IUTAM'19

Phase Transformations in Shape Memory Materials: Modeling and Applications

AT&T Conference Center
The University of Texas at Austin
April 28 – May 2, 2019

Scientific Committee

IUTAM Symposium

Phase Transformations in Shape Memory Materials: Modeling and Applications

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IUTAM Symposium

Phase Transformations in Shape Memory Materials: Modeling and Applications

The University of Texas at Austin

April 28 – May 2, 2019

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Organizational Details

Organizational Details

- The conference registration desk will be on the same floor as the hotel registration desk (M2)

- The conference will end at 5:30pm on Wednesday, May 1. On Thursday, May 2, there will be an optional round table discussion on future directions on SMA constitutive modeling issues from 9:00 to 11:00am. This can include remaining challenges, calibration and required experiments, evaluation of performance, and validation. Participants, feel free to prepare a few words or slides to seed the discussion.

- Breakfast will be available 7:30 to 8:30am on Monday, Tuesday, and Wednesday at the Tejas Dining Room in the AT&T Conference Center.

- Lunch will be served 12:00 to 1:30pm in the Tejas Dining Room on Monday, Tuesday, and Wednesday.

- The reception will take place on Sunday, April 28, 6:00 to 7:30pm in the Tejas room.

- The banquet will take place on Tuesday, April 30, 7:00 to 9:00pm in the Lavaca Room, 4th floor, at Rowling Hall (adjacent to the AT&T Conference Center).

Schedule at a Glance

IUTAM Symposium

Phase Transformations in Shape Memory Metals: Modeling and Applications

The University of Texas at Austin
April 28 – May 2, 2019

Program Summary

Time	Sun 4/28	Mon 4/29	Tue 4/30	Wed 5/1	Thu 5/2
7:30-8:10		Registration	Registration	Registration	
8:10-8:30		Welcome	Registration	Registration	
8:30-9:00		Sehitoglu	Elahinia	Sun	
9:00-9:30		Mirzaeifar	Karaman	Petryk	Roundtable
9:30-10:00		Sedlak	Heller	Wendler	Roundtable
10:00-10:30		***Break***	***Break***	***Break***	Roundtable
10:30-11:00		Feigenbaum	Chen	Welsch	Roundtable
11:00-11:30		Kiefer	Stebner	Purohit	Roundtable
11:30-12:00		Wang	Scalet	Lee	
12:00-1:30		***Lunch***	***Lunch***	***Lunch***	
1:30-2:00		Mabe	Shaw	Kazinakis	
2:00-2:30		Ben Zineb	Ley	Lagoudas	
2:30-3:00		Daly	Haghgouyan	Hartl	
3:00-3:30		***Break***	***Break***	***Break***	
3:30-4:00	Registration	Gall	Seiner	Solomou	
4:00-4:30	Registration	Plucinsky	Saint-Sulpice	Frost	
4:30-5:00	Registration	Bucsek	Kyriakides	Baxevanis	
5:00-5:30	Registration	Asle Zaeem	Posters	Landis	
5:30-6:00	Registration				
6:00-7:30	***Reception***				
7:00-9:00			***Banquet***		

Schedule

IUTAM Symposium on Phase Transformations in Shape Memory Materials: Modeling and Applications

Sunday April 28, 2019

3:30-6:00pm	Registration
6:00-7:30	Reception

Monday April 29, 2019

7:30-8:10am	Registration
8:10-8:25	Welcome from Chad Landis, Stelios Kyriakides, and Dimitris Lagoudas
8:25-8:30	IUTAM information from Henryk Petryk
Session 1	*Chair: Chad Landis*
8:30-9:00	Scientific understanding of interfacial plasticity in shape memory alloys, *Huseyin Sehitoglu*, University of Illinois
9:00-9:30	Mechanics of phase transformation in nickel-titanium shape memory alloys at macro-, micro- and atomistic scales, *Reza Mirzaeifar*, Virginia Tech
9:30-10:00	Simulations of coupled transformation and plasticity in NiTi, *Petr Sedlak*, Czech Academy of Sciences
10:00-10:30	Break
Session 2	*Chair: Ibrahim Karaman*
10:30-11:00	The effect of various model features on predicting the macro-scale magneto-mechanical behavior of magnetic shape memory alloys, *Heidi P. Feigenbaum*, Northern Arizona University
11:00-11:30	Local and global approaches to the modeling of magnetic shape memory alloys, *Björn Kiefer*, TU Bergakademie Freiberg
11:30-12:00	Effect of microstructural length scales in the multi-ferroic transformations in metamagnetic shape memory alloys, *Yuhao Wang*, Texas A&M
12:00-1:30pm	Lunch

Schedule

Session 3	*Chair: Huseyin Sehitoglu*
1:30-2:00	Shape memory alloy actuation technology for adaptive low boom supersonic transports, *James Mabe*, Texas A&M
2:00-2:30	Finite element and experimental structural analysis of endodontic application made of Cu-based single crystal SMA considering a micromechanical behavior model, *Tarak Ben Zineb*, Université de Lorraine
2:30-3:00	Experimental investigations of microstructure-transformation interactions in Nitinol, *Samantha Daly*, UCSB
3:00-3:30	Break
Session 4	*Chair: Samantha Daly*
3:30-4:00	Commercialization of NiTiNOL in large joint fusion: Basic Science to Clinical Results, *Ken Gall*, Duke University
4:00-4:30	Modeling branching microstructure and measuring interfacial energy in shape memory alloys, *Paul Plucinsky*, University of Minnesota
4:30-5:00	Unveiling shape memory alloy micromechanics with internal, in situ measurements of the local microstructure, *Ashley Bucsek*, University of Minnesota
5:00-5:30	Insights on deformation mechanisms of shape memory ceramics by multiscale scale modeling, *Mohsen Asle Zaeem*, Colorado School Of Mines

Tuesday April 30, 2019

7:30-8:30am	Registration
Session 5	*Chair: Stelios Kyriakides*
8:30-9:00	Additive manufacturing of shape memory alloys: key challenges and lessons learned, *Mohammad Elahinia*, University of Toledo
9:00-9:30	Engineering the transformation hysteresis by precipitation in NiTi and NiTiHf, *Ibrahim Karaman*, Texas A&M
9:30-10:00	Transformation-plasticity coupling in superelastic NiTi characterized by in-situ DIC, resistometry, IR thermography and DMA, *Ludek Heller*, Nuclear Physics Institute of the Czech Academy of Sciences

Schedule

10:00-10:30	Break
Session 6	*Chair: Henryk Petryk*
10:30-11:00	Rational design of shape memory alloys with low functional fatigue properties, *Sherry Chen*, Hong Kong University of Science and Technology
11:00-11:30	The multiaxial nature of thermomechanical constitutive relationships of shape memory alloys, *Aaron Stebner*, Colorado School of Mines
11:30-12:00	Recent advances on phenomenological and computational modeling of shape memory alloys, *Giulia Scalet*, University of Pavia
12:00-1:30pm	Lunch
Session 7	*Chair: Björn Kiefer*
1:30-2:00	Extension-twist responses of superelastic shape memory alloy tubes, *John Shaw*, University of Michigan
2:00-2:30	The Effect of Non-Metallic Inclusions on NiTiHf Actuation Fatigue Performance Using Advanced Charecterization, *Nathan Ley*, University of North Texas
2:30-3:00	Fracture toughness and crack growth behavior in NiTi and NiTiHf shape memory alloys, *Behrouz Haghgouyan*, Texas A&M
3:00-3:30	Break
Session 8	*Chair: Darren Hartl*
3:30-4:00	Microstructures in modulated martensites – experimental observations and theoretical models, *Hanus Seiner*, Czech Academy of Sciences
4:00-4:30	Prediction of low cyclic fatigue of NiTi structures using reduced techniques based on multi-scale modeling , *Luc Saint-Sulpice*, ENIB
4:30-5:00	Response of Pseudoelastic NiTi Tubes Under Combined Tension and Internal Pressure, *Stelios Kyriakides*, University of Texas at Austin
5:00-5:30	Poster Presentations
7:00-9:00pm	Banquet

Schedule

Wednesday May 1, 2019

7:30-8:30am	Registration
Session 9	*Chair: Dimitris Lagoudas*
8:30-9:00	Ultrahigh compressive fatigue life and fatigue mechanisms of superelastic NiTi in solid-state cooling technology, *Qingping Sun*, Hong Kong University of Science and Technology
9:00-9:30	Phase-field approach to microstructure evolution in SMA: size effects and rate-independent dissipation, *Henryk Petryk*, Polish Academy of Sciences
9:30-10:00	Mesoscale simulation of shape memory alloy thin film devices, *Frank Wendler*, Friedrich-Alexander-University of Erlangen-Nürnberg
10:00-10:30	Break
Session 10	*Chair: Aaron Stebner*
10:30-11:00	A fully-coupled simulation tool for elastocaloric air-cooling devices, *Felix Welsch*, Saarland University
11:00-11:30	Kinetics of phase boundaries in bistable chains in the isothermal and adiabatic regimes, *Prashant K. Purohit*, University of Pennsylvania
11:30-12:00	Characterization and actuation of nematic elastomers, *Victoria Lee*, Caltech
12:00-1:30pm	Lunch
Session 11	*Chair: John Shaw*
1:30-2:00	Effect of phase transformation on the stability of pseudoelastic NiTi tubes under bending, *Karlos Kazinakis*, University of Texas at Austin
2:00-2:30	A three-dimensional constitutive model for shape memory alloys considering the evolutionary material response and two-way shape memory effect at stress-free conditions, *Dimitris Lagoudas*, Texas A&M
2:30-3:00	Towards high power density solid/liquid metal composite actuators, *Darren Hartl*, Texas A&M
3:00-3:30	Break

Schedule

Session 12 *Chair: Hanus Seiner*

3:30-4:00 Bayesian materials discovery: Application on the discovery of precipitation hardened NiTi shape memory alloys through micromechanical modeling, *Alexandros Solomou*, Texas A&M

4:00-4:30 Macroscopic constitutive model tailored for polycrystalline NiTi shape memory alloys with localized phase transformation, *Miroslav Frost*, Czech Academy of Sciences

4:30-5:00 On the Mechanics of Overload and Fatigue Failure in Shape Memory Alloys, *Theocharis Baxevanis*, University of Houston

5:00-5:30 A new framework for phenomenological constitutive models for SMAs, *Chad M. Landis*, University of Texas at Austin

Thursday May 2, 2019

9:00-11:30am Round-table discussion on future directions for SMA constitutive modeling, experiments, and applications

Sehitoglu - M 8:30-9:00

Scientific Understanding of Interfacial Plasticity in Shape Memory Alloys

***H. Sehitoglu*, S. Alkan, M.S. Khan**

Department of Mechanical Science and Engineering University of Illinois at Urbana-Champaign Urbana, Illinois 61801(huseyin@illinois.edu)

Scientific studies of material interfaces (phase boundaries, grain boundaries and precipitation) are paramount to understanding the mechanical response of materials. Despite the need to understand interfaces, most analyses and experiments in engineering have focused on bulk properties and homogenous idealizations bypassing the presence of interfaces. Such an idealized treatment is unable to capture the local stresses leading to irreversibilities and localizations, hence does not lend itself to further development of new materials with unusual transformations, boundaries and strengthening phases. To achieve such an objective, we develop a theory for rapid assessment encompassing material anisotropy, crystal lattice types, defect structures and local strain fields. With such a formalism, the resultant dislocation and disconnection networks, steps at the interfaces that minimize the strain energy are established along with the internal stress fields. These internal stress fields at interfaces are of critical importance for the flow CRSS (Critical Resolved Shear Stress) prediction which are strongly orientation and stress-state dependent [1, 2]. Therefore, we map out the key parameters including the role of interfaces on modified flow behavior at interfaces. The theory is exercised on a number of metals and alloys to predict the misfit-induced defect networks and local strains utilizing anisotropic elasticity and molecular dynamics.

References

[1] Alkan S, Ojha A, Sehitoglu H. The complexity of non-Schmid behavior in the CuZnAl shape memory alloy. Journal of the Mechanics and Physics of Solids 2018;114:238-57.

[2] Alkan S, Sehitoglu H. Dislocation core effects on slip response of NiTi- a key to understanding shape memory. International Journal of Plasticity 2017;97:126-44.

Mirazaeifar - M 9:00-9:30

Mechanics of Phase Transformation in Nickel-Titanium Shape Memory Alloys at Macro-, Micro- and Atomistic Scales

Reza Mirzaeifar

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Shape memory alloys (SMAs), particularly NiTi (also called Nitinol), are widely used in a broad variety of applications in multiscale devices ranging from nano-actuators used in nano-electrical-mechanical systems (NEMS) to large energy absorbing elements in civil engineering applications. All these applications are based on either the Shape Memory Effect (SME), or the Pseudoelasticity (PE) in these materials. Both these amazing properties at macroscale are connected to the microstructural changes at the grains level in the material, which is itself governed by the phase transformations at the atomistic level. To have a precise description of the material response, and also to obtain an accurate prediction of the thermomechanical response of various devices made at different length scales, these materials need to be studied at macro-, micro- and nanoscales.

The complicated response of the material, particularly when accompanied with the solid-solid phase transformation makes multiple challenges to investigate the response and thermomechanical properties of the alloy at each length scale. In this work, a multiscale analysis for NiTi is performed for better understanding various aspects of martensitic phase transformation at different length scales ranging from macroscale to microscale, and nanoscale. At macroscale, phenomenological constitutive frameworks are adopted and developed by adding the effect of phase transformation latent heat. Analytical closed-form solutions are obtained for modeling the coupled thermomechanical behavior of various large polycrystalline SMA devices subjected to different loadings, including uniaxial loads, torsion, and bending. In order to study some important properties of polycrystalline SMAs that the macroscopic phenomenological frameworks cannot capture, including the texture and intergranular effects, a micromechanical framework is used. Generalized coupled thermomechanical governing equations considering the phase transformation latent heat are derived for polycrystalline SMAs. By considering appropriate distributions of crystallographic orientations in the grains obtained from experimental texture measurements of NiTi samples, the effects of texture and the tension-compression asymmetry on the thermomechanical response of polycrystalline SMAs are also studied.

