Appendix. SMA modeling.

A review on phenomenological shape memory alloy constitutive modeling approaches

The present appendix is organized in three parts. Part 1 considers various modeling methodologies, focusing on continuum thermodynamics with internal variables which is, in our opinion, the most suited approach for the development of reliable 3D SMA constitutive equations, able to describe material response under complex multi-axial thermo-mechanical loadings. Part 2 presents a detailed literature review for the approach selected in Part 1. Finally, Part 3 discusses possible future research directions. A list of references cited in the document is reported at the end.

PART 1: SMA phenomenological modeling approaches

From 1980 up to now, constitutive modeling of shape memory alloys has been an active research subject. The resulting models can be in general categorized as micro, micro-macro or macro.

Description of micro-scale features, such as nucleation, interface motion, twin growth, etc., is the main focus of micro models. They are useful to understand fundamental phenomena, occurring at the microscopic level, although they are not easily applicable at the structural/device scale.

Micro-macro studies combine micromechanics and macroscopic continuum mechanics to derive constitutive laws of the material. Their predictions are often successful, but the required time-consuming computations make them inappropriate for engineering applications.

Phenomenological or macro approaches use macroscopic variables to describe average material behavior and, in general, they are suitable to be used within numerical methods (such as the finite element method - FEM) in an efficient way to predict the effective behavior of structural components and devices.

In the following we review phenomenological SMA constitutive models. The available phenomenological constitutive modeling approaches can be categorized to as follows:

Models without internal variables

In such models the material behavior is described by strain, stress, temperature, and entropy without the introduction of quantities representing phase mixture.

Polynomial potential models

In this approach, constitutive information is provided by a polynomial free-energy, function whose partial derivatives provide constitutive equations for strain (or stress) and entropy. In 1980, Falk proposed a Landau-Devonshire like free-energy function based on the analogy between SMA uniaxial stress–strain curves and the electric field–magnetization curves of ferromagnetic materials.

Non-monotone stress–strain curves are obtained, and the unstable negative slope part is interpreted as the occurrence of the phase transition. The actual pattern followed during transformation is assumed to proceed at constant stress. The particular form of the Landau-Devonshire free energy accounts for the temperature dependence of the isothermal stress–strain behavior. We can address Falk (1980), Falk (1983) and Falk and Konopka (1990) as models in this group. The main advantage of these models is their formal simplicity, but they are not able to model complicated behavior of the material. They are also not adequate to describe accurately the evolutive nature of processes.

Hysteresis models

Hysteresis models seek to reproduce experimentally observed curves that involve high nonlinearity and complex looping. They have been widely used in several fields, in particular for magnetic materials. In this approach, constitutive equations are proposed directly on the basis of their mathematical properties, often without explicit focus on their link with the underlying physical phenomena of interest.

Reliability and the robustness of the model are favorably matched to experiments, and the resulting algorithm allows for the treatment of arbitrarily complex driving input. Two main algorithm classes have received special attention in the context of SMA phase transformation. The first one is based on tracking sub-domain conversion/reversion and lead to *integral based* algorithms. The most common of these is known as the Preisach algorithm and it has been used to describe uni-axial isothermal pseudoelastic stress–strain SMA response (Huo, 1989; Ortin, 1992). The second algorithm class involves *differential equations* with separate forms for driving input increase and driving input decrease. Differential equations of Duhem-Madelung form have been used to model SMA phase fraction evolution during thermally induced transformation (Likhacev and Koval, 1989; Ivshin and Pence; 1994). This allows reproducing phase fraction sub-loops for temperature histories. Under sustained thermal cycling, these sub-loops collapse onto a final limiting sub-loop, with the resulting shakedown behavior registering the fading influence of the initial phase-fraction state.

Models with internal variables

The key feature of this approach is to introduce appropriate *internal variables* describing the material internal structure. Internal variables, along with a set of mechanical and thermal *control variables*, define a collection of *state variables*. A general thermo-dynamically consistent approach then allows to derive evolution equations for the internal variables. Mechanical control variables can be either strain or stress, while thermal control variables can be either temperature or entropy. The internal variables typically include one or more phase fractions and/or macroscopic transformation strains. The first application of such an approach to SMA seems to be due to Tanaka and Nagaki (1982), where internal variables are employed to describe the development of the underlying phase mixture.

