

## Models for Shape Memory Alloy Behavior: An overview of modeling approaches

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### Abstract

Shape memory alloys (SMA) have been known for over five decades and modeling of their response has attracted much attention over the last two decades. Recent increase in the range of applications of these materials has lead to an increased focus on modeling their thermomechanical response. Various approaches ranging from macroscopic phenomenology to microscopic lattice based methods are being pursued to model SMA behavior. Models ranging from simple tools as design aids to complex thermodynamic based models to understand the characteristic martensitic transformation responsible for the shape memory and superelastic response exist. In this report, following a brief introduction to the SMA behavior and the underlying martensitic transformation, an overview of models for SMAs is provided. This is aimed at providing an understanding of the state of the art and also to identify possible future directions. In this review, models are classified both on the basis of the approach and the level (scale) of continuum they address. General methodology of each type of approach is presented briefly followed by a review of the models that fall under that category. Certain liberties are taken in classifying these models to facilitate understanding and thus the present classification is by no means either unique or completely rigorous. Also, while an attempt is made to cover most of the approaches, review of all the models that exist in literature is practically impossible. Finally, summarizing the literature on models for SMAs, several interesting and relevant problems are identified for possible future developments.

### 1 Introduction

Shape memory alloys (SMAs) exhibit two fascinating characteristic behaviors, viz., shape memory (SME) and superelasticity (SE) or pseudoelasticity (PE). Hence, they are also classified as ‘smart materials’ or ‘intelligent materials’ or ‘active materials’. Two broad classes of SMAs exist, viz., thermally activated and magnetically activated. The focus of the present review is on the more prevalent thermally activated SMAs. The key characteristic of SMAs is the martensitic phase transformation, brought about by temperature change and/or by application of stress. In SMAs, Martensitic Transformation (MT), is between a high-symmetric, usually cubic, austenitic phase (**A**) and a low-symmetric martensitic phase (**M**), such as their monoclinic variants. This reversible phase change can be brought about by much smaller temperature change compared to conventional phase transformation like solidification. MT is usually accompanied by significant changes in mechanical, electrical and thermal properties that render them as prime candidates for the development of smart structures and devices. Typical examples of SMAs are NiTi (commonly referred to as nitinol), NiTiCu, CuAlZn and CuAlNi. Extensive literature exists that explains the phase transformation and associated SME and SE behavior in these materials (Duerig et al (1990), Birman (1997) and Otsuka and Wayman (1998), Otsuka and Kakeshita (2002), Friend (2001), Bernardini and Pence (2002a), Ortin and Planes (2005)). SMAs, being smart materials, their modeling and applications, in general, require a multidisciplinary expertise involving material science, mechanical engineering and electronics.

In order to facilitate the discussion on constitutive models that attempt to explain the phenomena, it is useful to understand the characteristic features of the material behavior. A brief introduction to the material behavior is provided here highlighting the SME and SE and the underlying MT. Different phase transformations that occur are schematically illustrated in Figure 1. Depending on the nature of loading, different types or variants of martensites form leading to SME and SE. Generally, SMAs exist in a stable high symmetry Austenitic phase ‘A’ above a certain temperature, Martensitic start ( $M_s$ ). Under certain conditions of temperature and stress (to be elaborated later), **a** transforms to **M** with lower symmetry either in a single step or through and intermediate Rhombohedral phase (R-phase).

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Abbreviations	
A	Austenite
BVP	Boundary Value Problem
DSC	Differential Scanning Calorimetry
LPM	Lumped Parameter Model
M	Martensite
MT	Martensitic transformation
SE	Superelasticity or superelastic
SIM	Stress induced martensite
SMA	Shape Memory alloy
SME	Shape memory effect
TWSME	Two-way shape memory effect
$M_f$	Martensitic finish transformation temperature
$M_s$	Martensitic start transformation temperature
$A_f$	Austenitic finish transformation temperature
$A_s$	Austenitic start transformation temperature

This transformation is fully reversible and several interesting relevant features of this transformation are discussed in next section. A brief overview of the macroscopic features in SMA response viz., the shape memory and superelasticity is discussed below.

### 1.1 Shape Memory Effect

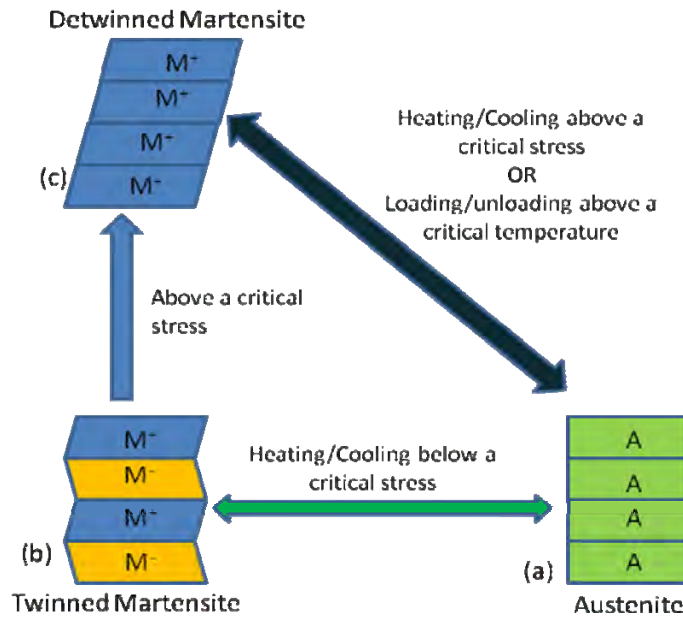


Figure 1: Schematic of phase transformation in SMAs; (a)-(b)-(c) is a typical shape memory cycle. (a)-(c) under stress cycling represents superelastic cycle; (a)-(c) under thermal cycling represents another shape memory path.

On cooling, below a critical temperature called Martensitic start ( $M_s$ ), in the absence of applied stresses, austenite starts transforming to several variants of the martensitic phase. This crystallographic transformation occurs in a self-

accommodating manner through twinning, resulting in no observable macroscopic shape change (path a-b in Figure 1). The transformation is complete upon reaching a critical temperature, Martensite finish ( $M_f$ ). Application of stress at this stage causes different self-accommodated twins to detwin (path b-c) into more stress preferred variants leading to significant macroscopic inelastic strains. For instance, upon tensile loading beyond a relatively small elastic regime, the 'M<sup>-</sup>' layers flip into 'M<sup>+</sup>' phase leading to considerable elongation or shape change (typically about 6% macroscopic strain). Upon unloading, only a small fraction of this strain is recovered leaving a large residual inelastic strain. Unlike plastic strains in conventional materials, this strain can be easily recovered. This is achieved by heating the material to a higher temperature ( $>A_s$ ) wherein the low-symmetry martensitic phase starts to revert to **A** (path c-a), and the inelastic strain is thus recovered (usually almost completely) upon reaching  $A_f$ . This transformation results in recovery of original shape and is responsible for the SME. The 'memory' here is referred to the ability of the material to remember a high temperature shape and to return to that shape upon heating after subjected to large inelastic deformation in low temperature martensitic phase. This is illustrated in Figure 2. The differences in the forward and reverse transformation temperatures lead to a hysteretic response. If the strain recovery is constrained, significant recovery stresses develop, typically in excess of 200-300 MPa. Another associated phenomenon is the two-way shape memory effect wherein in addition to remembering a high temperature shape, a low temperature shape is also remembered and it is possible to cycle the material between these two states without any stress. However, most of the applications of shape memory effect involve only the one-way (high temperature) shape memory.

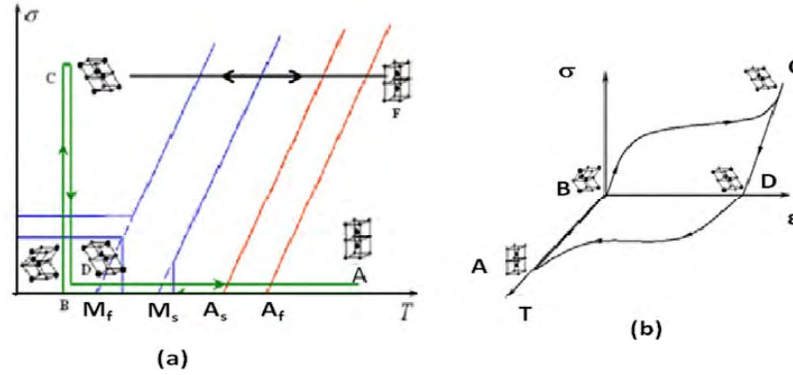


Figure 2: Shape memory cycle; (a) load path on stress-temperature diagram, A-B-C-D-A show stress-free recovery while F-C-F shows constrained recovery (b) stress-strain-temperature response for free recovery cycle.

### 1.2 Superelasticity

Pure mechanical loading can induce MT when the material is in the austenitic phase. Figure SE1 schematically illustrates this effect. Upon loading Stress Induced Martensite (SIM) is directly produced from **A** leading to large macroscopic strains which are recovered by unloading when the temperature is above  $A_f$ . This is referred to as Superelastic or Pseudoelastic effect and is illustrated in Figure 3. Critical stresses at which the forward and reverse transformation occurs again illustrate the associated hysteretic behavior. Most of the bio-medical and damping applications of shape memory materials exploit this effect.

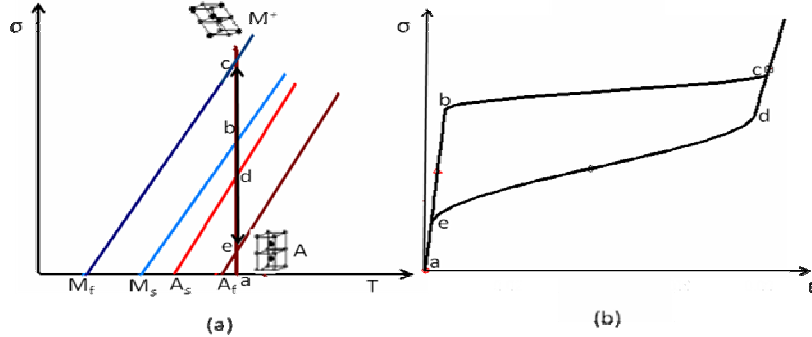


Figure 3: Superelasticity effect; (a) load path a-b-c-d-e-a on stress-temperature diagram; (b) stress-strain hysteresis response.

### 1.3 Two-way Memory Effect

An associated phenomenon is the Two-Way SME (TWSME) wherein, in addition to a high temperature shape, a low temperature shape is also remembered and it is possible to cycle the material between these two states without any stress (Perkins (1974)). This is schematically illustrated in Figure 4. However, most of the applications of shape memory effect involve only the one-way (high temperature) shape memory. It may be noted that at times, two-way memory is also attributed to the case of constant stress recovery. However, the authors feel that the distinguishing features in two-way is the presence of martensite either in a partially or completely detwinned state due to internal/residual stresses and not due to the application of (external) stress.

In order to better understand the mechanisms and associated theoretical aspects that lead to the SME and SE phenomena a brief overview of the MT along with the underlying mechanisms and driving forces is provided here.

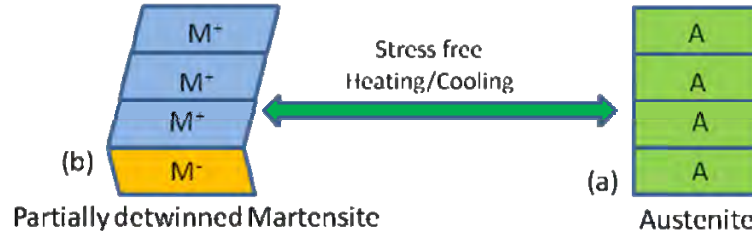


Figure 4: Schematic of two-way memory due to partial detwinning caused by internal stresses

## 2 Characteristics of the Martensitic Transformation in Shape Memory Alloys

Martensitic transformation (MT) which has several fascinating features has been investigated extensively in the context of both single and polycrystalline SMAs. Even after nearly four decades of effort, several unresolved and challenging aspects in MT make it still an open problem for active research. Thus, various disciplines in materials research ranging from molecular dynamics to continuum irreversible thermodynamics at macroscale are being employed. A brief discussion on several relevant aspects of MT in SMAs is presented here to facilitate better understanding of modeling approaches for SMA response.

### 2.1 Crystallographic Aspects in MT

As noted earlier, MT is a diffusionless reversible solid-solid phase transformation occurring by activation and/or nucleation and growth of the martensitic phase from a parent austenitic phase. Discussion on several important crystallographic features of MT is available in literature (Bhattacharya (2003), Otsuka and Ren (2005), James (1986), Otsuka and Wayman, Duerig et al (1990)). For brevity, only an outline of salient aspects is provided here. Generally inelastic shear or distortion associated with the crystal lattice is the dominant deformation mechanism with only cooperative and collective motion of atoms on distances smaller than the lattice parameters. The characteristic size of martensitic plates is very small, typically of the order of few microns. The deformation mode is twinning rather than slip (occurring during conventional plastic deformation) of the crystallographic planes which gives it the reversible nature. A lattice invariant strain-free plane, also called ‘habit plane’ exists at the interface between the product and parent phases. Depending on the alloy, the lattice vectors of the two phases possess well defined mutual orientation relationships (the Bain correspondences).

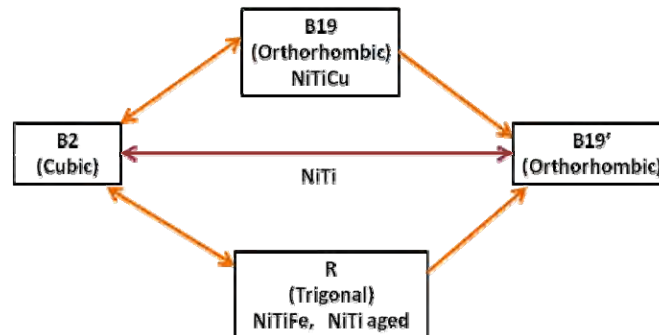


Figure 5: Different martensitic transformation pathways in NiTi based alloys

These bring out the coherency aspects of the two different microstructures and play a critical role in the kinetics and morphology of phase transformation process. The absence of diffusion makes MT almost instantaneous and also athermal or thermoelastic. Theoretically, the transformation occurs at the speed of sound in the material. However, in polycrystalline materials, it is possible that under certain conditions, the transformation occurs at much slower rates (Shaw and Kyriakides (1995)).

Crystallographically several different MT are possible, and in NiTi based SMAs; three different pathways are possible as illustrated in Figure 5 (Otsuka and Ren (2002)). Because of differences in crystal structure of the phases, the transformation strain(s) also varies. Generally monoclinic B19' yields maximum transformation strain, followed by orthorhombic (B19) with least transformation strain seen in trigonal (Rhombohedral- R) phase. The number of variants of the lower symmetry structure that can form from the parent cubic structure is determined by the nature of symmetry of the parent structure and the product structure. Hence, even in a single crystal parent, when there is transformation, the product is polycrystalline. For instance, in NiTi, 24 monoclinic variants can form from the parent cubic phase. One of the important aspects in MT is the arrangement of these multiple variants and the product and parent phases. In the absence of stress, these variants form 'twins' wherein the lattice strain is self-accommodated such that no macroscopic or long-range strain occurs. For instance, pure thermal cycling of SMA under no stress would lead to cyclic transformation between the parent austenite and twinned martensites. However, stress biases the type of variant that forms (detwins and/or reorients the variant) giving rise to net transformation strain. This is responsible for the SME and SE described above. In a single crystal, the transformation strains can be really large ( $>10\%$ ). However, in polycrystalline SMAs, presence of grain boundaries, defects, precipitates etc., influence the morphology of the evolving phase leading to higher complexity and heterogeneity. Thus, the reversible macroscopic strains are much less (typically 5-6% for NiTi). One of the important aspects in SMAs is the dependence of the phase morphology on the deformation history of the material; this will be discussed later in this section. This is microscopically related to the 'memory' or path dependency in the response of material giving rise to hysteretic response. In this context, in polycrystalline SMAs, the texture or the orientation of the grains in the material plays an important role in the transformation characteristics and hence in SE and SME. Concomitant to MT are significant changes in some of the material properties like moduli, specific heat, thermal conductivity, electrical resistivity, which influence the thermomechanical response.