For studying various aspects of the thermomechanical properties of SMAs at at the atomistic, molecular dynamics simulations, and density functional theory calculations are used. A broad range of NiTi properties at the atomistic level are investigated including; the martensite reorientation, austenite to martensite phase transformation, twinning mechanisms, energy and structure of grain boundaries in NiTi alloys, stacking fault energies, dislocation properties, energy dissipation through phase transformation and shock wave propagation in these alloys.

Sedlak - M 9:30-10:00

Simulations of coupled transformation and plasticity in NiTi

***P. Sedlak*[1], H. Seiner[1], M. Frost[1], L. Heller[2] and P. Sittner[2]**

[1]Czech Academy of Sciences, Nuclear Physics Institute & Institute of Thermomechanics, Czech Republic

[2]Czech Academy of Sciences, Nuclear Physics Institute & Institute of Physics, Czech Republic

Description of mechanisms of plastic deformation in NiTi shape memory alloy is far from trivial as basic understanding of these mechanisms is still missing. Traditionally, it was assumed that plastic deformation occurs dominantly in austenitic phase and it is less favorable in martensite because of lower symmetry and only a single slip system. However, recent experiments [1] showed that the deformation twinning in martensite also plays an important role in generation of plastic deformation; after the reverse transformation, it results in residual twins in austenite (B19' => $B2^T$).

In this contribution, we will present both experimental evidence of the B19' => $B2^T$ transition and its basic description by means of a macroscopic thermodynamic model. The model describes mutual interconnection of reversible transformation/reorientation processes and irreversible plastic deformation mechanisms. It is based on unique energetical and dissipation functions and captures properly plastic deformation of both austenite and martensite, and, at the same time, coupled phenomena as martensite stabilization by plastic deformation, change of thermo-mechanical coupling at elevated temperatures/stresses and the reverse B19' => $B2^T$ transition.

References

[1] Šittner, P., Sedlák, P., Seiner, H., Sedmák, P., Pilch, J., Delville, R., Heller, L., Kadeřávek, L., On the coupling between martensitic transformation and plasticity in NiTi: Experiments and continuum based modelling (2018) Progress in Materials Science, 98, pp. 249-298.

[2] Heller, L., Šittner, P., Sedlák, P., Seiner, H., Tyc, O., Kadeřávek, L., Sedmák, P., Vronka, M., Beyond the strain recoverability of martensitic transformation in NiTi (2019) International Journal of Plasticity, 116, pp. 232-264.

Feigenbaum - M 10:30-11:00

The Effect of Various Model features on Predicting the Macro-Scale Magneto-Mechanical Behavior of Magnetic Shape Memory Alloys

***Heidi P. Feigenbaum*, J. Lance Eberle, Constantin Ciocanel and Glen J. D'Silva**

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Ferromagnetic shape memory alloys (FSMAs or MSMAs) can exhibit the shape memory effect due to an applied magnetic field at room temperature. Under variable magnetic field and constant bias stress loading, MSMAs have been used for actuation applications. Under variable stress and a constant bias field, MSMAs can be used in power harvesting or sensing devices. This work focuses on modeling the macro-scale magneto-mechanical behavior of a Ni-Mn-Ga single crystal MSMA. In particular, several features of the model are individually varied in order to study the effect that each feature has on the predictions of the magneto-mechanical behavior under load typically seen for actuation or sensing/power harvesting applications.

The models discussed in this work are based on sufficient conditions to ensure the satisfaction of the laws of thermodynamics, and assume three types of internal state variables: the volume fraction of variants (ξ), the volume fraction of magnetic domains whose magnetic easy axis aligns with the i-direction within each variant (α_i), and the angle of rotation of the magnetization vectors away from the magnetic easy axis in each variant (θ_i). Each model makes a unique assumption regarding the evolution of the internal variables, the treatment of demagnetization, or material parameters to determine their impact on model predictions. Specifically, we consider three choices for demagnetization: zero demagnetization, piecewise constant demagnetization in each time step, and variable demagnetization that is included in the Gibbs free energy and used to calculate dissipation. Similarly, we consider three choices for α_i and θ_i: constant, piecewise constant such that two different values are possible, and continuously evolving. For the later, the evolution of the internal variable is found by ensuring that magnetic domain wall motion or magnetization rotation is a reversible processes. Finally, we consider three choices for the anisotropy coefficient (a material parameter associated with magnetization rotation): the value provided by the manufacturer of the material, a calibrated value, and a value in between these two.

Model predictions are compared to experimental data, collected on a Ni-Mn-Ga single crystal with a fine twin microstructure, to assess the performance of each model feature. The experiments include both stress-controlled loading with constant bias magnetic field load (which mimics power harvesting or sensing) and field-controlled loading with constant bias compressive stress (which mimics actuation). Each type of test was performed at several different load levels.

Comparing model predictions and experimental results suggest that higher accuracy is achieved by accounting for demagnetization in the Gibbs free energy, particularly at higher field levels. In addition, results suggest that $\alpha = 1$ predicts field controlled tests well, but stress controlled tests poorly. This might imply that the magnetic domains in the stress preferred variant can be affected by high fields in the perpendicular directions. Finally, results showed that including magnetization rotation is important, and model predictions could be improved significantly by properly calibrating the anisotropy coefficient.

Kiefer - M 11:00-11:30

Local and Global Approaches to the Modeling of Magnetic Shape Memory Alloys

Björn Kiefer[1], **Thorsten Bartel**[2], **Andreas Menzel**[2,3]

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Although shape memory alloy modeling has been an active topic in mechanics for about three decades, see for instance the overview provided in [1], open challenges remain as demands on comprehensiveness, fidelity, and efficiency of such models continue to rise. The same is true for magnetic shape memory alloys, a more recent discovery, which also show conventional shape memory behavior, but additionally exhibit strong magneto-mechanical coupling. This has fundamental implications on the conceptualization of constitutive models. Coupling exists in terms of the field equations (Maxwell's equations, balance laws of continuum thermodynamics) in terms of the constitutive properties of the individual phases (e.g., piezomagnetic, magnetostrictive) but also manifests itself in the driving forces for microstructure evolution (e.g., magnetic field-driven phase changes and variant switching). An important aspect in this context is that the formation of microstructure in ferromagnetic materials can be interpreted as a non-local effect, in the sense that the behavior at a material point—particularly the formation of domains—depends on the magnetostatic energy stored in the demagnetization field occupying the entire spatial domain. Most modeling approaches for MSMA behavior proposed in the literature, however, are local in nature. They often account for the sample shape dependence intrinsic to the magnetostatic problem through the demagnetization factor concept, but the magnetization of the solid material is either considered to be spatially homogeneous or can at least be locally computed at the material point level. In micromagnetics approaches [2], non-local aspects of magnetic domain evolution are naturally included, but these methods are typically unable to resolve the length- and time-scales required to describe realistic experimental settings.

In this contribution a recently established modeling framework is presented, cf. [3], that accounts for microstructure evolution in predicting the effective behavior of MSMAs and through its embedding into a newly formulated finite element framework can be applied to the analysis of spatially inhomogeneous problems. While we make use of the same general continuum thermodynamics framework as in earlier work [1, 4–7], in which the evolution of crystallographic and magnetic domains is captured via dissipative and non-dissipative internal state variables, the MSMA modeling approach presented here is fundamentally different. It relies on concepts of energy relaxation in the context of non-convex free energy landscapes whose wells define preferred states of straining and magnetization. The so-called constrained theory of magnetoelasticity developed by DeSimone and James [8] can be regarded as a point of departure for our model development. Their modeling framework

essentially combines the Ball and James theory of microstructure formation [9] with classical micromagnetics approaches [2]. It has successfully been demonstrated that this physically well-motivated and mathematically rigorous the- ory can be applied to the modeling of MSMAs and is able to predict important features of the magnetic shape memory effect (MSME), cf. [3, 10]. On the other hand, key response characteristics—e.g. the hysteretic nature, elastic effects, the linear magnetization response in the pre-variant reorientation regime, and the stress dependence of the maximum field induced strain, both of which are directly related to the rotation of magnetization vectors—are prohibited by the inherent assumptions of the constrained theory. To improve the energy relaxation-based modeling of MSMAs, the following ex- tensions are made: (i) elastic deformations are allowed and their distribution to the individual phases occurs in an energy minimizing fashion, (ii) the high, in fact infinite, magnetocrystalline anisotropy energy limit of the constrained theory is alleviated to allow for magnetization rotations away from easy axes, and (iii) dissipative effects are accounted for in an incremental variational setting for standard dissipative materials.

Moreover, to account for the non-local nature of magnetic microstructure evolution in macroscopically inhomogeneous problems, we propose a variational principle and associated finite element framework

in which three global fields are considered: the displacement field, the scalar magnetic potential, and an additional set of state variables parameterizing the magnetic and crystallographic microstructure—see [11] for a discussion of the purely magnetostatic subproblem. Contrary to conventional micromagnetics, however, the microscale is not spatially resolved and exchange energy terms introducing gradients of the magnetization are neglected in this approach, an assumption that is often referred to as the large body limit [8]. The influence of microstructure is instead incorporated in an effective sense—through appropriate mixture rules and underlying homogenization schemes—, which allows for relatively efficient computations of meso- and macroscale problems. This approach necessitates the development and implementation of novel mixed element formulations. It further requires the enforcement of inequality constraints at the global level. To handle the latter, we employ Fischer-Burmeister complementarity functions and introduce the associated Lagrange multipliers as additional nodal degrees-of- freedom. As a particular application of this general methodology, the energy-relaxation based model for magnetic shape memory behavior described above was implemented and tested. Special cases— considering ellipsoidal specimen geometries—are discussed and used to verify the magnetization and field-induced strain responses obtained from FE-simulations by comparison to calculations based on the demagnetization tensor concept. Following this verification step, we address response simulations with samples of arbitrary geometry—including prismatically-cut single crystals, that are often used in MSMA characterization experiments and actuator/sensor applications. With the presented approach we are able to overcome systematic errors usually introduced by the application of spatially-averaged demagnetization factors to problems exhibiting macroscopically inhomogeneous magnetization fields.

Kiefer - M 11:00-11:30

References

[1] Lagoudas, D. C. (Ed.), Shape Memory Alloys: Modeling and Engineering Applications, Springer- Verlag, 2008.

[2] Brown Jr., W. F., Micromagnetics, John Wiley & Sons, Interscience Tracts on Physics and Astronomy 18, 1963.

[3] Kiefer, B., Buckmann, K., Bartel, T., Numerical Energy Relaxation to Model Microstructure Evolution in Functional Magnetic Materials, GAMM-Mitteilungen, 38(1): 171–196, 2015.

[4] Kiefer, B., Lagoudas, D. C., Magnetic Field-Induced Martensitic Variant Reorientation in Mag- netic Shape Memory Alloys, Philosophical Magazine, 85(33–35): 4289–4329, 2005.

[5] Kiefer, B., Lagoudas, D. C., Modeling the Coupled Strain and Magnetization Response of Mag- netic Shape Memory Alloys under Magnetomechanical Loading, Journal of Intelligent Material Systems and Structures, 20(2): 143–170, 2009.

[6] Haldar, K., Kiefer, B., Lagoudas, D. C., FE-Analysis of the Demagnetization Effect and Stress Inhomogeneities in MSMA Samples, Philosophical Magazine, 91(32): 4126–4157, 2011.

[7] Kiefer, B., Bartel, T., Menzel, A., Implementation of Numerical Integration Schemes for the Simulation of Magnetic SMA Constitutive Response, Smart Materials and Structures, 21(9): 094007, 2012.

[8] DeSimone, A., James, R. D., A Constrained Theory of Magnetoelasticity, Journal of the Me- chanics and Physics of Solids, 50(2): 283–320, 2002

[9] Ball, J. M., James, R. D., Fine Phase Mixtures as Minimizers of Energy, Archive for Rational Mechanics and Analysis, 1987, 100(1): 13–52, 1987.

[10] Tickle, R., James, R. D., Shield, T., Wuttig, M., Kokorin, V. V., Ferromagnetic Shape Memory in the NiMnGa System, IEEE Transactions on Magnetics, 35(5): 4301–4310, 1999.

[11] Buckmann, K., Kiefer, B., Bartel, T., Menzel, A., Simulation of Magnetised Microstructure Evolution Based on a Micromagnetics-Inspired FE-Framework: Application to Magnetic Shape Memory Behaviour, Archive of Applied Mechanics, 2018. (doi:10.1007/s00419-018-1482-7)

Wang - M 11:30-12:00

Effect of microstructural length scales in the multi-ferroic transformations in metamagnetic shape memory alloys

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Meta-Magnetic Shape Memory Alloys (MMSMAs) undergo a martensitic transformation (ferroelastic transition) which is coupled with a strong decrease in the magnetic ordering from a ferromagnetic parent phase to a weak-magnetic product phase (ferromagnetic transition). The properties of this multi-ferroic transformation (MFT) have been shown to depend on composition, thermal history (including atomic ordering) and external applied stress and magnetic fields lending many tunable properties for applications. It is well-known that many of these MFT properties, like transformation hysteresis and transformation magnetization change which are crucial for the magneto-caloric effect, depend on the magnetic contributions to the thermodynamic energy balance between austenite and martensite. As consequence, these properties are a function of the difference between the characteristic temperatures of the ferromagnetic transition in the austenite, Tc, and of the multi-ferroic transformation, like Ms. However, the dependence of the Tc-Ms difference on thermal history is complex and not well understood. In particular, for some Ni-Co-Mn-In MMSMAs, the MFT Ms temperature presents unexpected non- monotonic dependence on the duration of thermal treatments when annealing below the order-disorder transition temperature.

Through preliminary in-situ high energy synchrotron and microstructural investigations, coupled with theoretical work, a possible explanation to these observations has emerged: microstructural features that evolve over long-range diffusive times––possibly Anti-Phase Boundaries (APBs)––may be the culprits for the observed complex, non-monotonic behavior of MT with annealing conditions. Notably, this non-monotonicity suggests that the microstructure-MT coupling occurs at the mesoscale. We present evidence from in-situ transmission x-ray diffraction using high energy synchrotron radiation, DFT-based atomistic/analytic simulations of ordering kinetics as well as theoretical/experimental analysis of the thermodynamics of the transformation and the kinetics of the microstructure evolution through combined high-resolution microscopy and atomistic phase field models. The combined theoretical/experimental work seems to confirm the role of mesos-cale microstructural features on the onset of the martensitic transformation in Ni-Co-Mn-In MMSMAs. While strong microstructure-MT couplings have been reported in conventional SMAs, this remains relatively unexplored in MMSMAs. Unraveling the microstructure-MT connection in MMSMAs is of scientific interest, as the ability to control the transformation behavior in these systems is seen as essential to any efforts to make practical use of these materials.