The models based on internal variables can furthermore be categorized into two groups:

Models with assumed phase transformation kinetics

Models with assumed phase transformation kinetics consider as internal variable the involved martensitic volumetric fraction, which is expressed as function of current values of stress and temperature. Several authors propose different functions to describe the volumetric fraction evolution. The model firstly developed by Tanaka and coworkers (Tanaka and Nagaki, 1982; Tanaka, 1985; Tanaka and Hayashi, 1993; Tanaka and Nishimura, 1994; Tanaka and Nishimura, 1995) was originally conceived to describe three-dimensional problems involving SMAs. Nevertheless, its implementation was naturally restricted to the one-dimensional context. The authors consider exponential functions to describe phase transformations. Since an exponential function is adopted, there should be an extra consideration for the phase transformation final bounds.

Boyd and Lagoudas (1994) rewrite Tanaka's original model, for a three-dimensional theory, while the relations used to describe phase transformation evolution remain the same as in

Tanaka's model. Liang and Rogers (1990) present an alternative evolution law for the volumetric fraction based on cosine functions. The authors also developed a three-dimensional model, in which they suggest that phase transformations are driven by the associated distortion energy. Brinson (1993) offers an alternative approach to the phase transformation kinetics, in which, besides considering cosine functions, the martensite fraction is split into two distinct quantities, the temperature-induced martensite and the stress-induced martensite. The authors also consider different elastic moduli for austenite and martensite.

Models with internal variable evolution equation

These models are developed within a more rigorous thermo-dynamical continuum approach. The theory is then composed of *physical laws*, i.e. the *constitutive equations* that characterize the features typical of each material, and *material behavior requirements* that ensure thermo-dynamical process restrictions.

Constitutive information is specified by two kinds of relations:

- *State equations* for the entities conjugate to control variables. These can be formulated directly or obtained as partial derivatives of a suitable free energy function after enforcing the Clausius-Duhem inequality for every process. If heat conduction is to be included, then a constitutive equation relating temperature gradient and heat flux (usually the Fourier equation) is also required.
- *Kinetic equations* for the internal variables. In view of phase transformation hysteresis, these equations generally depend on the material past history. Standard practice in most internal variable models is to specify this dependence through equations relating the rates of the internal variables to the current state and its time derivatives. The internal state then follows from the solution of differential equations in time.

Although sometimes employed formalisms are quite different, several models fitting into this basic framework have been proposed to describe SMA behavior. While most of the efforts are limited to modeling one-dimensional behavior of the material, in the last decade, motivated by extensive engineering applications as well as available multi-axial experimental data, considerable attention has been devoted to developing three-dimensional constitutive models. Nowadays, there are varieties of 3D phenomenological models trying to properly capture different aspects of SMA behaviors listed as follows:

> Asymmetric behavior under tension-compression; phase dependent mechanical properties; different material behavior in high and low temperature; subloops and return point memory effect; thermomechanical coupled and pseudo-rate dependent behavior; permanent transformation-induced plastic strains in cyclic loadings; variant reorientation under non-proportional loadings; finite deformations and nonlinear geometric effects; plasticity due to dislocation motions.

Compared with the extensive efforts in constitutive modeling, there have not been enough attention paid to the corresponding numerical implementation. This fact is partially due to unavailability of proper constitutive models which have a suitable form for the corresponding numerical implementation. High nonlinear behavior of material and complicated structure of models - compared to plasticity - are other obstacles in numerical implementation. It is generally accepted in the literature that in order to reach a computational tool for design and analysis of SMA devices and structures, 3D phenomenological constitutive models in framework of continuum thermodynamics with internal variables should be developed.

Micro-plane method

Another approach in constitutive modeling is based on micro-plane theory. This approach is interesting for its capability of extending a 1D constitutive model to a 3D constitutive model.

