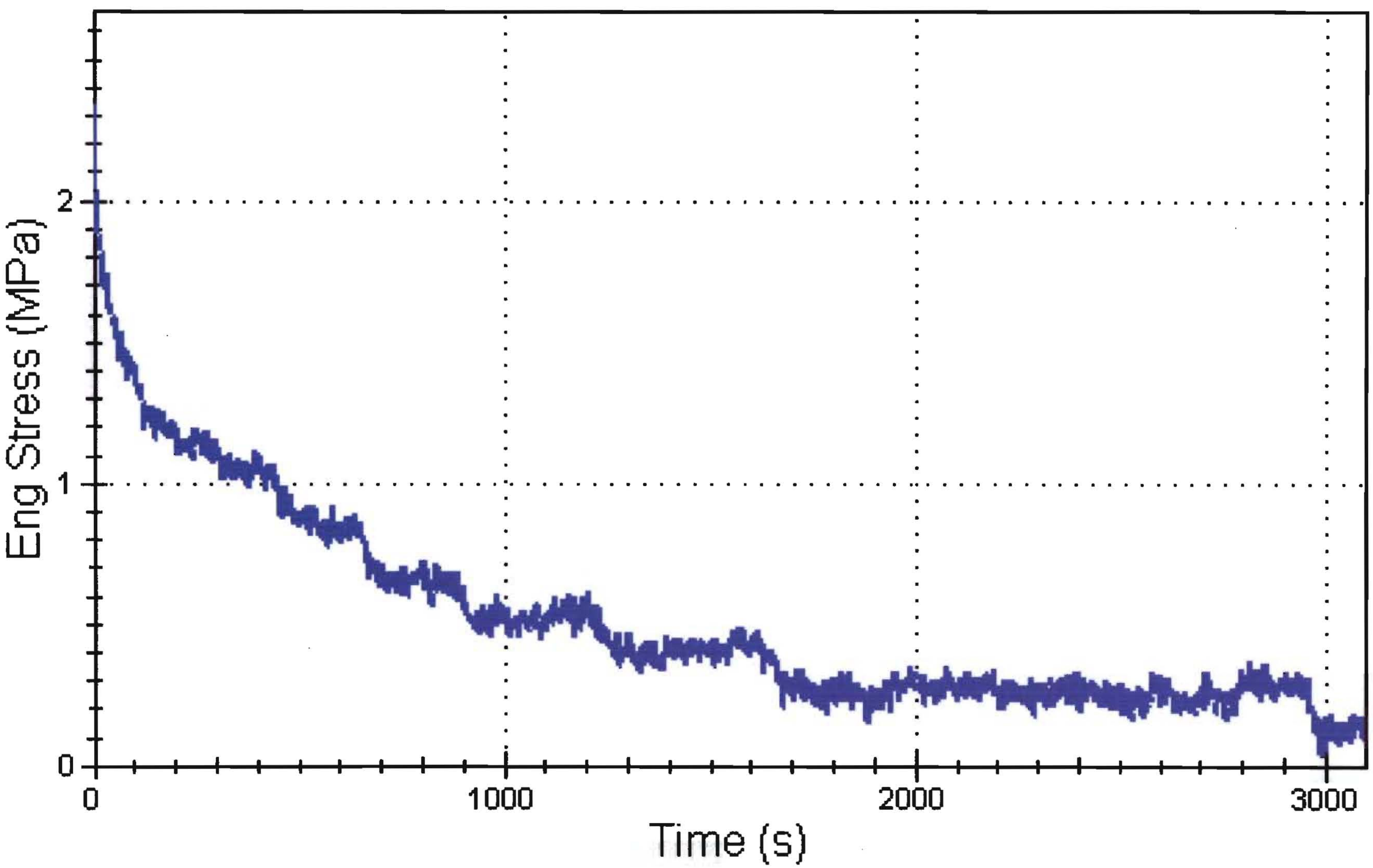
- **Dynamic Mechanical Analysis (DMA) Tests at different temperatures, strain ranges, and frequencies:**
  - Measure magnitude and phase of modulus as a function of frequency and temperature (and, when asked for, strain range)
  - Usually used to identify glass transition, crystallinity changes, and 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\pbxfrsw021803.001
Operator: MSC
Run Date: 18-Feb-03 16:34
Storage Modulus (MPa)
Tan Delta
Loss Modulus (MPa)
Beta Transition
GlassTransition
Binder Softening
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!