Mabe - M 1:30-2:00

Shape Memory Alloy Actuation Technology for Adaptive Low Boom Supersonic Transports

James H. Mabe[1], **Dimitris Lagoudas**[2] **and Darren Hartl**[2]

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For years the promise of Shape Memory Alloy (SMA) actuators as an enabling technology has seemed poised to revolutionize the design of adaptive structures and smart systems for aircraft. As far back as 2005 Boeing successfully integrated SMA actuators into the fan nozzle of a 777-300ER GE- 115B engine to modify nozzle geometry in flight for community and cruise noise reduction [1]. While the Variable Geometry Chevron (VGC) flight tests clearly demonstrated that SMA technology can enable solutions for challenging aerospace applications, it also exposed critical technology gaps and needs that would be essential to advancing SMA technology.

Since 2005 Boeing, Texas A&M, and numerous industry, academic, and government partners have made significant advances in the area of SMA actuation technology filling many of the identified gaps. Including improved materials, design and modelling tools, and approved test methods. [2]

Many of these advances in SMA technology and tools are currently being applied to the development of many SMA applications. One of these is adaptive aircraft structures in support of NASA's University Leadership Initiative (ULI) project led by Texas A&M University titled Adaptive Aerostructures for Revolutionary Civil Supersonic Transportation.

To enable the return to flight of civil supersonic transports, aircraft must be developed that meet noise and efficiency requirements across a range of operating conditions. A team of researchers, led by Texas A&M University, is investigating real-time aircraft geometry changes, driven by compact and lightweight SMA actuators, to minimize boom signatures across all flight phases including varying aircraft configurations and environmental atmospheres. [3]

In this presentation the ULI program will be described, including its goals and objectives. The characterization of improved SMA materials and alloys tailored for specified ULI applications will be presented. Strategies for integrated SMA design and design optimization tools, including fluid structure interaction will be discussed. Examples of hardware demonstrations of morphing structures for shock wave control in supersonic wind tunnel tests and structural shape control will be shown. [4]

Mabe - M 1:30-2:00

References

[1] J.H. Mabe, F.T. Calkins, G.W. Butler, "Boeing's Variable Geometry Chevron: Morphing aerostructure for jet noise reduction" 47nd AIAA Adaptive Structures Conference, AIAA-2006-2142, Newport RI, May 2006.

[2] F. Calkins, J. Mabe, "Shape Memory Alloy Based Morphing Aerostructures" Journal of Mechanical Design, NOVEMBER 2010, Vol. 132 / 111012-1

[3] https://engineering.tamu.edu/news/2017/06/researchers-working-to-create-a-quieter- transforming-supersonic-aircraft-for-commercial-use.html

[4] Mabe, James H., Darren J. Hartl, Nathan Tichenor, Murphy Zackery, Eric Blades, and Michael Nucci. "Fluid-Structure Interaction Modeling of a Shape-Memory Alloy Actuated Supersonic Wind Tunnel Model Alloy." In AIAA Scitech 2019 Forum, p. 0602. 2019.

Ben Zineb - M 2:00-2:30

Finite element and experimental structural analysis of endodontic application made of Cu- based single crystal SMA considering a micromechanical behavior model

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Shape Memory Alloys (SMAs) are widely used in endodontology area and particularly as instruments for root canal preparation namely endodontic files. Despite their high performances compared to stainless steel instruments, it is still possible to enhance their cutting efficiency by acting on their shape and material properties, such as the exhibited reversible martensitic transformation strain making them softer without decreasing their mechanical strength. Increasing the maximum martensitic transformation strain becomes possible with single crystal SMAs reaching values up to about 12% whereas it stagnates to about 6% for polycrystalline SMAs. Single crystal NiTi based SMAs are very rarely used because of their very complicated elaboration. On the contrary, Cu-based (Cu-Al-Be, Cu-Zn-Al) single crystal SMAs start to emerge and can reach about 12% of martensitic transformation strain, in addition to their interesting antimicrobial properties (Vincent et al. 2018).

Schema of bending-torsion loading setup

Endodontic file and its corresponding finite element model

Figure 1. Schematic Bending torsion loading and finite element model

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This study investigates, numerically and experimentally, the development of endodontic files made of single crystal Cu-based SMAs. The numerical analysis is carried out by finite element method using the Abaqus code. The geometry of the instrument is parametrized by considering as parameters the cross section shape, the taper, the tip diameter, the helical pitch and the length of the operative part. Applied boundary conditions represent a separated or combined bending-torsion loading by clamping the 3mm length part starting from the tip of file and applying separately or in a combined way two rotations to the top cross section around the file axis and/or its perpendicular direction. The geometry is meshed with continuum tetrahedral elements with quadratic interpolation (labeled in Abaqus C3D10). Small size elements are used in the area with highest stress state and martensitic transformation. This size progressively increase toward weakly loaded or unloaded areas. A micromechanical constitutive law initially developed by (Niclayes et al. 2002), improved by (Merzouki et al. 2010) and (Collard et al. 2012) and implemented in Abaqus via the subroutine

Umat allows to describe the thermomechanical behavior of the single crystal Cu-based SMA in the local coordinate system of the crystalline lattice oriented in the file axis direction. Its formulation derives from a thermodynamic approach at the lattice scale considering mechanical, thermal, chemical and interaction energies. It takes into account the different compatibilities and incompatibilities between martensitic variants. A given set, of habit plane and twinning direction, defines each martensitic variant. Corresponding volume fractions (domain volume occupied by each variant/ RVE volume) are the internal variables of this behavior model. The driving force for each volume fraction derives from the adopted free energy expression. Comparison to its corresponding yield force leads to the nonlinear constitutive equations that are solved implicitly with the Newton-Raphson scheme. A numerical analysis of the sensitivity to geometrical parameters allows to determine values corresponding to a maximum deformation with a minimum stress state, (Vincent et al. 2015). Corresponding material parameters are identified starting from tensile tests on wires made of the same single crystal Cu-based SMA.

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Figure 2. Comparison of numerical and experimental responses for bending, torsion and bending-torsion loadings

Coltene-Microméga company manufactured endodontic file prototypes made of Cu-Al-Be single crystal SMA with the obtained shape from the numerical simulation, figure 1. A specific setup applying the same boundary conditions of torsion-bending loadings, aforementioned for the numerical part, is used to characterize these SMA file prototypes. It applies controlled rotations and measures corresponding induced moments. Each bending, torsion and bending- torsion test is carried out for three samples in order to check the response repetitiveness and average values are adopted by giving the corresponding standard deviation. A cyclic preloading is applied in order to stabilize the superelastic response of the endodontic file and the analysis is based on the stabilized response. Figure 2, depicts a pretty good agreement between experimental and numerical responses, for a combined bending-torsion loading, proving the relevance of the proposed numerical approach. This modeling approach will be enriched by taking into account the cutting forces in the contact lines between the endodontic file and the cut dentine. Finally, fatigue life of these instruments will be investigated before considering them for clinical tests.

References

1. Marin Vincent, Raphaël Duval, Pascal Hartemann, Marc Engels-Deutsch, Contact killing and antimicrobial properties of copper, Journal of applied microbiology, 2018, Vol. 124, N°5, pages 1032-1046

2. Christophe Niclaeys, Tarak Ben Zineb, Shabnam Arbab-Chirani and Etienne Patoor, “Determination of the interaction energy in the martensitic state”, International Journal of Plasticity, 2002,Volume 18, Issue 11, Pages 1619-1647.

Ben Zineb - M 2:00-2:30

3. Tarek Merzouki, Christophe Collard, Nadine Bourgeois, Tarak Ben Zineb, Fodil Meraghni, “Coupling between measured kinematic fields and multicrystal SMA finite element calculations”, Mechanics of Materials, 2010, Volume 42, Issue 1, pages 72 – 95.

4. Christophe Collard, Tarak Ben Zineb, “Simulation of the effect of elastic precipitates in SMA materials based on a micromechanical model”, Composites Part B, 2012,Volume 43, Issue 6, pages 2560–2576.

5. Marin Vincent, Frédéric Thiebaud, Saifeddine Bel Haj Khalifa, Marc Engels-Deutsch, Tarak Ben Zineb, ”Finite element analysis of a copper single crystal shape memory alloy based endodontic instruments”, Journal of Materials Engineering and Performance, 2015, Vol. 24, Issue 10, pages 4128-4139.

Daly - M 2:30-3:00

Experimental Investigations of Microstructure-Transformation Interactions in Nitinol

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This talk will discuss experimental investigations into the stress-induced phase transformation of the shape memory alloy Nickel-Titanium (Nitinol). These investigations utilize a custom methodology to examine phase transformation at the sub-grain level, which is achieved by combining digital image correlation with scanning electron microscopy. The development of the methodology will be briefly discussed, including new SEM-DIC patterning techniques for the reduced length scale and approaches to collect high-resolution displacement fields (e.g. 100+ million data points) over mm-scale fields of view. Using the DIC-calculated displacements, the progression of phase transformation and its relation to the underlying crystallography is examined at the grain level in mechanically loaded tensile samples. The heterogeneous nature of phase transformation at the microscale, the effect of grain size and orientation on transformation characteristics, and the use of this data to identify CV and HPV formation will be discussed. Additional comments will be made on the opportunities and challenges that large data analysis of microscale deformation data enables in the study of phase transformations.

Gall - M 3:30-4:00

Commercialization of NiTiNOL in large joint fusion: Basic Science to Clinical Results

Ken Gall

Mechanical Engineering and Materials Science, Duke University

Does new basic materials knowledge drive technology innovation or do emerging technology needs motivate the creation of new knowledge and new materials? This answer to this question is simple: both. In this talk we will discuss the first path. Specifically, how basic science research aimed at understanding a vexing material phenomenon in NiTiNOL "unintentionally" created knowledge that enabled a shape memory alloy product breakthrough in large joint fusion. The resulting NiTiNOL device has changed fusion rates in this very high risk procedure from 50% to nearly 90%.

Plucinsky - M 4:00-4:30

Branching microstructure in shape memory alloys: A model and it application to experiments

Paul Plucinsky

Aerospace and Engineering Mechanics, University of Minnesota

In shape memory alloys, the branching of martensitic twins typically appears close to the interface between austenite and a first order laminate of two martensitic variants. In their seminal work, Kohn and Müller (1994) argue that this is the result of a delicate energy balance: The gradual refinement of the twins towards the interface reduces the elastic strain energy localized directly at the interface, but also partially localizes the surface energy. They showed—for a simplified 1-D model of shape memory alloys—that the balance of these competing effects can often result in lower total energy compared to that of a simple laminate for these characteristic microstrucutures.

Building on these ideas, we present an explicit construction of branching microstructure at the austenite-martensite interface in a fully non-linear, three-dimensional setting, and we show that branching using this construction leads to the expected reduction of the total energy. In addition, the construction can be directly applied—without any fitting parameters—to particular shape memory alloys with experimentally determined material parameters. This enables us to: 1) discuss the character of the elastic strain field in real branched microstructure, 2) suggest ways to reduce the overall energy stored in this microstructure, and 3) characterize the interfacial energy per unit length of a twin by making direct comparisons of the construction and analogous experiments.

This is joint work with Hanus Seiner, Vivekanand Dabade, Barbora Benesova and Richard D. James.

Bucsek - M 4:30-5:00

Unveiling Shape Memory Alloy Micromechanics with Sub-Surface, In Situ Measurements of the Local Microstructure

Ashley Bucsek[1], **Hanus Seiner**[2], **Hugh Simons**[3], **Phil Cook**[4], **Can Yildirim**[4], **Yuriy Chumlyakov**[5], **Carsten Detlefs**[4], **and Aaron P. Stebner**[6]

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It has become increasingly clear that local deformation events are directly influenced by individual microstructure features, and these local interactions contribute to the effective material properties and overall performance. For example, many functional materials including shape memory alloys owe their unique properties to a deformation mechanism called martensitic phase transformation wherein a high-symmetry austenite phase reversibly transforms to a low-symmetry martensite phase. Recent research has shown that martensitic transformation is directly influenced by local microstructure features such as oxide/carbide inclusions, grain boundaries, interfaces, and precipitates [1–4]. In some cases, the interaction between deformation and local microstructure features are detrimental to the overall material performance [1,2], and in other cases the interaction markedly improves the overall material performance [3,4]. These interactions provide an incredible opportunity to enhance macroscopic material properties via microstructure engineering. However, the exact nature of the relationships between deformation, microstructure, and overall performance is still poorly understood due, in large part, to a lack of direct experimental observation. To understand these relationships, it is essential to directly image the interactions between deformation and local microstructure features while measuring the effects of these interactions on the surrounding microstructure and on the macroscopic properties.

Toward these goals, we use a recently developed technique called dark-field X-ray microscopy (DFXM) to measure the evolution of the austenite microstructure sub-surface and in situ. DFXM offers the capability to spatially map internal microstructure features with a spatial resolution as low as 100 nm, and orientation and strain can be mapped with a sensitivity of 0.001° and 10^{-5}, respectively—superior to that of transmission electron

microscopy [5]. Using DFXM, we directly image the austenite microstructure beneath the sample surface while measuring local changes in the austenite phase fraction, misorientation, and elastic strain in a bulk nickel-titanium sample as it is cooled through martensitic phase transformation. The results show that some material defects (e.g., inclusions and stress concentrations due to polishing) consistently induce transformation, while other defects (e.g., grain boundaries) consistently impede propagating transformation fronts. The results also show that the austenite undergoes an orientation splitting wherein the austenite near the transformation front is constrained from rotating while the austenite far from the transformation front is free to rotate it. Finally, we measure interfacial strain fields at the transformation front that extend tens of micrometers into the material. We use an analytical model to show how these strain fields can be explained by kinematic incompatibility at the austenite–martensite interface. These results mark a new level of insight into the relationships between deformation and local microstructure features via direct experimental evidence.