The micro-plane modeling approach originated from the work of Taylor (1938), who studied the constitutive behavior of polycrystalline metals by developing relations between stress and strain vectors on generic planes of arbitrary orientations in the material and determining the macroscopic stress or strain tensors as a resultant of all these vectors. This concept was later modified by others and is commonly known as *slip theory of plasticity*. As slip is not the source of inelastic response for all types of materials, Bazant (1984) introduced a neutral term called the *micro-plane theory,* which can be used for general inelastic behavior. In this approach, a 1D constitutive law for one stress component and the associated strain component on each micro-plane is sufficient to generate a macroscopic 3D model by considering either of the two main formulations in micro-plane theory named *static constraint* and *kinematic constraint*. In static constraint formulation, it is assumed that the stress vector acting on each micro-plane is the projection of the macroscopic stress tensor. In kinematic constraint formulation, the strain vector on any micro-plane is considered as the projection of the macroscopic strain tensor. Moreover, there are some particular material laws where both static and kinematic constraints coexist. Such a case is called *double constraint* formulation. Brocca et al. (2002) present a model based on micro-plane theory, which can model both shape memory and PE. A micro-plane constitutive model for polycrystalline SMA is proposed in Kadkhodaei et al. (2007) by first deriving a 1D model and then generalizing it to 3D case. The proposed model also shows deviation from normality rule and interaction between stress components under non-proportional loading paths.

PART 2: A review on phenomenological SMA constitutive models based on continuum thermodynamics with internal variables

In this part we review phenomenological constitutive models based on continuum thermodynamics with internal variables. This is a general subject and it covers many aspects of SMA behavior. Although, it is possible to review the constitutive models in terms of research topics, we review them in terms of the corresponding research groups. The reason for this choice is that there are only few active groups in modeling SMA behaviors and most of the publications available in the literature belongs to these active groups. In this way, it is possible to cover most of the publications in a structured way, showing strategies and goals as well as research methods pursued by each group. It is clear that this approach does not cover non-group studies and we mention just few of them within a general group named *others*.

Considering available publications, we can identify followings as active groups:

- **Ferdinando Auricchio's group**. This is an active group located in Italy, University of Pavia, with main focus on numerical implementation as well as constitutive modeling of shape memory alloys.

  Web site: http://www-2.unipv.it/compmech/

- **Dimitris C. Lagoudas's group**. This active group is located in USA, Texas A&M University, and the main interest is constitutive modeling, although they have published some numerical papers.

  Web site: http://smart.tamu.edu/overview/overview.html

- **Christian Lexcellent's group**. This group is located in France, Franche-Comte University, and the main focus is experimental study, constitutive modeling and micro-mechanics based constitutive modeling for single crystals. Sylvain Calloch, Christophe Bouvet and Alexandre Vivet are members of this group.

- **Catherine L. Brinson's group**. This group is located in USA, Northwestern University, and their main interest is constitutive modeling both at micro and macro level. Brinson is one of the pioneers in this field.

  Web site: http://www.mech.northwestern.edu/fac/brinson/new

- **German group**. In Germany there are several groups active in SMAs modeling, all with contributions in the very large SFB459 project based in Ruhr-university, Bochum.

  Among others, we may mention Stefanie Reese (Technical university, Braunschweig), Otto Bruhns (Ruhr-university, Bochum), one of the well-known researcher in mechanics and continuum mechanics, Dirk Helm (Peter Haupt's PhD student, university of Kassel). This group has published most part of finite-strain constitutive models. While most of the group members are interested in constitutive modeling, several numerical papers have been published by Stefanie Reese.

Web site: http://www.ruhr-uni-bochum.de/sfb459/english/

- **Raniecki's group**: This is a group based in Poland and has published some of the first papers on SMA constitutive modeling.
- **Brazilian group**: This group is known by Marcelo Amorim Savi and Alberto Paiva. They have published some papers on constitutive modeling based on Fremond's method.
- **Mumni's group**. This group is based in France, Ecole Polytechnique, and they have recently published a series of papers within the framework of generalized standard materials with internal constraints (a method which is considered in the framework of continuum thermodynamics with the internal variables approach). Wael Zaki is a member of this group.
- **Prakash Thamburaja's group**. This group is based at the National University of Singapore. Thamburaja was Lallit Anand's PhD student at MIT university. The main interest is SMA constitutive modeling motivated by plasticity theory.

