A stochastic thermodynamic model for the gradual thermal transformation of SMA polycrystals

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Abstract. The martensitic–austenitic phase transformation of a polycrystalline shape memory alloys (SMA) occurs gradually over a range of temperatures even though the monocrystal undergoes a first-order transition (at a single temperature). Factors such as material inhomogeneities and internal stresses in a polycrystal are believed to cause the spread in transformation temperatures. In this work, we assume that the local regions of a polycrystal transform at a single temperature, characteristic of a first-order transition; this temperature is taken to vary from one region to another. The first-order transition of a generic local region is modeled with the Boyd–Lagoudas thermodynamic theory and a simple averaging process is used to derive the overall response of the polycrystal. The concept of a statistical distribution in the first-order transition temperatures is then introduced. By reducing the proposed stochastic thermodynamic theory to the special case of a pure thermal transformation in a polycrystal, it becomes possible to obtain the parameters of the statistical distribution from calorimetric data. This new approach renders unnecessary the customary practice in the SMA literature to artificially assign 'start' and 'finish' transformation temperatures to a SMA polycrystal. The statistical distribution is also used as a basis to correlate strain recovery against temperature measurements from repetitive cycles of a thermally induced transformation in untrained polycrystalline SMA wires.

1. Introduction

The accurate characterization of polycrystalline shape memory alloys (SMAs) is essential in order to realize the ultimate goal of successfully commercializing them for vibration and shape control. Theoretical modeling of the shape memory effect (SME) has been done by Tanaka (1986), Patoor *et al* (1987), Ortin and Planes (1988, 1989, 1991), Sato and Tanaka (1988), Berveiller *et al* (1991), Liang and Rogers (1990, 1991) Raniecki and Lexcellent (1994). Recently, Boyd and Lagoudas (1996) proposed a thermodynamic model which combines and extends the aforementioned work to account for non-proportional loading, simultaneous transformation and reorientation, adiabatic deformation and combined isotropic and kinematic hardening. The developed theories for the SMA constitutive response then can be used to address the question as to how a host material would respond when a SMA material is embedded in it. Theoretical studies of the inelastic response of such 'active composites' have been undertaken by micromechanical methods and periodic cell approaches (Lagoudas *et al* 1994). While

all the constitutive models are capable of modeling the effective response of SMA materials with varying degrees of success, these do make some assumptions for the SMA material response resulting in certain fundamental differences between the theoretical predictions and the experiments. We use a short discussion on experiments in the next paragraph to highlight the aforementioned difference in theory and experiment.

A monocrystalline SMA undergoes a stress-free thermal transformation from its high temperature phase of austenite (A) to a low temperature phase of martensite (M) on cooling. The transformation is exothermic and occurs at a single temperature; hence the phase change is a first-order phase transition (Delaey *et al* 1974). The thermal transformation in a polycrystalline SMA is characteristically different. A differential scanning calorimetric (DSC) measurement (shown in figure 1(a), and conducted at a constant temperature rate) gives the rate of heat gained by the calorimeter, $\dot{Q}_{cal} - \dot{Q}_{cal,0}$, during the transformation of the SMA during cooling (equal in magnitude and opposite in sign to that lost by the SMA) as a function of the temperature. It is seen that the evolution of the heat rate itself is gradual, and occurs over a range of temperatures. Owing to the gradual nature of