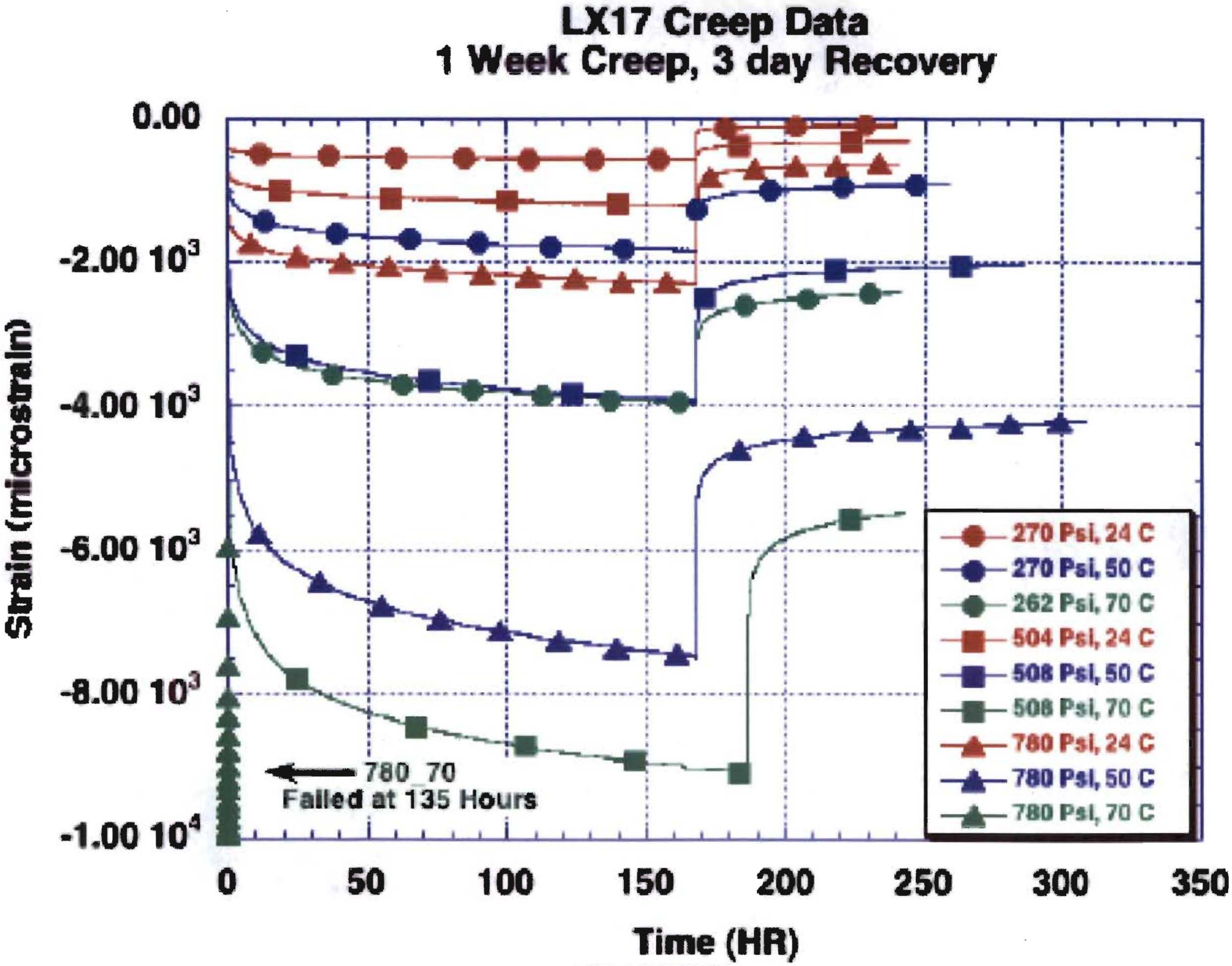


Eng Stress (MPa)
0
1
2
0
1000
2000
3000
Time (s)

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.

