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

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Presented
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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

- 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 ($T/T_m > 0.3$)

- Strain-rate sensitivity
- Creep
- Relaxation
- Thermal Recovery
- Dynamic Recovery
- Large "state" recovery
- Small strain recovery
- Small reversed inelastic strain

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
- Ratchetting Behavior

**Strain-controlled**

- Shakedown Behavior
- Nonrelaxation of mean stress
- Relaxation of mean stress
- Ratchetting Behavior
Material Behavior Can Significantly Impact Structural Response (e.g. Recovery Mechanisms)

Applied Compressive Stress/Euler Stress = 0.095
Normalized Initial imperfection – 0.01


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

- Severe thermomechanical loading conditions result in irreversible strains
- Unified viscoplastic models successfully predict the experimentally observed deformation trends
Multiscale Functional Framework for Deformation and Life Modeling

Characterization/Validation

Structural Analysis

Detection Techniques

Global
- NDE
- Sensors
- Analysis

Local
- NDE Techniques
  - Ultrasonic
  - X-Ray
  - CT
  - Eddy Current

LIFE

Test Methods
- Global (Component)
- Local (Coupon)

Experimentation

Data Reduction

COMPARE
- (Auto Parameter Est)
- Deformation Damage

Hereditary Deformation Modeling

Continuum Damage Mechanics

Mechanism Evolutionary Laws

Subdomain Solution Schemes for Nonhomogenous/Localized Fields

Structural Failure Criteria

Component Validation

Life Prediction Branch
Structures Division GRC
SMA 7/97
CONSTITUTIVE MODELING

Structural Mechanics Problem

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**

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

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

ABAQUS

Mathematical Characterization
Of
Material Behavior

COMPARE

Automatically write required input information

www.mdmc.net

FEA Analysis of component

ABAQUS

Source Code
Object Code

Implicit
GVIPS
UMAT

Large Scale Implementation

- Integration scheme
- Multimechanism Constitutive Relation

www.mdmc.net

Material Behavior

Mathematical Characterization

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Thermomechanical Testing in Support of Constitutive Model Development

Characterization Tests

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

Exploratory Tests

- 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

Constitutive Model Deformation & Damage

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

Validation Tests
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**
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**Experiments Indicated Existence of Reversible and Irreversible Threshold Surface**

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

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

<table>
<thead>
<tr>
<th>Technical</th>
<th>Practical Implication</th>
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</thead>
</table>
| 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

- Thermodynamic Variables “Force-Like”
- Thermodynamic Conjugates “Displacement-Like”

Equations of State

- Thermodynamic Potentials (e.g., Gibb’s, Helmholtz’s)
- Dissipation Potentials
  - Complementary Type $\Omega = \Omega$ (variables)
  - Free Energy Type $\Psi = \Psi$ (conjugates)

Evolution of Variables

- “Displacement-Like”
- “Force-Like”

Compliance Operators

Missing Link in past potential based theories
Advantages and Attributes of Potential Formulation

• Provides a consistent framework for deformation and damage modeling
  ➢ Nonisothermal and/or anisotropic extension straightforward
  ➢ Nonproportional loading histories automatic
  ➢ Automatic satisfaction of the Dissipation Inequity 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

Equations of State

\[ \Phi = \Phi_R + \Phi_{IR} \]

\( \Phi \) = \( \Phi^0 \) \( + \) \( \Phi^{IR} \)

“Displacement-Like”

Total = Stored + Dissipated

\[ \sigma e = \Phi + \Omega \]

Stored (\( \Phi \)) = Reversible + Irreversible

Lattice Distortion

Dislocation Pile-up

Reflects change in microstructure

Dissipation (\( \Omega \)) = Reversible + Irreversible

Dislocation bowing

Deformation & Thermally driven Mechanism

Reflects mobility/rate of evolution in microstructure

Irreversible = \( \Omega_1 \) (deformation) + \( \Omega_2 \) (diffusional; mass/vacancy)

Glide/plastic Slip

- Thermal recovery
- Dislocation/boundary interaction
- Formation of cell structure
General Multimechanism Hereditary Behavior Model of the GVIPS Class

Reversible

\[ \sigma = \sigma_s + \sum_{a=1}^{M} q^{(a)}; \quad \alpha = \sum_{b=1}^{N} \alpha^{(b)} \]

\[ \dot{\varepsilon} = \dot{\varepsilon}^{ve} + \dot{\varepsilon}^{vp} \]

\[ \Phi = \Phi_R + \Phi_{IR} \quad \Omega = \Omega_R + \Omega_{IR} \]

\[ \Phi_R = \Phi_R(\sigma, q^{(a)}) = \frac{1}{2} \sigma_s E^{-1} : \sigma_s + \frac{1}{2} \sum_{a=1}^{M} q^{(a)} : [M^{(a)}]^{-1} : q^{(a)} + \sum_{a=1}^{M} q^{(a)} : p^{(a)} \]

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

Eqs. of state:

\[ \varepsilon^{ve} = \left( \frac{-\partial \Phi_R}{\partial \sigma_s} \right) \]

Flow law:

\[ \dot{p}^{(a)} = \frac{\partial \Omega_R}{\partial q^{(a)}}, \quad a = 1, 2, \ldots, M \]

\[ \Phi_{IR} = \Phi_{IR}(\sigma, \alpha^{(b)}) = \sigma : \varepsilon^{vp} + \sum_{b=1}^{N} H_{(b)}(\alpha^{(b)}) \]

\[ \Omega_{IR} = \Omega_{IR}(\sigma - \alpha) + \sum_{b=1}^{N} \Omega^{(b)}_2(\alpha^{(b)}) \]