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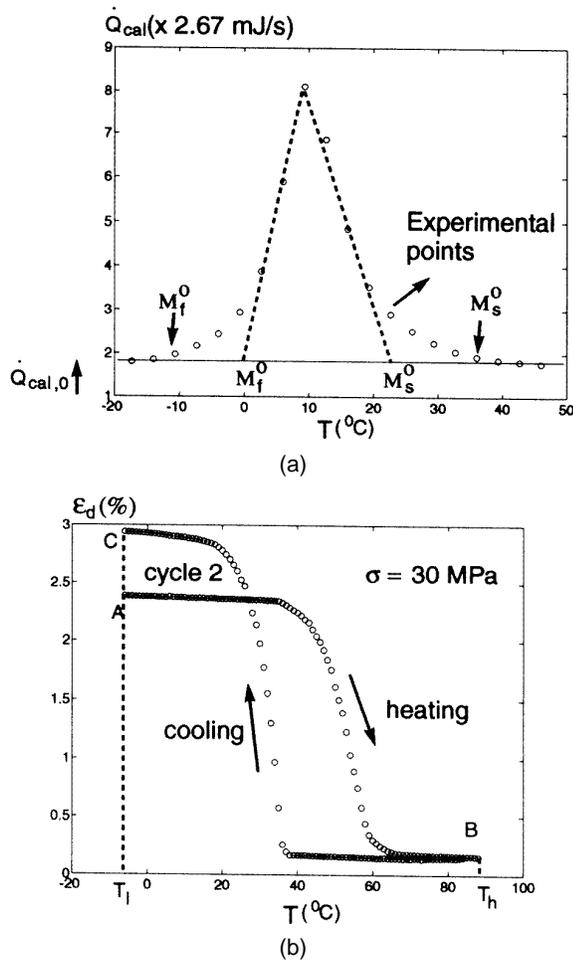
Figure 1. (a) Calorimetric data of latent heat for a stress-free thermal austenitic to martensitic transformation of a Nitinol SMA polycrystal. The mass of the sample used was 71.5 mg and $\dot{T} = -10\,°C\ min^{-1}$. The experiment was done by Dr M H Wu of Memry Corporation, Connecticut. (b) Strain–temperature response of a Nitinol SMA wire under dead load of 30 MPa. The experiment was carried out in the Active Materials Laboratory, Texas A & M University.

the transformation, the 'start' and the 'finish' temperatures cannot be clearly identified. The gradual nature of the phase change in the polycrystal is also evident during a thermally-induced transformation under dead load—shown in figure 1(b)—where the strain has been plotted as a function of temperature. It is seen that the 'onset' and 'finish' temperatures are not clearly identifiable. We shall return to a more detailed discussion of these data in the last section of the paper.

Several factors are responsible for the difference between the monocrystal and the polycrystal response. One of the reasons is that the range of transformation temperatures of a polycrystal is extremely sensitive to the ratio of alloying elements (Jackson *et al* 1972). It is quite likely that the alloy content in a local region of the polycrystal may be different from the nominal (or average) alloy content of the polycrystal. Thus a variation in the alloying content locally might cause different parts

of the polycrystal to transform at different temperatures, leading the polycrystal to transform gradually. A second reason is the result of the presence of an inherent defect structure in the polycrystal, leading to a non-uniform residual stress field in the material, even prior to phase transformation. This issue has been addressed by Chen (1979) and Cohen and Wayman (1981). According to their findings, under the influence of this stress field, it is conducive for certain regions in the polycrystal to transform at a temperature different from those of other regions, leading to a gradual transformation of the polycrystal. A third possible reason is the effect of orientation of grains with respect to the macroscopic loading of the polycrystal. Some grains are in a more favorable orientation (for the $A \rightarrow M$ transformation) with respect to the macroscopic loading than other grains (and vice-versa for the $M \rightarrow A$ transformation), causing the onset of transformation in the grains. The observable gradual response in a real SMA polycrystal is expected to follow from a synergistic effect of the aforementioned possible causes.

In the absence of clearly defined transformation temperatures, it has become customary in the literature to adopt certain rules based on which martensitic start and finish temperatures, M_s and M_f, respectively for the $A \rightarrow M$ transformation are identified. A common practice is to assume that the transformation 'starts' and 'finishes' corresponding to the points on the curve where it shows a noticeable departure from the base line, shown as M_s^0 and M_f^0 at the tails of the curve in figure 1(a) (the definition of what is 'noticeable' is obviously somewhat subjective) (Tanaka 1986). Another practice is to extend the two branches of the curve shown in figure 1(a) as straight lines and designate the points where these intersect the base line as M_s^0 and M_f^0 (Shaw and Kyriakides 1995). Similar procedures can also be adopted to determine the austenitic start and finish temperatures, A_s^0 and A_f^0, respectively for the reverse $M \rightarrow A$ transformation. While the former rule may appear more accurate than the latter in characterizing the onset and finish of transformation, both are nonetheless artificial. As the constitutive models incorporate the transformation temperatures as parameters, a certain amount of artificiality inevitably creeps into the models.