Issues of compatibility of microstructure (Ball and James (1987)), strain energy associated with lattice distortion, transformation strain and the stress that arises due to incoherency and heterogeneity play a vital role in determining the evolution of the MT. Since MT is treated as a first order transformation, notion of order parameter associated with breaking of symmetry is used to describe or characterize the transformation. Evolution of the phase can be related to 'evolution' of the order parameter and hence evolution of the inelastic strain associated with the transformation. Another aspect that influences MT is the generation, growth and stabilization of dislocations and/or defects in the material during transformation. These introduce complexities in the microstructure evolution and influence the macroscopic response. The crystallographic aspects outlined above give a brief sketch of the kinematics of MT and factors influencing it. In the following, thermodynamics of MT which governs the kinetics and associated aspects is briefly discussed.

## 2.2 Thermodynamics of MT

From the above discussion it is clear that both thermal and elastic energies play a vital role in phase transformation in SMAs. Further, there is a strong interaction or coupling between these two energies manifesting as a highly non-linear and coupled thermomechanical behavior. For instance, even when MT is purely stress induced, it is accompanied by exchange of latent heat of transformation. The forward ( $A \rightarrow M$ ) transformation is exothermic while the reverse transformation is endothermic. The amount of latent heat involved depends on the alloy composition and processing history. In addition, MT is dissipative in nature involving inelastic deformation. Hence, thermodynamics plays a critical role in describing MT and a good amount of literature on this exists (Wollants et al (1993), Shaw and Kyriakides (1995), Huo and Müller (1995), Müller and Seelecke (1999), Rajagopal and Srinivasa (1999), Ortin and Planes (2005), Chang et al (2006)). Though MT is essentially thermodynamically irreversible (dissipative), both equilibrium (reversible) thermodynamics and irreversible thermodynamics are used to investigate MT. A brief outline of some important thermodynamic aspects is provided here to facilitate the discussion on modeling of SMAs.

Kinetics of phase evolution in terms of conditions for onset, direction of transformation (forward  $A \rightarrow M$  or reverse  $M \rightarrow A$ ), depending on the nature of loading and the amount of phase evolution for a given load increment is central to understanding of MT. In this context, several thermodynamic concepts like free-energy, dissipation potential, entropy production and driving force are used extensively to describe MT. Usually, Helmholtz or Gibbs' form of free energy is used to explain MT in terms of the relative stability of the parent and product phases. The temperature at which the chemical parts of free energies of the two phases are equal is termed as equilibrium temperature ( $T_0$ ). In a defect free single crystal, the transformation occurs instantaneously at  $T_0$ , the direction of which is determined by the sign of  $\Delta T$ . This unstable transformation at the microscopic level manifests as jump in the stress-strain response. The slope of the

stress-strain curve during transformation is associated with the interaction between the parent and product phases and the thermal equilibrium due to latent heat (Bernardini and Pence (2002b), Chang et al (2006)).

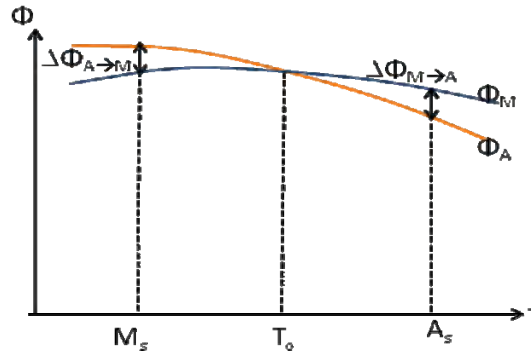


Figure 6: Potential for A and M phases as a function of temperature.  $T_0$  is the equilibrium temperature.

Due to friction and other internal factors, additional energy is needed to initiate transformation (undercooling to  $M_s$  or superheating to  $A_s$ ).

However, presence of defects, grain boundaries etc., alters the transformation temperature requiring either undercooling or superheating (Figure 6). Once initiated, the transformation is not self-sustaining (as in an initiation controlled process) and additional driving force is necessary for further transformation (propagation controlled process) (Rajagopal and Srinivasa (1995)). Additional driving force is needed to overcome friction and other dissipative forces that exist due to interaction energy. From a macroscopic perspective, MT is assumed to occur through a sequence of metastable states associated with athermal nature of kinetics. Minimization of free energy is used as the criterion to determine the state of SMA. For example, cubic austenite transforms into several energetically equivalent, yet crystallographically different variants of martensite. This fact is used to construct free energy forms applicable at different scales of continuum to model SMA response. For instance Falk (1985) constructed Landau's form of Gibbs and Helmholtz free energies as a polynomial of the order parameter.

Figure 7 shows the influence of stress on Landau's free energy parameter (based on Gibb's free energy). It shows two symmetric low energy wells corresponding to the two variants of martensite considered. Instead of the initial symmetry in the free energy structure corresponding to different self-accommodating variants (under a stress free condition) the direction of applied stress biases the free energy wells leading to the formation of martensites with specific orientations thereby accumulating large macroscopic strain. The isothermal stress-strain response shows two stable branches corresponding to the pure phases (A and M). During transformation, equilibrium of the phase mixture line gives a line with negative slope (corresponding to fully reversible and dissipation less transformation). Unstable branches at different temperatures are identified based on the free energy structure as a function of temperature and order parameter (in this case, the strain).

Thermodynamically, MT in SMAs is classified as either a weak first order or a second order transformation (Ehrenfest's criterion). First order transition requires only continuity of free energy of individual phases at the

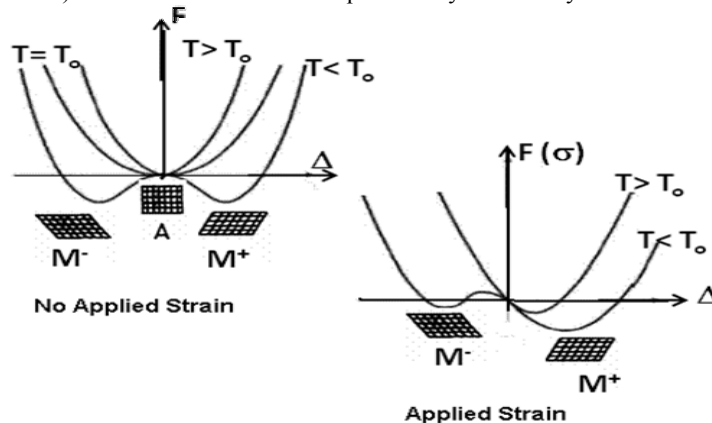


Figure 7 Schematic of free energy as a function of strain (order parameter) for a two variant martensite and austenite transformation.

equilibrium temperature ( $T_0$ ) whereas the second order transformation additionally requires continuity in gradient of free energy at  $T_0$ . In a regular first order phase transformation like solidification, there is a sharp change in the energy parameter with respect to a state variable like temperature. Also, there is long range movement of atoms (diffusion). However, in SMAs, though there is no diffusion, significant strains result in sharp change in the gradient of the energy parameter. Thus, the transformation in SMAs is displacive in nature and is a weak first-order or second order transformation. The transformation usually occurs over a temperature range ( $M_f < A_f$ ) and the start and end temperatures are affected by the stress. Generally, the transformation temperatures increase almost proportionately with stress. Further, the difference between the start and the end temperatures of martensitic and austenitic phases are approximately same. The interdependence of transformation temperature and stress is usually expressed using the Clausius-Clapeyron relation, in this context given by,

$$\frac{d\sigma}{dT} = \frac{-\Delta H}{T_0 \varepsilon_0} = \frac{-\Delta \eta}{v_0 \Delta \varepsilon}$$

where,  $\sigma$  is the stress,  $\Delta H$ , the change in enthalpy due to transformation and  $\varepsilon_0$ , the total inelastic strain,  $v_0$  is the molar volume,  $\Delta \eta$ , the change in entropy due to transformation. Usually the stress-transformation temperature relationship is obtained by conducting physical experiments.

The athermal aspect of kinetics in MT implies that, in general, the process depends on the instantaneous temperature (or stress) and not on the sweep rates of these driving parameters. This implies a certain rate-independence in MT. Apparent rate effects seen in macroscopic response like changes in shape of hysteresis due to rate of the loading parameter is more due to the latent heat effects associated with phase transformation. Due to unstable (metastable) nature of transformation, thermodynamic formulation based on equilibrium approach is useful only in bringing out some essential aspects of transformation. Heat transfer, diffusion and propagation effects that are not accounted for in the equilibrium approach are to be considered in order to fully describe the thermoelastic behavior.

### 2.3 Memory in MT

Path dependency in MT is attributed to the (rate of) entropy production in these materials. A suitable notion of ‘memory’ or information about the evolution for the load history within that transformation zone is essential while defining the kinetics under arbitrary loading. Ideally, due to history dependency, to predict the instantaneous state of the material during transformation, the information about the entire load-deformation history is essential. In order to capture the history dependency, suitable state variables are introduced into the free energy function. However, under arbitrary thermodynamic loading, definition of memory poses a significant challenge. Another aspect adding to the complexity is that the nature of memory changes during transformation history over many cycles. The response for arbitrary thermomechanical loading manifests as:

- Shakedown or training or stabilization of material (stability in the hysteretic response)
- Incomplete transformation (partial and inner hysteresis loops).

### 2.4 Stability in Material Response

An important aspect that governs the hysteretic response is the stabilization of the material behavior under cyclic thermomechanical loading. Under repeated loading, the material behavior is said to be stable, if the hysteresis for each load cycle is stable (shows no drift). Else, the behavior is said to be non-stabilized and this could typically manifest as remnant strain and/or stress at the end of each cycle, which could accumulate during subsequent cycles (ratcheting response). This leads to non-closure of hysteresis loops. Stability is desirable from a device or an application perspective and hence special thermomechanical treatments are imparted to the material to achieve the same. For instance, dislocations and defects are deliberately introduced and grown through thermomechanical process (Lin et al., 1991; Liu and Tan, 2000; Otsuka and Ren, 2005; Feng and Sun, 2007) to obtain desired levels and repeatability of SME and SE. Factors influencing stabilization are the load levels, history and number of cycles at the given load level. Due to history dependency of the material response, stability is observed only under loads ‘not greater’ than the previous maximum load levels. For higher loads, a certain number of additional cycles are necessary before stabilization occurs. Such transformation behavior can be interpreted as ‘imperfect memory’ which needs multiple cycles to become ‘perfect’.

### 2.5 Partial and Inner Loops

Load reversals before complete transformation lead to partial and internal or sub loops. These are complex hysteresis phenomenon that affects not only the material behavior but also the functional or device level behavior. Unlike MT associated with complete transformation, partial cycles have not been investigated in detail and several open issues relating to them exist; for instance, the nature of these loops (shape of these loops with respect to the outer or major loop). Aspects like MT with regard to return point memory and sink point memory (Huo and Müller (1993)) depicted in

Figure 8 is yet to be clearly understood (Seelecke and Müller (1999), Ortin and Planes (2005), Matsuzaki et al (2002), and Kishorekumar et al (2007)).

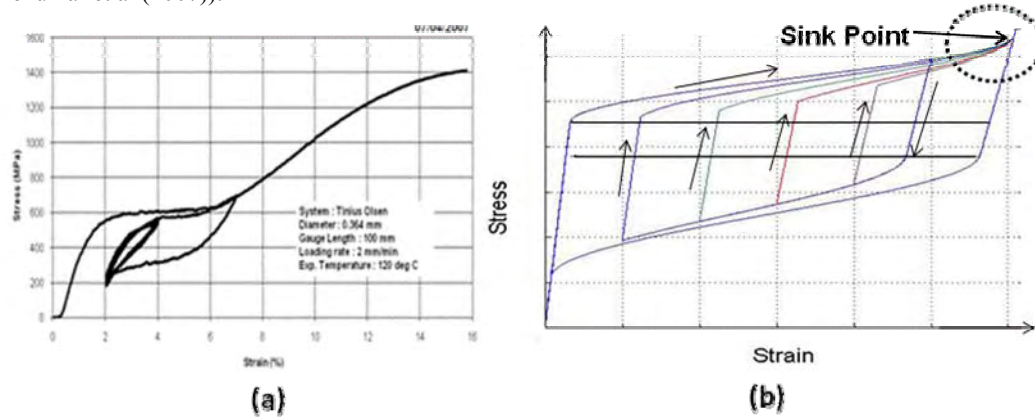


Figure 8: Different inner or partial loop behavior; (a) return point memory behavior in a commercially available NiTi; (b) Schematic sink point behavior.

Another aspect discussed below to facilitate discussion on modeling is the essential characterization of SMAs. While extensive literature exists on this aspect (Shaw and Kyriakides, Sittner et al (2000), Duerig et al (1990)), only essential aspects of this are briefly presented here.

## 2.6 Macroscopic Characterization of SMAs

### 2.6.1 Differential Scanning Calorimetry

Differential Scanning Calorimetry (DSC) is a thermo-analytical technique that is often used to characterize thermally induced stress-free transformation in SMAs. ASTM F2004 provides a standard procedure to conduct the tests and report the results. In DSC, essentially, the difference in the amount of heat required to increase the temperature of a small quantity of the sample (about 10 mg) and the reference are measured as a function of temperature. Both the sample and reference are maintained at nearly the same temperature during thermal cycling over the entire transformation temperature range at a typical rate of 10 °C/min. A typical output from DSC test on SMA with and without R-Phase in terms of heat flow rate versus temperature is shown in Figure 9. From these, the transition temperatures and the enthalpy of transformation ( $\Delta H$ ) associated with  $M \rightarrow A$  (heating) and  $A \rightarrow M$  (cooling) transformations are determined.  $\Delta H$  is measured as the area under the transformation peaks during the heating and cooling cycles. A more sophisticated test is the modulated DSC that can differentiate both the reversible and irreversible components of heat flow (Brantley et al (2002)). This is useful to resolve multimode transformations or other second order effects.

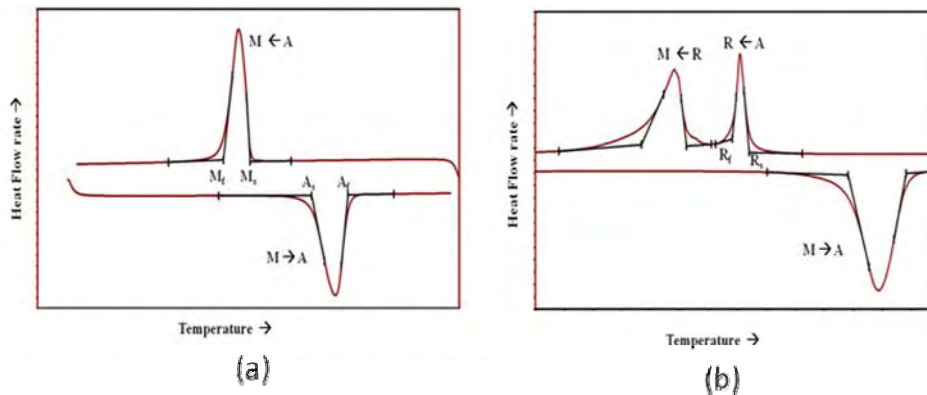


Figure 9: Heat flow vs temperature trace in DSC for SMAs (a) without R-phase and (b) with R-phase. Transformation temperatures are identified by drawing tangents as shown.



### 2.6.2 Stress-strain-temperature tests

Although DSC is an excellent experimental technique to obtain the SMA transition temperatures, it is suitable only under stress free condition. In order to characterize the thermomechanical hysteresis of SMAs, an experimental technique to study the material behavior under heating and cooling under a constant stress is required. Generally, two types of tests are frequently employed for this purpose.

1. Constant stress thermal cycling (iso-baric test)
2. Constant temperature mechanical cycling (isothermal test)

Several important material parameters like moduli, total transformation strain (both one-way and two-way), and Clausius-Clapeyron relation are estimated from these tests. This information is used to obtain the phase diagram (discussed in detail in next section).

#### 2.6.2.1 Isobaric tests

On either the tensile coupons or wires, constant stress is applied and the SMA is thermally cycled between the martensite and austenite conditions. This experiment is usually conducted with SMA under a dead weight or in a UTM under constant force mode. The rate of heating and cooling is kept sufficiently low (order of 5 °C/min). In this case, SMA shows a hysteretic strain-temperature ( $\epsilon$ -T) response. A typical  $\epsilon$ -T hysteresis response is plotted for a given stress level as shown in Figure 10. It is not always easy to identify the transformation temperatures from this plot. For engineering purposes, usually, tangents are drawn to the heating and cooling segments (Figure 10) to obtain the transformation temperatures ( $M_s$ ,  $M_f$ ,  $A_s$  and  $A_f$ ). More analytical methods such as numerical differentiation of the curve can be used to identify change in slope or curvatures and associate them with the critical temperature. Another parameter that is obtained from this test is the amount of transformation strain.

