Advances In High Temperature (Viscoelastoplastic) Material Modeling for Thermal Structural Analysis

Dr. Steven M. Arnold
Senior Research Engineer
Life Prediction Branch
NASA Glenn Research Center

and

Prof. Atef F. Saleeb
The University of Akron
Civil Engineering Department

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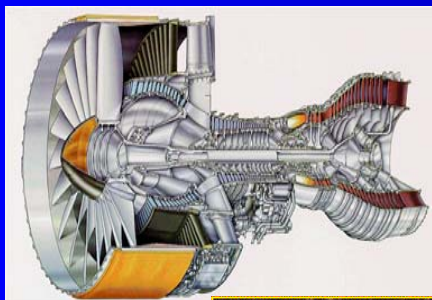
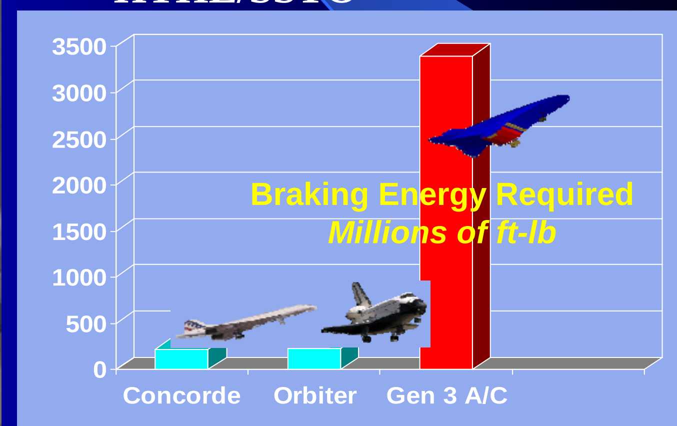
OUTLINE

- **Background/Philosophy**
  - Elevated Material Behavior
  - Impact on Analysis
  - Multiscale Framework/Vision
- **Recent Advances**
  - Theoretical Modeling/Testing
  - Numerical Integration
  - Material Characterization

Typical High Temperature Applications Demand High Performance Materials

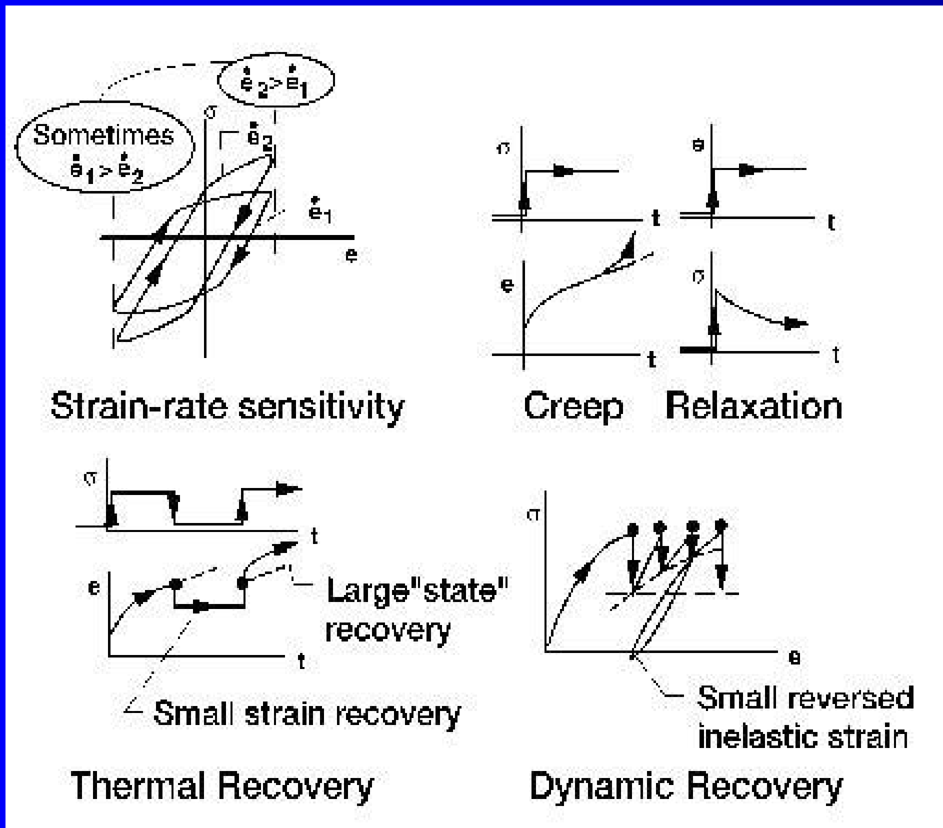


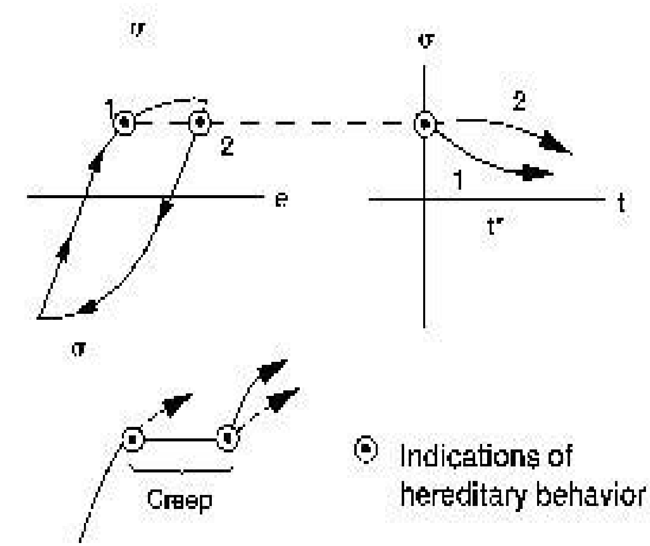
HTHL/SSTO



- Complex Thermomechanical Loading
- Complex Material response requires Time-Dependent/Hereditary Models: Viscoelastic/Viscoplastic
- Comprehensive Characterization (Tensile, Creep, Relaxation) for a variety of material systems

Important Phenomenological Observations of Behavior of Metals at High Homologous Temperatures (T/T_m>0.3)





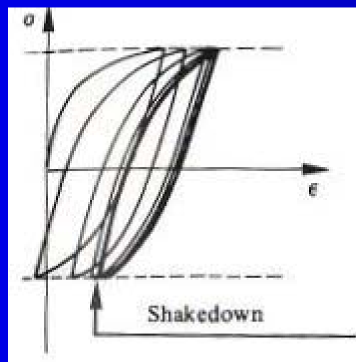
Creep-Plasticity Interactions

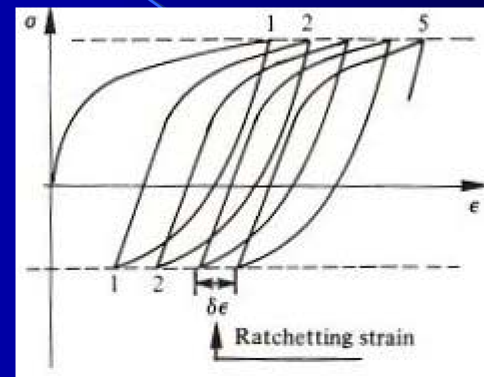
Classic Reason for Introducing Unified Viscoplastic Models (e.g., GVIPS Class)

Important Phenomenological Observations of Behavior of Metals at High Homologous Temperatures ($T/T_m > 0.3$)

Cyclic Behavior

Stress-controlled

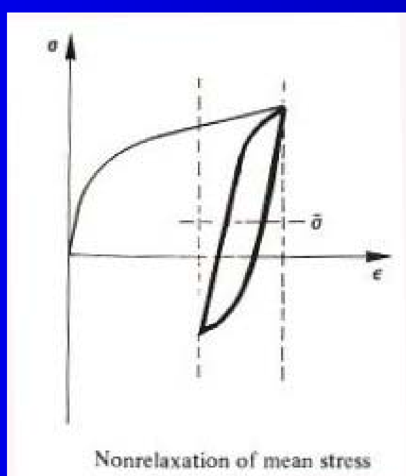


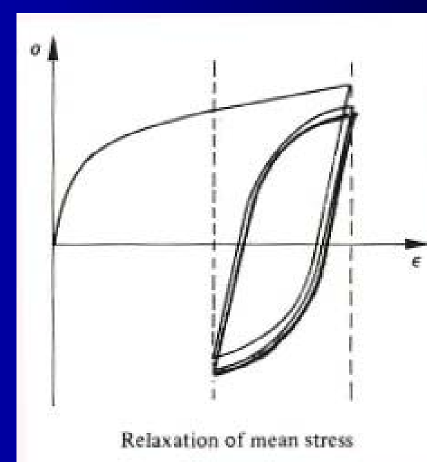


Shakedown Behavior

Ratchetting Behavior

Strain-controlled



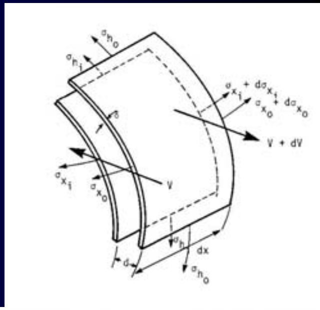


Material Behavior Can Significantly Impact Structural Response (e.g. Recovery Mechanisms)

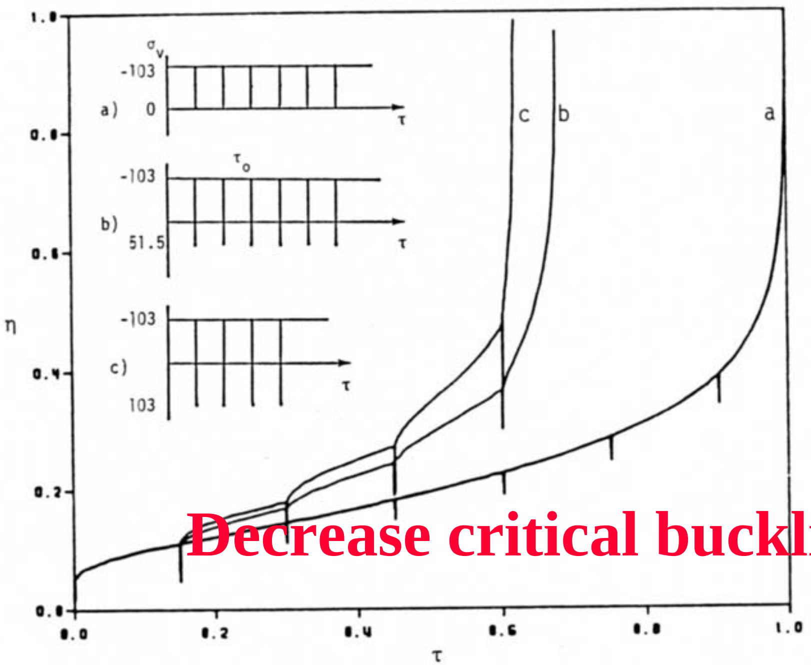
Applied Compressive Stress/Euler Stress = 0.095

Normalized Initial imperfection – 0.01

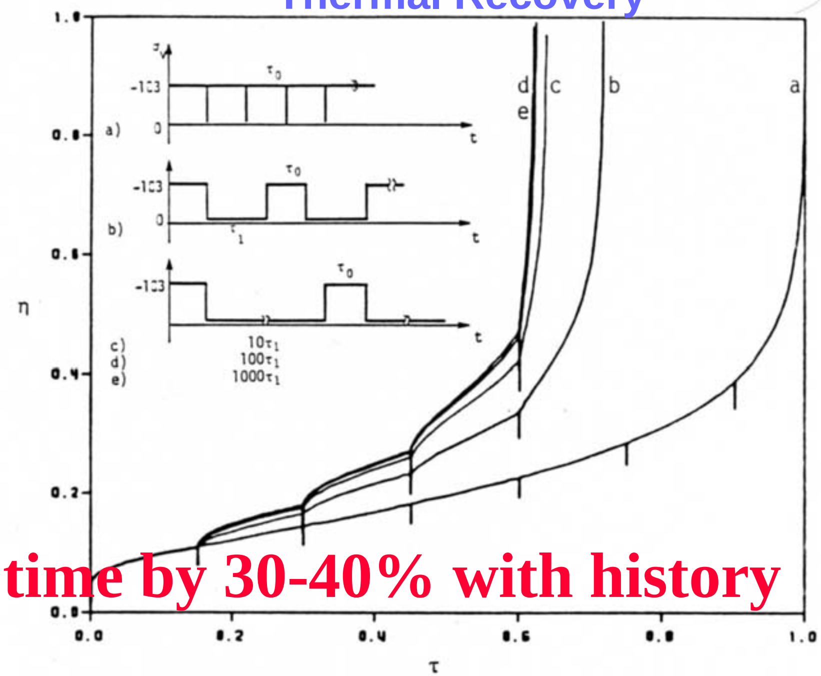
Arnold et al., " Creep Buckling of a Cylindrical Shell Under Variable Loading", Jnl of Eng Mech., ASCE, Vol. 115, No. 5, pp. 1054-1074, 1989.