The objective of this paper is to develop a theory which does away with the notion of having to determine the 'start' and 'finish' temperatures in a thermal transformation of a polycrystal (with and without dead loads). The issue of stress-induced phase transformation (where stresses change) will be addressed in a future communication. We assume that a cluster of grains residing in a polycrystalline environment undergoes a first-order transition. This cluster is thus taken to transform at a single temperature. The magnitude of the phase transformation temperature is taken to change from cluster to cluster. A statistical distribution in these phase transformation temperatures is introduced to capture this variation.

The paper is organized in the following manner. Experimental observations to motivate the theoretical development are discussed in the first part of section 2. The statistical distribution is then introduced in the

second part of that section. In section 3, the phase transformation in a generic cluster is modeled with the thermodynamic approach of Boyd and Lagoudas (1996) (any other constitutive model could have been used as well) and the overall polycrystalline response is obtained through a simple averaging scheme involving the response of the constituent clusters. We conclude in section 4 with numerical results of comparison of the theory with some available experimental data. All the constitutive theories incorporating the transformation temperatures of the polycrystal as parameters will be referred to as the deterministic constitutive theories whereas the current theoretical approach that incorporates the statistical distribution in a constitutive model will be referred to as the stochastic constitutive theory. In that light, Boyd and Lagoudas's (1996) approach will be referred to as the deterministic thermodynamic theory and its extension as given in section 3 will be referred to as the stochastic thermodynamic theory.

In the following, we shall use the symbolic notation unless mentioned otherwise. A second-order tensor will be denoted as a boldface letter whereas a fourth-order tensor will be denoted as a capital letter unless denoted otherwise. The deviatoric part of a second-order tensor, $\boldsymbol{\sigma}$, will be denoted as $\boldsymbol{\sigma}'$ and defined as $\boldsymbol{\sigma}' = \boldsymbol{\sigma} - \frac{1}{3}\,\mathrm{tr}(\boldsymbol{\sigma})\boldsymbol{I}$. Here, $\boldsymbol{I}$ is the second-order identity tensor and $\mathrm{tr}(\boldsymbol{\sigma}) = \sigma_{ii}$ (summation over repeated indices is implied). The inverse of a second-order tensor, $\boldsymbol{\sigma}$, where it exists, will be denoted as $\boldsymbol{\sigma}^{-1}$ (with a similar definition for fourth-order tensors). The inner product of a fourth-order tensor A and a second-order tensor $\boldsymbol{\sigma}$ is denoted as $A\boldsymbol{\sigma}$ and $A_{ijkl}\sigma_{kl}$ in indicial notation. The inner product of two second-order tensors $\boldsymbol{\sigma}^{(1)}$ and $\boldsymbol{\sigma}^{(2)}$ results in a second-order tensor and is $\boldsymbol{\sigma}^{(1)} \cdot \boldsymbol{\sigma}^{(2)}$ ($\sigma_{ij}^{(1)}\sigma_{jk}^{(2)}$ in indicial form). The trace of $\boldsymbol{\sigma}^{(1)} \cdot \boldsymbol{\sigma}^{(2)}$ is denoted as $\boldsymbol{\sigma}^{(1)} : \boldsymbol{\sigma}^{(2)}$. Their dyadic product yields a fourth-order tensor, A, indicated symbolically as $A = \boldsymbol{\sigma}^{(1)} \otimes \boldsymbol{\sigma}^{(2)}$ and, in indicial notation, as $A_{ijkl} = \sigma_{ij}^{(1)}\sigma_{kl}^{(2)}$. The transpose of A is denoted as A^t and is defined by the identity $(A\boldsymbol{\sigma}^{(1)})\boldsymbol{\sigma}^{(2)} = \boldsymbol{\sigma}^{(1)}(A^t\boldsymbol{\sigma}^{(2)})$ for all $\boldsymbol{\sigma}^{(1)}$ and $\boldsymbol{\sigma}^{(2)}$. Assuming that a scalar quantity, $\Pi(T, \boldsymbol{\sigma})$ is a function of another scalar T and a second-order tensor, $\boldsymbol{\sigma}$, two partial derivatives can be defined $-\nabla_T \Pi$ (a scalar) and $\nabla_{\boldsymbol{\sigma}} \Pi$ (a second-order tensor). In component form, the former is $\partial\Pi/\partial T$ whereas the latter is $\partial\Pi/\partial\sigma_{ij}$.