References

[1] A. N. Bucsek, D. Dale, J. Y. P. Ko, Y. Chumlyakov, A. P. Stebner, Measuring Stress-Induced Martensite Microstructures Using Far- Field High-Energy Diffraction Microscopy. Acta Crystallogr. A. **74** (2018) 425–446. [2] H. M. Paranjape et al., In situ, 3D characterization of the deformation mechanics of a superelastic NiTi shape memory alloy single crystal under multiscale constraint. Acta Mater. **144** (2018) 748–757.

[3] H. Gu, L. Bumke, C. Chluba, E. Quandt, R. D. James, Phase engineering and supercompatibility of shape memory alloys. Mater. Today. **21** (2018) 265–277. [4] Casalena Lee et al., Structure-Property Relationships of a High Strength Superelastic NiTi–1Hf Alloy. Adv. Eng. Mater. **20** (2018).

[5] H. F. Poulsen et al., X-ray diffraction microscopy based on refractive optics. J. Appl. Crystallogr. **50** (2017) 1441–1456.

Zaeem - M 5:00-5:30

Insights on Deformation Mechanisms of Shape Memory Ceramics by Multiscale Scale Modeling

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Phase-field modeling and multimillion-atom molecular dynamics simulations are used to investigate the deformation and failure mechanisms of single crystal and polycrystalline yttria-stabilized tetragonal zirconia (YSTZ) nanopillars and nanoparticles. Results show that the nanoscale plastic deformation of single crystal YSTZ has a strong dependence on the crystallographic orientation. [101] , [10 1] , [011] are [01 1] oriented single crystal YSTZ nanopillars only experience tetragonal to monoclinic transformation, whereas dislocation nucleation and emission is found to dominate the failure process of [001]□, [110] □ and [110] □ oriented nanopillars. Some particularly oriented nanopillars deformed by a combination of dislocation motion and tetragonal to monoclinic transformation is also detected. The dislocation-dominated deformation leads to the lowest strength for nanopillars, while phase transformation- dominated deformation results in the highest strength. Super elasticity and super plasticity are observed in the single crystalline YSTZ nanoparticles. The mechanisms of shape memory degradation are revealed including amorphous phase formation, self healing and accumulation.

In polycrystalline zirconia, phase transformation rather than dislocation motion is observed to be triggered at a lower stress and consequently dominates the plastic deformation. Partial dislocations are observed to nucleate from grain boundaries and propagate throughout the whole grain, which are finally absorbed by the opposing grain boundary. Our simulation results suggest that the formation of partial dislocations act as a splitter of large grain and plays a significant role on the rotation of grains, and it consequently promotes the amorphous-to-crystal transition in-between neighboring grains. A decrease in Young's modulus and strength is revealed with the decrease of grain size, and grain boundary density is identified to be responsible for the observed grain size-induced softening in polycrystalline YSTZ nanopillars. Furthermore, an inverse Hall-Petch equation is constructed to describe the relationship between grain size and yield stress for polycrystalline YSTZ nanopillar with grain size below 15 nm. In polycrystalline YSTZ nanoparticles, only super plasticity is observed and residual strain is left after thermal treatment. Amorphous phase formation and accumulation are observed to act as the dominant shape memory degradation mechanism.

Elahinia - T 8:30-9:00

Additive manufacturing of shape memory alloys: key challenges and lessons learned

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Shape memory alloys (SMAs) are now cover a wide variety of applications from biomedical to aerospace, automotive to oil industries. Both shape memory and/or superelasticity behavior make these alloys suitable for such applications, which is a result of a phase transformation between solid-state phases. However, SMAs are currently available in very simple geometries due to difficulties in their processing and machining. Hence, additive manufacturing(AM) of SMAs as a way to achieve complex shapes has been of interest to researchers for a while. In AM, a part is sliced into multiple layers, and then a laser melts down each layer upon the previous layer. There are multiple process parameters (PPs) involved in AM which needs to be optimized to achieve a successful built. Common PPs are laser power(P), laser scanning speed(v), hatch spacing (H), which is the distance between two consecutive laser passes, and powder layer thickness. As for a successful built, different criteria can be defined: density, dimensional accuracies, microstructural features, impurity pickups, mechanical behavior-recoverable, and irrecoverable strains, strength, modulus of elasticity-, and transformation temperatures (TTs) to name a few. Our team has been actively investigated the effects of PPs on the properties of final parts for years and achieved multiple goals in the fabrication of both low and high-temperature SMAs.

A parameter called Energy density defined as E= P/(v.H.d) found to be an essential factor to achieve fully dense NiTi. It is reported that a minimum E of 55 J/mm^3 is needed to achieve %99.9 of density. Then through changing, P and v, we have shown that the microstructure and properties of parts can be changed significantly. Based on the level of the P and v, AM fabricated parts showed different textures which result in different modulus of elasticity, critical stresses, and shape memory/superelasticity behavior and surprisingly different TTs due to the variation in composition, cooling rates and precipitate formations. However, a study on the effect of H showed that hatch spacing is a dominant factor that significantly alters the material texture. For example, the laser power of 250W, scanning speed of 1250 mm/s, hatch spacing of 80 μm, and layer thickness of 30 μm resulted in a textured microstructure along [001] direction which showed good superelasticity with stabilized %5.20 of recovery at room temperature. Hence, through variation in PPs not only one can manufacture dense complex-shape parts, but also tailoring the properties for different applications is feasible for different applications.

Despite considerable research on PPs in the literature, less attention was toward size effects, compositional variation, fabrication chamber parameters, and powder size effect, and grain growth mechanisms for AM of these alloys. In other words, AM fabrication of SMAs is not just about building fully dense material with superior strength but also the functionality of the final parts is very important. From the preliminary results, it was

shown that different sizes or even geometries could result in different properties such as ultimate tensile strength regardless of having the same PPs. This was mostly attributed to the fraction of fine to coarse grain sizes in different specimens. Another challenge toward AM of SMAs is the compositional variation due to Ni-loss in this high- temperature process. Not considering this may result in Ti-rich component out of a Ni-rich powder, for instance. Hence, it is very important to study the effect of these factors to come up with a better understanding of AM SMAs.

Karaman - T 9:00-9:30

Engineering the transformation hysteresis by precipitation in NiTi and NiTiHf

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The ability to control the transformation temperatures and thermal hysteresis of NiTi and NiTiHf shape memory alloys is of great importance for engineering applications. For example, pipe coupling applications require a wide hysteresis in order to maintain coupling forces in a wide temperature range, while actuator applications require a narrow hysteresis in order to improve response time and efficiency. Aeronautical, automotive, and oil-and-gas environments require higher transformation temperatures, while biomedical and space applications require lower transformation temperatures. In the current work, we performed a systematic study in order to explore how aging heat treatments in a wide range of binary NiTi compositions (50.7-52.4 at% Ni) can be used to control the transformation temperatures and the thermal hysteresis with and without the presence of external stress. Aging treatments between 200oC-550oC for durations between 30 minutes – 100 hours were performed, and differential scanning calorimetry was performed to determine the transformation behavior. The resulting data was used to demonstrate general trends in how aging conditions affect the transformation behavior. Additionally, 3-dimensional response surfaces and model fitting were used to generate tools to predict the aging time, temperature, and initial composition required to meet a set of transformation temperature requirements. Several selected conditions were subjected to isobaric-heating cooling in order to characterize the effect of these heat treatments on the transformation behavior under stress. Finally, we demonstrate some results from NiTiHf alloys to show that the same concepts can be extended to ternary NiTi alloys, which greatly extends the application space of heat treated NiTi based SMAs.

Heller - T 9:30-10:00

Transformation-plasticity coupling in superelastic NiTi characterized by in-situ DIC, resistometry, IR thermography and DMA

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The plastic deformation in superelastic NiTi has been considered as a primary cause for the cyclic evolution of the stress-strain response as well as for the low fatigue performance. It has been shown that besides commonly assumed slip in austenite, there are particular mechanisms of plastic deformation induced by martensitic transformation (MT). As a result, even in the case of NiTi wires with yield stresses higher than the actual transformation stress, the plastic deformation occurs at the austenite-martensite interface moving under the external loading with a magnitude exponentially depending on temperature and stress at which the MT proceeds [1]. Two mechanisms have been suggested for this MT-coupled plasticity [2]: i)dislocation slip proceeding at the habit plane during reverse MT, ii) austenite twinning proceeding during forward MT through sequential B2-B19'-$B2^T$ evidenced by lower martensite volume fraction after apparently complete forward MT. Besides the stress and temperature, the microstructure decides the magnitude of the plastic deformation and its mechanism i.e. homogeneous slip in austenite or localized MT-induced mechanisms. To identify the prevalent plastic deformation mechanism activated at given operating conditions in a particular NiTi microstructure and resulting in specific amount of stored deformation energy, there is a need for in-situ experimental methods that can spatially resolve strains to distinguish slip in austenite from MT-coupled plasticity, estimate the phase fraction to distinguish the slip-based mechanisms from MT-induced austenite twinning, and evaluate dissipated heat and mechanical hysteresis to estimate the energy stored in defects. As will be presented, we have applied digital image correlation (DIC), infra-red (IR) thermography, electrical resistometry (ER), and dynamical mechanical analysis (DMA) in order to investigate the role of thermomechanical conditions and microstructure in activation of above mentioned plasticity mechanisms in nanograined and micrograined superelastic NiTi wires with diatemers 0.1 mm and 1.78 mm, respectively. As shown in Fig. 1, ER and DIC allowed to identify temperature ranges at which different plastic deformation mechanisms are activated in medical graded NiTi [2]. IR thermography have been often used to spatially track the MT. It will be shown that IR thermography can also provide quantitative information about the total heat released during the MT. Our recent results show that the total heat energy released at the austenite-martensite interface evolves depending on activation of individual plastic deformation mechanisms as will be discussed during the presentation.

Heller - T 9:30-10:00

Figure 1: Tensile response of medical graded superelastic NiTi a) showing inhomogeneous and homogeneous deformation b) due to transformation and slip I, transformation coupled with austenite twinning II, and homogeneous slip in austenite depending on temperature range c) ($VFM^{UP/RES\text{-}O}$, $\varepsilon^{UP/RES\text{-}O}$ volume fraction of martensite and strain at the end of upper plateau (^{UP}), and after unloading and stress free heating ($^{RES\text{-}O}$)) [2].

References

[1] L Heller et al. On the plastic deformation accompanying cyclic martensitic transformation in thermomechanically loaded NiTi, International Journal of Plasticity, Volume 111, December 2018, Pages 53-71.

[2] L Heller et al., Beyond the strain recoverability of martensitic transformation in NiTi, International Journal of Plasticity, Volume 116, May 2019, Pages 232-264.

Chen - T 10:30-11:00

Rational design of shape memory alloys with low functional fatigue properties

Xian(Sherry) Chen

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Materials undergoing reversible solid-solid phase transformations provide emerging applications such as biomedical implants and stents, microelectronic actuators and sensors. The essential functionality of these materials is the ability to recover large deformation (i.e. 5~8%) before and after the structural transformation driven by temperature/stress/ electromagnetic fields. It has been theorized that the macroscopic behaviors depend strongly on the kinematic conditions at atomistic scales. A set of mathematical conditions (i.e. cofactor conditions) has been derived and proposed to predict the formation of microstructure for these materials, which has been proven by experiments that when the lattice parameters closely meet such conditions, the materials do not fatigue even under demanding loads up to millions of cycles. In this talk, I will briefly review the mathematical framework of these conditions, by which I will introduce a rational way to develop new phase-transforming materials with enhanced phase reversibility, thus low functional fatigue property. The theory underlies a material descriptor and the corresponding mechanics criteria by which we can algorithmically search for new materials. Finally, I will discuss the experimental platform we built to measure precisely and quantitatively the deformation gradient and the evolution of microstructure during phase transformation under external loads.

Stebner - T 11:00-11:30

The multiaxial nature of thermomechanical constitutive relationships of shape memory alloys

Aaron Stebner

Mechanical Engineering, Materials Science, Colorado School of Mines

Researchers have been challenged for nearly a century to directly measure the multiaxial nature of the thermomechanical constitutive relationships of crystalline materials. Recently, a new planar-biaxial experimental platform has been developed to meet these challenges. Coupling with far-field high-energy diffraction microscopy enables the direct assessment of elastic vs. inelastic deformation of the gauge sections of cruciform specimens subjected to plane stress loadings, without any a priori assumptions of the form of constitutive relationships. Results using this platform answer a long-standing shape memory alloy mechanics question: What is the mechanistic origin of path-dependence in superelastic nickel-titanium? Concluding remarks will be given to show the connections between the experimental data with micromechanical and continuum modeling frameworks.

Scalet - T 11:30-12:00

Recent advances on phenomenological and computational modeling of shape memory alloys

Giulia Scalet[1], **Fabrizio Niccoli**[2], **Carmine Maletta**[3], **Elena Bonetti**[4], **Ferdinando Auricchio**[1]

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The great and continuing interest in shape memory alloys (SMAs) is deeply stimulating the research on accurate constitutive models that can be efficiently integrated into numerical tools. Computer- based simulations become in fact extremely useful in predicting the mechanical and functional response of SMA-based devices under complex loading conditions, thus reducing the number of time- and cost-consuming experiments.

This work aims to present our recent results concerning 3D phenomenological modeling of SMAs, within the framework of continuum thermodynamics with internal variables. Particularly, the work first focuses on the formulation of a constitutive model describing both the one-way and two-way shape memory effects. Then, a more general model, including, among the others, the description of multiple phase transitions, martensite reorientation, and low-stress phase transformation, is presented. Model formulations are completed by a brief discussion on numerical implementation issues.

The developed models are used for the finite element simulation of several case-studies (specifically, fastening, coupling, and actuation systems) subjected to complex loading conditions. A comparison with experimental data is also presented. The obtained results demonstrate the effectiveness and the accuracy of the developed models and allow to discuss several features of SMA behavior under such complex loading conditions.

Shaw - T 1:30-2:00

Extension-Twist Responses of Superelastic Shape Memory Alloy Tubes

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While the tensile response of commercially-available superelastic shape memory alloys (SMAs) has been widely studied, detailed experimental studies of SMAs under multiaxial loading are relatively rare. There remains a definite need for experimental data under more complex loading conditions to advance the understanding of SMAs for the burgeoning range of structural applications and to inform general constitutive modeling.