Dynamic Recovery



Thermal Recovery



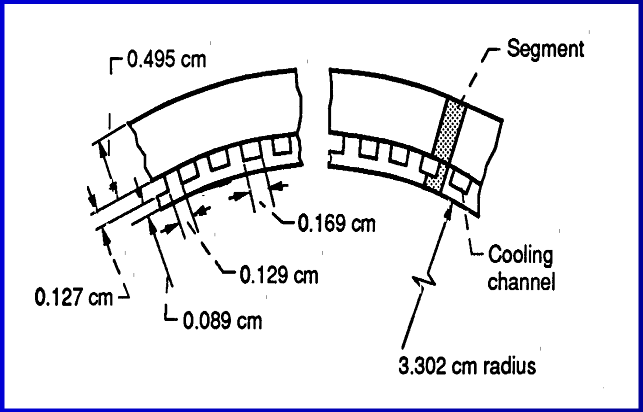
Decrease critical buckling time by 30-40% with history

Normalized radial displacement versus normalized time for variable loading histories given in inserts

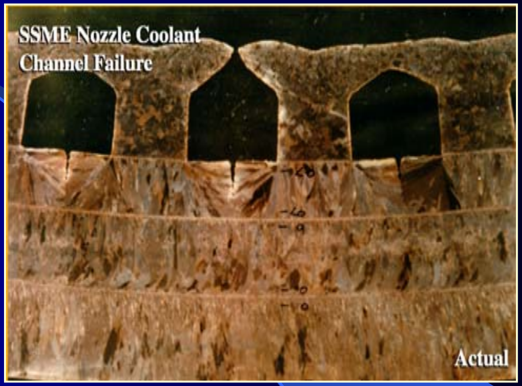
Unified Viscoplastic Models Capture Deformation Response in Rocket Engine Nozzle Liners

SSME

Nozzle Liner Geometry

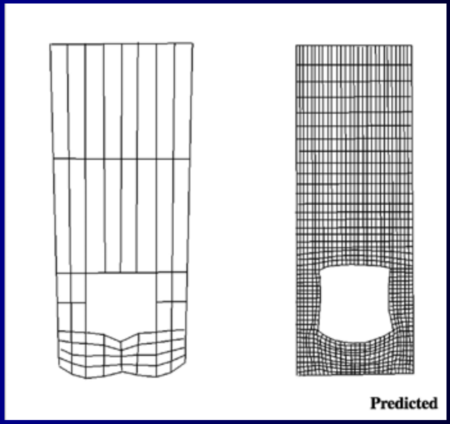


Experiment (GRC)



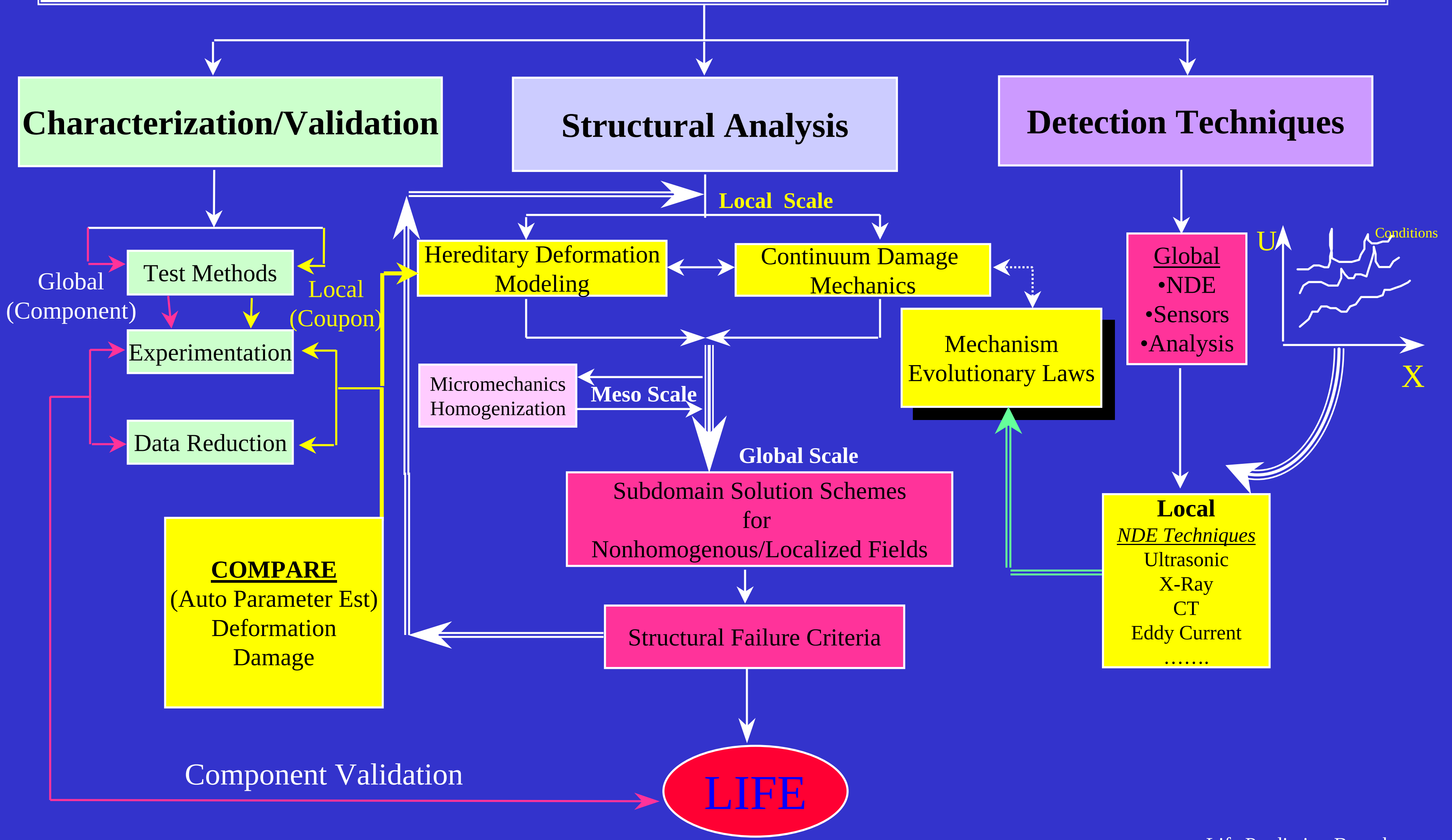
Prediction

Classical (Lockheed) Unified (GRC)



- Severe thermomechanical loading conditions result in irreversible strains
- Unified viscoplastic models successfully predict the experimentally observed deformation trends
  - Arya and Arnold, AIAA, Vol 30, No. 3, 1992

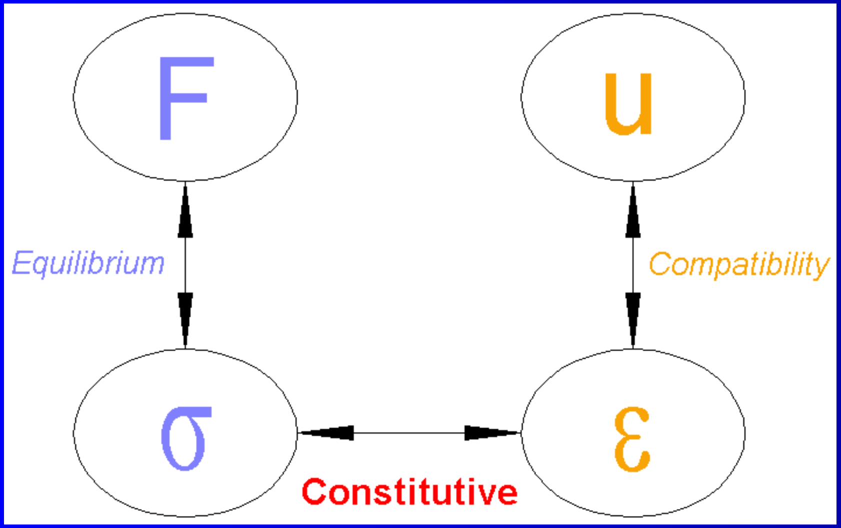
Multiscale Functional Framework for Deformation and Life Modeling



Life Prediction Branch
Structures Division GRC
SMA 7/97

CONSTITUTIVE MODELING

Structural Mechanics Problem



Knowledge of the material's life and constitutive behavior is a prerequisite for assessment of component performance/reliability

Need to **concurrently address** three important and related areas:

i) mathematical formulation for the accurate multiaxial representation **GVIPS Classes**

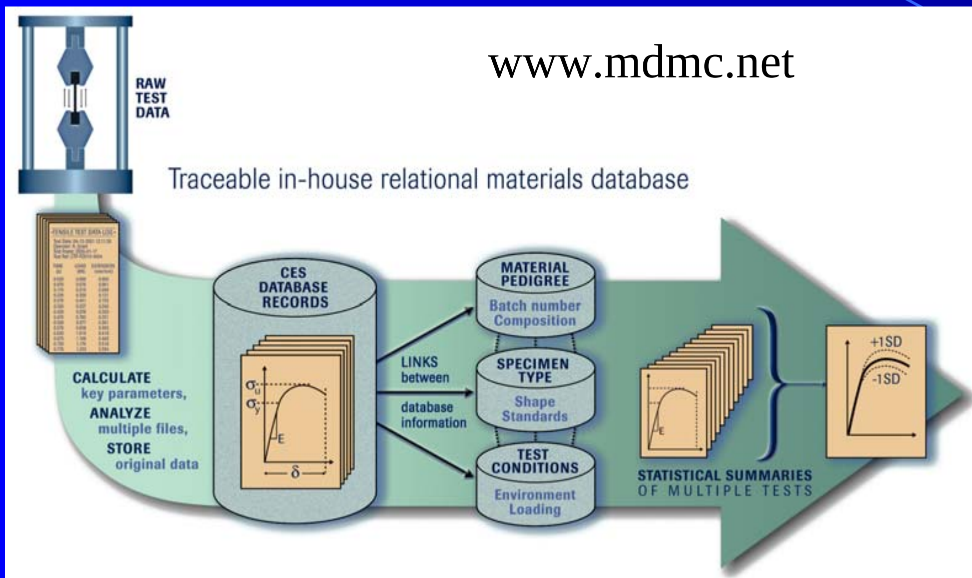
ii) algorithmic developments for the updating (integrating) of external and internal state variables -**FEA User Definable Subroutines**

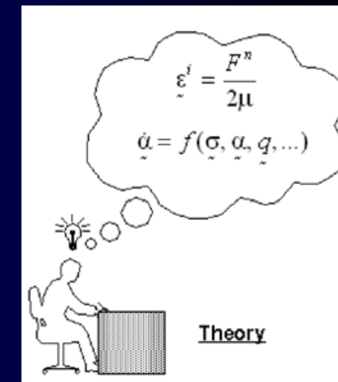
iii) parameter estimation -**COMPARE**

This approach allows one to **overcome** the **two major obstacles** for **practical utilization** of sophisticated time-dependent (hereditary) models:

1) lack of efficient and robust integration algorithms - FEA Linkage issues
2) difficulties associated with characterization of large number of material parameters and appropriate experimental "data content" - COMPARE & sensitivities