2. Experimental observations and the proposed statistical distribution in the stress-free transformation temperatures

2.1. Experimental observations

It has been observed that when a stress-free SMA polycrystal undergoes the $A \rightarrow M$ transformation, it does so gradually. The evolution of the latent heat per unit volume from the SMA is also gradual, depicted in terms of the energy release rate from the SMA in figure 1(a). This curve has been obtained from a differential scanning calorimetric (DSC) measurement of the latent heat during the transformation. An initially austenitic polycrystal with a volume V is cooled from an elevated temperature

sufficiently so that the $A \rightarrow M$ phase transformation takes place. If austenite and martensite possess identical specific heats and these are not sensitive to temperature (in the absence of transformation), then the latent heat of transformation, H_f, per unit volume of the polycrystal during the $A \rightarrow M$ transformation is defined as

$$H_f = -\frac{1}{\dot{T}V} \int_{-\infty}^{+\infty} [\dot{Q}_v - \rho V C_A \dot{T}]\,\mathrm{d}T \qquad (1)$$

when the temperature rate, $\dot{T}$, is held constant (as is the case in a DSC experiment). The parameter $\dot{Q}_v$ is the rate of heat lost by the SMA and C_A is the specific heat of austenite. The integral $\int_{-\infty}^{+\infty} [\dot{Q}_v - \rho V C_A \dot{T}]\,\mathrm{d}T$ follows from the area between the base line and the data points in a plot of a DSC measurement shown in figure 1(a), after identifying

$$\dot{Q}_v - \rho V C_A \dot{T} = -(\dot{Q}_{cal} - \dot{Q}_{cal,0}) \qquad (2)$$

where the first negative sign on the right indicates that the thermal energy per unit time lost by the SMA is exactly equal and opposite to that gained by the calorimeter. The value of $\dot{Q}_{cal,0}$ defines the height of the base line and is usually set arbitrarily in a DSC measurement, as only the difference $\dot{Q}_{cal} - \dot{Q}_{cal,0}$ is relevant for the phase transformation and not the base value. It is seen that the function $\dot{Q}_v$ is nonlinear, and with no clearly defined 'start' and 'finish' points. It is however customary to artificially assign a temperature, M_s^0, at which the transformation starts and the temperature, M_f^0, at which it finishes. Since the transformation temperatures are artificially chosen, it is desirable to develop a constitutive theory which does not rely on the notion of a 'start' and 'finish' temperature. The observed transformation behavior for a polycrystal being an outcome of a single to polycrystal transition, we give a short discussion regarding this transition next to motivate the theoretical development.

The phase transformation in a single crystal occurs over a narrow range of temperatures as opposed to the transformation in a polycrystal, where material heterogeneities and incompatibilities imposed by grain boundaries result in a wide temperature range for the phase transition. Therefore, the customary practice in the literature has been to assume that the martensitic transformation in a single crystal is a first-order transition (Delaey *et al* 1974). We shall make the same assumption here. The $A \rightarrow M$ stress-free transformation is then taken to occur at a single temperature, M_0^{si} (unlike that in a stress-free polycrystal which is assumed to start at the temperature, M_s^0 and end at M_f^0) whereas the $M \rightarrow A$ stress-free transformation is taken to occur at A_0^{si}. If the single crystal is subjected to mechanical loading, certain components of the stress tensor, σ_{ij}, are expected to influence the transformation. Thus a schematic of the combination of stress and temperature causing the transformation in a single crystal is depicted in figure 2(a).

A phase transformation in a SMA polycrystal can be induced thermomechanically. For the forward $A \rightarrow M$ transformation at a given stress, it progresses gradually as the temperature is decreased. The temperature at which the onset is assumed to have taken place is determined
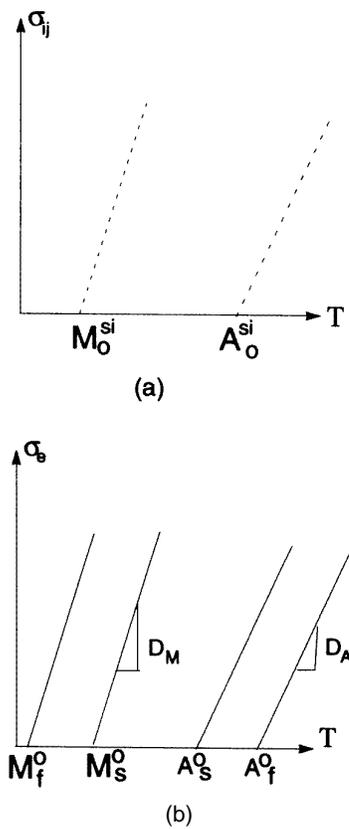
Figure 2. (a) The schematic of a first-order transition temperatures in a single crystal and (b) the transformation temperatures in a polycrystal.