  Web site: http://serve.me.nus.edu.sg/prakash/

There are also active groups in micromechanics-based modeling approaches as well as other groups that are less related to this subject and we don't consider them here.

Auricchio's group

This group publication starts from Auricchio's Ph.D. dissertation, which contains the first published SMA constitutive model in finite-strain regime (Lubliner and Auricchio, 1996; Auricchio and Lubliner, 1997; Auricchio and Taylor, 1997a,b; Auricchio, 2001). This group has published papers on different aspects of SMAs modeling as: rate-dependent behavior (Auricchio et al., 2008), two-way shape memory effect (Auricchio et al., 2003), permanent inelasticity (Auricchio et al., 2007), asymmetry and phase dependent properties (Auricchio and Sacco, 1997; Auricchio et al., 2009), cyclic loading of wires (Auricchio and Sacco, 2001), developing SMA beam model (Auricchio and Sacco, 1997;1999) and numerical implementation (Auricchio and Taylor, 1999; Auricchio and Petrini 2002;2004a,b; Auricchio and Stefanelli, 2004; Auricchio et al., 2009). This group has published the most cited numerical papers.

Lagoudas's group

This group has covered different aspects of shape memory materials including shape memory alloys, shape memory polymers and magnetic shape memory alloys. But we mention only the publications related to shape memory alloys. The first publication is the three-dimensional extension of Tanaka model (Boyd and Lagoudas, 1994), developed into the generalized model by Qidwai and Lagoudas (1996). Other contribution comes from SMA behavior modeling under cyclic loading in a four-part paper by Bo and Lagoudas (1999a,c,d) and Lagoudas and Bo (1999b), impact-induced phase transformation (Chen and Lagoudas, 2000) and dynamic loading of SMA rods (Lagoudas et al., 2003), transformation-induced plasticity (Entchev and Lagoudas, 2004; Lagoudas and Entchev 2004), 3D modeling of superelasticity and detwinning (Popov and Lagoudas, 2007), modeling porous SMA (Qidwai et al., 2001), transformation surface (Qidwai and Lagoudas, 2000) and a numerical paper on implementation of SMA constitutive model by Qidwai and Lagoudas (2000).

Lexcellent's group

This group has several important contributions on experimental studies, but we don't consider these types of contribution here since we are focusing mainly on constitutive modeling and numerical implementation. Two well-known papers in SMA phenomenological modeling are the works by Leclercq and Lexcellent (1996) and by Raniecki and Lexcellent (1998). Other contribution comes from Lexcellent and Tobushi (1995) in modeling and experimental study of sub-loops, cyclic behavior (Lexcellent and Bourbon, 1996), two-way shape memory effect (Lexcellent et.al, 2000), identification of phase transformation surface (Lexcellent et al., 2002; Lexcellent and Blanc, 2004; Taillard et al., 2006; Lexcellent and Schlömerkemper, 2007; Laydi and Lexcellent, 2008; Lexcellent and Thiebaud, 2008), SMA constitutive model, considering multiaxial loading conditions (Bouvet et al., 2004), equivalent transformation strain definition (Calloch et al., 2006; Taillard, 2008), and SMA modeling under anisothermal condition (Lexcellent and Boubakar, 2006). This group has proposed a model considering asymmetric behavior and temperature effects, and implemented it in the finite element method (Thiebaud et al., 2007).

Brinson's group

The first paper by Brinson is a well-known paper in which she introduces the concept of additive decomposition of martensite fraction into temperature-induced and stress-induced (Brinson, 1993). Brinson and Lammering (1993) implement this model into finite element method. In 1996, Brinson and Huang compare the available models and show that the difference between models is due to different kinetics of the phase transformation. The papers by Bekker and Brinson (1997,1998) present a constitutive model based on phase diagram description. The micro-plane model by Brocca et al., (2002) is another modeling paper in this group. Recent works of this group are a constitutive model by Panico and Brinson (2007) with focus on variant reorientation modeling under non-proportional loadings and computational modeling of porous SMAs (Panico and Brinson, 2008).