The Desired Vision For Design and Analysis





Mathematical Characterization Of Material Behavior

COMPARE

Automatically write required input information

ABAQUS ↔

Source Code

Object Code

UMAT: **Implicit** | **GVIPS**

Large Scale Implementation

- **Integration scheme**
- **Multimechanism Constitutive Relation**

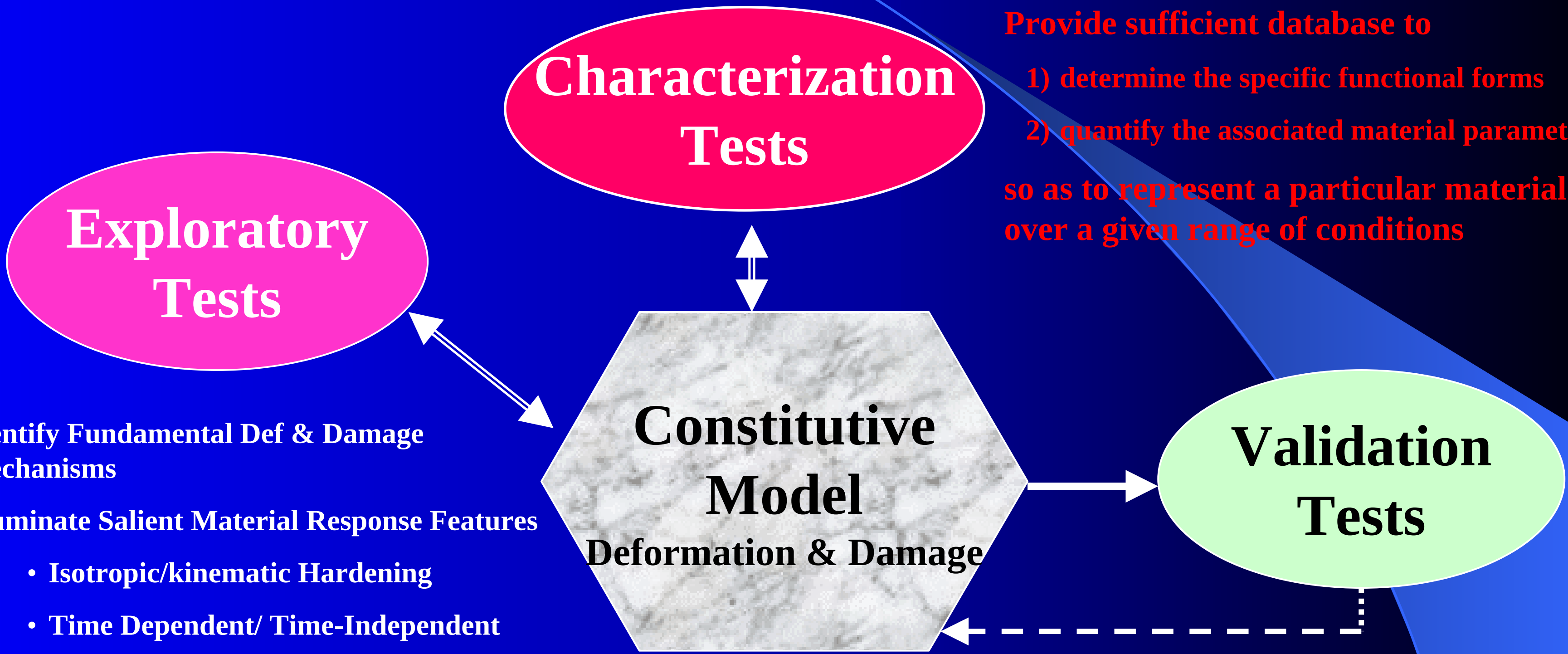
FEA Analysis of component

Thermomechanical Testing in Support of Constitutive Model Development

Provide sufficient database to

1) determine the specific functional forms
2) quantify the associated material parameters

so as to represent a particular material over a given range of conditions

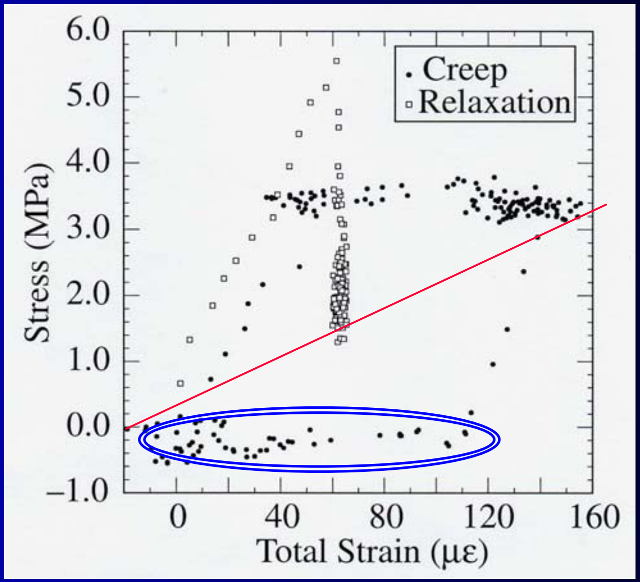


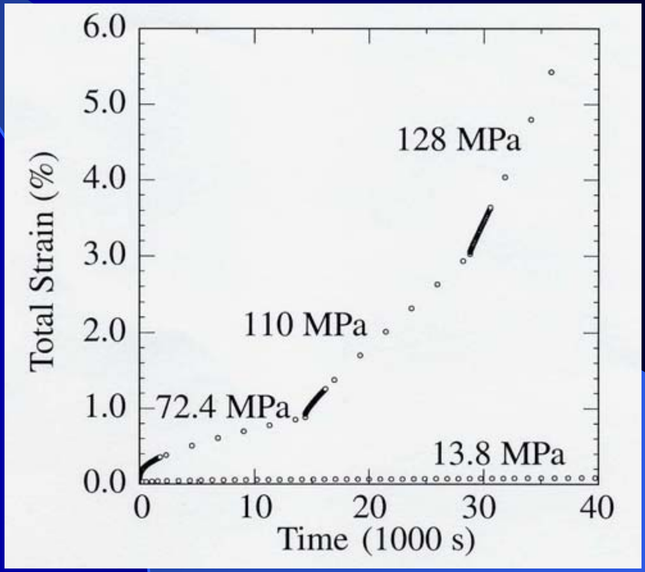
- Identify Fundamental Def & Damage Mechanisms
- Illuminate Salient Material Response Features
  - Isotropic/kinematic Hardening
  - Time Dependent/ Time-Independent
  - Sensitivity Hydrostatic Stress Field
  - Isotropic/Anisotropy Material Symmetry
- Guide Mathematical Structure of Model
- Guides Specimen design/ Test Method Development

- Often structural in nature
- Provide prototypical response data which is to be compared with model predictions
- Ideally provide feedback for subsequent model refinement

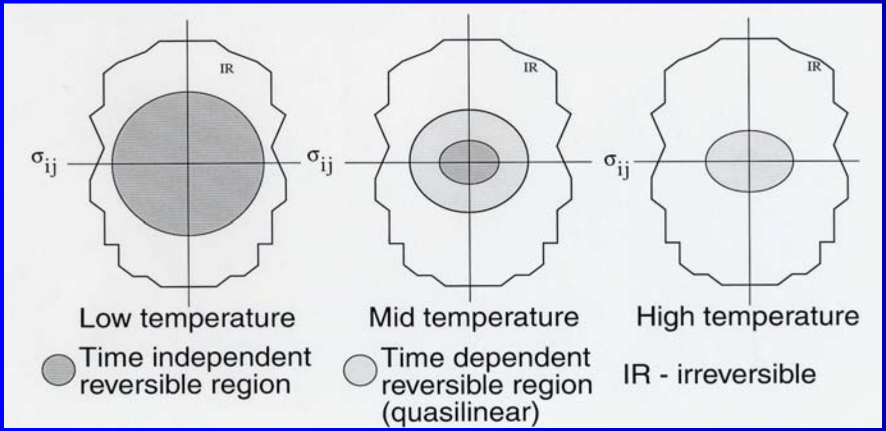
Experimental Observations

- **Reversibility**
  - rate-dependent instantaneous stiffness
  - transient creep/relaxation
  - limit equilibrium state
- Theoretical demarcation (Exp. Verified)
- **Irreversibility**
  - strain-stress dependent
  - nonlinearity
  - strain rate dependence
  - creep with steady-state
  - relaxation with finite residual state
  - creep/plasticity interaction
  - thermal recovery
  - nonlinear kinematic/isotropic hardening
- Anelastic recovery during reversal in both quasilinear and fully developed inelastic regions





Experiments Indicated Existence of Reversible and Irreversible Threshold Surface



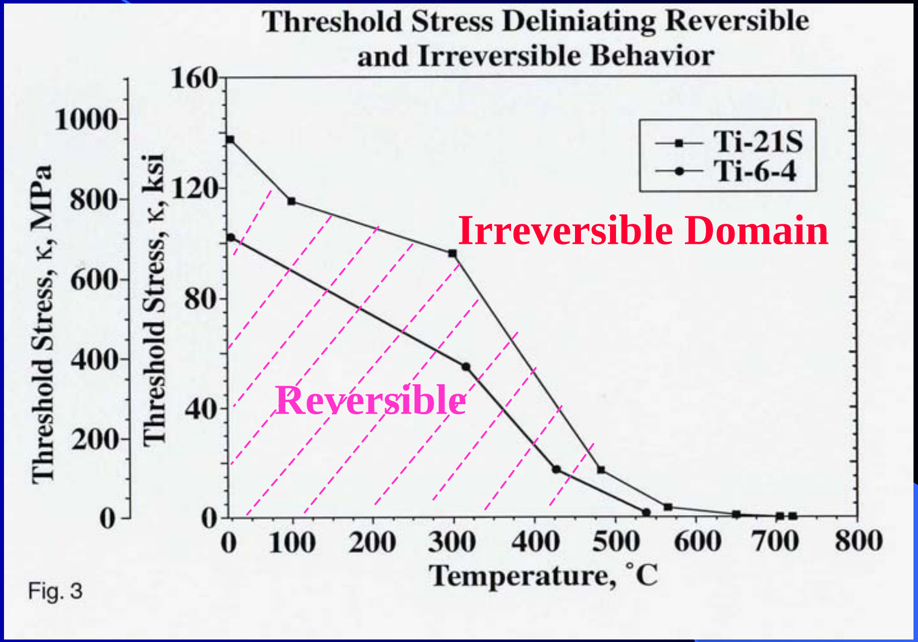
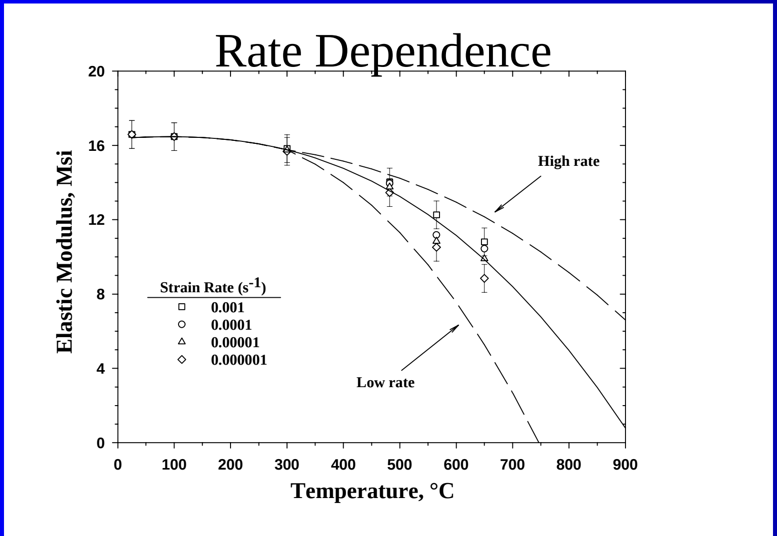


