Modeling Efforts in Multifunctional High Temperature Shape Memory Alloys

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Current and Future Directions in HTSMAs
Current research activities—Projects

- “Accelerating the Development of Phase Transforming Heterogeneous Materials: Application to High Temperature Shape Memory Alloys”, Designing Materials to Revolutionize and Engineer our Future, National Science Foundation.

- “Elucidating Actuation-Induced Failure Mechanisms in High Temperature Shape Memory Alloys”, Air Force Office for Scientific Research.

- “Fracture Mechanics in the Presence of Reversible Martensitic Transformation in High Temperature Shape Memory Alloys”, National Science Foundation.
“Accelerating the Development of Phase Transforming Heterogeneous Materials: Application to High Temperature Shape Memory Alloys”, Designing Materials to Revolutionize and Engineer our Future, National Science Foundation.

Ultimate goal is to develop a framework capable of addressing the following question:

- **given a set of desired performance requirements, establish the likely feasible set of processing + chemistry combinations with a minimal number of experimental iterations**
Optimizing the development cycle of shape memory alloys via predictive modeling

Motivation

- Given a set of desired SMA performance requirements, create a framework that can establish the likely feasible set of processing & chemistry combinations with a minimal number of experimental iterations.

Proposed Methodology

- Create necessary database on the effects of composition, heat treatment, and processing on the microstructure and effective thermomechanical properties.
- Augment database and accelerate the development cycle with numerical experiments, minimizing the required number of physical experiments.
- Solve effectively the forward problem and close the loop with a Bayesian framework.
- Optimal experiment design for identifying the compound with the desired properties.

Schematic of the Proposed Methodology

- Desired Performance Parameters
  - Synthesis
  - Processing
  - Precipitate Models
  - Uncertain Parameters
  - Model Calibration
  - Optimal Experiments

- Characterization
  - SMA Response
  - Uncertain Models
  - Uncertain Conditions
  - Experiment Design

Forward Modeling

- Experiments will fine tune the CALPHAD model to extract the precipitation distribution metrics...

...to create representative volume elements to predict the effective thermomechanical properties on the basis of composition, heat treatment, and processing.

Bayesian Framework

- Task: Derive robust predictions as well as objective-based uncertainty metrics under data uncertainty.
- Solution Strategy: Robust optimization, such as pessimistic or scenario optimization
- Challenges: Providing appropriate constraints based on data uncertainty.

DMREF: Accelerating the Development of Phase Transforming Heterogenous Materials: Application to High Temperature Shape Memory Alloys, Grant No: CMMI-1534534 (PM: Alexis Lewis)
Thermodynamic and Kinetic Model of Ni-Ti-Hf System

- Experiments:
  - Diffusion Multiples at different temperatures
  - Existing precipitation treatments

- Calculations:
  - Preliminary assessment of CALPHAD Ni-Ti-Hf system (using existing binaries)
  - DFT calculations to estimate ternary interaction parameters

- Calibration: Possible use of Bayesian methods for CALPHAD modeling

[Karaca, 2014]

[Zhao 2001]
Optimal Experimental Design

- Goal is to demonstrate framework
- Possible use of calibrated precipitation model for NiTi

[Graph of Heat Treatment Condition]

[Karaman Group]
Microstructure – Property Relations

1) RVE Generation

2) Coherency

3) Ni distribution

4) Thermomechanical Cycle
## Prediction Comparison

<table>
<thead>
<tr>
<th>Initial Composition [Ni at.%]</th>
<th>Aging Temp. [°C]</th>
<th>Aging Time [hr]</th>
<th>Estimated Precipitate VF [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>50.8</td>
<td>300</td>
<td>100</td>
<td>1.7</td>
</tr>
</tbody>
</table>

**Graphs:**
- **200 MPa**
- **150 MPa**
- **100 MPa**

- **Solutionized**
- **Experiment**
- **Prediction**

**Image:**
- Micrograph showing microstructure with a scale of 0.5 μm.
Role of Defects and Microstructure in HTSMA

- Interaction between transformation and viscoplasticity
  - Size effect (nanoprecipitates)
  - TRIP and TRIVP

Kondori, Needleman & Benzerga (2016) In preparation

Role of Defects and Microstructure in HTSMA

- Effect of temperature (dislocation creep)
- Effect of inhomogeneities (e.g., different CTE coefficients)

Greer & Benzerga (2016) In preparation
Stable crack growth under mechanical loading in SMA

- Stress-induced phase transformation and other dissipative mechanisms are responsible for the toughness enhancement associated with crack advance

R-curve behavior

Baxevanis et al., Int. J. Plast., 2013
Experimental Observations under Actuation Loading

Experimental setup for actuation experiments of double-notch SMA specimens under temperature-induced phase transformation and constant bias tensile load

Thermomechanical loading path
Experimental Observations (cont.)

How can a dissipative process such as phase transformation lead to crack propagation?