Here, we present isothermal responses of superelastic NiTi tubes for a series of axial extension-twist controlled histories, including radial paths and non-proportional paths, spanning pure tension to simple torsion to pure compression. All eight biaxial stress and strain surfaces for the onset and *saturation* of forward and reverse stress- induced transformations are quantified for the first time. Each transformation surface is well-captured by a smooth (three-parameter) ellipse in both strain and stress space. In addition, stereo digital image correlation (DIC) is used during each experiment to characterize the transformation kinetics and surface strain morphologies. Under tension at relatively low amounts of twist, strain localization occurs in helical bands that evolve into axial propagation of ring-like transformation fronts with fine criss-crossing fingers (similar to those seen by Q. P. Sun and co- workers in pure tension). However, at large amounts of twist, including simple torsion and pure torsion, we report a new and perplexing transformation morphology, involving strain localization along nearly longitudinal bands in the tube. Interestingly, strain localization is observed in all the tension-twist experiments, including the simple twist experiment, but aside from some momentary buckling, is largely absent in experiments that involve compression.

Ley - T 2:00-2:30

The Effect of Non-Metallic Inclusions on NiTiHf Actuation Fatigue Performance Using Advanced Charecterization

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High temperature shape memory alloys (HTSMAs) have many potential applications in the aerospace, automotive, and defense industries due to their ability to perform significant amounts of repeatable actuation work at elevated temperatures above 100 °C. While there has been initial early success with NiTiHf HTSMAs, several issues still exists that need to be resolved in order for NiTiHf to become a more viable alloy. One of the major issues is how different types of non-metallic inclusions (NMIs) formed during the melting and processing of the alloy affect the actuation fatigue life of NiTiHf. In this study, the actuation fatigue behavior of two different melts of NiTiHf were examined: one with apx. 1% and a second with less than 0.1% volume fraction of a (Ti,Hf)C phase. The material lots were characterized using differential scanning calorimetry (DSC), scanning electron microscopy (SEM), thermo-mechanical fatigue testing, and synchrotron radiation x-ray diffraction (SR-XRD).

Haghgouyan - T 2:30-3:00

Fracture Toughness and Crack Growth Behavior in NiTi and NiTiHf Shape Memory Alloys

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The unique properties of shape memory alloys (SMAs) such as shape memory and superelasticity stem from martensitic phase transformation. This solid-to-solid and diffusionless transformation can be triggered by appropriate mechanical and/or thermal inputs. SMAs like nickel-titanium (NiTi) with near-equiatomic compositions are being used in many applications. Driven mainly by the aerospace industry, there has been a recent interest in SMAs as a potential substitute for solid state actuators. However, limited knowledge on their failure mechanisms, in particular fracture behavior, has limited implementation of SMAs in such applications. Consequently, there is a need to understand and quantify fracture response of SMAs to fully exploit their huge potential. Based on experimental observations, high stresses near the crack result in a phase transformation zone in SMAs. The presence of this zone alters the near-tip mechanical fields, and cannot be neglected when its size is large compared to the characteristic dimensions of the crack configuration. However, the published fracture toughness data reported in literature is based on the premise of linear elastic fracture mechanics (LEFM). As shown by the authors in ref. [1] taking into account the effect of such non-linear crack-tip dissipation mechanisms results in a fracture toughness values for NiTi that are much greater than the ones reported based on LEFM. Moreover, it enables a more precise prediction for crack growth under various thermo-mechanical loading paths (Figure 1).

Figure 1. Load-displacement curves and strain (εyy) measurements corresponding to the load maximum under mode-I isothermal loading of NiTi SMA obtained from experimental measurements and finite element calculations [2].

The inherently low transformation temperatures (below ~100°C) has limited the applications of NiTi SMAs at elevated temperatures. Consequently, with the intent of

increasing transformation temperatures, high- temperature SMAs has been developed by alloying of NiTi with ternary elements. Although the thermo- mechanical constitutive behavior of the high-temperature SMAs has been studied in recent years, there is very little understanding of their fatigue and fracture properties, which is crucial for their successful integration into commercialized applications. To address this, fatigue crack growth and fracture behavior of a NiTiHf high-temperature SMA is investigated. Preliminary results showed that unlike NiTi SMAs, transformation is confined to a small region at the crack-tip, resulting in unstable crack growth and relatively small fracture toughness.

References

[1] Haghgouyan, Behrouz, et al. "Fracture toughness of NiTi–Towards establishing standard test methods for phase transforming materials", *Acta Materialia* (2019).

[2] Haghgouyan, Behrouz, et al. "Stable crack growth in NiTi shape memory alloys: 3D finite element modeling and experimental validation", *Smart Materials and Structures* (2019).

Seiner - T 3:30-4:00

Microstructures in modulated martensites – experimental observations and theoretical models

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Modulated martensites of Ni-Mn-Ga ferromagnetic shape memory alloys are able to form complex, hierarchical microstructures of twins and macro-twin interfaces. Some of the macro-twins in this material exhibit a very unique property called supermobility, i.e. such interfaces can be set into motion by as small mechanical stress as 0.01MPa and can be also easily driven by external magnetic fields. The origin of the supermobility is not fully understood yet. It is, however, believed that this phenomenon may be related to the the ability of Ni-Mn-Ga to form martensitic microstructures at very fine spatial scales, and thus, to specific lattice parameter and crystal structure of this alloy. The talk will summarize the recent experimental observations of microstructures in 10 M modulated Ni-Mn-Ga, and outline the main theoretical tools used for describing their formation. It will be shown that these microstructures exhibit several unique features, not observed in any shape memory alloy before, which open a discussion whether other alloys with supermobile interfaces could be, in future, designed based on the knowledge gained on Ni-Mn-Ga.

Saint-Sulpice - T 4:00-4:30

Prediction of low cyclic fatigue of NiTi structures using reduced technics based on multi-scale modeling

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NiTi shape memory alloys are used in several applications for their specific properties such as super-elasticity or shape memory effect. Furthermore, those applications often subject the alloys to cyclic loadings generally inducing failure by fatigue. Low cycle fatigue must then be studied in order to insure the reliability of applications.

However, only few studies concern the low cycle fatigue of NiTi shape memory alloys. Indeed, in order to predict the low cycle fatigue life of a structure, non-linear 3D finite element simulations are generally used. These simulations require a very long processing time which is often prohibitive.

In this study, we propose to use reduced technics in order to predict the low cycle fatigue life of structures. These technics are based on a localization operator. It permits to estimate the stress at critical point(s) using only finite element simulation of half a cycle [1, 2]. From this estimated local stress and a non-linear behavior model of the alloy, it is then possible to estimate rapidly the total and transformation strains at critical point(s) during cyclic loadings. These technics have been applied to austenitic or martensitic hourglass samples under traction and rotary bending loadings as well as endodontic files under rotary bending loadings. The results have been validated with non- linear 3D finite element simulations.

Then, by using an adapted fatigue criterion, the fatigue life of the considered structures has been estimated. It is then possible to have the estimated fatigue life in function of the stress amplitude. These results have been compared with the ones obtained by fatigue tests realized on hourglass samples under traction and rotary bending loadings and on endodontic files under rotary bending loadings.

References

[1] Herbland, Thibault, Georges Cailletaud, and Stéphane Quilici. “Evaluation of Local Stress and Strain State at Notch Root by Means of a New Method Valid for Multiaxial Random Loadings.” In *International Conference on Fracture*, 10 p. Ottawa, Canada, 2009.

[2] Darlet, Adrien. “Estimation rapide en surface de la triaxialité des contraintes et de la plasticité : application aux disques et aux aubes de turbine de turboréacteurs.” Theses, École Normale Supérieure de Cachan - ENS Cachan, 2014.

Kyriakides - T 4:30-5:00

Response of Pseudoelastic NiTi Tubes Under Combined Tension and Internal Pressure

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Nearly equiatomic NiTi can be strained in tension to several percent and fully recover upon unloading (*pseudoelastic* behavior). This property is derived from solid-state transformations between the *austenitic* (A) and *martensitic* (M) phases, which can be induced by either changes in temperature or stress. It is well established that stress-induced phase transformation leads to localized deformation associated with the nucleation and propagation of the M-phase during loading and the A-phase during unloading. It has been demonstrated that this partially unstable material behavior strongly influences the stability of NiTi structures (e.g., [1]). A crucial requirement for the analysis and design of such structures is constitutive models that capture this instability. Most efforts on modeling SMA behavior to date are based on uniaxial experiments. In an effort to expand knowledge to the multiaxial setting we present results from a series of experiments on pseudoelastic NiTi tubes loaded under combined axial load and internal pressure. Specimens were loaded under radial stress paths in the axial-hoop stress space using stereo digital image correlation for full-field monitoring of the evolution of transformation-induced deformation. Results spanning axial-to-hoop stress ratios from -1.0 to uniaxial tension revealed that, but for a narrow region near equibiaxial tension, transformation leads to localized helical deformation bands with helix angles that depend on the stress ratio. In the process, the stresses remain nearly constant until transformation is completed. In the vicinity of equibiaxial tension, the material exhibits hardening and homogeneous deformation. Loci of the transformation stresses, while exhibiting very modest anisotropy, traced an elongated trajectory in the axial-hoop stress space not captured by a von Mises representation. By contrast, the transformation strains exhibit significant anisotropy between axial and hoop dominant stress paths. Moreover, strains around the equibiaxial stress state, where material hardening and homogeneous deformation was observed, are significantly smaller than in the rest of the stress space. The strain anisotropy has a corresponding reflection on the energy dissipated during transformation with axial dominant stress paths dissipating significantly more energy than hoop dominant ones, with less dissipation observed in the neighborhood of equibiaxial stress.

References

[1] D. Jiang, S. Kyriakides, S., N.J. Bechle, C.M. Landis, "Bending of pseudoelastic NiTi tubes." *Int'l J. Solids & Structures* **124**, 192-214, 2017.

[2] N. Bechle, S. Kyriakides, "Evolution of localization in pseudoelastic NiTi tubes under biaxial stress states." *Int'l J. Plasticity* **82**, 1-31, 2016.

Sun - W 8:30-9:00

Ultrahigh Compressive Fatigue Life and Fatigue Mechanisms of Superelastic NiTi in Solid-State Cooling Technology

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Superelastic NiTi shape memory alloy (SMA) has been identified recently as a promising refrigerant in solid-state green refrigeration technology due to its large latent heat and cooling capacity in reversible phase transformation driven by external mechanical and/or thermal field. One of the key challenges in developing the solid-state cooling is the required high fatigue resistance of the NiTi material to ensure a reliable long term operation of the cooling system. About $10^7 \sim 10^8$ phase transition cycles is expected for a refrigeration device working over a ten-year lifespan. Unfortunately, under cyclic tensile working mode, bulk commercial superelastic NiTi alloy wires, strips and tubes have very limited fatigue life (about $10^2 \sim 10^4$ cycles) and are almost impossible to meet such stringent requirement. Cyclic compression of NiTi rod and tubular structures was used instead in the bulk cooling system prototypes, mainly for an enhanced fatigue performance and more efficient heat transfer with the fluid media. This talk reports fatigue behavior of superelastic NiTi shape memory alloy rods and tubes under cyclic compressive phase transition. Fatigue crack nucleation and propagation and the resulting ultrahigh fatigue life under compression and their dependence on the microstructure are investigated. Recent advances in developing nano-structured NiTi shape memory alloys with improved fatigue performance through microstructure engineering, modelling and characterization techniques will be presented.

Petryk - W 9:00-9:30

Phase-field approach to microstructure evolution in SMA: size effects and rate-independent dissipation

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Stress-induced martensitic transformation in shape memory alloys (SMA) typically proceeds through the formation and evolution of martensitic microstructures. Competition between interfacial energy contributions at different levels provides a natural intrinsic length scale and makes the microstructures size-dependent. In the numerical simulations presented, the phase-field approach is used, where the interfaces are diffuse and mobile, so that no a-priori assumption on the microstructure topology is needed. The evolution of a microstructure is governed by two thermodynamic potentials of the free energy and dissipation rate. Calculations are performed by using realistic material parameters for a CuAlNi SMA and assuming quasi-static isothermal transformations. Differences and similarities between size-dependent laminate microstructures calculated earlier by using a sharp-interface model and more recent phase-field modelling results [1] are discussed.

The usual phase-field approaches that involve only a purely viscous dissipation are not capable of simulating rate-independent dissipative effects, commonly observed experimentally in SMA in the form of hysteresis loops of finite width for arbitrarily small rates of cyclic loading. Recently, the rate- independent dissipation, corresponding to a finite threshold value for a thermodynamic driving force, has been introduced into the phase-field framework for modelling displacive transformations like twinning or phase transformation in SMA [2]. Theoretical and numerical aspects of this novel approach are discussed. Simulation results for two- and three-dimensional boundary value problems representative for SMA are presented.

References

[1] K. Tůma, S. Stupkiewicz and H. Petryk. Size effects in martensitic microstructures: finite-strain phase field model versus sharp-interface approach, *J. Mech. Phys. Solids* **95**, 284-307 (2016).

[2] K. Tůma, S. Stupkiewicz and H. Petryk. Rate-independent dissipation in phase-field modelling of displacive transformations, *J. Mech. Phys. Solids* **114**, 117-142 (2018).

Wendler - W 9:30-10:00

Mesoscale Simulation of Shape Memory Alloy Thin Film Devices

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Shape memory alloys (SMAs) are characterized by a high cyclic work density and large latent heat, which renders them ideal materials for both solid state cooling and vibration damping. Until now, the latter is exploited in large-scale applications like the protection of buildings against seismic loads. NiTi thin-film-based miniature devices in form of tensile loaded bridge suspensions enable fast heat exchange, and have the potential to provide vibration damping and micro-cooling in portable electronics.

For damping, we apply both pseudoelasticity and the one-way shape memory effect to dissipate energy using passive and active strategies. The complex thermo-mechanical coupling with mutual conversion of elastic into chemical (phase state) and thermal energy leads to changing stress-strain cycles during temperature evolution in the material. Here, a previously developed FEM material model which implements transition state kinetics for the martensite-austenite (M-A) transformation and contributions for the M-A interface energy from a phase-field approach [1] is applied as a mesoscale description. The external spring- mass suspension is treated as a discrete system represented by ODEs coupled to the finite element domain in form of boundary conditions [2]. For parameterization, macroscopic as well as local material properties are evaluated by a set of tensile testing, DIC (digital image correlation), thermal IR and DSC experiments. Additionally, we develop a test protocol to identify model parameters under dynamic conditions.