Fig. 3



Experimentally verified for both TIMETAL 21S and Ti-6-4

GRCop-84 doesn't appear to exhibit strong viscoelastic response

Theoretical/Computational Motivation

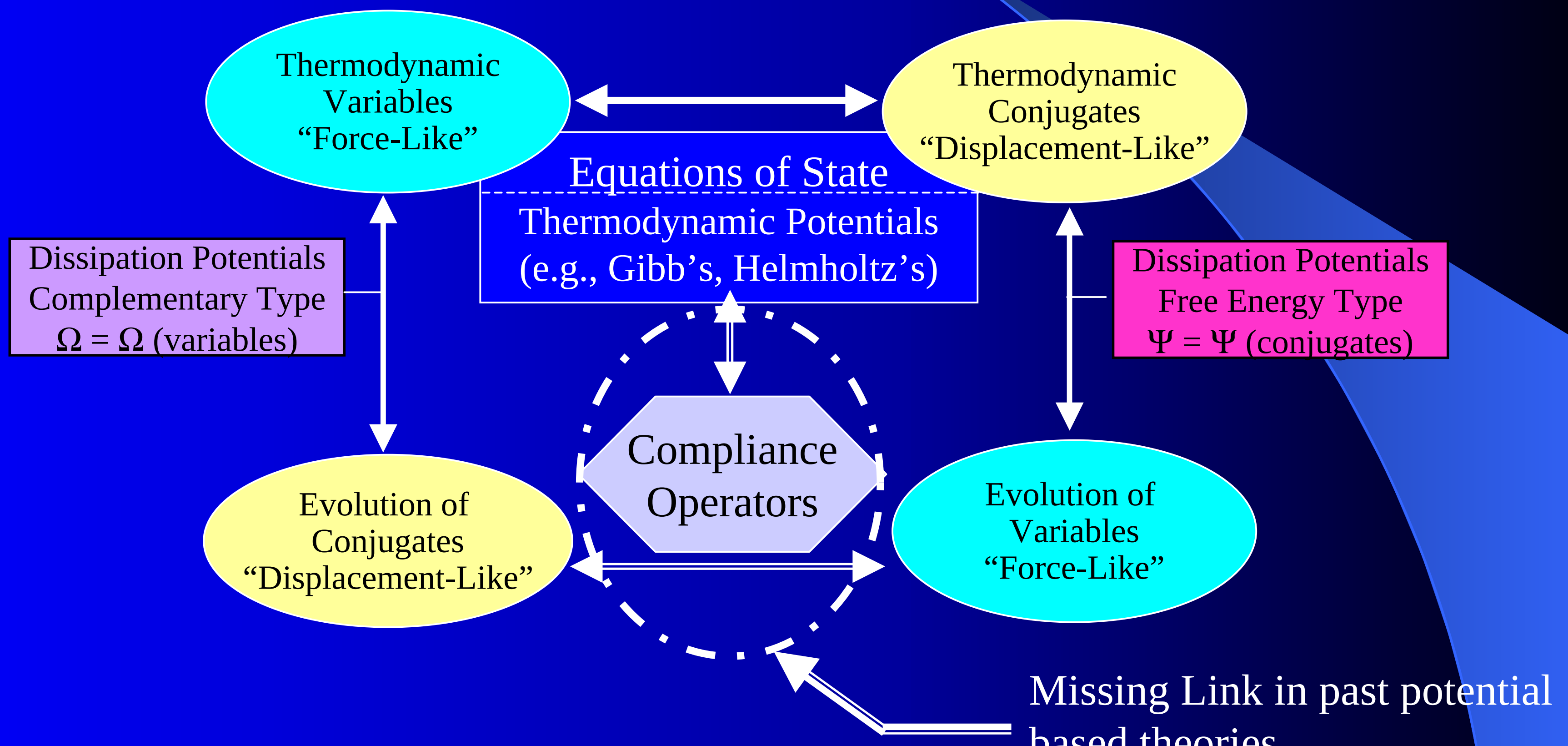
In view of **four + decades** of active research in the area of inelastic behavior modeling, the **need** still exists for an:

Accurate representation of material response details over an extensive domain of time, stress, temperature, loading conditions ...

Assessment

Technical	**Practical Implication**
Non-associative - Nonsymmetric Tangent Stiffness - Coupled system of Stiff Diff. Eq.	⇒ Non-uniqueness of solution ⇒ Implementation into large scale FEA codes problematic ⇒ Difficult to integrate
Numerous nonphysical material parameters	⇒ Requires expertise to characterize model
Single-mechanism models	⇒ Qualitatively capable, yet quantitatively limited in response spectrum

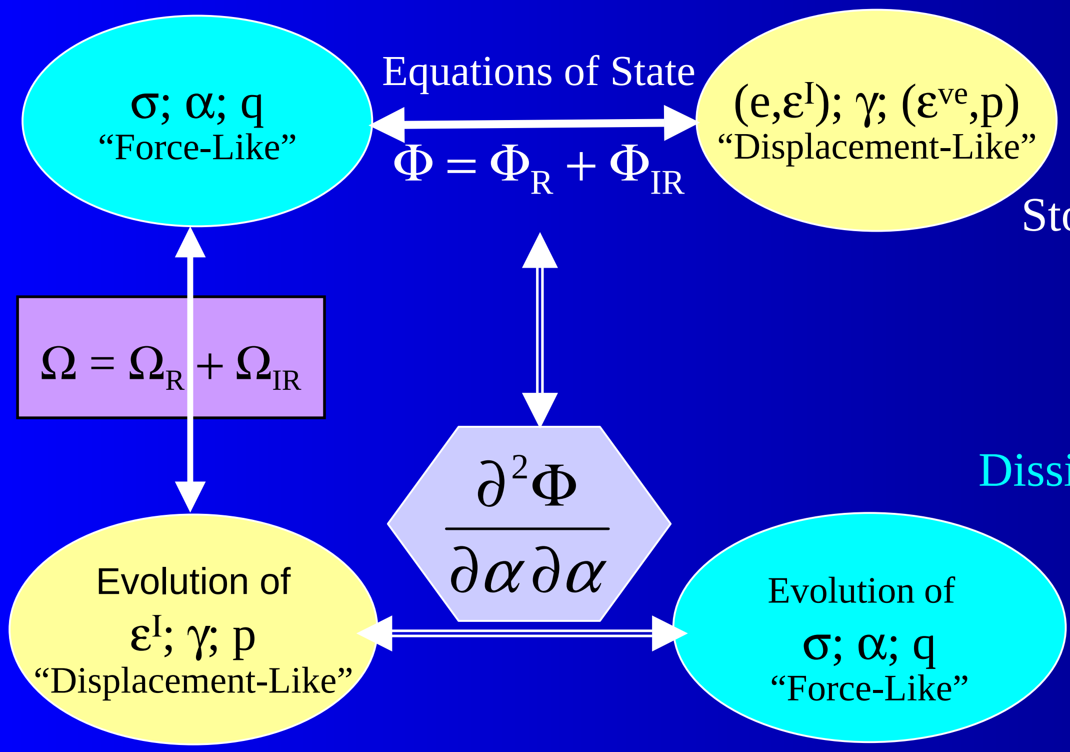
Utilize Concept of Thermodynamic Internal State Variables to Obtain Constitutive Equations



Advantages and Attributes of Potential Formulation

- Provides a consistent framework for deformation and damage modeling
  - Nonisothermal and/or anisotropic extension straight forward
  - Nonproportional loading histories automatic
  - Automatic satisfaction of the <u>Dissipation</u> <u>Inequity</u> of Thermodynamics
- Eliminates the “ad-hoc” nature of model development
- Provides sufficiently general variational structure.
- Constitutes cornerstone of regularity and bounding (or limit) theorems in plasticity and viscoplasticity.
- Lends itself to robust numerical implementation

Physical Mechanisms Underlying The Partitioning of Energy : Complementary Type



Total = Stored + Dissipated

$\sigma e = \Phi + \Omega$

Stored (Φ) = Reversible + Irreversible

Lattice Distortion — Dislocation Pile-up

Reflects change in microstructure

Dissipation (Ω) = Reversible + Irreversible

Dislocation bowing — Deformation & Thermally driven Mechanism

Reflects mobility/rate of evolution in microstructure

Irreversible = Ω_1 (deformation) + Ω_2 (diffusional; mass/vacancy)

Glide/plastic Slip

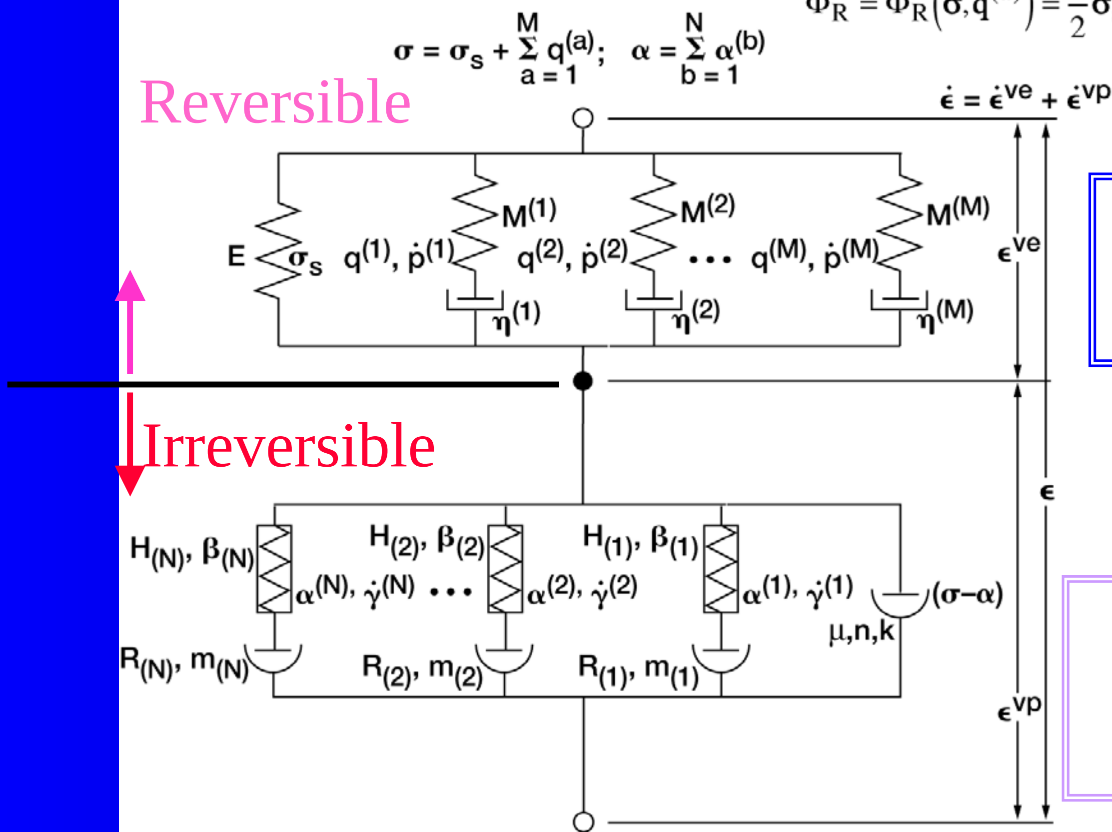
- **Thermal recovery**
- **Dislocation/boundary interaction**
- **Formation of cell structure**

General Multimechanism Hereditary Behavior Model of the GVIPS Class

$$\Phi = \Phi_R + \Phi_{IR} \qquad \Omega = \Omega_R + \Omega_{IR}$$

$$\Phi_R = \Phi_R\left(\boldsymbol{\sigma}, \mathbf{q}^{(a)}\right) = \frac{1}{2}\boldsymbol{\sigma}_s : \mathbf{E}^{-1} : \boldsymbol{\sigma}_s + \frac{1}{2}\sum_{a=1}^{M} \mathbf{q}^{(a)} : \left[\mathbf{M}^{(a)}\right]^{-1} : \mathbf{q}^{(a)} + \sum_{a=1}^{M} \mathbf{q}^{(a)} : \mathbf{p}^{(a)}$$

$$\Omega_R = \frac{1}{2}\sum_{a=1}^{M} \mathbf{q}^{(a)} : \left[\eta^{(a)}\right]^{-1} : \mathbf{q}^{(a)}$$



Eqs. of state: $\varepsilon^{ve} = \left(\dfrac{-\partial \Phi_R}{\partial \sigma_s}\right)$

Flow law: $\dot{p}^{(a)} = \dfrac{\partial \Omega_R}{\partial q^{(a)}}; \qquad a = 1, 2, \ldots, M$

$$\Phi_{IR} = \Phi_{IR}\left(\boldsymbol{\sigma}, \alpha^{(b)}\right) = \sigma : \varepsilon^{vp} + \sum_{b=1}^{N} \overline{H}_{(b)}\left(\alpha^{(b)}\right)$$

$$\Omega_{IR} = \Omega_1(\boldsymbol{\sigma} - \boldsymbol{\alpha}) + \sum_{b=1}^{N} \Omega_2^{(b)}\left(\alpha^{(b)}\right)$$

Flow law:

$$\dot{\varepsilon}^{vp} = \frac{\partial \Omega}{\partial \sigma} = \frac{\partial \Omega_1}{\partial \sigma}$$