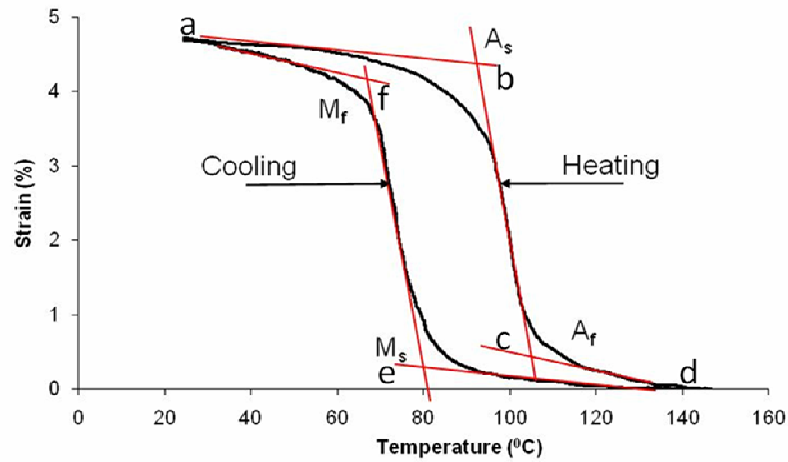


Figure 10: Strain-temperature hysteresis at 100 MPa stress for a commercially available NiTi.

#### 2.6.2.2 Isothermal tests

Tensile tests involving complete load-unload cycle covering the range of SIM and its reverse transformation are often performed to characterize SMA response. The tests have been done in a controlled thermal environment at different constant temperatures; the range depending on the transformation temperatures. The strain rates are typically small to obtain quasistatic response (order of 0.001 /s). Typical stress-strain curves at a few temperatures are given in Figure 11. Critical transformation stresses for both forward and reverse transformation are obtained from this test as shown in Figure 11. The transformation strain can also be determined from this test.

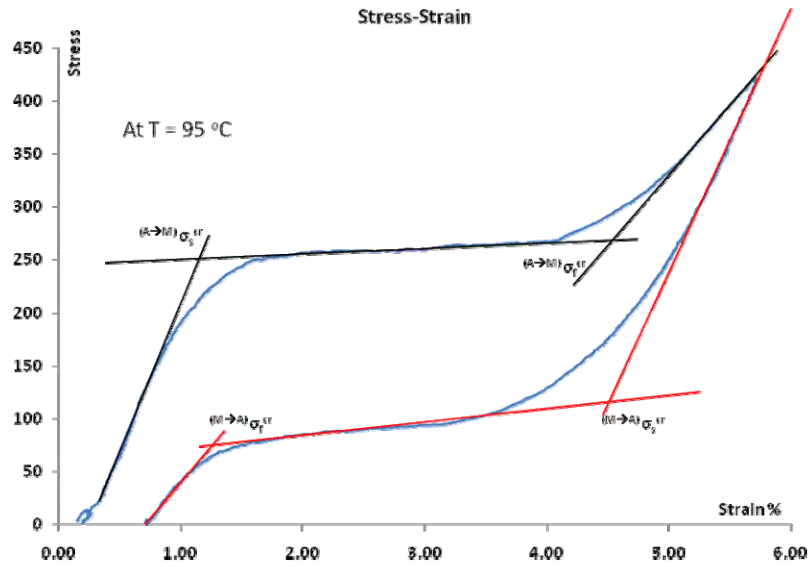


Figure 11: Stress-strain response and tangents drawn to determine critical transformation stresses for a commercially available NiTi.

The above discussion briefly introduced salient aspects underlying SMA response to motivate the need to model them. It is clear that MT, with its characteristic microscopic features is responsible for the macroscopically observed SME, SE and other related effects. This poses a challenge in terms of bridging the continuum scale between the microstructure and the bulk form of SMA that is exploited in several different applications. Different continuum scales that are of interest are schematically illustrated in Figure 12. However, from an application development perspective, 1-D form of SMA like bar, rod and more prominently wire are the preferred forms of SMA (Duerig et al 1990). Hence, most of the model development also focuses on the 1-D behavior. A broad overview of the modeling literature on SMAs is provided here. Recognizing the vastness of literature on SMAs in general and on modeling them in particular, this review is by no means exhaustive and is aimed at giving a perspective of the development of models for SMAs at different continuum scales. At the outset, it may be mentioned that since the focus here is on thermomechanical behavior of SMAs, several aspects related to MT in SMA like the R-phase and changes in resistivity are not covered. Further, for convenience, discussion is made based on the development of modeling approaches by groups (wherever possible). This is preferred over the chronological basis. A snapshot of both macroscopic and microscopic approaches is provided in tabular form for quick comparative assessment.

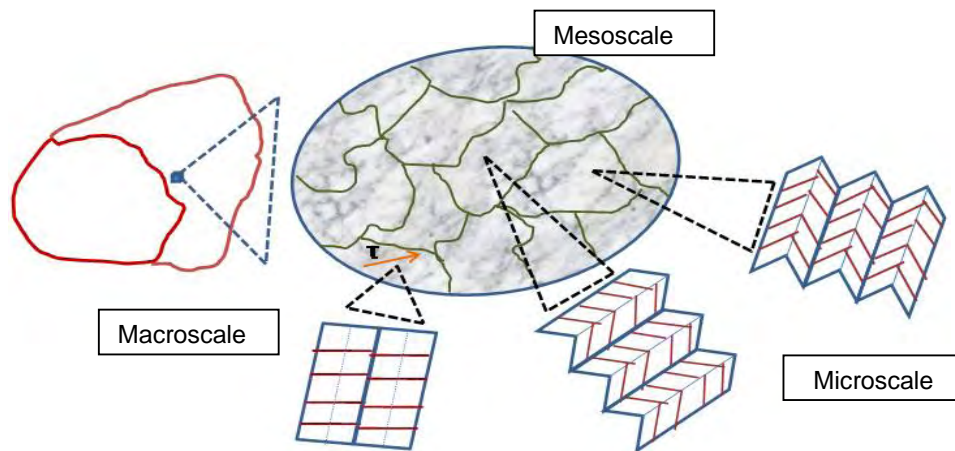


Figure 12: Schematic of continuum scales for investigating SMAs

### 3. Models for SMA Behavior

A survey of existing models for SMA behavior yields a rich amount of information pertaining to the models aimed at capturing the essential hysteretic response in SMAs. As can be readily recognized, it is an uphill task to cover the entire gamut of available models for SMAs. A quick glance at these models suggests that a plethora of approaches exist. Birman (1994), Bernardini and Pence (2002a) and Paiva and Savi (2005), Smith (2005) and Lagoudas (2008) have reviewed models for SMA. Noting the increasing attention of research community over the last decade, a brief review of modeling approaches and models for SMA response is attempted here. To facilitate this, some liberties are taken in classifying these approaches wherein the classification is made to facilitate understanding, albeit compromising scientific rigor. A classification of the models in terms of the scale of the continuum that is of primary focus is presented in Figure 13. A broad classification of some of the salient approaches to modeling SMA response is given in Figure 14.

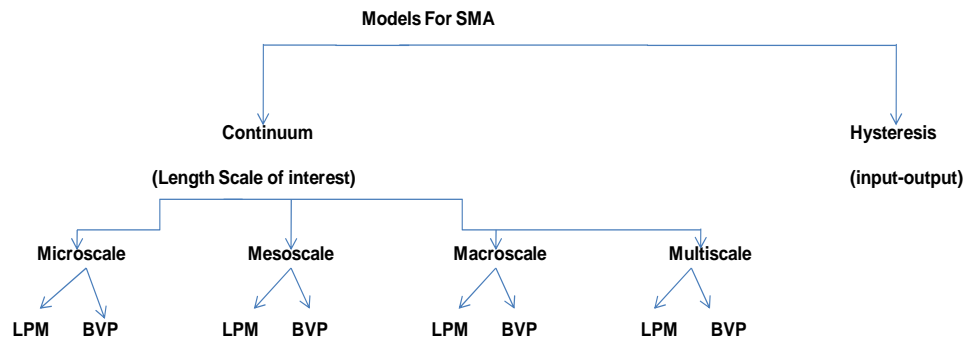
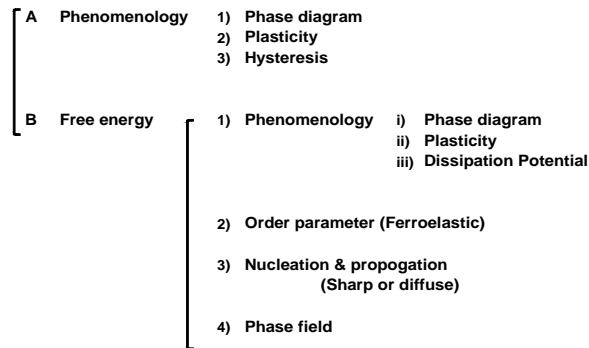


Figure 13: Classification of types of models for SMAs

At this juncture, it may be useful to note that modeling of SMAs is attempted for a variety of purposes and in particular, for the following.

1. Understanding of the underlying physics and mechanisms that cause the observed effects; helps in explaining the observed phenomena
2. Identify the material properties or processing parameters that can yield desired effects in terms of SME, SE, TWSME etc., - helps in material development
3. Predict the material response in conjunction with the smart device or a system that is under investigation- helps in application development

#### I Macroscopic Approach



#### II Microscopic Approach

- A Free energy
- B Micromechanics
- C Crystal plasticity
- D Lattice dynamics

Figure 14: Classification of types of modeling approaches

Further, different modeling approaches are suited for different purposes. Hence, depending on the objective(s), selection of a suitable modeling approach(es) is made. For instance, macroscopic thermodynamic based models are suitable for capturing several macroscopic effects and explain the underlying physics. Microscale or lattice scale models are suitable for identifying the underlying mechanisms. This also facilitates tailoring the material and/or process parameters to arrive at a suitable material composition and processing that yield SMA with desired characteristics. However, it may be noted that such a modeling approach could be mathematically quite rigorous and computationally intensive. Alternatively, empirical or phenomenological models are relatively much simple and serve as design aids in the development of smart devices and systems. However they may not be able to adequately capture all the associated effects. In the following review these aspects are highlighted.

Following the classification in Figure 14, a brief discussion on the macroscopic approach and some of the existing models based this approach are presented.

#### 4. Macroscopic Modeling Approaches

Macroscopic models, as the name suggests, attempt to capture the SMA response at a macroscopic scale (typically  $>100$  microns). Suitable assumptions and approximations are made to account for its macroscopic effects. The nature of assumptions and the approximations usually characterize a given model. Most of these approaches use phenomenology. The extent and the nature of phenomenology they use form the basis of their classification here. Another important aspect is the use of thermodynamic principles. While some models possess such a thermodynamic framework, others rely significantly on phenomenology, assuming that the thermodynamic laws are satisfied *a priori*. In the following, models which draw heavily on phenomenology are termed phenomenological models, while those with a significant amount of thermodynamic framework are classified as free-energy based models. Another class of models attempts to capture the hysteretic input-output response without explicitly accounting for underlying physics. These models use different types of hysteresis operators to predict specific stress-strain-temperature response. Macroscopic approaches and models based on them are discussed briefly in the following.

##### 4.1 Phenomenological Models

Simplicity, coupled with a fair degree of success in capturing the macroscopic SMA response, at least in a 1-D setting, has resulted in large number of phenomenological models. Commonly used phenomenological descriptions are discussed herein. Phenomenological models separate out the two aspects of modeling mentioned below.

- Constitutive stress-strain-temperature relationship due to elastic forces, thermal expansion and phase transformation;
- The driving forces and the evolution (kinetics) of the phase transformation in terms of onset and completion of transformation and the rate of evolution of internal variables or phase fractions.

In general, most of the salient differences in approaches stem from the choice of internal variables and the description of their evolution in terms of the thermomechanical driving forces. Some of the frequently encountered approaches are discussed below.

##### Phase diagram based models

Several models for evolution kinetics in SMAs use a  $\sigma$ -T phase diagram to identify appropriate transformation (active) and dead zones. A typical phase diagram and its construction was discussed earlier (Secn. 2). The phase diagram illustrated in Figure 15 is representative of the equilibrium or quasistatic response in SMAs and that the start and finish transformation lines are rate-independent. In each active zone appropriate evolution functions are defined to compute the extent of phase transformation. The functions commonly used are linear, cosine or exponential, describing either the evolution of martensitic fraction  $\xi$  or its rate form ( $\dot{\xi}$ ). Time is only notional since these models describe rate independent (quasistatic) evolution. Subsequently, a constitutive relationship that uses the phase fraction describes the thermomechanical behavior. Depending on the nature of the phenomena being modeled, the model can have multiple internal variables representing, schematically, different martensitic fractions that are of interest. This approach is also classified in literature as an internal variable based approach. While most of these models are 1-D in terms of uniaxiality of stress and strain, some 3-D models exist that accounts for multi-axial stress using a suitable equivalent 1-D driving function. It may be noted that the Cauchy stress is used in the construction of phase diagram. This approach leads to simplified models facilitating their use as design tools.

Anaka (1990) was among the first to use this approach for SMA to study superelasticity with stress induced martensitic fraction ( $\xi_s$ ) as an internal variable. Analogous to the exponential Koistinen-Marburger relation, an evolution law is deduced in terms of stress and temperature. Further, using strain and temperature as the control variables, a constitutive relation was derived for constant material functions.

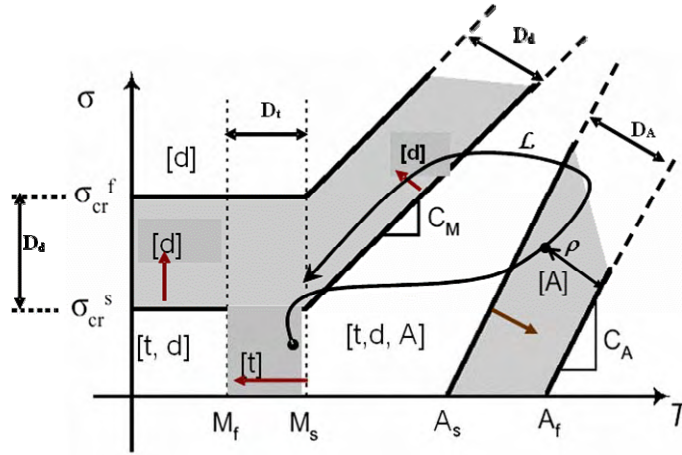


Figure 15: Idealized phase diagram for typical NiTi SMA material under uniaxial stress condition showing the dependence of transformation temperature on stress and regions with different phase mixtures. L is the load path, [A]- Austenite, [t] – twinned martensite; [d] – detwinned martensite. The shaded region represents the region where transformation is said to occur.

To obtain a better fit to the experimental data, Liang and Rogers (1990) modified the phase kinetics to a cosine based function. Both Tanaka (1996) and, Liang and Rogers (1990) were successful in capturing the superelastic behavior. Based on the broad framework of Tanaka (1990) and Liang and Rogers (1990), Brinson (1993) proposed a modified model to also account for the shape memory effect. The distinguishing feature in Brinson (1993) model is splitting the martensitic phase fraction into two parts, viz., temperature induced twinned fraction ( $\xi_T$ ) and stress induced detwinned fraction ( $\xi_S$ ). This differentiation of the phase fractions is used to capture recovery stress/strain. One of the important simplifying assumption is that the twinned martensite does not contribute to the recovery stress. A phase diagram was constructed to describe phase transformation involving austenite and the two martensite variants. To describe the constitutive behavior, the constitutive model with Voigt type non-constant material functions are used. Prahlad and Chopra (2001) and Brinson and Huang (1996) provide a comparative assessment of these models. In these models the kinetics is given in the piecewise integrated (or algebraic) form for the phase fraction(s). Wang et al (2006) proposed a model for materials wherein the detwinning transformation boundaries also has non-zero slopes (negative slope for  $T < M_s$ ). They modified the kinetics proposed by Brinson (1993) to capture the temperature dependence of the detwinning stress. It may be mentioned that Brinson (1993) model has been used widely for modeling SMAs. Further, Buravalla and Khandelwal (2007) proposed modified material definitions which yield consistent rate form of constitutive equation for the Brinson (1993) model. The kinetics for the co-evolution zone (Figure 15) where austenite transforms into both twinned and detwinned martensites as given by Brinson (1993) needed appropriate constraints to obtain physically admissible volume fractions. This is addressed independently in Chung et al (2007), Gao et al (2007) and Khandelwal and Buravalla (2008). Buravalla and Khandelwal (2008) show that the rate form of kinetics inherently has appropriate constraints that cater to co-evolution zones. The rate form of kinetics for SMAs follows from the analogy of flow-rule in rate independent plasticity. Models that follow this approach are described below.