Figure1: Evolution of mass displacement (a) and martensite/temperature evolution (b) of a thin film SMA damping device (c) during free vibration. FEM simulations show local strain bands for two times.

Wendler - W 9:30-10:00

Computational studies of the micro-devices under free and forced harmonic excitation are carried out. Experimentally observed martensitic strain bands, which correlate to thermal patterns in tensile loading are resolved in the simulations, where higher loading frequencies above 10 Hertz favour quasi-homogeneous band nucleation. A strong dependency of the mechanical response on prestrain and applied amplitudes and the nonlinear vibration characteristics is found, and helps to optimize the damping capacity using active control.

References

[1] F. Wendler, H. Ossmer, C. Chluba, E. Quandt, M. Kohl, Mesoscale simulation of elastocaloric cooling in SMA films, Acta Mater. 136, 105-117 (2017).

[2] S. Ahmadi, K. Jacob, F. Wendler, M. Kohl, Shape Memory Alloy Film Damping for Smart Miniature Systems, Int. J. Smart and Nano Mat. 9(3), 199-215 (2018).

Welsch - W 10:30-11:00

A Fully-Coupled Simulation Tool for Elastocaloric Air-Cooling Devices

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Shape memory alloys (SMA) are generally known for biocompatibility, high energy density, and self-sensing properties. In addition to being used in lightweight actuator systems and biomedical applications, these alloys exhibit excellent cooling properties. Superelastic Nickel-Titanium (NiTi) enables a novel environment-friendly cooling technology without global warming potential with growing interest in the last few years [1].

Elastocaloric cooling uses solid-state NiTi-SMA as a non-volatile cooling medium compared to vapor compression-based cooling systems. Due to the high latent heats activated by mechanical loading/unloading, large temperature changes can be generated in the material. Accompanied by a small required work input, a high coefficient of performance is achievable. The potential of these alloys can be accessed by the use of an appropriate thermodynamic cooling cycle [2] and optimized elastocaloric materials [3], as well as efficient system design. Economic development of an efficient SMA based cooling device also requires the understanding of the material behavior supported by experimental investigations [4], and predictive system simulation tool including effects of local material behavior [5].

This contribution introduces a fully coupled thermomechanical simulation tool that will aid in the systematic design of such machines. It combines heat transfer analysis between the fluid flow and the cam-driven mechanical loaded SMA material, leading to release and absorption of the latent heats finally responsible for heating and cooling. The mathematical structure and computational implementation of the simulation tool is discussed in detail along with a first analysis of how operational parameters such as rotation frequency and air flow rate impact COP and cooling power.

Device

During the DFG Priority Program SPP 1599 a continuous operating elastocaloric fluid cooling system using tensile-loaded SMA wires has been developed and successfully demonstrated [6]. A special cam drive allows the implementation of thermodynamically optimal cycles, identified in previous lab experiments, to operate the device in continuous rotatory operation. The system, presented in Figure 1a, consists of the heat transfer system

designed for fluid cooling and a mechanical system for individual loading and unloading multiple SMA wire bundles. The versatile realization of the device allows the independent variation of process parameters like loading profile, rotation frequency, duct geometry, heat transfer characteristics, fluid flow rate, flow direction, inlet temperatures as well as material parameters. Rotation frequency, fluid flow rate, and inlet temperatures are adjustable at the running device. The first realization is equipped with 24 bundles, consisting of 30 single wire with a diameter of 200 µm and a total length of 300 mm. For the first experimental tests NiTiCo#3, produced by Fort Wayne Metals, is used and loaded up to 3 % with a symmetric 40°-load profile for loading and unloading. The in- and outlets of the airflow are arranged symmetrically around the loading and unloading with an angle of 68°.

Simulation tool with GUI

To assist the design process of the device with an optimized parameter set for the desired performance and efficiency, a fully coupled thermomechanical system level simulation tool of the multi-wire elastocaloric cooling unit is developed. The tool, implemented in MATLAB, represents the interacting subunits of the device: The mechanically driven kinematics, the thermal values with fluid transport and heat transfer unit, as well as multiple SMA models. Numerous vectorized SMA- models, based on Mueller-Achenbach-Seelecke model using Boltzmann statistics with a multi-well free energy function, support the thermo-mechanical coupling between the loading function and the heat transfer unit, allowing a drive torque and thermal power calculation. Reproducing the heat transfer between SMA and fluid and the heat transport in the fluid, the flow channel is discretized with finite differences. The resulting compact simulation tool is qualified for massively parallel computation on modern multi-core computers, which allows economic comprehensive parameter scans, due to the short computation time. To enable parameter studies and investigate parameter spans for different input and design parameters, the simulation tool is linked to a parameter table defining the parameter set with the material specification for each simulation.

In addition to the detailed results, each simulation returns key values like stationary output temperatures, thermal and mechanical power and COP to the parameter table, supporting the meaningful analysis of the parameter studies. The graphical user interface, implemented in MATLAB, offers the possibility to arrange the results of the parameter sweep in an individual illustration to point out trends and relationships of different device parameter sets. Improving the understanding of the results the simulation can be visualized as a video, a still frame is presented in Figure 1b.

Simulation setup and results

Imitating the first experiments of the developed machine prototype, the parameter sweep in Figure 1c uses rotation frequencies of 0.05...0.6 Hz and flow-rates of 10...40 m^3/h. The geometry is chosen consistent with the device configuration mentioned before. Further, the mechanical material parameters are fitted to NiTiCo#3 with Young's modulus for austenite to 53.8 GPa, martensite to 22.6 GPa, a plateau height of austenite to 542.5 MPa, martensite to 423.3 MPa, the transformation strain is set to 3.712 %, and the Clausius-Clapeyron

coefficient to 7 MPa/K. Additionally, a density of 6317 kg/m^3, the heat capacity of 463 J/kg/K and the latent heats of 15.6 J/g are used. The inlet temperatures at the hot and cold side are set to 22°C.

With rising rotation frequency, the number of loading and unloading cycles increases and thus the temperature differences between in- and outlets rise. The maximum temperature difference of 10.4 K is reached while operating at a flow rate of 10 m^3/h and a rotation frequency of 0.1 Hz.

Figure 1: a) Schematic view of the first continuous operating elastocaloric cooling device based on tensile loaded NiTi wire bundles. b) Screenshot of the visualization tool. c) Simulation results of a parameter sweep.

Conclusions

A fully coupled thermomechanical system level simulation tool is presented to predict the system performance under various operating conditions. The model captures the mechanical and thermal device characteristics required for the identification of an optimized parameter set for high-efficient and high-performance cooling at large temperature spans. Also, the model can be used for systematic and comprehensive parameter studies. Further, an animated visualization tool is implemented to support the fast evaluation of the complex system behavior. First results of the simulation and visualization tool are presented using this computationally efficient, parallelized thermo-mechanical model. Additionally, a first parameter study with varying rotation frequency and flow rate is executed to find an optimized parameter set. In the next step, a direct comparison between the simulation and the real device will be conducted to validate the performance and predictive power of the model.

Acknowledgments

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References

[1] S. Fähler, “Special Issue on ‘Ferroic Cooling,’” *Energy Technol.*, vol. 6, no. 8, 2018.

Welsch - W 10:30-11:00

[2] M. Schmidt, "Elastokalorisches Kuhlen mit Ni-Ti-basierten Formgedachtnislegierungen: Thermodynamische Analyse, experimentelle Untersuchungen, Prozessoptimierung," PhD thesis, Saarland University, 2017.

[3] J. Frenzel, G. Eggeler, E. Quandt, S. Seelecke, and M. Kohl, "High performance elastocaloric materials for the engineering of bulk and micro cooling devices.," *MRS Bull.*, vol. 43(4), 2018.

[4] N. Michaelis, F. Welsch, S.-M. Kirsch, M. Schmidt, S. Seelecke, and A. Schütze, "Experimental Parameter Identification for Elastocaloric Air Cooling," *Int. J. Refrig.*, 2019.

[5] F. Welsch *et al.*, "Numerical simulation and experimental investigation of the elastocaloric cooling effect in sputter-deposited TiNiCuCo thin films," *Contin. Mech. Thermodyn.*, vol. 30, no. 1, pp. 53–58, 2017.

[6] S.-M. Kirsch *et al.*, "NiTi-based elastocaloric cooling on the macroscale - from basic concepts to realization," *Energy Technol.*, no. Ferroic Cooling, pp. 1567–1587, 2018.

Purohit - W 11:00-11:30

Kinetics of phase boundaries in bistable chains in the isothermal and adiabatic regimes

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The use of one dimensional chains of masses and bistable springs as models for phase transforming materials is well-established in the mechanics literature [1]. These models can be thought of as discrete representations of a one-dimensional bar whose Helmholtz free energy function has multiple wells corresponding to different phases. The equations of motion of the masses in the chain can be derived from Newton's second law after accounting for the interactions of each mass with its neighbors. Numerical impact experiments on tri-linear and bi-linear chains have revealed that sonic waves and phase boundaries that are known from the continuum dynamics of phase transitions in bars are seen also in mass-spring chains [2]. However, the solutions involving phase change in a bar are non-unique, and this non-uniqueness can be remedied by supplying a *kinetic relation* for phase boundaries as constitutive information. On the other hand, solutions involving phase change in a mass-spring chain are uniquely determined by the energy landscape of the springs and the equations of motion of the masses. This suggests that a kinetic law relating the driving force on the phase boundary to its speed in the reference configuration can be deduced from the mass-spring chain. The form of this kinetic law has been obtained analytically and has been verified through numerical experiments [2]. This kinetic law corresponds to a purely mechanical problem with no consideration of the effects of temperature.

Inspired by the success of mass–spring chains with only extensional degrees of freedom in predicting the kinetic laws for phase boundaries, we added rotational degrees of freedom to the masses in a chain and studied the dynamics of phase boundaries across which both the twist and stretch can jump. We solved impact and Riemann problems in the chain by numerical integration of the equations of motion and showed that the solutions are analogous to those in a phase transforming rod whose stored energy function depends on both twist and stretch. From the dynamics of phase boundaries in the chain we again extracted a kinetic relation whose form is familiar from earlier studies involving chains with only extensional degrees of freedom. However, for some combinations of parameters characterizing the energy landscape of our springs we found propagating phase boundaries for which the rate of dissipation, as calculated using isothermal expressions for the driving force, was negative [3]. This suggests that we cannot neglect the energy stored in the oscillations of the masses in the interpretation of the dynamics of mass–spring chains. Keeping this in mind we defined a local temperature of our chain and showed that it jumps across phase boundaries, but not across sonic waves. Hence, impact problems in our mass–spring chains are analogous to those on continuum thermos-elastic bars, and the phase boundaries propagate adiabatically in the chain with no energy lost to the surroundings.

Purohit - W 11:00-11:30

Having addressed kinetic laws for phase boundaries in the purely mechanical and adiabatic settings it remains to address the kinetic law for a phase boundary propagating isothermally. We accomplish this by immersing our mass-spring chain in a heat bath and integrating Langevin's equations of motion for the masses [4]. We can estimate the dissipation at the propagating phase boundary by performing an energy balance on the chain while taking account of the fluctuation-dissipation theorem of statistical mechanics. This time we find that the kinetic law is of the 'stick-slip' type and is dependent on the bath temperature. We use this kinetic law to solve continuum boundary value problems for a bar with a moving phase boundary and find that the force-extension relation for the bar is fully consistent with that of the mass- spring chain except that thermal fluctuations seen in the chain cannot be captured in a continuum theory.

The size of these fluctuations can be estimated using principles from statistical mechanics. Thus, mass- spring chains can be used as a vehicle to model features of kinetic laws that are known from experiments on shape memory alloys.

References

[1] R. Abeyaratne and J. K. Knowles, *Evolution of phase transitions*, Cambridge University Press, New York, (2006).

[2] Q. Zhao and P. K. Purohit, "Extracting a kinetic relation for the dynamics of a bistable chain", *Modeling and simulation in materials science and engineering* **22**, 045004 (20 pages), (2014).

[3] Q. Zhao and P. K. Purohit, "(Adiabatic) phase boundaries in bistable chains with twist and stretch", *J. Mech. Phys. Solids* **92**, 176-194, (2016).

[4] C. Sun and P.K. Purohit, "Stick-slip kinetics in bistable bar immersed in a heat bath", submitted, (2019).

Lee - W 11:30-12:00

Characterization and actuation of nematic elastomers

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Nematic elastomers are a type of liquid crystal elastomer that lie at the forefront of programmable soft materials because they can reversibly deform under an external stimulus such as a change in temperature or light, are capable of undergoing large deformation, and can be tuned for repeatable, predictable actuation. In thermotropic nematic elastomers, the order of anisotropy in the material is controlled by the temperature governing a nematic-isotropic phase transition, which makes them promising materials for applications in aerospace for deployable structures, in the biomedical engineering as a soft peristaltic pump, and in communications applications for the actuation mechanism in a reconfigurable antennae. Due to the cyclic nature of actuation applications, a better understanding of the viscoelastic behavior is necessary to optimize design and performance. This talk describes a custom-built temperature-controlled tensile test apparatus that characterizes the material and a continuum-level constitutive model to de- scribe the viscoelastic behavior of thermotropic nematic elastomers. Additionally, the solutions to quasi-static elastic phenomena in this material will be presented, such as the deformation of a cylindrical balloon and its application as a peristaltic pump, the cavitation of a disk, and the bending of a block.

Kazinakis - W 1:30-2:00

Effect of Phase Transformation on the Stability of Pseudoelastic NiTi Tubes Under Bending

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Bending of tubes induces ovalization to the cross section, a nonlinearity that reduces the bending rigidity and may precipitate additional instabilities leading to collapse. Stress-induced phase transformation of NiTi in the pseudoelastic temperature regime is characterized by inhomogeneous deformations with coexisting martensite at strain of about 7% and austenite at less than 1%. This paper presents experiments followed by analysis that examine how the geometric nonlinearities and this inelastic behavior of NiTi interact in tubes under bending. An experiment with a diameter-to-thickness ratio of 18.7 shows that transformation causes the nucleation of several dispersed high strain banded patterns of martensite on the tensioned side of the tube. The zone where the bands coalesce into intersecting diamonds undergoes excessive local ovalization causing catastrophic buckling at a relatively low overall tube curvature. A recently developed constitutive model of pseudoelastic NiTi has been implemented within a finite element framework in order to simulate the bending experiments [1]. The analysis captures the level of the moment-curvature response, the nucleation and evolution of the high strain diamond shaped patterns, the influence of those patterns on ovalization, and the resultant buckling and collapse of the tube. Parametric studies have shown that as the tube D/t increases, the interaction between the material and geometric nonlinearities becomes stronger making buckling more imperfection sensitive.