Evolutionary law:

$$\dot{\gamma}^{(b)} = \frac{-\partial \Omega_{IR}}{\partial \alpha^{(b)}}; \qquad b = 1, 2, \ldots, N$$

Internal State Rate Eqs.:

$$\dot{\alpha}^{(b)} = L\dot{\gamma}^{(b)}; \quad L = \left[\frac{-\partial^2 \Phi_{IR}}{\partial \alpha^{(b)} \partial \alpha^{(b)}}\right]^{-1}$$

Specific Choice of Energy Potentials and Material Functional Forms

$$\Phi_R = \Phi_R(\boldsymbol{\sigma}_{ij}, \mathbf{q}_{ij}^{(a)}) = \frac{1}{2}(\boldsymbol{\sigma}_s)_{ij}\, \mathbf{E}^{-1}_{ijkl}(\boldsymbol{\sigma}_s)_{kl} + \frac{1}{2}\sum_{a=1}^{M} \mathbf{q}_{ij}^{(a)}[\mathbf{M}_{ijkl}^{(a)}]^{-1}\mathbf{q}_{kl}^{(a)} + \sum_{a=1}^{M}\mathbf{q}_{ij}^{(a)}\mathbf{p}_{ij}^{(a)}$$

$$\Phi_{IR} = \Phi_{IR}(\boldsymbol{\sigma}_{ij}, \boldsymbol{\alpha}_{ij}^{(b)}) = \boldsymbol{\sigma}_{ij}\boldsymbol{\varepsilon}_{ij}^{vp} + \sum_{b=1}^{N} \bar{H}_{(b)}(G^{(b)})$$

Stored Energy

and

$$\Omega_R = \frac{1}{2}\sum_{a=1}^{M} \mathbf{q}_{ij}^{(a)}[\boldsymbol{\eta}_{ijkl}^{(a)}]^{-1}\mathbf{q}_{kl}^{(a)}$$

$$\Omega_{IR} = \Omega_1(F) + \sum_{b=1}^{N} \Omega_2^{(b)}(G^{(b)})$$

Dissipation

where

$$F = \frac{1}{2\kappa^2}(\boldsymbol{\sigma}_{ij} - \boldsymbol{\alpha}_{ij})\mathcal{M}_{ijkl}(\boldsymbol{\sigma}_{kl} - \boldsymbol{\alpha}_{kl}) - 1$$

$$G^{(b)} = \frac{1}{2\kappa_{(b)}^2}(\boldsymbol{\alpha}_{ij}^{(b)}\mathcal{M}_{ijkl}\,\boldsymbol{\alpha}_{kl}^{(b)})$$

and the specific functions :

$$\Omega_1(F) = \int \frac{\kappa^2 F^n}{2\mu} dF \qquad \Omega_2^{(b)}(G^{(b)}) = \kappa_{(b)}^2 \int \frac{r(G^{(b)})}{h(G^{(b)})} dG^{(b)} \qquad \bar{H}_{(b)} = \kappa_{(b)}^2 \int \frac{1}{h(G^{(b)})} dG^{(b)}$$

$$r(G^{(b)}) = R_{(b)}[G^{(b)}]^{m_{(b)}}$$

$$h_{nonsat}(G^{(b)}) = \frac{H_{(b)}}{[G^{(b)}]^{\beta_{(b)}}}$$

$$h_{sat}(G^{(b)}) = H_{(b)}\left\langle 1 - \sqrt{G^{(b)}} \right\rangle^{\beta_{(b)}}$$

Results Illustrating Recent Improvements Made to the Hardening Functional Form in GVIPS Model

Previous Non-saturating

$g(G)=H / G^{ß}$

Current Saturating Form

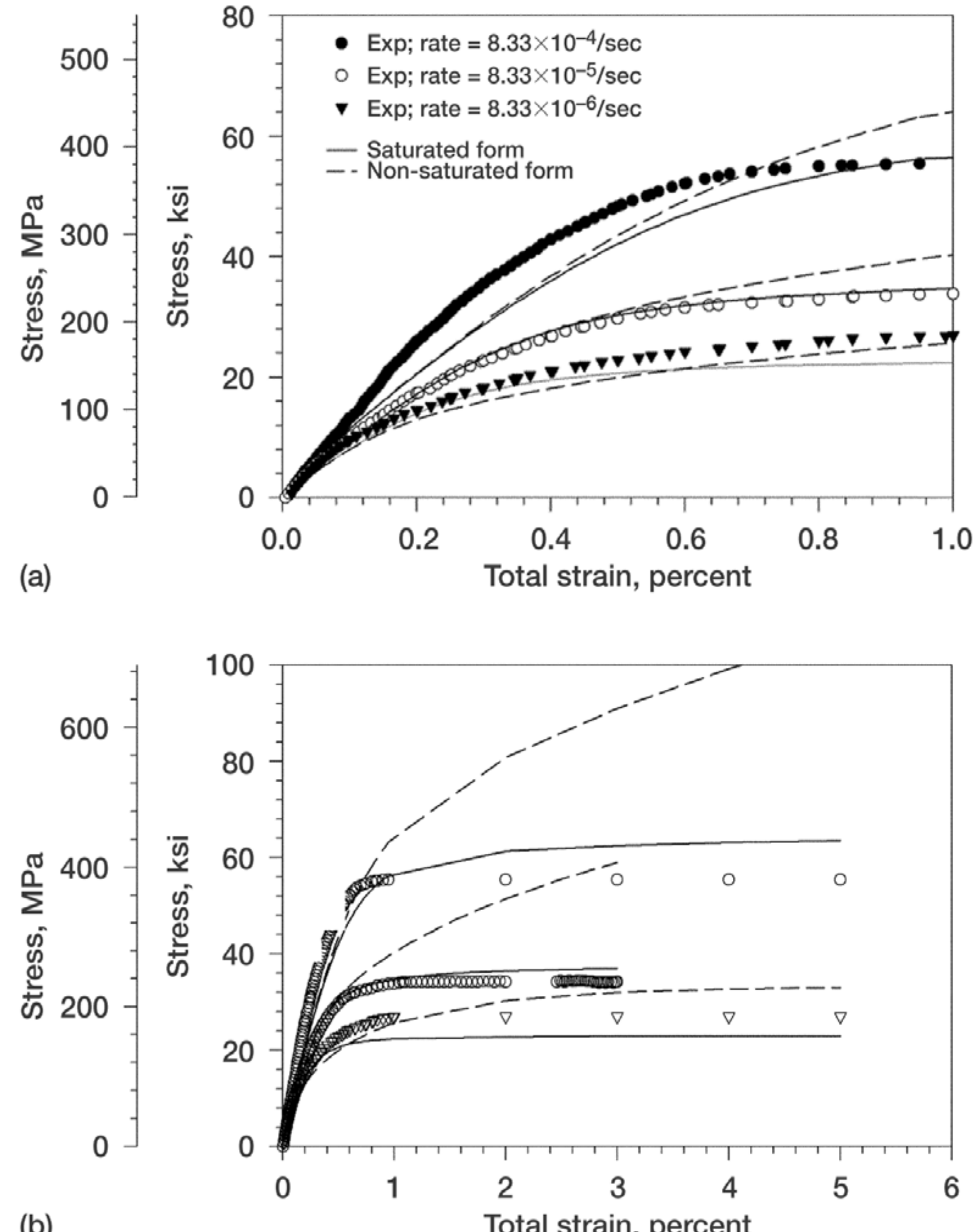
$g(G)=H(1-G)^{ß}$

$G = [½(\alpha_{ij}\ \alpha_{ij})/\ \kappa^{2}_{(b)}]^{0.5}$

TIMETAL 21S: 650°C

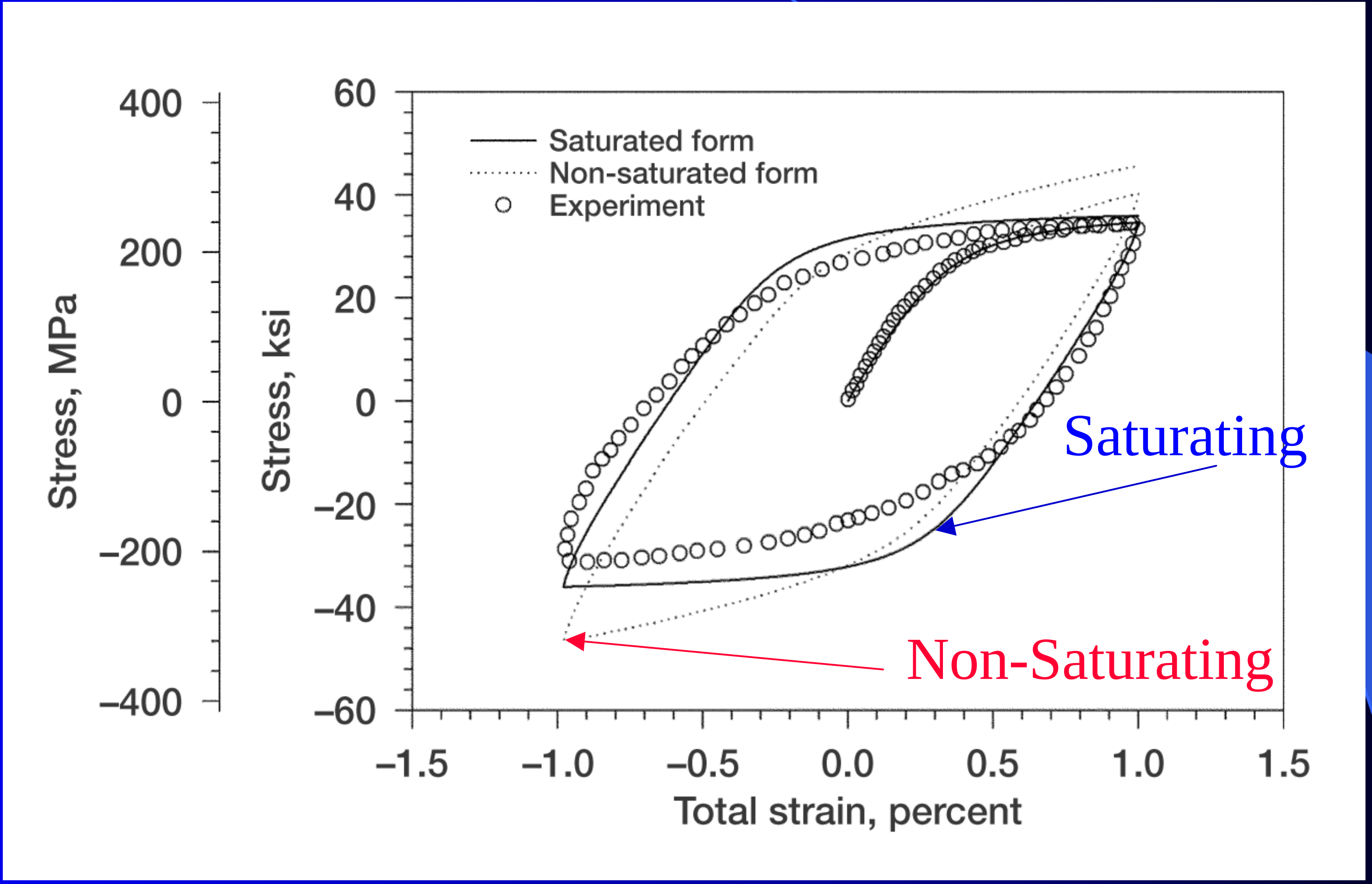
Strain Controlled Tensile

Single Mechanism



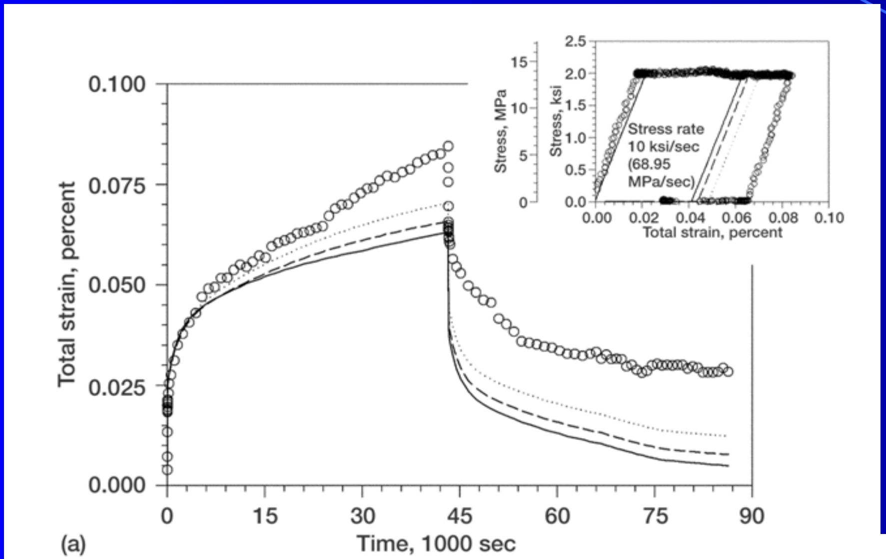
Demonstrates how scale-abuse can be used