#### 4.1.1 Plasticity based models using phase diagram

A more consistent thermodynamic description relates the rate of entropy production to  $\dot{\xi}$  rather than to  $\dot{\xi}$ . Thus, it may be more suitable to assume a functional form of  $\dot{\xi}$ . In conjunction with the phase diagram, the notion of flow rule in rate independent plasticity is generalized to describe the kinetics in the rate form ( $\dot{\xi}$ ). Lubliner and Auricchio (1996) present a generalized plasticity based model for single variant MT, capable of simulating SE. Auricchio and Lubliner, (1997) extended this by considering two internal variables representing multi-variant (similar to twinned martensite) and single variant (similar to stress-induced) martensite. In order to consider multi-axial state of stress, a Drucker-Prager type of loading function is employed by Auricchio et al (1997). They present an algorithm to solve the 3-D BVP involving momentum balance equation and illustrate the effect of stress multi-axiality through several case studies for superelastic response. However, this algorithm is limited to the stress-induced single variant transformation and hence is not suitable for SME. To facilitate the implementation of this constitutive model in a displacement based finite-element approach, Auricchio and Sacco (1999) give a strain based flow-rule with linear kinetics.

Table 1. Summary of macroscopic phenomenological models

Model	Model for Elastic Modulus	Evolution kinetics			Inner/partial loops	Twin / Detwin distinction
		Representation		Functional description		
		Form	Nature			
Tanaka (1985)	$E=E_A=E_M$	Algebraic	Global	Exponential	No	No
Liang and Rogers (1990)	$E=E_A=E_M$	Algebraic	Global	Cosine	Compression model	No
Brinson (1993)	Voigt	Algebraic	Global	Cosine	Compression model	Yes
Ivshin and Pence (1994)	Reuss	Rate	Global	General tanh	Compression	No
Boyd and Lagoudas (1994)	Voigt	Rate	Global	Exponential	No	No
Bekker and Brinson (1998)	Voigt	Algebraic	Local	Cosine	Yes	No
Govindjee and Kasper (1999)	Voigt	Algebraic	Global	Linear	Yes	No
Aurricchio and Lubliner (1997) Aurricchio and Sacco (1999)	Voigt and Reuss	Rate	Global	Exponential	Yes	Yes
Wu and Pence (1998)	Reuss	Algebraic	Local	Cosine	Yes	Yes
Chenchiah and Sivakumar (1999)	Voigt	Algebraic	Local	exponential	No	No
Matsuzaki ( et. al. 2002	Reuss	Algebraic	Global	Polynomial	Priesach	Yes
Ikeda et. al. 2004	Reuss	Algebraic	Global	Exponential	Shift-skip Model	Yes

An iterative scheme is necessary to translate a given temperature and strain increment into the equivalent stress-temperature loading that is used with the stress-temperature phase diagram. Auricchio (2001) proposed a robust return mapping algorithm incorporating finite strains in a single variant MT. This is implemented in a finite element framework to study SE. Typical SE applications like orthodontic wires are modeled using this approach. Auricchio et al (2003), modeled the effects of training and TWSME by introducing an additional empirical variable called, addition irreversible residual martensite. This is defined as a material parameter, representing the ability of the material to be trained and is used to scale the transformation strain during cycling (shakedown) and to capture the evolution of two-way strain.

Several enhancements to the phase diagram based approach exist. For instance, the phase diagram shown in Figure 15 can also be extended to consider compressive stress (Gao et al (2001)). Further, to account for stress multi-axiality, Brocca and Brinson (2002) proposed a model based on the habit plane or microplane theory. Using the notion of microplanes at a macroscopic level, they deduce a form for macroscopic transformation strain due to 3-D loading employing a modified 3-D transformation onset criteria. As a summary, some of the salient aspects of phenomenological models are listed in Table 1.

#### 4.1.2 Phase diagram based models for arbitrary loading

Most of the models reviewed above are applicable to cases wherein the transformation is monotonic and complete. In cases where the loads are arbitrary, partial and/or inner hysteresis loops may occur and hence suitable memory parameters are necessary to capture them. Bekker and Brinson (1997) recognize the need for models capable of predicting SMA response under arbitrary thermomechanical loading. They introduce the notion of switching points to incorporate memory into the transformation kinetics. Defining different types of switching points, a given load path is discretized into segments where either the transformation occurs (active) or not (dead). They additionally associate the concept of distance of a point on the load path from a reference point (called the base-point) to determine the extent of

transformation. For each active segment, local kinetics are defined to describe evolution of  $\xi$ . A scheme to construct global kinetics for loading involving different regions of phase-diagram using the local kinetics is presented. Bekker and Brinson (1998) later extend this model and present three different algorithms viz., Y-Algorithm, Z-Algorithm and YF-Algorithm, based on different ways in which the distance information is used to determine the transformation. They have studied a few specific types of arbitrary load cases and have highlighted several effects that could be predicted using their model. It may be mentioned that for certain types of cyclic loading the model predicts unlimited ratcheting (refer Figures. 8 and 13 in Bekker and Brinson, 1998). This is not usually seen in many polycrystalline SMAs which exhibit either a limited (non-stabilized) or non-ratcheting (stabilized) response. Recently, Gao et al. (2007) used the Z-Algorithm to obtain a finite element implementation of the Bekker and Brinson (1998) model.

Govindjee and Kasper (1999) introduced a memory parameter in terms of the extremum value of  $\xi$  already achieved in the current active zone. The choice of maximum or minimum is made depending upon the transformation zone. The memory is 'erased' when the path enters the reverse transformation zone. This is adequate only for a single variable (either only stress or only temperature) loading and linear kinetics. If the kinetics is nonlinear, additional memory parameter(s) like the associated values of  $(\sigma, T)$ , corresponding to extremum of  $\xi$  for the load history within the transformation zone becomes necessary. This would then be like a 'Restart' switching point in Bekker and Brinson (1998) model. The rate based kinetics proposed by Auricchio and Lubliner (1997) is more suitable and simple to implement and can be used for predicting response under arbitrary loading. The concept of switching points is implicit in the rate form of kinetics. However, even this model can predict unlimited ratcheting for certain certain types of loading such as repeated excursions between active and dead zones.

Recently, a simple distance based algorithm for describing kinetics for arbitrary loading in a phase diagram setting is proposed by Buravalla and Khandelwal (2008). In this work, discussing the importance of appropriate memory in the kinetics, they introduce suitable memory parameter, defined as the distance of a point on the load path inside the transformation zone from the finish boundary, to capture the extent of transformation under load excursions. This information is used to stipulate additional transformation conditions which prevent spurious evolution. The notion of fading memory (Coleman (1964)) is used to alter the memory parameter during stabilization. Limited validation of this approach is provided for stress induced transformation under arbitrary mechanical loading. The approach presented above is shown to involve reduced 'book-keeping' compared to other existing phase diagram based models for arbitrary loading.

Depending on the alloy composition, processing and load-deformation history, SMA exhibits different types of hysteresis that lead to different types of phase diagrams. One of the characteristic features in phase diagram based models is the nature of Clausius-Clapeyron relation, given by the slope of the transformation boundaries. It may be noted that usually the slopes of the start and finish boundaries (Figure 15) are assumed to be same, though they are different for martensite ( $C_M$ ) and austenite formation ( $C_A$ ). In a polycrystalline case, apart from the stored elastic energy, the interaction energy plays a significant role in determining the onset of transformation. The interaction energy, rate of dissipation, and the thermal balance associated with the latent heat of transformation determine the nature of hardening and hence the finish transformation boundary. In principle, for polycrystalline SMAs, depending on the nature of interaction energy and dissipation rate, the slopes of start and finish boundaries could be different. Further, even if  $M_s < A_s$  for some range of stress, beyond a certain stress, it is possible that  $M_s > A_s$  which reflects as intersection of  $M_s$  and  $A_s$  lines. Such a phase diagram represents drastically different shapes of hysteresis in the response. Models for such complex phase diagrams do not exist in literature. Extension of the existing phase diagram models to such cases could be one of directions for further research.

#### 4.1.3 Hysteresis models

Broadly two types of approaches exist in literature that model the complex hysteresis response in SMAs without necessarily going into the underlying physics. They are similar to input-output models wherein a suitable transfer function is constructed that captures the observed hysteresis between a forcing function and the response variable. Such models are commonly used in modeling magnetic and ferroelectric materials and are frequent in control literature. Noting several similarities in the SMA response, attempts are made to adopt them for modeling SMAs. Smith (2005) gives a detailed discussion on this approach for modeling SMAs. There are two main types of hysteresis models viz.,

1. Preisach type models
2. Duhem-Madelung models.

These models differ in terms of the nature of the hysteresis operator that is used to track the response through a series of relays.

Preisach models follow an integration of the response of individual relays that switch between two fixed states, each representing in this case, the type of transformation. Critical driving forces are prescribed for switching in both the directions. Though the traditional Preisach models do not have interaction between individual relays, a suitable form of interaction between the neighboring relay elements can be prescribed that yields the observed response,  $v(t)$ . The multi-

valued response is captured using the information from the response history. Ortin (1992), Ortin and Delaey (2002) have used this approach to capture the SE and SME hysteresis in SMAs. One of the advantages in this approach is the facility to model inner loops and return point memory. The Preisach operator  $P[w]$  is defined as follows using a linear superposition of relay operators.

$$w(t) = \int_0^\infty \int_{-\infty}^\infty w(r, s) \mathcal{R}_{s-r, s+r} [v](t) ds dr, \quad (1)$$

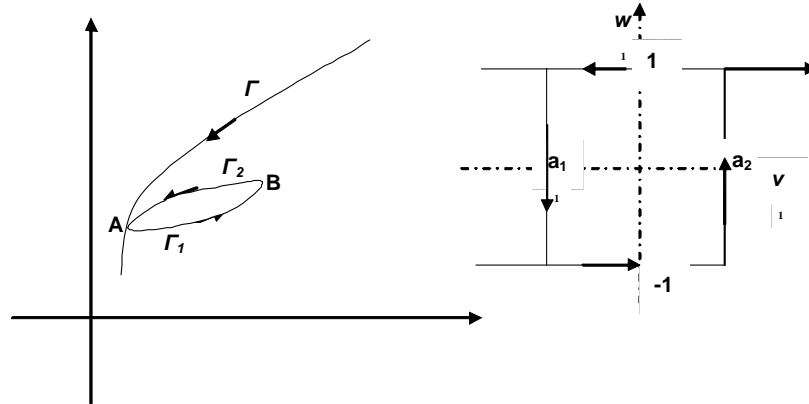
where  $w(r, s)$  is a density function, assumed to vanish for large values of  $r$  and  $s$ .  $\mathcal{R}_{s-r, s+r}$ , is the relay operator, with initial values of -1 for  $s < 0$  and +1, otherwise. It may be noted that Preisach models cannot account for dead zones in the hysteresis models and hence need suitable modifications. Matsuzaki et al (2002) used this approach to model inner loops in the SMA response. This is later adopted by Ikeda et al (2004) along with a suitable thermodynamic transformation energy barrier concept to develop a shift-skip model.

Unlike the Preisach operator, Duhem-Madelung models capture the hysteresis using differential equations. In general, two differential operators, one for the loading segment and the other for the unloading segment of the load path are used to capture the response in an incremental manner. For ferromagnetic type hysteresis three rules exist, viz (refer. Figure 16.),

1. Any curve  $\Gamma_1$  emanating from a turning point A of the input-output graph (Figure 16) is uniquely determined by the coordinates of A.
2. If any point B on the curve  $\Gamma_1$  becomes a new turning point, then the curve  $\Gamma_2$  originating at B leads back to point A.
3. If the curve  $\Gamma_2$  is continued beyond the point A, then it coincides with the continuation of the curve  $\Gamma$  which led to the point A before the  $\Gamma_1$ - $\Gamma_2$  cycle was traversed.

These rules are used to capture the SMA response. Ivshin and Pence (1994) used this approach to capture the hysteresis in SMAs. Using this model they show that the stabilization in hysteresis due to cyclic loading can be captured. It may be noted that the YF Algorithm proposed by Bekker and Brinson (1998) is an integrated form of the Duhem-Madelung model.

Due to its simplicity, this approach is used in real time control of SMA devices and also to predict inner-loop response. However, the approach becomes tedious when effects like TWSME, changes in hysteresis and multiple variants are considered. This approach is not amenable to design the material or a system since they do not provide sufficient insight into the phase transformation process in the material. Moreover, for materials with more complex hysteresis, significant tailoring of the operator may be needed. Lack of physical basis makes this tailoring a challenging task.



**Figure: (HOP) Branching from an arbitrary path showing rejoining after a partial loop;(b): Relay  $\mathcal{R}_{a_1, a_2}$  operator**

Figure 16: Hysteresis showing (a) different branches; (b) Relay operator



#### 4.2 Macroscopic free energy based models

As briefly discussed in Section 2, MT can be defined using appropriate free-energy function and additional thermodynamic notions for dissipative processes. In this approach, a more consistent attempt is made to identify a suitable form of free energy or potential that represents the state of the system and introduce the phase transformation related effects through either the changes in free energy itself or through generalized constitutive function like dissipation potential. The choice of field or state variables determines the type of free energy like, Gibbs, Helmholtz, or phenomenological Landau-Devonshire forms. It may be noted that it is possible to interchange the Gibbs and Helmholtz forms using appropriate Legendre's transforms. In the Landau form, internal variables like an order parameter(s) or phase fraction(s) are introduced. Since MT is considered a first order transformation, generally order parameters can be directly associated with the transformation strain either at the level of crystal or at the macroscale (Falk 1980, Ortin and Planes 2005). To account for the non-local effects like phase fronts, gradient terms are introduced either as state variables or used to modify the form of free energy. Table 2 lists the types of free energies that are commonly used and associated formalism. In general, the free energy takes the form:

$$\phi = \phi(\mu^{Mech}, \mu^{Th}, \mu^{PT}, \mu_{,x}^{PT}); \quad (2)$$

where,  $\mu^{Mech}$  is a set of mechanical state variables (like stress or strain),  $\mu^{Th}$  is temperature,  $\mu^{PT}$  is a set of internal variables and  $\mu_{,x}^{PT}$  is the set of spatial derivatives of the internal variables.

The fundamental form of free energy is then given by:

$$d\phi = F^{Mech} d\mu^{Mech} + F^{Th} d\mu^{Th} + F^{PT} d\mu^{PT} + F_x^{PT} d\mu_{,x}^{PT} \quad (3)$$

where,  $F$  represents the corresponding generalized forces or work conjugates associated with each of the state variables. Necessary restrictions on the choice of constitutive functions using second law of thermodynamics in the form of Clausius-Duhem (C-D) inequality are imposed. In the strong form, each of the four terms in the RHS of Eq. 3 is assumed to independently satisfy the C-D inequality. Further, due to the dissipative nature of the phase transformation,

$$\begin{aligned} -F^{PT} \dot{\mu}^{PT} &\geq 0; \\ -F_x^{PT} \dot{\mu}_{,x}^{PT} &\geq 0. \end{aligned} \quad (4)$$

In the absence of any phase transformation, the inequality in Eq. (4) reduces to the equality condition (as in thermoelasticity).

The kinetics which tracks the dissipation through the evolution of internal variable(s) during the transformation process may be captured in two ways. A simple way is to independently assume a functional form for the rate of evolution of internal variables (i.e.,  $\dot{\mu}$ ) or the evolution of the internal variable itself ( $\mu$ ) such that Eq. (4) is satisfied. Alternatively, another potential that dictates the dissipative process in the material called dissipation potential is assumed (Huo and Müller (1993), Rajagopal and Srinivasa (1999), Bernardini and Pence (2002b)). Clausius-Clapeyron relation is implicit in this potential. The total derivative of this potential is used to derive the functional form of kinetics. For instance, neglecting the second expression in Eq. (4),

$$F^{PT} - \Pi = 0 \quad (5)$$

where,  $\Pi$  is the critical driving force which will decide the onset or occurrence of phase transformation. The rate form in Eq.(4) provide the evolution kinetics. It may be noted that  $\Pi$  could be a function of state variables. In the case of Ginzburg-Landau formalism (Levitas and Preston (2005)), the kinetics is derived using the following relation.

$$\dot{\mu}^{PT} = A F^{PT} + B \nabla^2 \mu^{PT}; \quad (6)$$

where,  $A$  and  $B$  are material functions. During simultaneous evolution of multiple variants, appropriate constraints like conservation of mass and self consistency or St.Venant compatibility are used to fully describe the evolution process.