Flow law:

\[ \dot{\varepsilon}^{vp} = \frac{\partial \Omega}{\partial \sigma} = \frac{\partial \Omega_{IR}}{\partial \sigma} \]

Evolutionary law:

\[ \dot{\alpha}^{(b)} = -\frac{\partial \Omega_{IR}}{\partial \alpha^{(b)}}, \quad b = 1, 2, \ldots, N \]

Internal State Rate Eqs.:

\[ \dot{\alpha}^{(b)} = L \dot{\gamma}^{(b)} \]

\[ L = \left[ -\frac{\partial^2 \Phi_{IR}}{\partial \alpha^{(b)} \partial \alpha^{(b)}} \right]^{-1} \]
Specific Choice of Energy Potentials and Material Functional Forms

\[ \Phi_R = \Phi_R(\sigma_{ij}, q_{ij}^{(a)}) = \frac{1}{2}(\sigma_{ij})_0 E_{ijkl}(\sigma_{kl})_{kl} + \frac{1}{2} \sum_{a=1}^{M} q_{ij}^{(a)} \frac{1}{M_{ijkl}^{(a)}} q_{kl}^{(a)} + \sum_{a=1}^{M} q_{ij}^{(a)} p_{ij}^{(a)} \]

\[ \Phi_{IR} = \Phi_{IR}(\sigma_{ij}, \alpha_{ij}^{(b)}) = \sigma_{ij} \varepsilon^{up}_{ij} + \sum_{b=1}^{N} H(b)(G^{(b)}) \]

and

\[ \Omega_R = \frac{1}{2} \sum_{a=1}^{M} q_{ij}^{(a)} \frac{1}{M_{ijkl}^{(a)}} q_{kl}^{(a)} \]

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

where

\[ F = \frac{1}{2\kappa^2}(\sigma_{ij} - \alpha_{ij}) M_{ijkl}(\sigma_{kl} - \alpha_{kl}) - 1 \]

\[ G^{(b)} = \frac{1}{2\kappa_{(b)}^2}(\alpha_{ij}^{(b)} M_{ijkl}^{(b)} \alpha_{kl}^{(b)}) \]

and the specific functions:

\[ \Omega_1(F) = \int \frac{\kappa^2 F^m}{2\mu} dF \]

\[ \Omega_2^{(b)}(G^{(b)}) = \kappa_{(b)}^2 \int \frac{r(G^{(b)})}{h(G^{(b)})} dG^{(b)} \]

\[ \bar{H}(b) = \kappa_{(b)}^2 \int \frac{1}{h(G^{(b)})} dG^{(b)} \]

\[ h_{\text{non}}(G^{(b)}) = \frac{H(b)}{G^{(b)}} \]

\[ h_{\text{sat}}(G^{(b)}) = H_{(b)} \left( 1 - \sqrt{G^{(b)}} \right)^{\beta_{(b)}} \]

\[ r(G^{(b)}) = R_{(b)} |G^{(b)}|^{m_{(b)}} \]
Results Illustrating Recent Improvements Made to the Hardening Functional Form in GVIPS Model

Previous Non-saturating
\[ g(G) = \frac{H}{G^\beta} \]

Current Saturating Form
\[ g(G) = H(1-G)^\beta \]

\[ G = \left[ \frac{1}{2} \alpha_{ij} \alpha_{ij} / \kappa^2(b) \right]^{0.5} \]

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 least two 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

<table>
<thead>
<tr>
<th>Method</th>
<th>Number of Load Steps</th>
<th>CPU Time</th>
<th>GIT</th>
<th>LIT</th>
</tr>
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<tbody>
<tr>
<td>Explicit</td>
<td>10,000</td>
<td>180.0</td>
<td>3</td>
<td>0</td>
</tr>
<tr>
<td>Implicit</td>
<td>100</td>
<td>5.0</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
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<td>1.05</td>
<td>4</td>
<td>10</td>
</tr>
<tr>
<td>Implicit</td>
<td>5</td>
<td>1 (54 s)</td>
<td>10</td>
<td>20</td>
</tr>
</tbody>
</table>

**Explicit Failed**

Under cyclic conditions

Under nonproportional loading conditions
Key to Accurate Characterization of GVIPS
Involves Sufficient “Data Content”

Viscoelastic Material Parameters
2+2M number, i.e., \(E_s, \nu, (M_{(a)}, \rho_{(a)})\)

Viscoplastic Material Parameters
- Flow \(\kappa, \mu, n\)
- Hardening \(H_b, \kappa_b\) and \(\beta\),
- 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

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Comprehensive Characterization of The Deformation Response of TIMETAL21S

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

"DATA CONTENT" IS HUGE ISSUE
Characterization of IN738LC @ 850 °C

Elastic + 4 Viscoplastic Mechanisms

Final characterized parameters using four Viscoplastic mechanisms for IN738LC @850°C:

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

* the value between parentheses was determined in the FE simulation of the experiment
Correlation of GRCop-84 Utilizing Multimechanism GVIPS Model

1 VE mechanisms
4 VP mechanisms

Relaxation Tests

Strain controlled Tensile Tests

Creep Tests
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

- 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)

- Automated Material Model Characterization
  - via COMPARE
  - Materials thus far:
    - Ni based; Cu based; Ti
    - MMC and PMC

- Now Commercially Available
  - COMPARE
  - GVIPS – via UMATs
Multiple Experiments produce data

Data

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

www.openchannelfoundation.org
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