- End of Mechanical Loading
- At Failure

$\varepsilon_{yy}$

- 0.025
- 0.0225
- 0.02
- 0.0175
- 0.015
- 0.0125
- 0.01
- 0.0075
- 0.005
- 0.0025
- 0

Materials Science & Engineering
Texas A&M University
Driving Force for Crack Growth


\[ dK_I = \frac{1}{\sqrt{8\pi}} \frac{EdA}{1 - \nu^2} r^{-3/2} M (\varepsilon_{\gamma \delta}^t, \beta) \]

where

\[ M (\varepsilon_{\gamma \delta}^t, \beta) = \varepsilon_{\alpha \alpha}^t \cos \frac{3\beta}{2} + 3\varepsilon_{12}^t \cos \frac{5\beta}{2} \sin \beta + \frac{3}{2} (\varepsilon_{22}^t - \varepsilon_{11}^t) \sin \frac{5\beta}{2} \sin \beta \]

Energy release rate vs Temperature
Crack Growth during Actuation

Jape et al, Shape Mem. Super., 2015

Normalized temperature vs. normalized crack growth for varying bias loads

R-type curve behavior
Research Challenges in HTSMAs

- Design of Stable Microstructures for Multiple Actuation Cycles at High Temperatures and Stresses
- Interaction between Phase Transformation and Inelastic Phenomena (Plasticity and Creep)
- Fracture Mechanics in the Presence of Phase Transformation and Inelasticity
- Actuation Fatigue and Failure
- Corrosion at High Temperatures under Multiple Actuation Cycles
Multicomponent, equiatomic solid solutions

Michael J. Demkowicz

4-component Lennard-Jones model

Distortions up to 10% of lattice parameter

Motivation:
- Single phase
- Thermally stable
- High strength and toughness
- Radiation resistant

Challenge:
current understanding of metal behavior is not able to account for the enormous atomic-level distortions in these materials

How do crystal defects behave in materials with such highly distorted crystal structure?
What are the consequences for behavior and potential applications under extreme environments?
Capabilities for Comprehensive exploration of equiatomic solid solution behavior

Experiments
- Crystal growth (Karaman)
- PVD (CINT)

Synthesis
- First principles (DFT, Qian)

Mechanical testing
- Micropillar compression (Pharr, Karaman)
- Nano-indentation (Pharr)

Characterization
- TEM (Pharr)
- SEM (Pharr, Karaman)

Modeling
- Molecular dynamics (MD, Demkowicz)
- Dislocation dynamics (DDD, Benzerga)

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Capabilities for modeling of radiation effects

Atomistic modeling of damage processes


Phase field models of microstructure evolution


Discrete dislocation models of structure and properties of solid-state interfaces

Abdolrahim N, Demkowicz MJ. Determining coherent reference states of general semicoherent interfaces. Computational Materials Science 118, 297 (2016); Editor’s choice for Vol. 118.

Kinetic Monte Carlo modeling of long-time material response

Inelastic Constitutive Behaviors

Numerical Methods (FEA-Based)

Active/Morphing Aerospace Structures

High-Throughput Structural Design Methods

Active Structural Design Across Scales

High-Throughput Multiscale Analysis

Current

Novel Morphing Structural Concepts

Capabilities

Structural Design Across Scales
High-Throughput Multiscale Analysis

Darren Hartl

...is used to initialize
calibration of the
same highly efficient
phenomenological model...

\[
\hat{\Phi}(\sigma) = \sqrt{3} \left[ (J_2^C)^{\frac{3}{2}} - cJ_3^C \right]^{1/3} \\
\{a_{ax}, a_{shr}, b_{ax}, b_{shr}, b_{11}, c\}
\]

...used for the high-throughput analysis of precipitates within
single crystals...

...and the calibrated analysis of
textured polycrystals...

...and the calibrated analysis of
engineering components.

Full predicted/measured crystalline transformation anisotropy...
Novel Morphing Structural Concepts

Self-folding structures via novel origami-based design methods

The “Stanford Bunny” test model

The “Stanford Bunny” test model (Hartl / Lagoudas; TAMU)

Bio-inspired multifunctional structures design via genetic programming

Bio-inspired multifunctional structures design via genetic programming (Hartl, Reich & Beran; AFRL/RQ)
Objective: establish a recurring, international summer school in multi-scale computational materials science

Unique Features:
- Theoretical and Practical sessions for all topics
- 4 Editions (next one in July 2016)
- Over 80 students from the US and across the world have participated
- Over 30 instructors, leaders in the field (from around the world)
- Lecture materials publicly available worldwide
IIMEC School

- 10 days
- 7 hours/day
  - 4 hours - Theory
  - 3 hours - Computer Labs
- Access to HPRC Resources
- Dissemination:
  - Website (Videos, Lecture Notes, Interactive Forum)
  - Virtual Machines (with everything installed beforehand)
  - Attending students and instructors become part of the IIMEC Computational Materials Science Group
  - Continuing education and advising