Several different forms or decomposition of free energy is used in literature. One way of decomposition is through the assumption of suitable energy well structure in terms of the internal variables (for instance Falk (1980)). Alternatively, a more mechanistic decomposition like that proposed by Fred and Gurtin (1994) and Rajagopal and Srinivasa (1999), shown schematically in Figure 17 can be adopted.

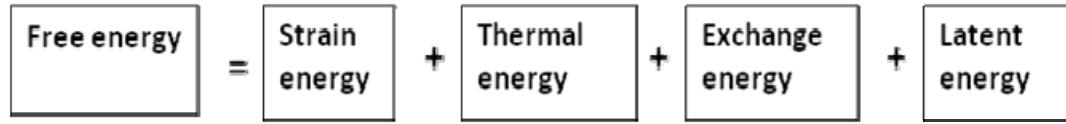


Figure 17: Schematic of free energy decomposition

The interaction energy or the exchange energy is a function of volume fraction and it usually determines the nature of kinetics through dissipation potential. In general, this includes both the bulk form and the surface or interfacial form due to inhomogeneities between different phases. Since martensite variants are assumed to have the same moduli, usually, the interaction between individual variants of martensite is ignored and only the interaction between martensite and austenite is considered. The interaction energy also determines the nature of hysteresis and memory in the material response. In realistic polycrystalline materials, the interaction energy could vary with load or deformation history due to creation, growth and stabilization of dislocations etc.. Thus, making a suitable choice on the nature of interaction energy becomes a daunting task.

Different ways of mechanistic decomposition of free energy lead to different modeling approaches and an overview of these is attempted here. The classification given in Figure 14 is used here. A brief discussion on some of the literature on macroscopic free energy based models is given below. Table 2 presents a snapshot of the salient aspects of the features in these models.

#### 4.2.1 Order parameter based models

As discussed briefly in Section 2.2, Falk (1980) proposed one of the first free energy based model for SMA using shear strain in a reference crystallographic plane [110] as an order parameter. Several parallels are drawn between comparing MT with ferroelasticity. The observed stress-strain response with stable and unstable branches was used to construct a free energy function. A sixth degree polynomial with even powers of strain is used to represent Helmholtz free energy as a function of strain and temperature. The choice of even degree polynomial is motivated by the symmetry in the crystal structure considered. The stable and unstable branches in stress-strain response are explained in terms of the energy wells and condition for stability. Both stress induced and temperature induced transformations are discussed. The stress-free transformation temperatures are predicted for a defect-free single crystal. A generalized free energy function is presented in terms of non-dimensional parameters (as a special material) and an experimental procedure to obtain the material parameters is discussed. A comparison for  $\text{Au}_{23}\text{Cu}_{30}\text{Zn}_{47}$  SMA is also provided. It may be noted that this model does not show hysteresis in the conventional sense.

Levitas and Preston ((2002a), (2002b) and (2003)) have used generalized Landau theory to model SMAs. As a first step, a 3-D theory for reversible SIM transformation is presented which is then extended to the transformations between the martensitic variants viz., detwinning and reorientation. To model the kinetics, gradients of the order parameter are introduced into the free energy to account for interfacial effects (Ref. Eq. 6). The free energy structure is similar to Falk (1980). In addition to the entropy and enthalpy, the activation barrier concept is used to deduce the constitutive coefficients in the free-energy polynomial. The curvature of the free energy well is used to stipulate the onset criterion. Full 3-D stress-strain tensor is used in the model and the transformation strain tensor has a general nonlinear relationship with the order parameters. They discuss the contribution of the linear and nonlinear terms in order parameter relating them to the 'proper' and 'improper' MT. When extending this model to cover transformation between the variants, they introduce additional interaction potentials. A cubic to tetragonal transformation is considered for investigating thermally induced transformations. An equilibrium phase diagram in terms of deviatoric stresses is constructed to illustrate the transformation process. Inclusion of the interactions results in a dead zone in the phase diagram. In Part III they explicitly investigate certain microstructural effects like grain size and dislocations using an additional potential called alternative potential. They discuss the curvature of the wells in different forms of free energy with respect to the stability and grain growth. However, as noted by them, this model does not capture the transformation from austenite to twinned martensite. It may be noted that this can be achieved by suitably coupling the transformation of twin variants while describing their kinetics.

Table 2. Summary of macroscopic free energy based models

Model		Form of free Energy	State variables	Product phase Variants	Type of Kinetics	Onset Criterion	
						Nature	Derivation
Falk (1980)		Landau, Gibbs (Explicit)	( $\epsilon$ , T)		Not specified	Fixed	G''
Achenbach and Müller (1985)		Landau	( $\epsilon$ , $\xi$ , T)	{ $\xi_s$ }	Jump condition	Fixed	G''
Abeyratne and Knowles (1993)		Gibbs and Helmholtz	( $\sigma$ , $\xi$ , T) Or ( $\epsilon$ , $\xi$ , T)	{ $\xi_s$ }	Thermally activated phase transitions	Fixed	Driving force
Boyd and Lagoudas (1994)	M <sub>0</sub>	Gibbs	( $\sigma$ , $\xi$ , T)	{ $\xi_i$ all variants}	Crystallographic	Fixed	Crystallographic
	M <sub>1</sub>	Gibbs	( $\sigma$ , $\xi$ , T)	{ $\xi_s$ , $\xi_T$ }	Driving Force	Varying	Dissipation potential
	M <sub>2</sub>	Gibbs	( $\sigma$ , $\xi$ , T)	{ $\xi_s$ }	Driving Force	Varying	Dissipation potential
Leclercq and LExcellent (1996) LExcellent et al (2000)		Helmholtz (notional)	( $\epsilon$ , $\xi$ , T)	{ $\xi_s$ , $\xi_T$ }	Independent	Varying	Yield function
Bekker and Brinson (1997)		Gibbs (explicit)	( $\sigma$ , $\xi$ , T)	{ $\xi_s$ , $\xi_T$ }	Independent	Fixed	Phase diagram
Bo and Lagoudas (1999)		Gibbs (notional)	( $\sigma$ , $\xi$ , $e^{tr}$ , $\eta$ , $\alpha$ , T)	$\eta$ and $\alpha$ are back and drag stress respectively. Single variant of martensite	Independent	Fixed and Varying	Dissipation potential
Rajagopal and Srinivas (1999)		Gibbs (Explicit)	( $\sigma$ , $\xi$ , T)	{ $\xi_s$ }	Driving Force	Varying	Dissipation potential
Qidwai and Lagoudas (2000)		Gibbs (explicit)	( $\sigma$ , $\xi$ , T)	{ $\xi_s$ }	Independent	Fixed	Yield function
Govindjee and Hall (2000)		Helmholtz	( $\epsilon$ , $\xi$ , T)	{ $\xi_i$ all variants}	Crystallographic	Fixed	KT condition on Yield function
Govindjee and Miehe (2001)		Helmholtz	( $\epsilon$ , $\xi$ , T)	{ $\xi_i$ all variants}	Driving Force	Fixed	Dissipation potential
Müller and Seelecke (2001)		Helmholtz (notional)	( $\epsilon$ , $\xi$ , T)	{ $\xi_s$ }	Driving Force	Fixed	Dissipation potential
Levitas and Preston (2002)		Landau (explicit)	( $\sigma$ , $\eta$ , T)	{ $\eta_i$ are order parameters representing all possible variants }	Ginzburg Landau	Fixed	G''
Bernardini and Pence(2002)	M <sub>0</sub>	Helmholtz (Explicit)	( $\epsilon$ , $\xi$ , T)	{ $\xi_s$ }	Driving Force	Fixed	Zero dissipation
	M <sub>1</sub>					Varying	Constant dissipation
	M <sub>2</sub>					Varying	Varying dissipation
Shaw (2002)		Hemholtz (Explicit)	( $\epsilon$ , $\epsilon_x$ , $\xi$ , T)	{ $\xi_s$ }	Independent	Fixed	Clausius Clapeyron
Chang et al. (2006)		Helmholtz (Explicit)	( $\epsilon$ , $\epsilon_x$ , $\xi$ , T)	{ $\xi^+$ , $\xi^-$ }	Independent	Fixed	Clausius Clapeyron
Savi et. al. (2002)		Helmholtz (notional)	( $\epsilon$ , $\epsilon^p$ , $\xi^+$ , $\xi^-$ , T)	{ $\xi^+$ , $\xi^-$ , $\xi^A$ }	Independent	Fixed	Yield function
Helm and Haupt (2003)		Helmholtz (notional)	( $\epsilon$ , $\xi$ , T)	{ $\xi_s$ }	Driving Force	Varying	Dissipation potential

Matsuzaki and Naito (2004)	Helmholtz (explicit)	$(\epsilon, \xi, T)$	$\{\xi_s\}$	Curve fitting	Varying	Dissipation potential
Aurichio and Petrini (2004)	Helmholtz (notional)	$(\epsilon, e^{\text{tr}}, T)$	$\{e^{\text{tr}}\}$	Associative evolution law	Fixed	Driving force/ yield function
Vedantam (2006)	Phase field (Explicit)	$(\epsilon, \xi, \xi_x, T)$	$\{\xi_s\}$	Micro-force balance	Varying	Micro-force balance
Zaki and Moumni. (2007)	Lagrangian	$(\epsilon, \xi, T)$	$\{\xi_s\}$	Driving force	Varying	Yield function
Panico and Brinson (2007)	Helmholtz (notional)	$(\epsilon, \xi, T)$	$\{\xi_s\}$	Driving Force	Varying	Dissipation potential
Popov and Lagoudas (2007)	Helmholtz (notional)	$(\epsilon, \xi, T)$	$\{\xi_s, \xi_r\}$	Independent (Linear)	Fixed	Yield function
Kishore Kumar et al (2007)	Helmholtz (notional)	$(\epsilon, \xi, T)$	$\{\xi_s\}$	Driving force	Varying	Dissipation potential

#### 4.2.2 Mechanistic decomposition based models

Models that use mechanistic decomposition of free energy (Figure 17) are referred to herein as mechanistic decomposition based models. They are classified here based on the methodology of arriving at the kinetics.

##### 4.2.2.1 Dissipation potential based Models

Huo and Müller (1993) were one of the first to discuss the importance of dissipative processes and use the notion of dissipation potential to describe the kinetics in SMAs. Hence an irreversible thermodynamic framework is used to obtain a macroscopic model for SMAs. The Helmholtz free energy is expressed in terms of the free energies of **A** and single variant **M** and an additional term related to coherence energy associated with the strain mismatch between the phases at the interface. Both SE and SME are modeled including partial and inner hysteresis loops. The notion of dissipation-less transformation in single crystals is used to arrive at suitable memory through the introduction of additional interaction terms. The phase transformation is obtained by solving the governing equation for isothermal process. The Clausius-Clapeyron relation is linear due to the assumption of constant entropy production. In this model, the modulus of **A** and **M** phases is same, thus leading to a simplified form of interaction energy. Earlier, Achenbach (1989) had derived a form for free energy based on the probabilistic argument that the surface energy attains a maximum half-way through the transformation. Thus, for the case of single variant transformation, the interaction term is taken to be proportional to the product  $\xi(1-\xi)$ . Several interesting experiments on single crystals of CuZnAl are reported in Huo and Müller (1993) showing the nature of partial transformation (partial hysteresis loops).

Building on the work of Achenbach (1989) and Huo and Müller (1993), Müller and Seelecke (2001) postulate that the interfacial energy arising out of coherency mismatch is responsible for the hysteresis. They introduce a form of interaction energy using coherency of interfaces and number of interfaces. Using a shear parameter they construct Helmholtz free energy for individual phases (**A**, **M+** and **M-**). Statistical considerations are used to determine the number of particles in a given state which gives the extent of phase evolution. The curvature of the free energy well is used to discuss the relative stability of phases and kinetics. Apart from the complete transformation under SE and SME, they also discuss response involving inner and partial loops. They show that in their model the Clausius-Clapeyron relation is, in general, depends on the phase fraction suggesting non-static phase boundaries. They construct phase diagrams to explain the hysteresis behavior under different conditions. Postulating different types of equilibrium scenarios they describe the plausible equilibrium configurations and associated energy landscape. Both single step (unstable) and multiple step (metastable) transformations are discussed. They show that the observed behavior shows both metastability associated with the dynamic equilibrium of individual phases and unconstrained phase equilibrium. Influence of coherency condition on the forms of the energy landscape is highlighted. The intermediate states between the stable **A** and **M** branches on the stress-strain response are unstable and could trigger the further phase evolution. Treating the evolution as an activated process, they also discuss the non-equilibrium aspects of phase transformation. In this context they provide the rate laws for evolution of phase fraction in terms of transition probabilities for the jumps to occur on the energy wells. This is also referred to as Eyring model for first order transitions under thermomechanical loading. Rajagopal and Srinivasa (1999) extended discussion on the importance of dissipative processes by Huo and Müller (1993). They used the concept of multiple natural configurations to describe the kinematics of transformation. Each possible lattice structure (that the material is capable of exhibiting) is associated with a natural configuration and the material response depends upon the deformation from all these configurations. For a single variant transformation,

the macroscopic kinematic response is derived by scaling the maximum deformation gradient with the amount of product phase. The transformation conditions are obtained using the notion of driving force for the rate of entropy production derived from the dissipation potential. An explicit constitutive equation is provided for the rate at which the input power is converted into heat by dissipative mechanisms. The displacement and temperature fields are obtained from the momentum balance and the rate of entropy production, respectively. As a special case, they discuss the dissipation-less transformation and obtain the ‘trilinear’ stress-strain response. Both complete and partial hysteresis loops are discussed. Use of non-dissipative transformation path as a feature that dictates the memory for partial and inner loops is illustrated. They state that from a thermodynamic perspective, the memory in the material can be linked to a single scalar (like the volume fraction), when the driving force for transformation is zero. They show that the history dependency or memory does not affect the free energy (Helmholtz potential) but influences only the rate of dissipation. Extraction of model and material parameters from test data is discussed using the experimental data from Huo and Müller (1993). Kishore Kumar et. al. (2007) have extended this model to study the behavior of partial transformation cycles. Bernardini and Pence (2002b) extended the above approach and proposed a free energy function which neglects the thermal strains and also assumes identical elastic moduli and specific heats for the **A** and **M** phases. Hence, for a single variant transformation, the interaction energy is taken as a function of the product  $\xi(1-\xi)$ . Further, the dissipation potential / driving force for transformation is obtained using Ziegler-Green-Naghdi approach. Three types of models are formulated:

- a) dissipation-free model (model M0)
- b) dissipation function independent of phase fraction (model M1)
- c) dissipation function varying linearly with  $\xi$  (model M2)

Three types of phase transforming processes are considered:

- (i) prescribed temperature under constant stress,
- (ii) prescribed stress under constant temperature,
- (iii) Prescribed stress in non-isothermal conditions, including adiabatic and convective environments.

Closed form solutions for these processes using these three models are obtained. The effect of rate of thermomechanical loading is discussed in terms of changes to the nature of process and hence on the shape of hysteresis. In this paper, attention is paid to the comparison among the various models with respect to the determination of explicit expressions for transformation stresses and temperatures, the stress–temperature phase diagram, transformational heating, adiabatic temperature change and material parameter identification.