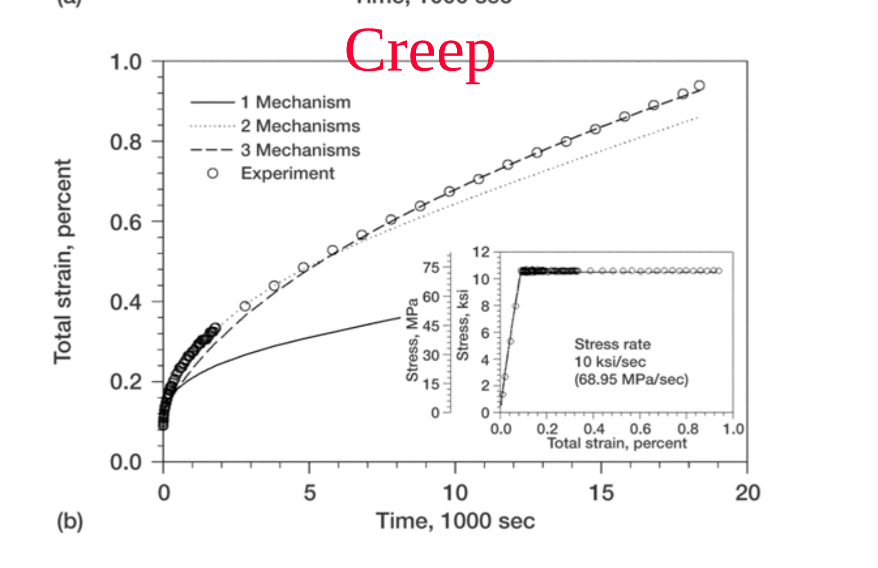
Comparison of Specific Hardening Forms Under Cyclic Loading

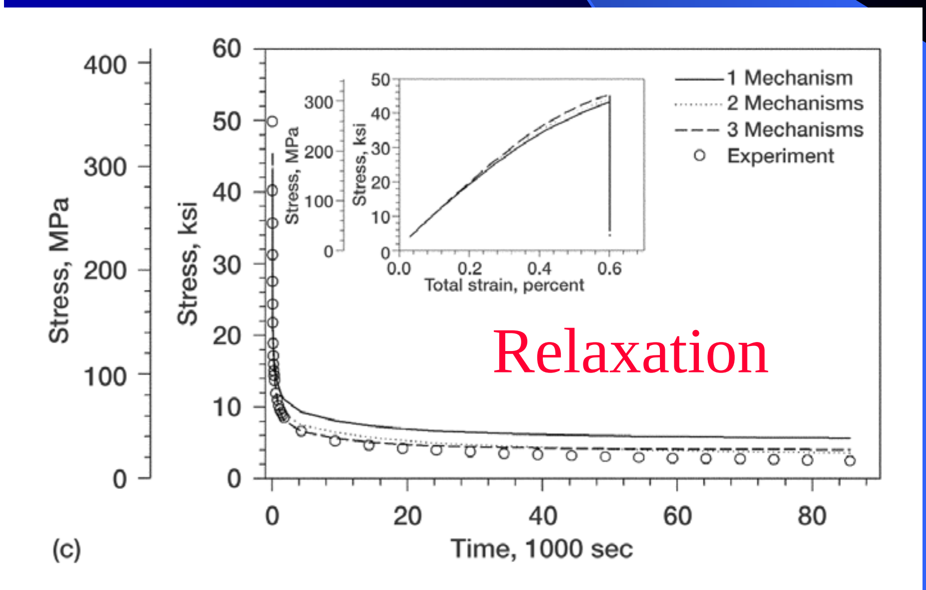


TIMETAL 21S: 650°C   Strain Controlled

New Saturating Form Does Not Adversely Impact Ability to Represent Creep/Relaxation







- But need at <u>least two</u> mechanisms to capture both creep and relaxation well

Robust Integration Scheme Key For Efficient Inelastic Finite Element Analysis

Common approaches for integration of rate equations:

1) Non-Iterative: explicit; semi-implicit

No local iterations ☑ less overhead stability problems

2) Iterative: fully-implicit

Requires local iterations ☑ additional overhead

Unconditional stability

Consistent Tangent Stiffness ☑ Quadratic Convergence of global Newton-Raphson Iterations

Advantages of Implementation

- Directly applicable for 3-D and sub-space loading(plane strain, axisymmetric, etc)
- Generalized Material Symmetry Operators (which influence flow, hardening, recovery, relaxation spectrum, etc.)
- Efficiency (through explicit algorithmic tangent stiffness)
- Robustness (through “slack” line search)

Selected:

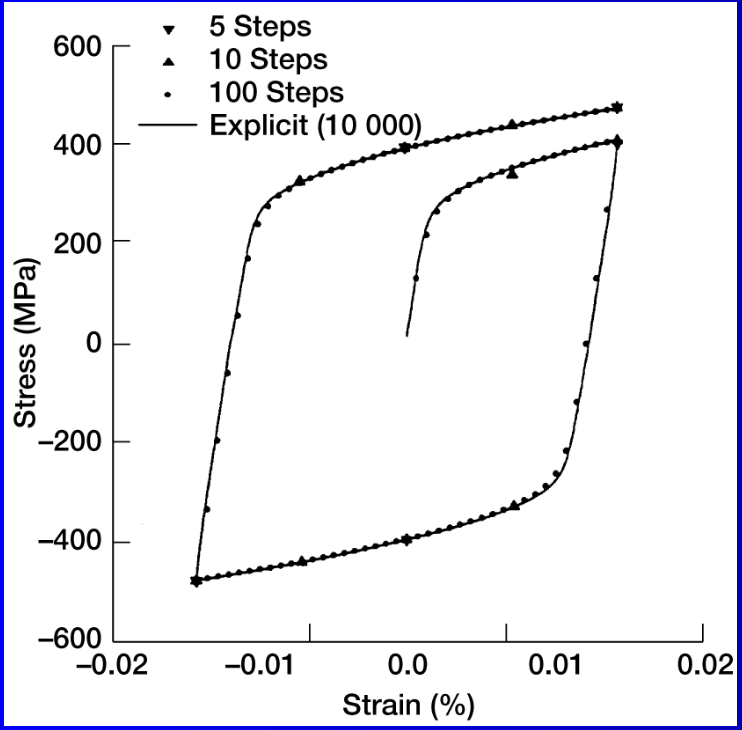
Backward Euler with Line Search

Results Illustrating the Efficiency of The Numerical Implementation of GVIPS

Backward Euler with Line Search

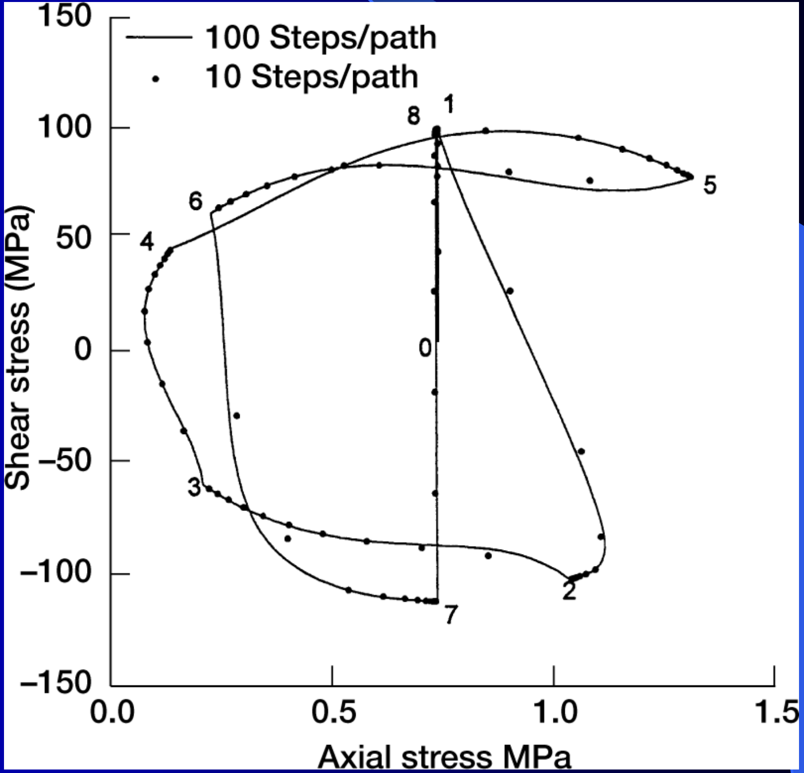
W/Kanthal , $\dot{\varepsilon}$=2x10^{-3}/s , ε_{max}=0.0144

method	number of load steps	CPU time	GIT	LIT
explicit	10,000	180.0	3	0
implicit	100	5.0	2	4
implicit	10	1.05	4	10
implicit	5	1 (54 s)	10	20



Under cyclic conditions

**Explicit Failed



Under nonproportional loading conditions

Key to Accurate Characterization of GVIPS Involves Sufficient "Data Content"

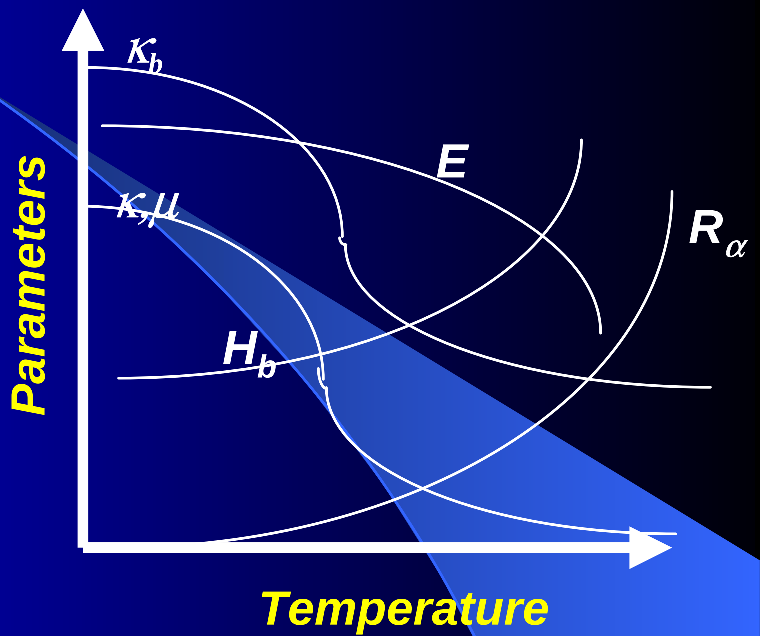
Viscoelastic Material Parameters

2+2M number, i.e., E_s, ν, $(M_{(a)}, \rho_{(a)})$

Viscoplastic Material Parameters

- Flow κ, μ, n
- Hardening H_b, κ_b and β,
- Recovery: R_b and m_b

3 + 5N irreversible material constants



Types of Experimental Tests

Strain controlled Tensile Tests (multiple rates)
Creep Test (Monotonic and/or step)
Relaxation (Monotonic and/or step)
Cyclic Tests (Fully reversed, ratcheting)
Biaxial Tests (tensile, creep, relaxation, cyclic)

Desire a mixture (rather than numerous of one type) of tests at numerous temperatures

Quality vs. Quantity

COMPARE CORE

Optimizer

Sequential Quadratic Programming (SQP)