German group

This group covers most part of the more recent finite-strain constitutive models. The first paper is by Helm and Haupt (2003) on modeling within continuum thermodynamics. This paper is part of Helm dissertation and is extended by Reese and Christ (2008) to finite-strain regime. Comparison of small and finite strain has been presented in Christ and Reese (2008). Recently they have generalized the finite-strain model to include thermo-mechanical coupling and asymmetric behavior (Christ and reese, 2009). The first paper by Bruhns extends the RL model of Raniecki and Lexcellent to finite strain regime (Muller and Bruhns, 2006). In a paper by Luig and Bruhs (2008), they emphasize the use of tensorial internal variables in SMA modeling. Series of paper have been published by Grabe and Bruhns (2008a,b; 2009) presenting extensive experimental study on SMA behavior under non-proportional thermo-mechanical loadings. They have shown that for the studied alloy, material behavior is rate-independent and the pseudo-rate effect is due to thermo-mechanical coupling effects.

Raniecki's group

The model by Raniecki and Lexcellent named RL-model is one of the well-known models in SMA constitutive modeling (Raniecki and Lexcellent, 1998). Other contributions comes from studying hysteresis loops (Raniecki et al., 2001), modeling and experiment of SMA beams (Rejzner et al., 2002), stress-induced martensite transformation (Ziolkowski et al., 2004) and a finite-strain constitutive model by Ziolkowski (2007).

Brazilian group

Paiva and Savi has published several papers on SMA modeling using Fremond's method (Baêta-Neves et al., 2004; Paiva et al., 2005; Savi et al., 2008) considering asymmetric behavior and plasticity.

Mumni's group

This group is trying to model SMA behavior using generalized standard materials with the internal constraints approach. They have used this method in modeling thermo-mechanical behavior of SMAs (Zaki and Moumni, 2007a) as well as cyclic behavior (Zaki and Moumni, 2007b). Theoretical and numerical study of solid-solid phase transformation is the subject of paper by Moumni et al. (2008). In a recent paper (Zaki et al., 2009), they have proposed a model to capture plastic deformations.

Thamburaja's group

This group's activity started with research on texture effects (Thamburaja and Anand, 2001, 2002, 2003). Martensite reorientation and detwinning is the subject of papers by Thamburaja (2005), Thamburaja et al. (2005) and Pan et al. (2007a,b). The recent paper (Thamburaja and Nikabdullah, 2009) presents a constitutive model as well as a finite element implementation.

Others

We also mention the model proposed by Souza et al. (1998) which is a 3D model capable to capture both SME and PE in small strain regime. The model by Evangelista et al. (2009) is the finite-strain extension of Souza's model.

PART 3: Current activities and future plans

According to the literature review and considering the rapidly increasing number of SMA applications, it is required to develop effective constitutive models as well as corresponding numerical implementations. To this end, it is required to develop constitutive models with emphasis on the following aspects:

- Finite deformations
- Reorientation (ability in predicting material behavior under non-proportional loading)
- Asymmetric behavior under tension-compression
- Phase dependent properties
- Numerical implementation robustness

So far, we have developed some finite-strain constitutive models considering reorientation as well as their numerical implementation. Future plans include extending the models to capture asymmetry and phase dependent material properties as well as thermo-mechanical coupling. We hope to be finally able to develop a constitutive model to satisfy the above mentioned requirements. As a main goal, based on the developed constitutive model we will develop a robust and efficient computational tool which can be used in design, analysis and optimization of various SMA structures. To validate the constitutive model's capability, it should be compared with experimental data available in the literature, while for validation of the numerical model, it is necessary to evaluate its robustness and efficiency for a number of complex benchmark problems which are available in the literature. Finally, the model's capability in simulating boundary value problems in real engineering applications can be demonstrated by simulating different SMA structures such as medical stents.

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