Boyd and Lagoudas (1996) develop a thermodynamic framework using certain concepts from micromechanics. They propose three models for SMA behavior with varying degree of fidelity. At the outset, they propose a microscopic continuum model with for multi-variant transformation motivated by micromechanics of in-homogenous inclusions. Though this model is essentially a microscopic model, it serves as a basis for the development of two simplified models for macroscale behavior. The Gibbs free energy is decomposed into the contributions from pure species and the mixture. The Eigenstresses and Eigenstrains due to inhomogeneous inclusions contribute to the free-energy due to mixing. Treating the transformation between the variants as chemical reactions and using the stoichiometric considerations for the rate of these reactions, the kinetics for the evolution of the phases are written. Appropriate constraints like conservation of mass are imposed. Following Patoor (1993)<sup>1</sup>, the kinematics of these reactions is written to obtain the transformation strain. Using thermodynamics, the constitutive expressions are deduced. Edelen’s Maximum dissipation formalism (Edelen, 1994) is used to define a dissipation potential for the total entropy production due to phase transformation and heat conduction. Using the C-D inequality, an expression for rate of entropy production is derived. Defining a material parameter representing the threshold driving force, the kinetics for individual phase evolution is provided using Lagrange multiplier method. For stable reactions, Kuhn-Tucker conditions serve to maximize the dissipation in a rate-independent transformation. Quadratic form of dissipation potential is assumed for each reaction to obtain explicit relations for phase fractions. Using the above framework developed for microscopic scale, two simplified models (similar to Huo and Müller (1993)) with three and two species are derived. Assuming constant driving force which corresponds to linear kinematic hardening in plasticity, the macroscopic response in SMAs is simulated. Isothermal and adiabatic stress-strain response and constant stress thermal cycle response are simulated. This approach is extended to model SMA composites.

#### 4.2.2.2 Plasticity based models

Using the “maximum dissipation postulate” of classical plasticity, an analogy between the dissipation potential and the rate-independent yield function can be established. Macroscopic free energy models inspired from plasticity utilize this fact. Boyd and Lagoudas (1994a, 1994b), Bo and Lagoudas (1999 a-c), Qidwai and Lagoudas (2000) were one of the first to propose and utilize this idea.

<sup>1</sup> This work is discussed in the next section on microscopic modeling approaches.

Lagoudas and Bo (1999) and Bo and Lagoudas (1999a-c) utilized this approach to study SMA response under cyclic loading. Effects like stabilization, TWSME and inner loops are modeled and the model is compared with experiments. Over a Representative Volume Element (RVE) of a polycrystalline SMA, they decompose the Gibbs free energy into elastic and chemical parts. The strain is decomposed into four components, viz., elastic, thermoelastic, transformation and the plastic strain. The plastic strain generation and accumulation is due to cyclic loads. Though the plastic strain does accumulate over cycles, within each cycle, they assume it to be much smaller than the transformation and elastic counterparts and hence are treated to be essentially a constant. The internal stresses due to this plastic deformation contribute to strain hardening affecting in turn the transformation driving forces. This is accounted for by introducing additional internal variables in the form of back and drag stress. The internal variables in the model are the stress, temperature, transformation strain, volume fraction, back stress and drag stress. Explicit expressions for changes in Gibbs free energy due to incremental evolution of martensite are derived. Assuming proportional loading and ignoring reorientation effects, they parameterize the rate of evolution of all internal variables into single martensitic fraction as pseudo-time. For uniform stress and temperature field within the RVE they write a general form of evolution kinetics for the rate of evolution of martensitic fraction. This is used to provide the incremental change in free energy as a function of incremental change in phase fraction. The interaction energy or mixture energy is expressed as functions of back and drag stresses, transformation strain and martensitic phase fraction. The expressions for back and drag stresses are first derived for proportional loading and then generalized for non-proportional thermomechanical loading. Defining a dissipation potential and using C-D inequality, they derive the driving forces and explicit kinetics for martensitic fraction following the procedure used in Boyd and Lagoudas (1996a). The model can account for residual stresses due to heterogeneity arising from processing and thermomechanical history by suitably specifying the back and drag stress. Further, the contributions to the back and drag stress due to the transformation induced heterogeneity is also included. This is decomposed into the strain incoherency due to martensitic variants at the grain boundary and the stresses due to transformation Eigen strains. This model is extended for cyclic loading and to include partial and inner hysteresis loops.

Qidwai and Lagoudas (2000) modified the Gibbs free energy structure in the above model by changing the internal variables in the model to account for only a single variant of martensite; i.e., the back and drag stresses are not included as internal variables. A quadratic asymmetric hardening function for forward and reverse transformation as a function of martensitic fraction is given. They investigated several aspects of numerical implementation comparing two different algorithms viz., convex cutting plane and close-point projection algorithms. To study multiaxial state of stress, they solve BVP for momentum balance in an isothermal setting. Both SE and SME are investigated. Popov and Lagoudas (2007) consider two-variant martensite transformation. Motivated by experimental observations, they stipulate different transformation temperatures for austenite formation from twinned and detwinned martensite. They extend this to modify the phase diagram for five different types of transformation. Following the framework of Boyd and Lagoudas (1996a), they provide a free energy structure and a set of generalized yield functions (transformation surfaces) akin to Leclercq and Lexcellent (1996)<sup>2</sup>. Two practically relevant cases involving BVP with simultaneous thermomechanical loading are investigated. Initially, constrained cooling of a solid SMA is investigated followed by SMA plate with a hole under plane strain conditions are studied to show the efficacy of this model.

Leclercq and Lexcellent (1996), using the framework of irreversible thermodynamics, propose a macroscopic model with two internal variables representing self accommodating and oriented martensite. The inelastic strain due to phase transformation is linearly scaled with the stress induced or oriented martensite fraction. Helmholtz free energy with these two internal variables, strain and temperature is decomposed into free energy of phases and that due to mixing. The interaction energy due to mixing is conceptually similar to configurational energy (Raniecki et al 1992). The yield function is derived using the continuity criterion for the free energy, which is also called as method of Lagrange multiplier. Further, they stipulate five yield functions, one for each type of phase transformation. Linear kinetic equations are then obtained through the consistency condition. Further, kinetics for inner loops is provided based on the dissipation-less transformation condition. They extend the model for a nonlinear kinetic description. The predictions based on exponential form of kinetics compare well with the experiments. Lexcellent et al (2000) extended this approach to model TWSME in SMAs by introducing a term dependent on the thermomechanical training. This additional term in the free energy requires additional thermodynamic state variable, conjugate of which represents stress due to cycling. Experiments are used to estimate the material parameters and the results compare well with experiments.

Differing from the above discussed work, Souza et al. (1998) used transformation strain as a state variable instead of martensitic fraction and proposed a 3-D macroscopic model using generalized standard material formalism. The state variables are elastic strain, transformation strain and temperature. Helmholtz free energy function contains a quadratic function of transformation strain, equivalent to the energy associated with configuration and also the work done by thermal Maxwell stress (representing the entropy change during phase transformation). An additional indicator function which signifies the occurrence of transformation is introduced to track the evolution of transformation strain. Keeping

<sup>2</sup> Described under macroscopic models

only the transformation strain as the state variable is equivalent to considering single martensite phase fraction. Based on the C-D inequality, the driving force is given here in terms of the transformation stress. This is equivalent to a generalized thermomechanical yield function. The associated consistency condition provides the flow rule. In this model, the Young's modulus is treated as invariant.

Auricchio and Petrini (2004a) have used the above thermodynamic formulation and the resulting constitutive equation to solve stress and thermal induced phase transformation in SMAs. This approach is different from their earlier generalized plasticity based approach discussed earlier. A generalized solution algorithm for thermomechanically coupled BVP is proposed. Three dimensional finite element simulations are performed with uniaxial and biaxial state of stress and non-proportional loading. Auricchio and Petrini (2004b) have further extended this approach to solve a coupled thermomechanical problem on SMA based hybrid composites.

Panico and Brinson (2007) have used the approach of irreversible thermodynamics to propose a three dimensional model which can take into account non-proportional loading. The model is based on the work of Leclercq and Lexcellent (1996) and is extended for general non-proportional loads. This is achieved by distinguishing the transformation into two types, viz., detwinning and reorientation of martensite along the loading direction. The inelastic strain has contributions from the detwinning as well from reorientation, whereas the volume fraction of martensite is linked only to the transformation (detwinning) component. An important aspect in this work is the derivation of the parameters involved in phenomenological phase diagram from the free energy based thermomechanical yield functions. Due to the logarithmic nature of the yield function, complete reorientation is not achieved. Numerical simulations using these models show good agreement with the experimental results. It may be noted that derivation of some of the parameters associated with the yield function are not explicitly provided.

Zaki and Moumni (2007a, b) propose a 3-D model introducing two state variables to describe several effects exhibited by SMAs. Standard quadratic form of interaction energy is assumed while constructing the Lagrangian for the system. Extremum principles are used to derive the state equations. Using the notion of yield surface and flow-rule, they describe the kinetics. Orientation effects of the martensitic variants and the kinematic hardening arising due to their interaction is shown to influence the slope of the stress-strain response during transformation. They extend this model to discuss training or shakedown due to cyclic SE loading by introducing an additional variable to track the irreversible martensitic fraction that accrues due to cycling. A SE stent is modeled to discuss the 3-D effects.

Govindjee and Hall (2000) proposed a macroscopic model using the Helmholtz free energy structure developed by Lagoudas and Bo (1998) for three species viz.,  $M^+$ ,  $M^-$  and  $A$ . Following Müller and Achenbach (1995), statistical methods are used to specify independent kinetics. The phase front velocity is explicitly modeled to incorporate rate effects. A BVP with momentum balance equation is solved using predictor-corrector method. Several interesting structural problems involving SMAs are solved. Hall and Govindjee (2002) proposed a model for macroscopic behavior using Lagrange potential. The interaction energy is used to define the partially relaxed free energy and optimizing this over the space of possible volume fractions gives the approximate quasistatic free energy. Crystallographic Bain strain is used to obtain macroscopic transformation strain. Kuhn-Tucker (KT) conditions are used to derive the condition for onset of transformation. The model includes complete stress and strain tensors and hence has 3-D capability.

#### 4.2.2.3 Phase diagram based models

As noted earlier, Bekker and Brinson (1997) extended the Brinson (1993) model to investigate the influence of arbitrary loading on the nature of memory and kinetics. To solve a nonlinear BVP in SMAs using the proposed kinetics it is necessary to have a free energy structure. Hence they derive a Gibbs free energy form using heuristics. Coupled non-stationary energy balance and quasi-stationary momentum balance equations are solved to obtain the SMA response. Three finite difference based numerical schemes using total enthalpy are proposed for the solution of mixed BVP. An interesting case wherein a tapered SMA rod is heated via a convective medium with cold isothermal end conditions is solved. The varying cross section introduces stress variation which is reflected in non-homogenous martensitic distribution. This aspect can be used to investigate propagation of martensitic fronts. Incompressibility conditions are assumed to incorporate changes in radial dimensions. Importance of spatial and temporal discretizations on the performance of the algorithm is discussed.

#### 4.2.3 Dynamic phase transition models

##### 4.2.2.4 Sharp interface model

One of the most cited works on modeling of SMAs is Abeyaratne and Knowles (1993). They were one of the first to investigate explicitly the nucleation of a phase and its propagation in SMAs. They introduce the displacement gradient as a field and construct Helmholtz free energy function based on trilinear stress-strain relation at fixed temperature. The

trilinear stress-strain function is integrated to obtain stress varying part of Helmholtz function. Since strain is used as an independent variable, the temperature dependence of strain is brought through specific identity of thermodynamics which is equivalent to the Clausius-Clapeyron relation. Nucleation criterion is expressed as a jump or discontinuity in the Gibbs free energy. This manifests as a generally non-zero traction or driving force across the interface. Driving traction equation is obtained using the stability criterion similar to C-D inequality. Explicit kinetic relation and nucleation criterion are developed. Kinetics developed here has form  $\dot{s} = V(f, \theta)$ , based on classical notion of thermally activated phase transitions. The velocity  $\dot{s}$  of the phase boundary is the macroscopic measure of the net rate at which the atoms change from the low-strain phase to the high-strain phase and is taken to be the difference between the average rates associated with the two atomic transitions. This kinetics takes the form of product of error functions and hyperbolic sine. This implies that the rate has monotonic increasing nature, unlike that obtained from cosine kinetics for the phase fraction. Exploiting the smallness of driving traction due to the quasistatic and reversible nature of the process, the kinetics is then linearized in temperature. The nucleation criterion is derived from Gibbs free energy and the sign of the latent heat is used to distinguish the forward and reverse transformation direction. They also discuss how the model parameters concerning nucleation can be derived from  $M_s$  and  $A_s$ . Finish of transformation depends upon the process. They investigate both SE and SME at constant stress. They also show the relationship between the phase boundary velocity and driving traction at various temperatures.

Abeyaratne and Knowles (1997) extended this approach to solve a BVP wherein a CuAlNi SMA single crystal is subjected to impact loading. This is posed as a Riemann problem, which consists of a conservation law together with a piecewise constant field having a single discontinuity. It may be noted that the Riemann problem is useful in investigating hyperbolic partial differential equations because properties like shocks and rarefaction waves appear as characteristics in the solution. It also yields an exact solution to complicated, non-linear equations like the Euler equation. They show the relationship between the impact velocity and the phase front velocity for different values of impact angles representing different tangential and longitudinal velocities. Abeyaratne and Kim (1997) generalized this approach to include effects due to cyclic loading. An additional internal variable is introduced to track the changes due to defects that get precipitated during cycling. These defects are shown to ease formation of transformation fronts.

A time discrete Ginzburg-Landau formalism is used by Wang and Kachaturyan (1996) to build 3-D stochastic kinetic field model of 'improper' martensitic transformations which explicitly takes into account the transformation-induced elastic strain. The model is able to predict the major structural characteristics of martensite during the entire MT process including nucleation, growth and eventually formation of internally twinned plates. Numerical simulations are performed for a generic cubic-tetragonal martensitic transformation in a single crystal  $ZrO_2$  which is elastically isotropic and homogeneous. The simulation results are in good agreement with experimental observations. This work has led to the development of several models for the dynamics of MT in SMAs.

#### 4.2.2.5 Diffuse interface model

Models with sharp interface have computational difficulties in tracking multiple moving interfaces. Hence as an alternative, diffuse interface theories are used to investigate the propagation characteristics. As the name suggests the sharp jump like interfaces are treated in a weaker set-up wherein the changes in properties are assumed to vary in a more continuous and diffuse manner across the phase boundaries. Hence, theories like phase field theory are used. Vedantam (2006) proposes a diffuse interface theory for SMA based on the formalism proposed by Fried and Gurtin (1994) using an order parameter field which has rapid, but continuous change across phase boundary. Evolution of this order parameter is specified through an equivalent Ginzburg-Landau equation. In addition to the strain energy, latent energy and exchange energy, the free energy includes gradient energy due to the phase jump. Gradient energy penalizes the presence of interfaces. An additional material parameter is introduced as constant of proportionality in the gradient energy term, which needs experimental evaluation. Exchange energy reflects the energetic preference for each phases. One of the key aspects of this approach is the notion of micro-force which can be treated as generalized force at the microscale with following characteristics.

1. Micro-force balance supplements the usual balance laws of linear and angular momentum
2. Micro-forces are distinct from classical Newtonian forces and perform work against changes in order parameters
3. Micro-force balance supplied with an appropriate constitutive equation provides an evolution equation for the order parameter.

For a 1-D SMA rod, momentum balance equation and micro-force balance are coupled and cast as a system of nonlinear partial differential equations which is solved using finite difference scheme. The model is able to capture the nucleation peak in the stress-strain response. Also, the model can capture effects due to the rate of elongation. However,



this model is valid for modeling the pseudoelastic effect only since temperature is only a parameter. Numerical simulation for tracking dynamics of phase transition is investigated giving relevant details.

Shaw and coworkers (Shaw (2000), Iadicola and Shaw (2002) and Chang et al (2006)) have studied the effects of nucleation and propagation of transformation fronts. Both experiments and numerical investigations are performed. To capture the diffuse interface in polycrystalline SMA wires, a 1-D model with strain gradient as an additional state variable is developed. The model is especially aimed capturing the Lüder like transformation bands or propagation effects seen in SMAs. Helmholtz free energy is adopted since the experiments are in displacement (strain) control mode. The rate of evolution of the phase fractions has been independently assumed. A 1-D coupled BVP in terms of both thermal and momentum balance equations are formulated and solved to elicit the SMA response. They discuss several aspects that govern the response in terms isothermal and adiabatic effects that alters the nature of hardening. They also discuss the influence of nature of interaction energy on the stability. They state that the nucleation in the macroscale manifests due to loss of stability in the microstructure. Elaborate experiments on wires are used to show the thermal and strain gradients that exist due to transformation and the influence of loading rate on the number and nature of transformation fronts. The complexities observed regarding the nucleation and propagation of transformation fronts even at relatively low strain rates are discussed.