artificially (just like the temperatures, M_s^0 and M_f^0, in the stress-free case). The operating temperature is known commonly as the martensitic start temperature, M_s. The transformation is assumed to have finished when the polycrystal reaches the martensitic finish temperature, M_f. Regarding the influence of the stress on the transformation, it is assumed that the transformation is insensitive to the hydrostatic stress; the transformation temperatures are then taken to depend linearly on the effective stress, $\sigma_e = [\frac{3}{2}(\sigma' : \sigma')]^{1/2}$, which in turn is computed from the deviatoric stress, σ'. Based on experiments (Delaey *et al* 1974), it is reasonable to assume that M_s and M_f are linear functions of the effective stress, σ_e. These are

$$M_s = M_s^0 + \frac{1}{D_M}\sigma_e \qquad \text{and} \qquad M_f = M_f^0 + \frac{1}{D_M}\sigma_e \quad (3)$$

and depicted in figure 2(b). The M_s^0 and M_f^0 are the stress-free martensitic start and finish temperatures for the polycrystal and D_M represents the change in the effective stress needed to cause a change in the M_s or M_f by 1 °C. Similarly, the onset and finish temperatures for the reverse $M \to A$ transformation are designated as A_s and A_f. These are

$$A_s = A_s^0 + \frac{1}{D_A}\sigma_e \qquad \text{and} \qquad A_f = A_f^0 + \frac{1}{D_A}\sigma_e. \quad (4)$$

The effective response of polycrystals is substantially different from those of its constituent single crystals. In the

stress-free case, for example, there is the range $M_s^0 - M_f^0$ over which the transformation occurs as compared to the first-order transition for the single crystal occuring at M_0. Three possible reasons for such a range could apply. The first possible reason for the observed gradual transformation in a polycrystal is due to the sensitivity of the transformation temperatures of a polycrystal to alloying elements. It is known that a 0.3% change in the titanium content in a nickel–titanium (Ni–Ti) SMA causes a shift in the transformation temperatures by as much as 30 to 55 °C (Jackson *et al* 1972). Since it is quite likely that the proportions of alloying elements in a local region of a polycrystal might differ from the nominal (or average) value, even a modest variation could result in significant differences in the transformation temperatures of the local regions. Thus, in the absence of a defect structure, different regions could conceivably transform at different temperatures, leading to a gradual transformation. The second reason is the existence of a defect structure in a polycrystal. A polycrystal contains an inherent distribution of defects in the form of grain boundaries, dislocations etc leading to an initial residual stress field in the polycrystal. A useful insight into the role of defects in martensitic transformations is provided by Chen (1979). She studied the evolution of martensitic transformation in a two-diimensional (2D) macroscopically stress-free austenitic crystal owing to a decrease in the temperature. A random distribution of defects in the form of elementary martensitic particles (EMPs) were introduced in the crystal. Assuming that the temperature field was uniform over the entire crystal, it was found that the stress field created by the defects enabled the early onset of transformation as opposed to a situation in which a single EMP in an otherwise 'perfect' austenitic crystal necessitated a considerable reduction in the temperature before the transformation could begin. It is then demonstrated that the pre-existing defects actually interfere with continued transformation at a given temperature and hence a further decrease in the temperature is necessary to continue the transformation. The model thus suggests that the transformation occurs over a range of temperatures. Although within the context of an idealized model, such an outcome bears a striking resemblance to the transformation in a polycrystal. The important role of the defect structure in the phase transformation is also underscored by Cohen and Wayman (1981) who have reported that the martensitic nucleation is heterogenous, starting from the so-called pre-existing nucleation sites (or defects). They also mention that these pre-existing sites have a tendency to transform at different temperatures. Raghavan (1992) has discussed some attempts to experimentally measure the distribution of these sites.