References

[1] Jiang, D., Kyriakides, S., Bechle, N.J., Landis, C.M. (2017). Bending of pseudoelastic NiTi Tubes. *Int'l J. Solids & Structures* **124**, 192-214.

Xu - W 2:00-2:30

A Three-dimensional Constitutive Model for Shape Memory Alloys Considering the Evolutionary Material Response and Two-way Shape Memory Effect at Stress-Free Condition

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Shape memory alloys (SMAs), since the discovery of their shape memory effect, have been intensively investigated as actuators for the past several decades. Due to their high actuation energy density compared to other active materials, their current and potential applications in the biomedical, aerospace, automobile and energy fields are expanding rapidly. Experimental evidences indicate that the response of SMAs subjected to cyclic thermomechanical loading condition is evolutionary rather than stable, during which TRansformation-Induced Plastic (TRIP) strains and internal stresses are usually generated. The evolutionary TRIP strains are generated because the repeated phase transformations induce significant distortion located at the austenite-martensite interfaces and grain boundaries, especially during the very first thermomechanical cycles as shown in figure 1. This distortion drives dislocation activity resulting in an observable macroscopic TRIP strain, which occurs at effective applied stress levels much lower than the plastic yield limit of the material. As a result, untrained SMAs components are usually subjected to a training process (i.e. thermal cycling under isobaric conditions) to stabilize their material behaviors before they are used as actuators. After the training procedure, the generated internal stresses inside the material along with a potential thermal loading provide the driving force to induce the oriented phase transformation so that the SMA-based actuators are able to exhibit the Two-Way Shape Memory Effect (TWSME) without applying external bias load. To predict these intrinsic phenomena, a three-dimensional constitutive model for untrained SMAs is developed. The proposed model utilizes the martensitic volume fraction, transformation strain, TRIP strain, and internal stress as internal state variables so that it is able to account for the evolution of TRIP strains and the TWSME for untrained SMAs under cyclic thermomechanical loading conditions. Boundary value problems considering untrained SMA materials subjected isothermal/isobaric cyclic loading are solved and the predicted cyclic response is compared against available experimental data to demonstrate the proposed capabilities.

Xu - W 2:00-2:30

Figure 1. TEM images showing the microstructure changes of an untrained NiTi matrial after 10 loading cycles. Sittner et al. 2018.

Figure 2. The 1st and 50th pseudoelastic stress-strain response of the untrained NiTi under 550 MPa uniaxial tensile loading, simulation and experimental results.

Hartl - W 2:30-3:00

Towards High Power Density Solid/Liquid Metal Composite Actuators

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Shape memory alloys (SMAs) provide the highest actuation density of all active materials and found in a wide variety of industrial sectors such as aerospace, automotive, biomedical, and oil exploration. [1] The thermal energy needed to drive actuation is most often generated electrically via resistive heating (Joule heating), though new concepts such as electromagnetic induction heating from an alternating current are being explored. [2] Despite SMA actuators being of great interest recently, there are still limitations preventing them from being used more widely. One issue is that SMA actuators suffer from a low actuation frequency. Joule heating allows rapid, on-demand heating, though only for SMA components of sufficiently small cross-sectional area for which electrical current limitations are not a concern. Further, there are not many attractive options for rapid, on-demand cooling, which is required to increase the actuation frequency of SMA actuators.

Previous research by Coppola et al. [3] has examined integrated cooling mechanisms for SMA actuators having small channels using water and oil. Water and polyalphaolen were flowed through vascular channels in the actuator system and convectively remove heat from the SMA component. Expedited cooling can be further advanced using fluids with higher thermal conductivity. A category of fluids with higher thermal conductivity is room-temperature liquid metal (LM), with viable candidates being non-toxic, gallium-based LMs. Gallium-indium eutectic (GaIn, 75.5/24.5 wt.%) have solidification temperatures below room-temperature, and thermal conductivity higher than water and oil. [4]. Furthermore, since a LM coolant is electrically conducting, multifunctionality becomes possible. Instead of designing cooling channels solely optimized for removing heat, one can orient these electrically conductive channels into resistive heater traces or into a coil to enable electromagnetic induction. With an alternating current applied to this LM coil, induction creates eddy currents in the bulk SMA, generating distributed heat fluxes to actuate the system. Subsequently, cooling is driven by flowing LM through the vascular channel, removing the heated LM from the actuator domain and replenishing it with cooler LM. In this way, a unique multifunctional mechanism to heat and cool an SMA actuator can be presented, modeled, and tested. To address the critical issue of LM-induced corrosion, focused studies have shown that NiTi is relatively unaffected by this phenomenon at up to 220°C for extended periods of time [5].

A number of thermo-electrical modeling studies have been performed considering an SMA beam with a simple spiral pattern cut into both its top surface and at its midplane. Liquid metal channels in a coiled configuration having an outer diameter of 32 mm and a semicircular or circular channel cross-section with a 2mm diameter have been considered. The electrical operation assumed a 12 A oscillating current applied at 150 kHz through the stationary LM channel for 60 s. Resulting inductive heating of the SMA beam has been

predicted. Further, 1-D pipe flow modeling methods have been used to assess the effect of embedded channels on SMA actuator cooling speed, and the modeling of both heating and cooling has carefully quantified the effect of LM coil placement. Physical prototypes having the channels described have been manufactured through selective laser melting, the channels have been electrically coated, and LM (gallium-indium eutectic) has been passed through the channel. An induction heater power supply has been used to provide the appropriate electrical input to the system and embedded induction heating of the SMA beam has been experimentally demonstrated. Subsequent flow of near 0°C LM through the channels leads to expedited cooling of the actuator. These prototype actuators prove the viability of using LM vascular channels for both inductive heating and integrated cooling in SMA actuator components.

Acknowledgments
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References

[1] D. Lagoudas, ed., Shape Memory Alloys: Modeling and Engineering Applications, Springer-Verlag, 2008

[2] R. N. Saunders, J. G. Boyd, D. J. Hartl, J. K. Brown F. T. Calkins, and D. C. Lagoudas, A validated model for induction heating of shape memory alloy actuators. Smart Materials and Structures 25(4), 045022, 2016.

[3] A. M. Coppola, L. Hu, P. R. Thakre, M. Radovic, I. Karaman, N. R. Sottos, and S. R. White, Active Cooling of a Microvascular Shape Memory Alloy Polymer Matrix Composite Hybrid Material: Active Cooling of a Microvascular Shape Memory, Advanced Engineering Materials vol. 18, pp. 11451153, July 2016.

[4] M. D. Dickey, R. C. Chiechi, R. J. Larsen, E. A. Weiss, D. A. Weitz, and G. M. Whitesides, Eutectic Gallium-Indium (EGaIn): A Liquid Metal Alloy for the Formation of Stable Structures in Microchannels at Room Temperature, Advanced Functional Materials 18, 10971104, 2008.

[5] Mingear, J. and Hartl, D., Corrosion of Nickel-Titanium, C110, and Al6061 in Gallium-based Liquid Metal Alloys, in the Proceedings of the TMS 2017 146th Annual Meeting and Exhibition, San Diego, CA, Feb-Mar, 2017.

Solomou- W 3:30-4:00

Bayesian Materials Discovery: Application on the Discovery of Precipitation Hardened NiTi Shape Memory Alloys through Micromechanical Modeling

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Shape memory alloys (SMAs) are unique materials with the ability to undergo and recover moderate to large inelastic deformations. Therefore, SMAs are suitable for applications in aerospace, oil and gas and biomedical industries where they are utilized as high performance solid state actuators. Experimental studies in aged NiTi SMAs have shown that the generated Ni4Ti3 precipitates in the microstructure of the material due to aging, affect significantly the phase transformation characteristics such as hysteresis size and transformation strain and temperatures [1]. To this end, careful manipulation of the composition of the SMA matrix and the volume fraction of precipitates can effectively control the material's behavior. Thus, an appropriate selection of the SMA aging conditions can be a key factor to acquire materials with the desired microstructural characteristics that meet the performance requirements of targeted applications. However, a purely experimental, intuition-based approach is not sufficient due to the high cost and preparation time required to synthesize and characterize the material. The present work aims to address the aforementioned issue by developing an integrated framework, to expedite the discovery of SMAs with desired performance, based on the concept of optimal experimental design. To this end, a micromechanics based Finite Element (FE) model is used to model the NiTi SMA material system behavior and capture its effective response and properties based on its composition and microstructure [1].

Solomou- W 3:30-4:00

Figure 1. Discovery of NiTi SMAs with targeted properties using a micromechanical model and a Bayesian optimal experimental design framework.

Subsequently, an optimal experimental design framework, based on the Bayesian approaches, is utilized to minimize the required computational experiments performed by the SMA micromechanical model (Fig. 1) in order to efficiently discover materials with targeted properties [2]. The results demonstrate the increased time efficiency of the proposed framework, in discovering the targeted materials, compared to the exhaustive model-driven exploration of the materials design space.

References

[1] A. Cox, B. Franco, S. Wang, T. Baxevanis, I. Karaman, and D. C. Lagoudas, "Predictive Modeling of the Constitutive Response of Precipitation Hardened Ni-Rich NiTi", *Shape Memory and Superelasticity*, (2017).

[2] A. Solomou et al., "Multi-objective Bayesian materials discovery: Application on the discovery of precipitation strengthened NiTi shape memory alloys through micromechanical modeling", *Materials & Design*, (2018).

Frost - W 4:00-4:30

Macroscopic constitutive model tailored for polycrystalline NiTi shape memory alloys with localized phase transformation

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Having found many applications in medicine, civil engineering or aerospace industries, NiTi-based alloys are a prominent class within SMAs usually utilized in the form of thin structures, e.g. wires, strips or tubes. In such structures, the martensitic transformation often does not occur in a spatially homogeneous manner; instead, localized "martensitic bands" form within the austenitic sample and their fronts propagate leaving a material with modified dimensions and microstructure behind. In a simple tension of a bar, the phenomenon resembles the well-known Lüders bands: the onset is usually accompanied by a stress overpeak and followed by a stress plateau, material rehardens after exhausting the available portion of inelastic strain and the formation of bands depends on microstructure of the material. Various localization patterns appearing in NiTi samples have been documented in many experimental works recently.

Because localization gives rise to high gradients of strain concentrated in small volumes of material, it is supposed to be one of critical factors for the fatigue lifetime. Hence, an effective constitutive model capable to reproduce (and even predict) occurrence of localization patterns is desirable. If the model is to plausibly reproduce common practical loading scenarios, it should also cover the specific features of NiTi alloys, e.g. reversible and strongly loading mode-dependent maximum attainable inelastic (transformation) strain, loading mode-dependent elastic properties of martensite or the strong stress-temperature coupling in the phase transformation.

In this talk we will introduce a well-established constitutive model for NiTi SMA [1, 2] and suggest its extension aiming at the above-mentioned challenge. By particular tuning of parameters of both the internal energy with a term motivated by an "austenite matrix – martensite inclusion" notion and the dissipation function it is possible to impose strain-softening in tension and strain-hardening in compression simultaneously [3]. Finite element implementation into Abaqus FEA software then allows to study localization patterns in common sample geometries (wires, ribbons, tubes) and loading modes (tension, bending, torsion) and compare them with available experimental data (DIC, XRD, optical methods).

References

[1] Sedlák, P., Frost, M., Benešová, B., Ben Zineb, T., Šittner, P., "Thermomechanical model for NiTi-based shape memory alloys including R-phase and material anisotropy under multi-axial loadings," *Int. J. Plast.* **39** (2012), 132–151.

Frost - W 4:00-4:30

[2] Frost, M., Benešová, B., Sedlák, P., "A microscopically motivated constitutive model for shape memory alloys: Formulation, analysis and computations", *Math. Mech. Solids* **21** (2016), 358–382.

[3] Frost, M., Sedlák, P., Heller, L., Kadeřávek, L., Šittner, P., "Experimental and computational study on phase transformations in superelastic NiTi snake-like spring", *Smart Mater. Struct.* **27** (2018), 095005.

Baxevanis - W 4:30-5:00

On the Mechanics of Overload and Fatigue Failure in Shape Memory Alloys

Theocharis Baxevanis

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Since the discovery of Shape Memory Alloys (SMAs), the SMA industry has been dominated by products for biomedical applications with geometrically small feature sizes, especially endovas- cular stents. For such products, emphasis is being placed on preventing crack nucleation rather than controlling crack growth. However, the successful integration of SMAs into commercial actuation, energy absorption, and vibration damping applications requires understanding and practice of fracture mechanics and fatigue damage-tolerant concepts in SMAs. The development of such concepts is rather complex owing to the reversibility of phase transformation, detwinning and re-orientation of martensitic variants, the possibility of overload and transformation-induced plastic deformation, and the strong thermomechanical coupling. Large-scale phase transformation under actuation loading paths, i.e., combined thermo-mechanical loading, and the associated configuration dependence complicate the failure response even further and question the applicability of single parameter fracture mechanics theories. In this talk, the existing knowledge base on the mechanics of failure of SMAs under mechanical loading will be briefly reviewed and recent developments in actuation-induced SMA overload and fatigue failure will be presented along with deficiencies of the classical elastic-plastic fracture mechanics theories and standards to treat the observed response and possible remedies to overcome those deficiencies.