A snapshot of the models discussed is presented in Table 2 that summarizes the key aspects in these models. From this discussion it is seen that a large variety of approaches exist for modeling macroscopic response in SMAs. Some of the models are simple and capable of capturing essential response like SME and SE and are suitable to be used to design and analyze specific device-level behavior.

The models covered in this subsection do not cater to several important aspects of MT in sufficient detail to make them flexible for application in wide range of scenarios. For instance predicting the amount of two-way, shakedown and partial loops require more sophisticated models. Some of the free energy based models described earlier are suitable for such cases. Another way to obtain better description of MT is to model the behavior at the microstructure level. Several approaches that attempt to accomplish this are discussed below.

## 5 Microscopic Modeling Approaches

As mentioned in Section 2, the length scale of martensitic plates is typically of the order of few microns. Several modeling approaches to capture the phenomena at this and slightly higher scales (mesoscale of the order of 10-100 microns) exist in literature. A brief overview of these approaches is presented here. The reader is reminded that the following classification of approaches is only illustrative and not necessarily rigorous or unique. Most of the microscopic models have a notion of unit cell or Representative Volume Element (RVE). Suitable assumptions are made regarding the nature of transformation (in terms of number of martensitic variants) and suitable volume averaging schemes are introduced to capture the overall effect. It may be noted that the martensitic variants introduced into the model could be either notional or actual crystallographic variants. Another aspect is that generally, multiple true crystallographic variants are considered in the microscale and after analysis, an equivalent single or multiple (reduced) variant macroscopic description of the phenomena is provided. This serves as a basis for more meaningful macroscale description of the underlying microscale effects, which can lead to a hierarchical framework for model development. From a mechanics perspective, usually the two phase mixture is treated as inclusion of the product phase in the parent matrix. Further, this inclusion can be treated either simply as a homogeneous inclusion or otherwise. Effective constitutive properties are determined using suitable Eshelby-Kroner or Mori-Tanaka approach and solving a BVP.

Another important aspect is the choice of internal variables and the kinetics for their evolution. Typically, internal variables represent some measure of strain at the micro-level in the form of either Bain strains or order parameters. In order to determine the strain due to the MT at the microstructure level, kinematics of crystallographic transformation like those proposed by Bhattacharya and Kohn (1996) is used. Assuming defect free and small strain conditions, self consistency or an equivalent principle like St. Venant condition given below is applied to establish the strain for a single crystal as

$$\bar{\nabla} \times (\bar{\nabla} \times \varepsilon)^T = 0;$$

where,  $\varepsilon$  is the small strain tensor. The influence of stress is considered in the preferential growth of variant(s).

A third aspect in the microscale modeling is arriving at suitable free energy structure to derive appropriate state equations. Ball and James (1987) have systematically studied the energetics of MT at the microstructure level and the methodology proposed by them is usually adopted. To a large extent, the microstructure evolution is governed by the nature of interaction between the parent and the product phases like self-accommodation or the lack of it. Models for microscale response for SMAs differ due to the differences in the aspects briefly discussed above, like the choice of internal variables and the form of interaction energy that is assumed. This also provides a link to the modeling of

macroscopic response. An overview of some of the salient models for microscale response of SMA follows. One of the key features in the microscale models is that important aspects like texture, defects and locked or irreversible phase pockets can be incorporated to investigate their effects on the SMA response at both the micro and macro scales. It may be noted that due to strong history dependency, these effects play a significant role in TWSME, shakedown and functional degradation.

### 5.1 *Micromechanics Based Models*

This class of models considers true crystallographic variants of martensites as compared to schematic or idealized variants considered in most of the other class of models. Micromechanics is used extensively to account for the behavior of the mixture of phases in terms of inclusions in an elastic matrix. This serves to define the form of interaction energy for macroscopic description.

Patoor et al (1988) proposed a model using transformation strain of a single crystal based on crystallography parameters. Instead of using the Eshelby-Kroner approach, a simplified interaction matrix was used to formulate the interaction energy. An averaging scheme was subsequently invoked to model the polycrystalline behavior. This model can describe SE; however, the simplistic form of interaction energy chosen prevents it from modeling temperature induced transformation. This work has lead to development of several microscopic models.

Following Patoor et al. (1988), Goo and Lexcellent (1997) proposed micromechanics-based Helmholtz free energy. Using the framework of irreversible thermodynamics, kinetics and criteria for nucleation and reorientation of martensitic variants are obtained. These relationships are applicable for 3-D proportional or non-proportional mechanical loading or a combination of mechanical and thermal loading. TWSME is simulated based on the assumption that mechanical dissipation of active variants decreases during cycling (training). Simulation results are compared with experimental results. A set of general equations are obtained which are used to explain some of the phenomenon. These equations are quite complex and no general solution methodology for these equations is proposed. Lu and Weng (1997) developed a model similar to that of Goo and Lexcellent (1997) with only one active variant of martensite. Exponential form of interaction energy is used which is also used to describe the kinetics. The phenomenological description of interaction energy shows some interesting facts about the phase diagram like the nonlinearity in Clausius-Clapeyron relation. Relaxing the traditional assumption of constant entropy change during phase transformation, a linear dependence of entropy on temperature contributing to the chemical free energy is introduced. They also show that the onset transformation stresses could depend on the amount of source phase availability.

Nicleays et al (2002) have formulated a form for interaction energy for 24 habit plane variants of martensites in Cu based SMAs. Presence of self-accommodating variants requires modifications to the form of coefficients of the interaction terms between different variants. A detailed discussion of this is given in this paper.

Sun and Hwang (1993a,b) and Sun et al (1991) proposed a model based on Mori-Tanaka theory. Multiple martensitic inclusions are treated as a single variant, ignoring relative orientations. The effective transformation strain is derived using concepts from transformation plasticity wherein suitable relation between the local transformation strain and an average stress is introduced. The model can account for SE and SME. Reorientation effects are captured by introducing another internal variable. It may be noted that local transformation strain is not strictly the crystallographic strain and the model is not adequate for complex loadings which combine transformation and reorientation.

Huang and Brinson (1998) proposed a micromechanics based model for single crystal NiTi SMA. They assumed that each martensite plate is formed by a single variant and the resulting wedge like microstructure. Similar to Patoor et al (1987), for a RVE with random distribution of variants treated as spherical inclusions, they derive a form of chemical part of free energy. Using Eshelby-Kroner approach they derive the interaction energy for multiple variants. The interaction energy is taken to be zero for self accommodating variants. The two-variant version of this model is capable of capturing both stress and temperature driven transformations. Tension-compression asymmetry is also captured. Influence of loading axis on the transformation response is also predicted. Gao et al (2000a,b) extended the above model for other SMAs and for penny shape inclusions. Also, all the 24 habit plane variants are considered in CuZnAl. They examine both Type-1 and Type-2 twins. If the twin plane normal and the twinning direction are parallel, the twin is set to be a compound twin. Type-1 twin is a twin wherein the twin-plane normal is rational and not the twinning (loading) direction. Type-2 twin is the case wherein the twinning direction is rational and not the twinning plane. Several aspects of crystallographic differences between different variants are discussed. Effects of polycrystallinity are investigated by homogenizing the assembly of non-textured spherical grains using self-consistent method.

Zhang and McCormick (2000a) considered the asymmetric change in free energy between the forward and reverse transformation. The change in free energy contains an irreversible component incurred during phase transformation associated with plastic deformation. This is included through Eshelby's macroscopic elastic analysis by defining a net transformation strain equal to the difference between the crystallographic transformation strain and the associated plastic strain. The remnant plastic strain due to cyclic mechanical loading results in a residual stress field. The associated residual strain influences subsequent transformation behaviour and provide the driving force for TWSME. It

is shown that linking the plastic and elastic component of strain (and associated energy) leads to a self consistent model for two variants which can capture SE, SME and TWSME. This approach is extended to include thermal loading in Zhang and McCormick (2000b) by introducing self accommodating variants. Numerical simulations show several aspects of shakedown due to cyclic loading like the built up of residual stresses, TWSME and decrease of critical transformation stresses.

Bernardini (2001) used a variational approach to formulate the free energy for SMA with inhomogeneous inclusion. On the basis of variational formulation of the problem of behaviour of a linear elastic heterogeneous material with prescribed Eigenstrains, macroscopic free energies for SMA are derived. The general structure and the dependence on the macroscopic state variables of such functions are discussed and formal expressions in terms of concentration tensors are given. In the case of an underlying two-phase microstructure, exact connections between the quantities (Young's modulus) that determine the free energies (macroscopic transformation strain, interaction energy, effective thermal expansion tensor) and the effective elastic compliance are derived. Estimates of the SMA macroscopic free energies based on Reuss, Voigt and Hashin-Shtrikman bounds for the effective elastic moduli are explicitly calculated and compared in the specific case of a NiTi alloy.

Vedantam and Abeyaratne (2005) used a quartic term in the irreducible Lagrangian strain polynomial in terms of the invariant of strain components to formulate Helmholtz free energy for CuAlNi. The strain invariants are like order parameters. The continuum kinematics is used to describe of crystal structure change in CuAlNi involving variants of the orthorhombic martensite and cubic austenite. This is used along with Cauchy-Born hypothesis to obtain continuum free energy. Experiments are used to evaluate the temperature dependent coefficients of the free energy polynomial. They also derive the parameterized expression for strain to describe the location of multiple wells in the free energy. The stress-strain relation obtained from the free energy is used to investigate the shear in twinning direction. Also, they propose a way to obtain appropriate constitutive model for macroscopic SMA behavior.

Mahapatra and Melnik (2006) proposed a methodology to combine the continuum description of the kinematics of microstructure change with the Landau theory. The free energy proposed by Levitas and Preston (2002a,b) is augmented with an additional term  $G_0$  to take the deformation/ processing history into account. The notion of activation barrier is used to arrive at a polynomial structure for free energy in terms of the order parameter. This is derived for the case of cubic to tetragonal phase transformation for NiAl. In order to avoid the computational difficulties associated with minimization of quasi-convex nature of energy, additional constraints in terms of the compatibility condition for microstructure evolution are stipulated. The concept of non-equilibrium thermodynamics and a consistent variational approach is used to develop a 3-D finite element procedure which couples the following three governing equations;

- a) Dynamics of phase transition through Ginzburg –Landau kinetics. This includes thermal fluctuations due to phonon-contribution.
- b) Energy balance: The Cattaneo-Vernotte equation for energy balance considering thermal inertia.
- c) Momentum balance: Cauchy stress obtained using Cauchy-Born hypothesis

This mixed variational formulation can be seen as a multi-scale technique since it bridges the information from microscale to the macroscale behavior. Numerical case studies are carried out to elucidate both stress and temperature induced transformation. Also, the critical transformation temperatures and stresses are evaluated by solving a 3-D BVP. The benefit of this approach lies in modeling effects of rate dependent material behavior, initial microstructure and non proportional three dimensional loading.

Guthikonda et al (2007) proposed a sequential laminate type microscopic approach at crystal level which is suitably bridged with smeared microscopic model. Stress induced martensite transformation for CuAlNi single crystal is numerically simulated. It is shown that different types of martensitic plates form for different loading axis. The shift in the preference of martensite plate formation is explained by 'criss-crossing' of critical stresses for different plates as the transformation progresses. Further, a homogenization technique like Taylor model or Sach's model is used to predict macroscopic polycrystalline SMA behavior. It has been shown that stress induced MT in polycrystalline SMA leads to a continuous stress-strain behaviour rather than a piecewise continuous behavior as obtained in some macroscopic models. This feature is explained with the major and minor loop formation in hysteretic stress-strain response.

From the above discussion, it is seen that a distinguishing feature among these models is the way the microstructure is modeled viz., true microstructure or an equivalent description based on macroscopic response. Crystal plasticity based approach attempts to describe MT using notion of habit plane variants and plastic deformation (or flow) along them. Some of the models based on this is discussed in the following.

## 5.2 Crystal Plasticity Based Models

As the name suggests, these models are based on observed phenomena of plasticity in crystals wherein the deformation of a single crystal is determined in terms of possible deformation modes like the number of slip systems that exist for the given crystal. In the case of SMAs, due to the nature of MT, the slip systems are replaced with either the actual number of habit planes or a reduced number of habit planes that are of interest. This class of models assumes

'n' number of martensite natural systems corresponding to habit plane variants that may be favored depending on the nature of deformation under a particular loading. The evolution kinetics for crystal mechanics based model from the following expression for the inelastic deformation rate  $L^{in}$ :

$$L^{in} = \sum_i \dot{\xi}^i \gamma_T \bar{a}^i \otimes \bar{n}^i$$

where  $\bar{n}^i$  is normal to the interface plane between austenite and  $i^{th}$  martensite (habit plane),  $\xi^i$  is the martensitic fraction of the  $i^{th}$  variant and  $\bar{a}^i$ , the polarization/slip direction which denotes the average transformation direction. In SMAs  $\gamma_T$  is assumed to be constant for all habit plane variants. Using the second law of thermodynamics, the driving force for evolution is associated with the dissipation at the crystal level.

Gall and Sehitoglu (1999) used crystal plasticity based approach to investigate the effect of texture in SMA sheets. They provide a methodology of associating the Bain strain with the transformation strain by providing an expression in terms of  $\bar{a}^i$  and  $\bar{n}^i$ . Also, they tabulate the interaction coefficients between the 24 correspondent variant pairs (habit plane variants) for NiTi required to evaluate the critical transformation stress. The micromechanical model predicted the critical transformation stresses and is seen to be in good accord with experiments. The phase transformation is correlated with Luder's type deformation in their experiments. The initiation of transformation is favoured under tension in the direction which has majority of grains oriented. They show the importance of texture in tension-compression asymmetry in the SMA sheets. Sehitoglu et al (2001) have used this approach to study the strain-temperature behavior for NiTiCu single crystal. Also, they discuss the changes in crystallographic structure due to addition of Cu in NiTiCu as compared to NiTi. They show that in NiTiCu, a two-stage transformation with different crystallographic transformation strains occurs under certain circumstances, which is reflected in the macroscopic transformation strain response.

Thamburaja and Anand (2001, 2002 and 2003) investigated MT in NiTi using crystal plasticity. They assumed a constant dissipation function and the interaction between the parent and product interfaces as well as that amongst the product interfaces is neglected. A crystal mechanics based finite element procedure is developed in order to model an initially textured material. One element in their FE model represents one crystal. The single crystal model using the 24 habit plane variants of martensite is used to capture the pseudoelastic response of a polycrystalline aggregate with random initial crystallographic texture. They also give a methodology to discretize the FE mesh of an aggregate based on the pole figure for SMA sheets obtained through texture measurements. A good accord between the experiments and their model is shown for SE test under uniaxial and multiaxial loading such as simple tension, simple compression and tubular torsion. Also, they discuss the engineering simplification of their model by using the homogenization technique called as Taylor's approach. Further, they conducted some experiments on different types of tension and torsion loading on a tubular SMA structure and have shown the efficacy of their model under such non-proportional loading scenario. Subsequently they have extended the FE algorithm to include the energy balance equation in order to come up with a thermomechanically coupled FE algorithm. This algorithm is used to predict the SE as well as SME for initially textured SMA sheets. The thermomechanically coupled analysis strategy enables capturing the resulting inhomogeneous deformation associated with the nucleation and propagation of transformation fronts. This is also the 'apparent hardening' of the nominal stress-strain curves observed in the experiments due to non-isothermal conditions.

Anand and Gurtin (2003) have provided free energy structure to the model developed by Thamburaja and Anand (2001) using the axioms of continuum thermomechanics. In their generalization, they associate the free energy formulation for single and polycrystalline SMA with the phase field model. Further, the flow rule or onset of evolution is derived from the microforce imbalance or the flag inequalities rendering the approach consistent with the laws of thermodynamics. They extend the methodology to consider non-isothermal loading in the SMA material in order to study thermal effects. Numerical studies show the development of martensite-austenite phases due to mechanical and thermal loading. This model facilitates tracking of the inhomogeneities in the microstructure during phase transformation. Qualitatively, they match the experimentally observed results of Shaw and Kyriakides (1997).

Thamburaja (2005) has extended their crystal mechanics approach to model the reorientation and detwinning. This is done by introducing an additional flow rule for the reorientation strain. This is made consistent with the flow of evolution of martensitic variants. The approach is experimentally validated with that of initially textured SMA sheets as shown by Thamburaja et al (2005). Pan et al (2007) have extended this approach to model the isotropic plasticity like phenomenon observed in SMA behavior. In this work they also numerically simulate BVP of practical relevance, like bio-medical arterial stent section and SMA based micro gripper.