Sensitivity

Direct Differentiation Approach

Analyzer

Implicit Integration for Primal Analysis

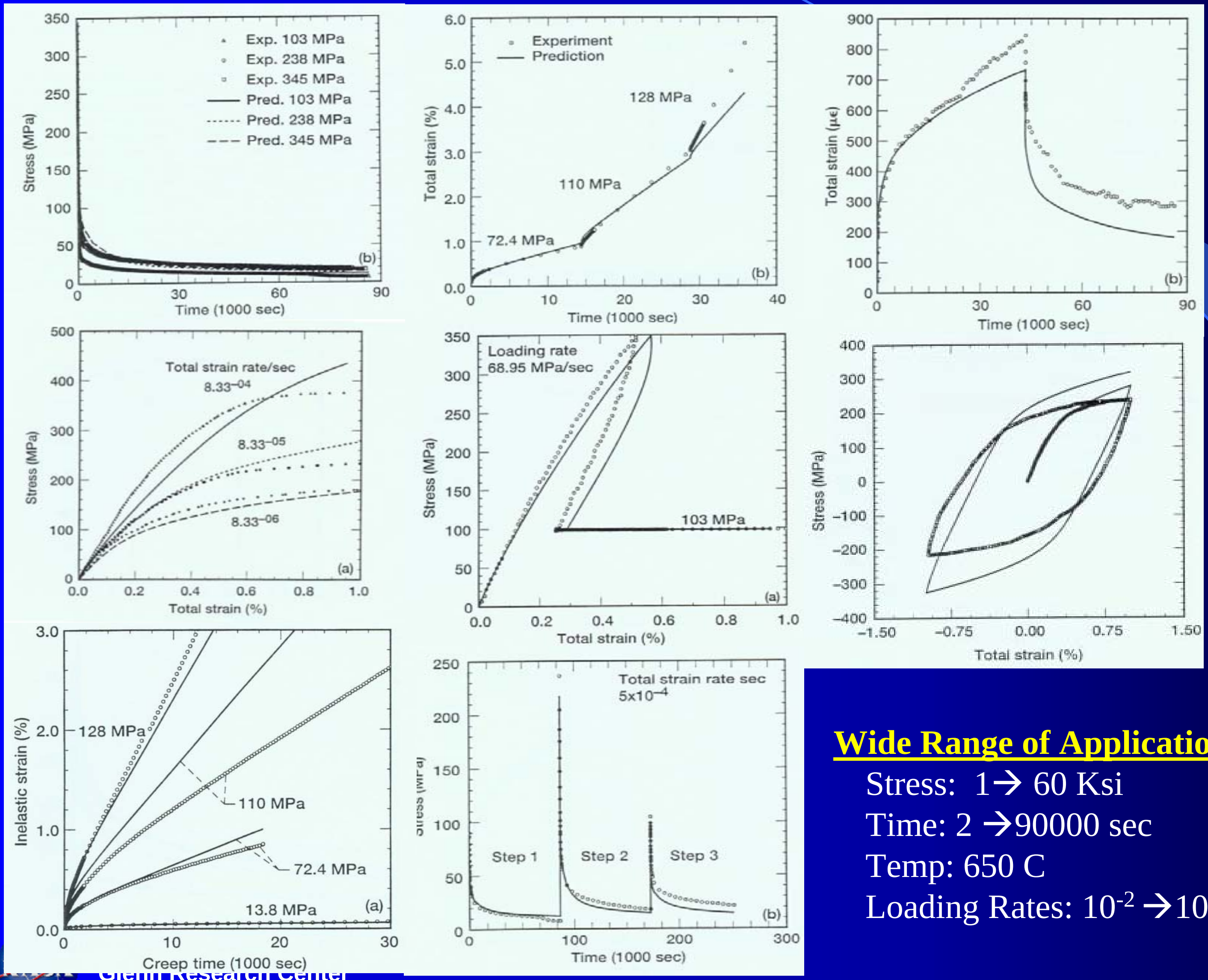
COMPARE (driver)

- Identify active/passive variables for a test
- Scaling design variables and objective function
- Formulating a single design optimization problem
  weighted objective function.
  Constraints
  sensitivities

Results

- Final Optimum Material Parameters
- Combined & Individual Error Functions

Comprehensive Characterization of The Deformation Response of TIMETAL21S

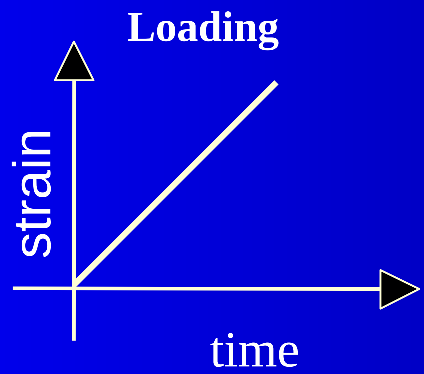


"DATA CONTENT" IS HUGE ISSUE

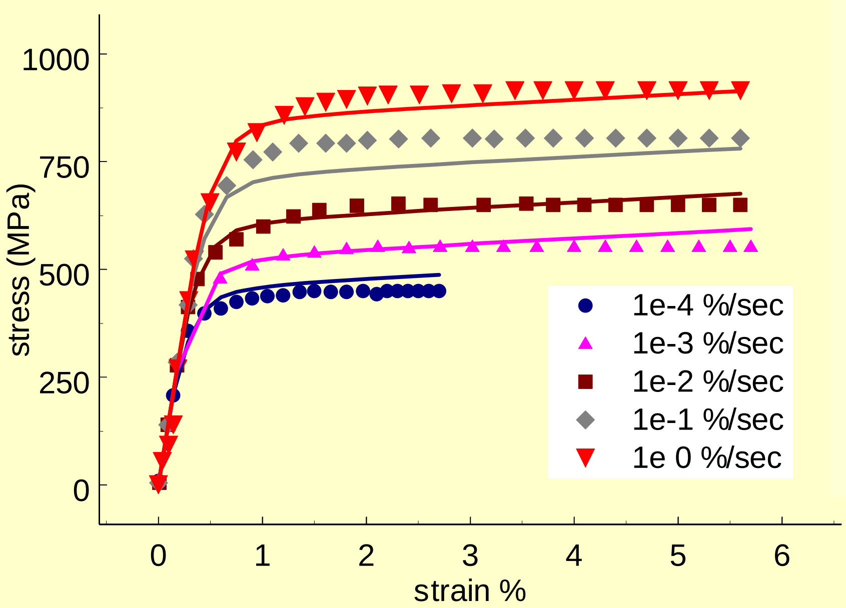
Wide Range of Application

- Stress: 1 → 60 Ksi
- Time: 2 → 90000 sec
- Temp: 650 C
- Loading Rates: $10^{-2} \rightarrow 10^{-10}$

Characterization of IN738LC @ 850 ^{0}C



Elastic + 4 Viscoplastic Mechanisms

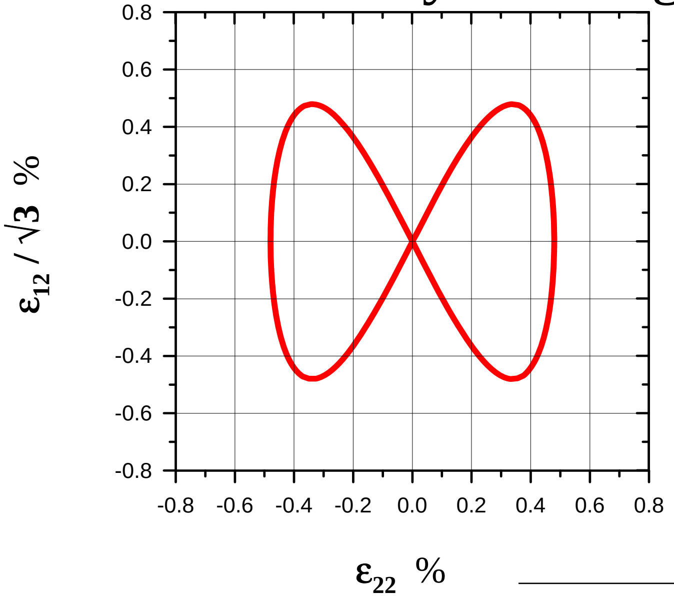


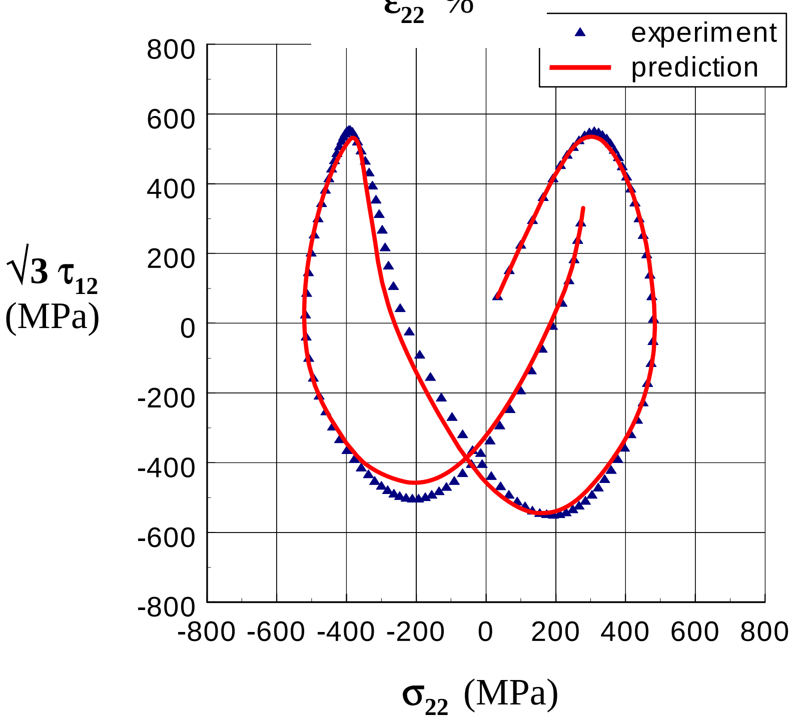
Final characterized parameters using four Viscoplastic mechanisms for IN738LC @850^0 C

Material Parameter	Units	Value	Material Parameter	Units	Value
E	MPa	$1.5x10^5$	β_1	-	1 (6)*
ν	-	0.33	β_2	-	1 (6)*
κ	MPa	0.1	β_3	-	1 (6)*
κ_1	MPa	61.43	β_4	-	1 (6)*
κ_2	MPa	64.37	R_1	1/s	$1.0x10^{-21}$
κ_3	MPa	62.30	R_2	1/s	$1.0x10^{-21}$
κ_4	MPa	75.08	R_3	1/s	$1.0x10^{-21}$
n	-	1.486	R_4	1/s	$1.0x10^{-21}$
μ	MPa -s	$3.79x10^{14}$	H_1	MPa	$4.6x10^4$
m_1	-	0.001	H_2	MPa	$5.13x10^4$
m_2	-	0.001	H_3	MPa	$8.33x10^7$
m_3	-	0.001	H_4	MPa	$9.458x10^7$
m_4	-	0.001			

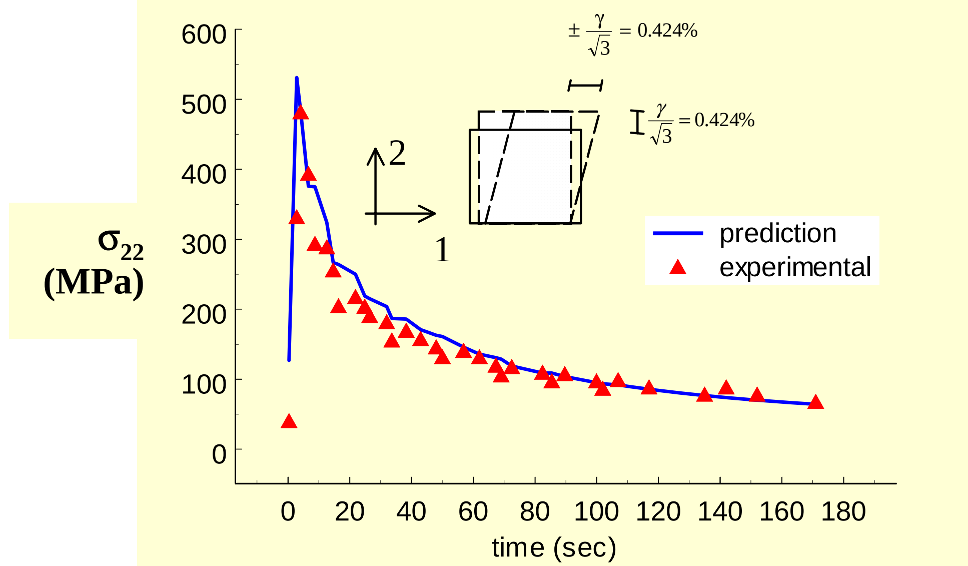
* the value between parentheses was determined in the FE simulation of the experiment