Landis - W 5:00-5:30

A new framework for phenomenological constitutive models for SMAs

Chad M. Landis

Aerospace Engineering and Engineering Mechanics, University of Texas at Austin

I will present recent work on a new constitutive model that captures pseudoelastic transformation induced recoverable deformation in SMAs that includes the strong asymmetries in the tensile and compressive responses [1]. The model is based on a J_2-type transformation surface and a nonlinear kinematic hardening framework with the back stress represented through a weighted mix of two potential functions that are calibrated to the tensile and compressive stress-strain responses of the material. I will illustrate the details of the model and how they admit J_3 dependence in the apparent transformation surfaces while implementing a model surface without J_3 dependence. How the back stress potential is able to produce the asymmetry in transformation strain, softening versus hardening, and asymmetry in the transformation stresses in tension and compression will be discussed. The constitutive model has been used to simulate numerically the interaction of these complex material behaviors with structural nonlinear behavior observed in experiments. The necessity of incorporating these asymmetries into the model for reproducing structural responses is seen in the problem of the buckling and recovery of NiTi tubes under axial compression and is shown in Figure 1, [2]. To close I will discuss how this modeling framework can be extended to include non-isothermal behaviors and show some preliminary results.

Figure 1. Comparison of simulation results to experimental measurements of the compression of a SMA tube.

References

[1] D. Jiang and C.M. Landis, 2016. "A Constitutive Model for Isothermal Pseudoelasticity Coupled with Plasticity", *Shape Memory and Superelasticity* **2** 360-370.

[2] D. Jiang, C.M. Landis, and S. Kyriakides, 2016. "Effects of Tension/Compression Asymmetry on the Buckling and Recovery of NiTi Tubes Under Axial Compression", *International Journal of Solids and Structures* **100** 41-5

Posters - Ulff - T 5:00-5:30

Finite element analysis of hydrogen effects on the thermomechanical response of NiTi orthodontic applications

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Nowadays, it is well known that NiTi Shape Memory Alloys (SMAs) exhibit a martensitic transformation, which induces a recovery deformation at constant force widely of interest for orthodontic treatments. After few months in buccal cavity, some fractures are observed (Yokoyama et al., 2001), due to a degradation of the mechanical properties of NiTi arches related to the presence of hydrogen. Indeed, the maximum strain decreases, the area of the hysteresis becomes smaller and the fatigue behaviour is degraded (Sheriff et al., 2004). Accounting for effects of hydrogen diffusion on the NiTi SMA behaviour, a coupled chemo-thermo-mechanical constitutive model needs to be formulated. Based on the work of (Lachiguer et al., 2016), a first step consists in introducing material parameter dependencies (transformations temperatures, maximum transformation strain, hysteresis size …) to the normalized concentration of hydrogen in the NiTi constitutive law developed by (Chemisky et al., 2011). Based on experimental results, it allows to formulate a first hydrogen concentration dependent SMA behaviour model.

The main limitation of this model is that the hydrogen concentration can only be considered in an averaged way as homogeneous. As nano-indentation tests reveal a heterogeneous distribution of hardness (which is indirectly related to the hydrogen concentration), it becomes necessary to take into account the gradient of hydrogen distribution from the surface to the cross section center. The thermal effect is also considered due to its influence on the mechanical response and the hydrogen diffusion.

To this end, we have to write equilibrium equations for each field (thermal, mechanical and chemical fields). These equations are then discretized to be solved numerically by finite element method. A 2D continuum special finite element with coupled degrees of freedom (displacements, temperature and hydrogen concentration) was first developed and implemented in the Abaqus finite element software through the UEL subroutine. The obtained numerical results (see Fig 1) showed the ability of the developed approach and completed the preliminary works, which only considered an homogeneous hydrogen concentration distribution (Ulff et al., under review).

Posters - Ulff - T 5:00-5:30

Figure 1: Heterogeneous distribution of concentration.

Figure 2: Formulation of the 3D element with five DOF.

For a realistic design of SMA archwires considering the effect of hydrogen diffusion, a 3D continuum special finite element with coupled degrees of freedom (displacements, temperature and hydrogen concentration) is now considered and implemented through the UEL subroutine (see Fig 2). The discretized form of nonlinear system to solve can be written:

$$\mathbf{R}_{\mathbf{e}}^{\mathbf{u}} = -\int_{\Omega_e} \left[B^u\right]^T \{\Sigma\} d\Omega_e + \int_{\partial\Omega_{e\Sigma}} \left[N^u\right]^T \left\{T^\Sigma\right\} dS + \int_{\Omega_e} \left[N^u\right]^T \{f_v\} d\Omega_e = \mathbf{0}$$

$$\mathbf{R}_{\mathbf{e}}^{\mathbf{th}} = -\int_{\Omega_e} \left[B^{th}\right]^T \{q\} d\Omega_e + \int_{\partial\Omega_{eq}} \left[N^{th}\right]^T \left\{\Phi_q\right\} dS + \int_{\Omega_e} \left[N^{th}\right]^T \left[N^{th}\right] \rho C_p \frac{\Delta T}{\Delta t} d\Omega_e = \mathbf{0}$$

$$\mathbf{R}_{\mathbf{e}}^{\mathbf{ch}} = -\int_{\Omega_e} \left[B^{ch}\right]^T \{j\} d\Omega_e + \int_{\partial\Omega_{ej}} \left[N^{ch}\right]^T \left\{\Phi_j\right\} dS + \int_{\Omega_e} \left[N^{ch}\right]^T \left[N^{ch}\right] \frac{\Delta C}{\Delta t} d\Omega_e = \mathbf{0}$$

where $\{\Sigma\}$ is the stress tensor , $\{q\}$ the heat flux and $\{j\}$ the hydrogen flux. Ω_e is the volume of the finite element and $\partial\Omega_e$ its boundary. $([N^u],[N^{th}],[N^{ch}])$ are the interpolation matrices. Thanks to the matrix $([B^u],[B^{th}],[B^{ch}])$, the strain tensor $\mathbf{E}$, the gradient ∇T or ∇C are computed. $\{f_v\}$ is the body forces vector applied to Ω. $\{T^\Sigma\}$ is the surface forces applied to $\partial\Omega_\Sigma$. $\{\Phi_q\}$ is the surface heat flux applied to $\partial\Omega_q$. $\{\Phi_j\}$ is the surface chemical flux applied to $\partial\Omega_j$. C_p is the heat capacity and ρ the density of the material.

This numerical tool allows to access to the local information in a given material point with a given local hydrogen concentration (stress state, transformation state…). Such information are mandatory for the design of SMA archwires considering the effect hydrogen diffusion. It is applied to the analysis of the effect of hydrogen diffusion on the performance of SMA-based orthodontic arches. Mechanical and chemical boundary conditions representative of the archwire fixation and the buccal environment are applied and the stress state and martensitic transformation are analysed in order to optimize its performance.

References

[1] Y. Chemisky, A. Duval, E. Patoor and T. Ben Zineb. "Constitutive model for shape memory alloys including phase transformation, martensitic reorientation and twins accommodation". *Mechanics of Materials*, 43(7) : 361-376, (2011).

[2] A. Lachiguer, C. Bouby, F. Gamaoun, T. Bouraoui and T. Ben Zineb. "Modeling of hydrogen effect on the superelastic behavior of Ni-Ti shape memory alloy wires". *Smart Materials and Structures,* 25 115047, (2016).

[3] J. Sheriff, A.R. Pelton and L.A. Pruitt. "Hydrogen effects on NITINOL fatigue". *Proceedings of the International Conference on Shape Memory and Superelastic Technologies* , 111–116, (2004).

[4] K. Yokoyama, K. Hamada, K. Moriyama and K. Asaoka. "Degradation and fracture of Ni-Ti superelastic wire in an oral cavity". *Biomaterials 22*, 2257–2262, (2001).

[5] N. Ulff, C. Bouby, A. Lachiguer, T. Ben Zineb, T. Bouraoui. "Modelling of hydrogen effects on the thermomechanical behaviour of NiTi-based shape memory alloys". *Shape Memory and Superelasticity – ESOMAT 2018 Special Issue,* (under review).

Heat dissipated at moving austenite-martensite interfaces in superelastic NiTi wires

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Superelastic NiTi wires undergoes critical deformation processes at the moving austenite-martensite interfaces, where the constrained stress-induced localized transformation proceeds. The material at the interface is subjected to simultaneous martensitic transformation (MT), martensite twinning, and coupled plastic deformation processes [1,2]. In this work, we experimentally quantify the total heat released/absorbed at the moving interface during cyclic forward and reverse MT in differently heat treated superelastic NiTi wires of diameter 1.78mm. The ultimate aim of this work is to correlate the dissipated heat with the propensity of NiTi wires to transformation-coupled plasticity, which varies according to applied Joule-heating-based heat treatment. The method for resolving the total heat dissipated at the moving interface from in-situ recorded thermograms will be explained. The method relies on axial symmetry of the interface [3], hence, the heat sources are resolved in 1D – along the wire axis. The total heat released/absorbed at the interface is then calculated as a spatial or time integral of the heat source at given time or material point. The total heat has been found to depend non-monotonously on the propensity of the microstructure to plastic deformation expressed in terms of unrecovered strains induced by superelastic cycling. Non-monotonic evolution is correlated with the evolution of martensite volume fraction at the end of the plateau indirectly evaluated by electrical resistometry and dynamical mechanical analysis. Finally, two estimates of the dissipated heat and latent heat are evaluated from the total heat under assumptions of i) symmetric dissipation in forward and reverse MT, ii) asymmetric dissipation considered in forward MT only.

References

[1] L Heller et al. On the plastic deformation accompanying cyclic martensitic transformation in thermomechanically loaded NiTi, International Journal of Plasticity, Volume 111, December 2018, Pages 53-71.

[2] L Heller et al., Beyond the strain recoverability of martensitic transformation in NiTi, International Journal of Plasticity, Volume 116, May 2019, Pages 232-264.

[3] Sedmák, P. et al., Grain-resolved analysis of localized deformation in nickel-titanium wire under tensile load. Science, 353(6299), 2016.

Posters - Zhang - T 5:00-5:30

A Finite Strain Constitutive Model for Polycrystalline Shape Memory Alloys accounting for Pseudoelasticity, One Way Shape Memory Effect, Orientation, Reorientation, "Ferroelasticity", and latent heat effects

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A finite strain, thermomechanically-coupled, constitutive description of the deformation response of polycrystalline Shape Memory Alloys (SMAs) is presented. The proposed model can describe efficiently–as depicted by detailed comparison of simulations with available experimental data– various deformation processes in SMAs (superelasticity, one-way shape memory effect, orientation, reorientation, "ferroelasticity", thermal expansion, tension-compression asymmetry, latent heat effects, and finite deformation assuming isotropic material responses, neglecting plasticity, cyclic evolution, and irreversible strains due to retained martensite) in a simple and thermodynamically- consistent manner. In most of the phenomenological constitutive models of SMAs, the set of in- ternal variables to describe the growth, orientation, and reorientation of variants includes at most one tensorial and two scalar variables. In many of the proposed models, the inelastic strain has been considered as a unique internal variable. In these approaches, the magnitude of the inelastic strain represents the volume fraction of martensite and its direction represents the average direction of different variants (or preferred direction of variants). Other models differentiate between the inelastic strain and up to two of the following as internal variables: (i) its magnitude, (ii) its orientation, and (ii) the martensite volume fraction. Most, if not all, of these models can efficiently describe a number of the aforementioned inelastic processes associated with the thermomechanical deformation response of SMAs but not all of them. The proposed model that can efficiently describe all these deformation processes by including all four of the aforementioned internal variables, allowing for an implicit description of the volume fraction of oriented martensite. In the developed numerical implementation, all the tensorial variables are cast in a corotational configuration for finite deformation analysis, based on the framework proposed by Xiao and Brunhs (1997, 1998), to achieve frame objectivity at each loading increment.

Posters - Joy - T 5:00-5:30

Estimation of Representative Volume in Micromechanical Modeling of Precipitation Hardened SMAs

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The Representative Volume Elements (RVEs) are central in micromechanical modeling to predict the material response. Although larger RVEs are more representative of the microstructure, optimum sized RVEs are desired for efficient modeling and lesser computational cost. The RVE size and the number of realizations has to be optimized based on the accuracy requirement in the response prediction. In the present work, an RVE based study is carried out on precipitation hardened NiTi SMAs with Ni_4Ti_3 precipitates. The RVEs considered consist of homogeneous SMA matrix with periodically arranged ellipsoidal precipitates. The actuation response of the resultant RVE is solved by means of a full-field micromechanical model using a recently developed Fast Fourier Transform variational approach for SMAs. An extensive study is conducted on these RVEs with changing volume fraction and increasing number of precipitates to understand the dispersion in the material response prediction. The convergence of the RVEs with respect to the effective response is studied and relations to determine the RVE size according to the desired accuracy in the effective response are presented.

a) RVE with volume fraction 4.2% of precipitates

b) RVE with volume fraction 20% of precipitates

Figure 1. Representation of RVEs considered in the study.

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a) Dispersion in the effective response from 10 RVE realizations of a fixed microstructure.

b) The maximum strain from RVE realizations are compared for increasing number of precipitates. The response converge with large RVEs.

Figure 2. Dispersion in the effective response and convergence with larger RVEs [1].

References

1. Joy, Jobin K., et al. "Representative volume size in micromechanical modeling of precipitated SMAs." *Smart Structures and NDE for Energy Systems and Industry 4.0*. Vol. 10973. International Society for Optics and Photonics, 2019.

Posters - Mohajeri - T 5:00-5:30

Mechano-Electrochemical Behavior of NiTi Shape Memory Alloy

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The effect of the change in crystallographic orientation of Nickel-Titanium shape memory alloy (SMA) on the electrochemical behavior at different load levels was characterized. Electrochemical techniques showed the global influence on the SMA surface during the change in crystallographic orientation due to the loading conditions. This change in crystallographic orientation affected the surface of Nickel-Titanium SMA locally. These local effects could be sensed by the global interfacial changes with electrochemical measurements, such as Electrochemical Impedance Spectroscopy (EIS), Open Circuit potential (OCP) and Linear polarization (LPR) methods.

The passive layer formation includes Ni and Ti oxide based composition following exposure in Rings solution. The increase in the loading parameter resulted in the breakdown of the passive layer while passivation stage could be reached due to the strain effect on the bonding or physical characteristics of the passive layer. Mechanical characterization is performed by tensile testing at room temperature to obtain elastic and inelastic regions. Strain distribution at each stress level is defined by Digital Image correlation. Differential Scanning Calorimetry is used as a thermal analysis technique to identify the phase transformation temperature for this alloy. NiTi-SMA showed the high polarization resistance under zero loading (160.7 $k\Omega\ cm^{-2}$) and the polarization resistance decreased to (49.8 $k\Omega\ cm^{-2}$) following loading to plastic region.

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