From the above discussion on models that use crystal plasticity approach, it is seen that it offers flexibility to incorporate several important aspects related to SMA microstructure like true crystallographic variants and texture into the model and assess their impact on the SMA response. It may be noted that in order to describe the dynamics of twin boundary motion during the phase transformation discrete models are more suitable as compared to continuum based models. In the following one such approach is discussed.

### 5.3 Lattice Dynamics Based Models

One of the key aspects of lattice based models is that mechanics of SMA crystal lattice forms the basis to determine the type of structure that evolves during transformation. Either a suitable atomic potential or a continuum free energy is used to investigate several aspects of MT. Müller and Achenbach (1985) (discussed here under the macroscale models) use the lattice cell mechanics while formulating the free energy and the kinetics based on probability and the relative stability of phases. However, lattice cell concept used by them is more notional than the lattice of a single or polycrystalline SMA material. A lattice dynamical model is proposed by Abeyaratne and Vedantam (2003) to obtain macroscopic kinetic law for Cu-Al-Ni shape memory alloy. This model is intended to capture the dynamics of twin boundary motion (at a microscale) due to detwinning of multiple self accommodating variants of martensite into a macroscopic single stress preferred variant. They also describe different types of twin formation viz. compound, type 1 and type 2 twins. The model is developed for compound and type-1 twins. To describe the lattice scale dynamics a Frenkel–Kontorowa type inter-atomic potential is used, which helps in deriving the governing multiple well energy structure. Further, a quasi-continuum approximation is used to determine the continuum-scale kinetics. This leads to a governing partial differential equation in terms of displacement field, the roots of which gives the multiple well locations of free energy. With suitable analytical approximation they correlate the propagation speed of twin boundary with the critical stresses for both compound and type 1 twin and are found to be in good agreement with the experimental results.

A snapshot of various microscopic models discussed here is provided in Table 3. From the above discussion it is clear that in spite of several differences that exist in modeling MT at microscopic level, these approaches have achieved a fair amount of success in capturing salient aspects of MT. However, there is significant scope to enhance the modeling capability at the microstructure level, like modeling the effects of defects and dislocations on MT. As in many other instances of material modeling, advances in computing power and numerical and statistical techniques have led to incorporation of nanoscale effects and build up the level of complexity in material response. One of the critical aspects in modeling at micron or sub-micron level is to have experimental techniques standardized to obtain relevant material data for both model development and validation. In the case of SMAs, currently standard procedures are available only for a few types of tests, that too for macroscopic characterization.

## 6. Summary and Possible Future Research Directions

An overview of the models that capture the SMA response and the underlying MT was presented. The models were classified based on the scale of continuum under consideration and the approach. It is seen that from a former consideration, the range of interest is from submicroscopic range lattice dynamics to macroscale (bulk) form. From the latter perspective, a wide variety of modeling approaches ranging from atomistic potential to macroscale thermodynamics are used to capture the essence of MT. While most of the approaches discussed herein have achieved a fair amount of success in modeling SMAs, several unresolved issues still exist that attracts further interest. One of the foremost challenges yet to be resolved is the bridging of scales of continuum that are involved in modeling SMAs. One of the critical issues here is the reduction of the number of martensitic variants into those that are significant under given circumstances (1-D or 2-D or 3-D behavior). Reorientation effects between these variants also play an important role in transformation behavior. These aspects were highlighted at several places in this review. A few other important aspects, particularly relevant to application development and fundamental understanding of the response at a macroscale are listed here.

Complexity in phase diagram:

The stress dependence for each of the four transformation temperatures can be different (and nonlinear), as shown schematically in Figure 18. This could be due to significant amount of remnant cold work or thermomechanical history (seen in actuator materials). From a phase diagram based modeling perspective, more model parameters are necessary to capture this, even to a limited extent. From a thermodynamic perspective, this suggests a more complex form of interaction energy that needs to be identified. One of the aspects seen in such cases is the asymmetric hysteresis. In addition, more rigorous ways of constructing phase diagrams, especially under multivariant transformation are needed. This is so since the phase diagram obtained from isobaric tests may not always match with that obtained from isothermal tests due to lack of consistent definition of critical temperatures and stresses.

Role of texture: Another aspect that alters the interaction energy or the nature of response is the texture (initial microstructure due to processing). For instance, in the wire form, the grains could be deformed significantly in the longitudinal direction and thus alter the transformation strain in different directions, leading to different macroscopic transformation strain. Crystal plasticity based models have addresses this issue to a certain extent.

**Table 3.** Summary of microscopic models

Models	Approach	Formulation	Evolution kinetics	Interaction energy	Type of crystal struct.	Material	Scalability to macrolevel
Patoor et al (1988)	Micromechanics	Crystallographic theory	Selfconsistent approach	Interfacial operator method by Hill	Poly	NiTi	Suitable (Computationally expensive)
Fischer and Tanaka (1992)	Micromechanics	Thermodynamics	Dissipation potential	Assumed exponential kinetics	Single and poly	Generic	Non-suitable
Raniecki et al (1992)	Micromechanics	Thermodynamics	Crystallographic		Poly	Generic	Non-suitable
Sun and Hwang (1993)	Micromechanics	Microstructural physical mechanism	Dissipation based	Mori-Tanaka inclusion	Poly	Generic	Suitable
Lu and Weng (1997)	Micromechanics	Irreversible thermodynamics	Dissipation potential	Exponential interaction	Single	Ti(49.8%Ni)	Suitable
Goo and Lexcellent (1997)	Micromechanics	Thermodynamic (Helmholtz free energy)	Irreversible thermodynamics	Surface energy on the interface	Single	CuZnAl	Non-suitable
Huang and Brinson (1998)	Micromechanics	Thermodynamic (Gibbs free energy)	Jump condition	Eshelby Kroner approach	Single	NiTi	Non-Suitable
Gao et al (2000)	Micromechanics	Thermodynamic (Gibbs free energy)	Dissipation potential	Self accommodating group hypothesis	Poly	NiTi	Suitable (Computationally expensive)
Zhang and McCormick (2000)	Micromechanics	Thermodynamic	Linear	Modified Eshelby theory of inclusion	Poly	Generic	Suitable
Bernardini (2001)	Micromechanics	Variational energy approach	Dissipation potential	Eshelby theory of inclusion	Poly	Generic	Suitable
Thamburaja and Anand (2001, 2002, 2003)	Crystal mechanics based	Finite element	Phenomenological	Phenomenological	Poly	NiTi	Suitable
Anand and Gurtin (2003)	Continuum crystal plasticity	Continuum thermomechanics	Micro instability	Quadratic interaction through asymmetric interaction coefficient	Poly	NiTi	Suitable
Hall and Govindjee (2002)	Micromechanics	Lagrangian potential	KT condition	Quadratic interaction	Poly	NiTi	Suitable
Levitas and Prestion (2002 b)	Micromechanics	Modified Gibbs free energy	Second derivative of free energy	Quadratic interaction through asymmetric interaction coefficient	Poly	NiAl	Suitable
Abeyaratne and Vedantam (2003)	Lattice dynamics	Effective interatomic potential (Frenkel–Kontorowa type)	Suitable derivative	Not considered	single	CuAlNi	Suitable (quasi-continuum approximation)
Vedantam and Abeyaratne (2005)	Micromechanics	Thermodynamic (Helmholtz free energy)	Not modeled	Not modeled	Single	CuAlNi	Non-suitable
Mahapatra and Melnik (2006)	Micromechanics	Non-equilibrium thermodynamics	Second derivative of free energy	Quadratic interaction through symmetric interaction coefficient	Poly	NiAl	Suitable (Bridging technique)
Guthikonda et al (2007)	Micromechanics of crystal	Thermodynamic (Helmholtz free energy)	Dissipation potential	Quadratic interaction	Single and Poly	CuAlNi	Suitable

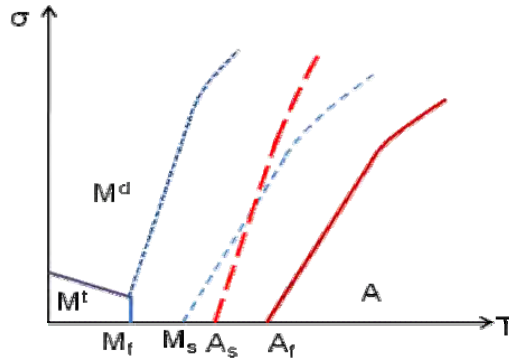


Figure 18: Schematic of phase diagram with different stress dependence for all the four transformation temperatures.

Modeling of shakedown or stabilization of hysteresis is another area that has not attracted sufficient attention compared to experimental investigations. Stabilization has several important implications like reliability of SMA applications and hence modeling tools that can capture it can be quite useful. Additional internal variables are necessary to account for the ‘residual’ martensite that reduces the amount of austenite available for further transformation. It may be noted that part of this martensite can be recovered if heated to a much higher temperature. This aspect is also alluded to as ‘healing’ in SMA literature. Figure 19 shows a SE elastic shakedown in a commercially available NiTi with a complex phase diagram and asymmetric hysteresis.

Partial and internal loops: The nature of memory that is responsible for the characteristics of partial or inner loops is still an open topic of research. While return point memory (RPM) is seen in most of the materials, sink-point memory is also observed in some cases (Figure 8). The reasons behind this are not clearly understood and models that adequately explain the underlying phenomena are not yet available.

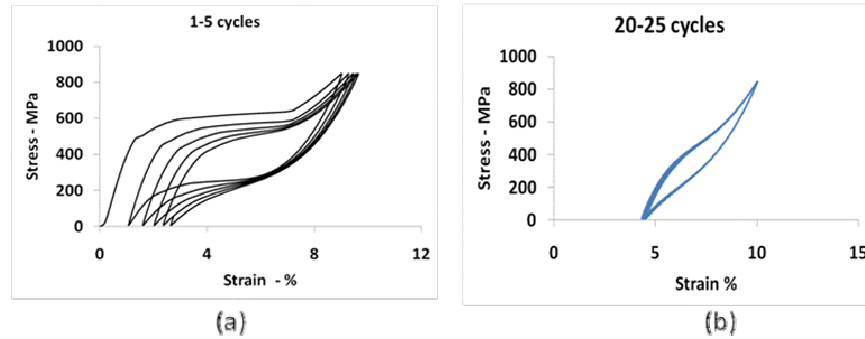


Figure 19: Shakedown seen in stress cycling of a commercially available NiTi; (a) First 5 cycles showing large strain accumulation; (b) Stable but drastically narrow hysteresis between cycles 20-25 cycles. Asymmetry in forward and reverse transformation paths is also evident.

**Thermal Arrest Memory Effect (TAME):** A fascinating feature seen in SMAs when the transformation is interrupted due to partial thermal cycling is the Thermal arrest memory (also called as Stepped Martensitic transformation (SMART)). Significant amount of experiments has been done investigating this effect (Madangopal (1994, 2005), Wang et al (2006)). However, several questions remain in terms of the cause of such a behavior and the role of interaction energy in TAME. Development of models that capture this satisfactorily is still an open area.

**R-phase related effects:** Though the presence of R-phase is well investigated, it has not attracted much attention by the modeling community. This might be attributed to the lack of applications or minimal SME and SE due to low transformation strains (typically less than 1 %) associated with R phase. Further, the presence of R-phase at higher stresses is diminished, if not completely absent. However, the electrical resistivity of R-phase is much higher than the martensite and austenite and hence, when present, R-Phase plays a crucial role in changes in resistivity during transformation. This aspect needs further investigations. Coupled electro-thermomechanical field problems arise when SMAs are heated resistively (Joule heating). Hence, models that captures the changes in resistivity due to R-phase may be useful in development of SMA based applications.

SMA composites: Embedding SMA in either wire or ribbon form into a suitable matrix to obtain SMA composite offers several advantages in terms of directionality of actuation force and strain, structural conformity of SMA wires etc.. However, they also pose several limitations in terms of the amount of transformation strain that is recoverable due to reduced flexibility of the matrix material. Issues related to the interface of SMA and matrix assumes importance in developing good SMA composites. Modeling the SMA composite has been attempted by Berman and White (1986) and Gao et al (2005). Much work still needs to be done to model them and facilitate development of realizable SMA composites for applications.

Effect of defects: An important aspect of processing history and stabilization is the presence of defects in the material. Some of these defects become 'dead materials' since they do not undergo transformation. However, apart from the well known effects of stress and/or strain concentrations that they introduce, they significantly influence the nature of MT, like biasing the growth of variants. Use of micromechanics to determine their effect on transformation and relating this effect suitably to the macroscopic response is an important area that can be pursued.

Functional and Mechanical fatigue in SMAs: Loss in shape memory or superelasticity (extent of phase transformation) due to thermomechanical cycling leads to functional degradation. From an application perspective, though the material may not have failed by conventional fatigue, functional fatigue is undesirable since it affects reliability. Recently this has attracted attention of researchers to investigate critical issues like causes of degradation and role of nature of thermomechanical loading on loss of SME and SE. In this context, modeling functional degradation attains importance. Another aspect is related to the mechanical failure or fracture due to cyclic loading. Understanding of the mechanisms, both at microscopic and macroscopic level, that cause fatigue damage under thermomechanical loads is still inadequate. This is attributed to the complexities associated with microstructural changes due to the repeated microstructural transformation leading to defect generation and growth.

Table 4. Summary of models with solution to boundary value problem

Models	Type	State of stress	Temperature field	Nature of BVP solved	Purpose
Abeyratne and Knowles (1993)	Macroscopic	1-D	1-D	Coupled non stationary momentum and energy balance	Sharp interface
Bekker and Brinson (1997)	Macroscopic	1-D	1-D	Quasistationary momentum balance and non-stationary energy balance	
Aurichio and Taylor (1997)	Macroscopic	3-D	As a parameter	Non-stationary momentum balance	
Amalraj et al (2000)	Macroscopic	Not considered	1-D	Non-stationary energy balance	
Qidwai and Lagoudas (2000)	Macroscopic	3-D	As a parameter	Non-stationary momentum balance	
Zlolkowski (2001)	Macroscopic	1-D	1-D	Coupled non stationary momentum and energy balance	Wave front propagation
Hall and Govindjee (2002)	Microscopic	3-D	As a parameter	Non-stationary momentum balance	
Thamburaja and Anand (2001)	Microscopic	3-D	As a parameter	Non-stationary momentum balance	Finite element based crystal mechanics
Shaw (2002)	Macroscopic	1-D	1-D	Coupled non stationary momentum and energy balance	Nucleation and Wave front propagation
Sadek et al (2003)	Macroscopic	1-D	1-D	Non-stationary energy balance with constant state of stress	
Liew et al (2004)	Macroscopic	3-D	1-D	Momentum balance	
Aurichio and Petrini (2004)	Macroscopic	3-D	1-D	Coupled non stationary momentum and energy balance	
Thamburaja (2005)	Macroscopic	3-D	As a parameter	Non-stationary momentum balance	
Kloucek and Reynolds (2006)	Macroscopic	1-D	1-D	Coupled non stationary momentum and energy balance	
Mahapatra and Melnik (2006)	Microscale	3-D	3-D	Non-stationary energy and momentum balance	Multiscale bridging approach



Solution of coupled BVP for realistic actuator scenarios: From an application perspective, solution of a coupled BVP involving a combination of energy, momentum and mass balance with appropriate boundary and initial conditions is extremely useful to analyze the performance of the SMA device. Formulation and numerical solution of such mixed field problems with reasonably realistic boundary and initial conditions is still a challenging task. A quick assessment from the view point of solution of BVP can be obtained from Table 4. For instance, contact conditions of SMA, especially in wire form, wherein the attachments like crimps introduce complex state of stress and transformation is still not well understood. Possible failure modes that occur due to such conditions is another aspect that needs detailed investigations.

In this work an overview of the various approaches to modeling SMAs was attempted. An extensive review of large number of models that exist in open literature was presented. The authors wish to repeat their earlier remark that this review is not exhaustive and that the classification of models provided here is not necessarily scientifically rigorous. The authors hope that this work has provided a useful overview of the plethora of approaches to modeling SMAs and that any further work in this direction would benefit from this review.

### Acknowledgements

Authors thank Dr. Prakash D. Mangalgiri, Amol G. Thakare and Dr. Ravikumar Karumanchi for their valuable inputs in the preparation of this manuscript.

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