Butterfly Loading

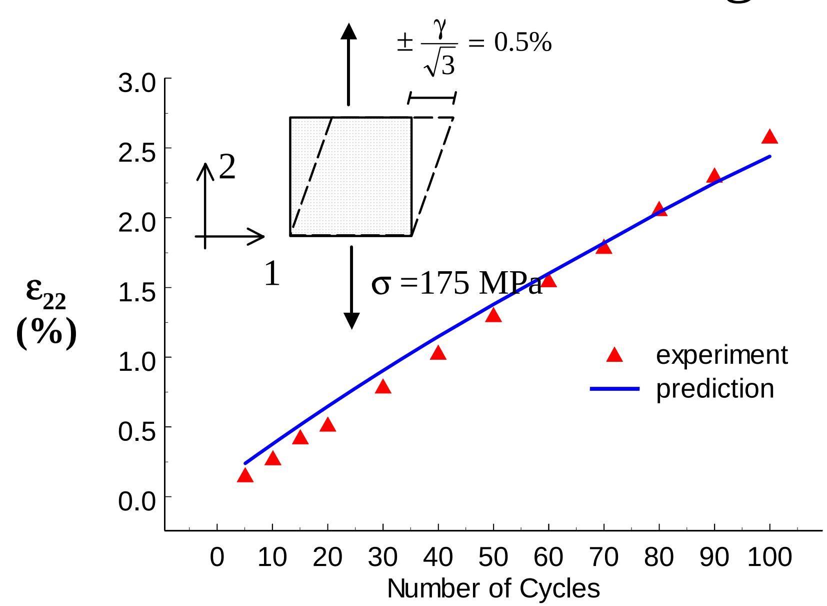




Multiaxial stress relaxation



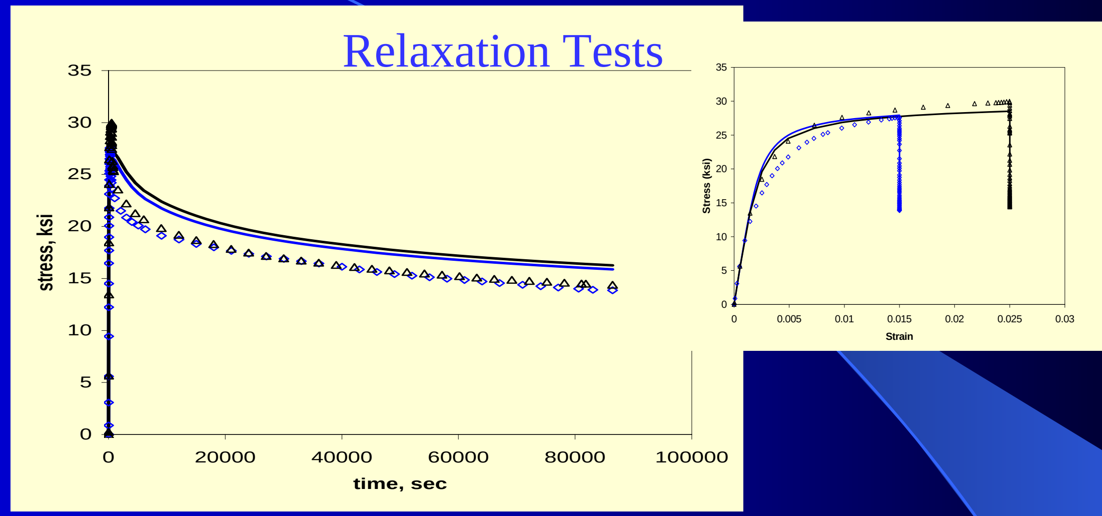
Multiaxial ratchetting

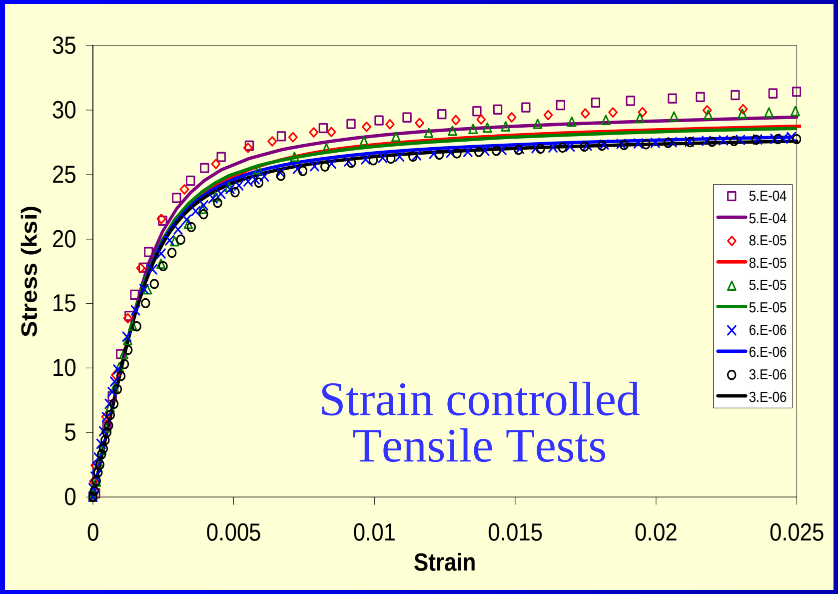


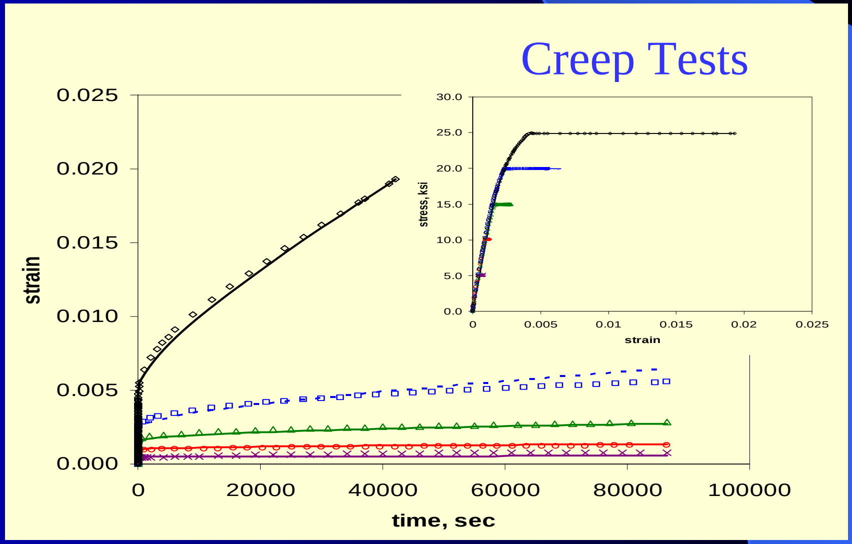
Correlation of GRCop-84 Utilizing Multimechanism GVIPS Model

1 VE mechanisms

4 VP mechanisms







Structural Verification Testing

- Ideally should provide feedback for subsequent model refinement
- Provide prototypical response data which is to be compared with model predictions

Consequently:

- Need accurate temperature, strain and load information at a variety of locations - required for any true validation
- Number of cycles to failure (alone) not enough
- Instrumentation incredibly challenging (sever environment)

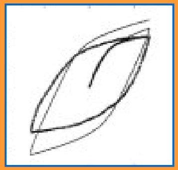
Summary of Advances in Material Modeling (Synergistic Technology)

- Generalized, Fully Associative, Multimechanism, Viscoelastoplastic Model Available
  - Reversible/Irreversible Regimes
  - Spanning wide time, stress, temperature spectrum
  - Nonlinear Hardening with Saturation
  - Ability to capture ratcheting
  - Stiffness and/or Strength Reduction
- Automated Material Model Characterization
  - via **COMPARE**
  - **Materials thus far:**
    - **Ni based; Cu based; Ti**
    - **MMC and PMC**
- Implicit Integration Algorithms
  - Directly applicable for 3D/sub-space loading
  - Generalized Material Symmetry Operators (which influence flow, hardening, recovery, relaxation spectrum, etc.)
  - Efficiency (through explicit algorithmic tangent stiffness)
  - Robustness (through “slack” line search)
- Now Commercially Available
  - COMPARE
  - GVIPS – via UMATs

Open Channel Software

www.openchannelfoundation.org

Experiments



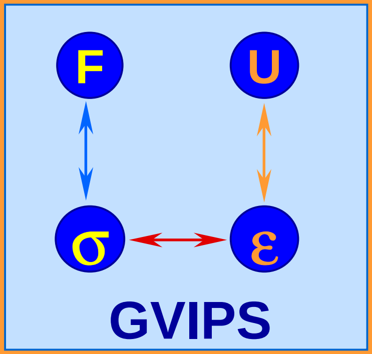
Multiple Experiments produce data

37446.27292	0.838069
37448.29514	1.320609
37450.27153	1.793447
37453.27222	1.005082
37455.28194	1.068973
37457.26597	1.040952
37460.45486	1.268637
37461.67014	1.357503
37462.34931	1.089025
37464.27778	1.13265
37467.28403	1.096359
37469.27153	1.064865

Data

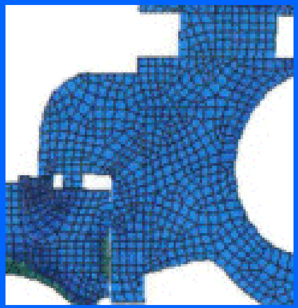
COMPARE σ ε GVIPS

COMPARE fits the GVIPS material parameters to experimental data within minutes.



User Definable Material Model

The resulting UMAT can be immediately accessed by the Finite Element Analysis



Finite Element Analysis

Future Work

- Extend formulation to account for
  - Coupled Nonisothermal Issues
  - Probabilistic Material Behavior
- Characterize additional material systems
- Verify under prototypical loading histories
- Implement softening (damage) mechanisms into COMPARE – theory complete
  - Characterize strength/stiffness reduction parameters to account for softening effects

Thank You

Questions?

Selected References

- Arnold, S. M., and Saleeb, A.F., ‘‘On the Thermodynamic Framework of Generalized Coupled Thermoelastic-Viscoplastic -Damage Modeling”, Jnl of Int. Plasticity, Vol. 10, No. 3.,pp. 263-278, 1994
- Arnold, S. M.., Saleeb, A.F. and Wilt, T.E., ‘‘An Investigation of the Modeling of Thermal/Dynamic Recovery and Nonlinear Hardening in Potential Based Viscoplasticity”, Int. Jnl. of Engng. Mat. & Tech., Vol. 117, No. 2, pp. 157-167, 1995
- Arnold, S. M., Saleeb, A.F., Castelli, M.G., ‘‘A Fully Associative, Nonisothermal, Non-Linear Kinematic, Unified Viscoplastic Model For Titanium Based Matrices”, *Thermo-Mechanical Fatigue Behavior of Materials: Second Volume*, ASTM STP 1263, M. Verrilli and M.G. Castelli, Eds. , 1996, pp.146-173.
- Saleeb, A.F. and Arnold, S. M.; ‘‘A General Reversible Hereditary Constitutive Model: Part I Theoretical Developments”, JEMT, Vol. 123, 2001, pp.51-64.
- Arnold, S. M., Saleeb, A.F., Castelli, M.G.; ‘‘A General Reversible Hereditary Constitutive Model: Part II Application To Titanium Alloys”, JEMT, Vol. 123, 2001, pp. 65-73.
- Saleeb, A.F., Arnold, S.M., Castelli, M.G , Wilt, T.E., and Graf, W.E., “A General Hereditary Multimechanism-Based Deformation Model With Application to The Viscoelastoplastic Response of Titanium Alloys, Int. Jnl. Of Plasticity, Vol. 17, No. 10, pp. 1305-1350. Oct. 2001
- Saleeb, A.F. and Arnold, S.M. ; “Specific Hardening Function Definition and Characterization of A Multimechanism Generalized Potential-Based Viscoelastoplasticity Model”, accepted *Int. Jnl of Plasticity, 2003*