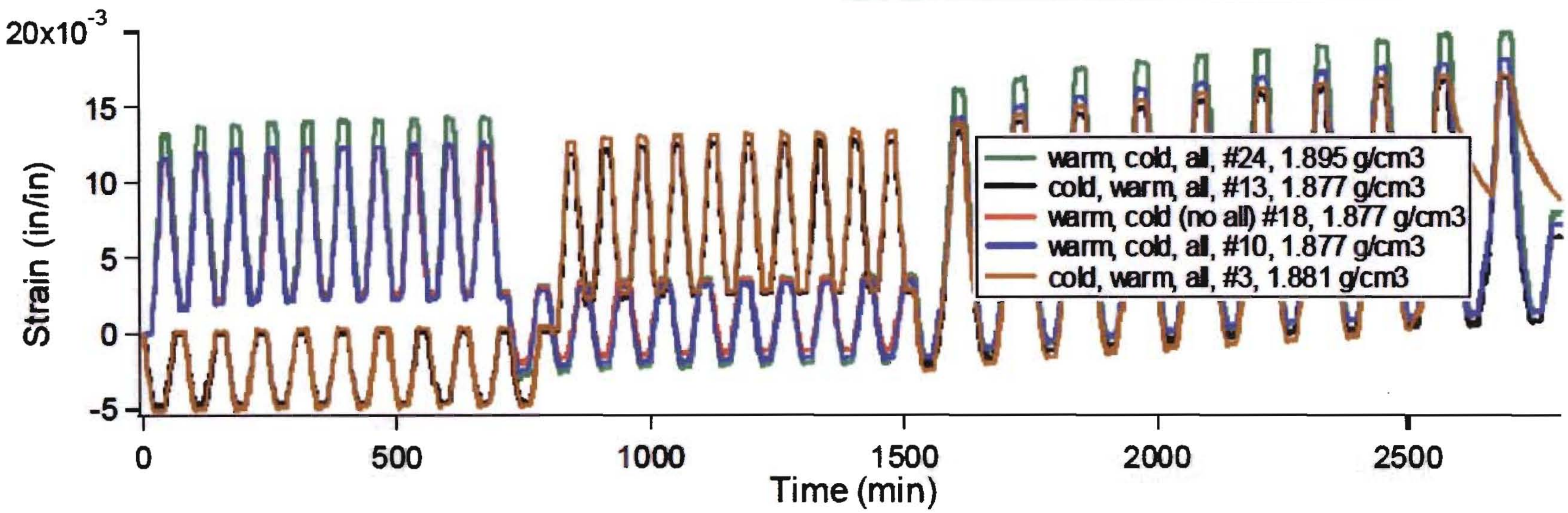
200 μm



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

Verification and Validation

Definition:

Verification is proving that the coded version of a model is operating as it is intended.

Requires known solutions and proof that the model *as coded* converges to the known solution when called with the right argument history and smaller increments are taken.

Should be done with all element types expected to be used and with a large number of elements to make sure that memory management is proper.

A metric is some measure of the error between the known solution and the code solution.

"Solving the equations correctly"

Verification and Validation

Definition:

Validation is proving that a model captures the right physics for a given material and relevant applications.

Requires well-characterized and controlled experiments (preferably repeats) that have not been used to tune the model parameters.

A metric is some measure of the difference between the model predictions and the range of measured response. A more sophisticated take on this identifies model parameter uncertainties and prediction sensitivities to the parameters.

"Solving the correct equations"

Verification and Validation

We further specialize this concept to *calculation validation*, where the model as implemented in the analysis code is validated along with the solution approach of the analysis code.

Point: It is possible to validate a material model on its own *only for cases where the stress or strain is known and controlled (typically uniform).* In order to validate in cases where there are gradients in these quantities requires validation *of the model implementation.*

In all of our applications, gradients exist. For this reason, it is appropriate to focus our validation efforts on *calculation validation of the material model implementation.*

Roles and Responsibilities

MODEL DEVELOPER MODEL IMPLEMENTER MODEL USER

Model Developer
- Develop model
- Document model
  - Words describing model (basis of model, data from which a first fit for a material was developed, parameters, fitting procedure)
  - Relevant equations
  - List of state variables and appropriate initial values
  - Verification problems and solutions
  - Best estimated range of applicability of the model

Roles and Responsibilities

MODEL DEVELOPER MODEL IMPLEMENTER MODEL USER

Model Implementer

- Implement model
- Verify implemented model response
  - Developer supplied problems + arbitrary rotations
  - User-specified element types and dimensionalities, different numbers of elements
- Document model implementation
  - Initial equations and their incremental form
  - Solution algorithm
  - Verification problems and results, list of elements used and numbers of elements (input files and graphical and numerical comparisons to known solutions)
  - User guide (parameters, known issues, caveats)

Roles and Responsibilities

MODEL DEVELOPER MODEL IMPLEMENTER MODEL USER

Model User

- Provide target code to implementer
- Provide list of element types and dimensionalities to implementer
- Provide information about neighboring materials and element types, contact types, and other relevant analysis information to implementer so that these can be tested with implementation
- Provide information about target application to developer and implementer (anticipated strain rates, strain ranges, temperatures, pressures if known)
- Define appropriate validation problems not already performed but necessary as part of analysis process
- Perform calculations of validation problems and compare to experimental data

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?

1um
5kV 25mm

Issues

- There are a wide variety of issues that need to be addressed in the 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.

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.

Path Forward

Use all available appropriate data (visiting with Bruce Cunningham and Ian Darnell on 9502 creep and ratchet growth data next week)

NNSA (and possible DoD) Workshop on appropriate characterization tests for Energetic Materials model development (Winter/Spring 2010)

Re-baseline 9502 uniaxial response (similar to recent work) BUT include lateral strain measurement and/or densitometry and unloading response

- Develop intermediate rate (0.1-100/sec) capability

Develop better triaxial testing capability

- Not a high pressure driver, but low temperature and better measurement technology capability is needed