A third possible reason is that some of the constituent grains in a local region of the polycrystal are at an orientation different from other grains. This will tend to favor the $A \to M$ transformation in some grains as compared to that in others (the opposite will be true for the $M \to A$ transformation). We shall refer to this as the orientation effect. The observed behavior in a real polycrystal is, however, expected to be an outcome of all three causes.
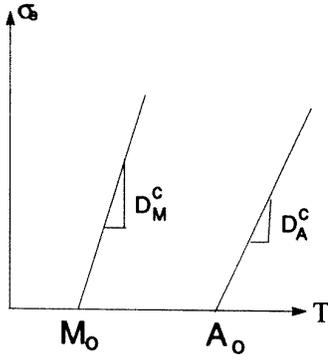
Figure 3. The transformation temperatures for a cluster of grains.

While the study of Chen (1979) on the defect structure is useful, it must be remembered that it is an idealization; the modeling of a 'real' polycrystal with a large number of initial defects and a variation in alloying content is an extensive 3D problem. The computational effort involved in characterizing such a polycrystal and tracking the evolution of martensite numerically seems to be an impossible task. An alternative approach is to suggest a phenomenological approach which allows incorporating the effect of the aforementioned possible reasons for the gradual transformation in constitutive models of polycrystalline SMAs. We incorporate the effect of the defect structure using a phenomenological model to be introduced next.

2.2. The statistical distribution in transformation temperatures

It is assumed that a cluster of grains in a SMA polycrystal undergoes the $A \rightarrow M$ transformation at a single temperature, $M(\sigma_e)$, as depicted in figure 3. We have assumed a functional dependence of the transformation temperature on the effective stress, σ_e, of that region. Such an assumption leads to a stress–temperature dependence intermediate between that of the single crystal and the polycrystal, depicted in figure 2(a) and (b).

The following relation for the martensitic transformation temperature is suggested for a generic region (cluster) of the polycrystal

$$M = M^0 + \frac{1}{D_M^c}\sigma_e \qquad (5)$$

and an austenitic temperature,

$$A = A^0 + \frac{1}{D_A^c}\sigma_e \qquad (6)$$

where the effective stress, σ_e is computed from an average deviatoric stress, σ', in that cluster as $\sigma_e = (\frac{3}{2}\sigma' : \sigma')^{1/2}$. The parameters D_M^c and D_A^c are the slopes of the transformation lines in figure 3. The underlying implication here is that all the grains in the cluster not only possess the same M_0 (or A_0) but also D_M^c and D_A^c. The latter implies that all grains in the cluster are equally sensitive to the

effect of stress on phase transformation. This might not be true, in general.

It can be anticipated that some grains in the cluster undergo the $A \rightarrow M$ transformation with relative ease (or the $M \rightarrow A$ transformation with relative difficulty) compared to other grains in the cluster owing to a higher resolved component in those grains of the macroscopic loading on the polycrystal. This orientation effect can be captured by considering a distribution in the slopes of transformation lines, D_M^c and D_A^c. While such a possibility could be included in the model, we shall assume in this work that applications will be restricted to moderate levels of stress (or the dead load), such that the distribution in D_M^c and D_A^c will not play as important a role as the one in M_0 (or A_0). Instead of distributions, we shall use single parameters, D_M^c and D_A^c; these can be viewed as some 'averaged' values of their underlying distributions. However, we propose to incorporate the distributions in these parameters in a forthcoming work on stress-induced transformations.

We now assume that the polycrystal contains clusters of grains where the stress-free transformation temperatures M_0 (or A_0) change from cluster to cluster. This will reflect the tendency of certain regions of the polycrystal to transform before others owing to defects and variability in alloying elements. Assuming the effective stress dependence of the transformation to be identical in each cluster (slopes of the lines in figure 3 remain unchanged from cluster to cluster), it is the distribution in M_0 (or A_0) that controls the gradual transformation. A defect free polycrystal will then possess the same M_0 (or A_0) everywhere.

Thus in a polycrystal of total volume V, the region (or cluster of grains) of the polycrystal possessing transformation temperatures in the range $M_0^a \leq M_0 \leq M_0^b$ is taken to have a volume $V(M_0^a \leq M_0 \leq M_0^b)$. The volume fraction of this region then is $V(M_0^a \leq M_0 \leq M_0^b)/V$, which also is the probability, $Pr(M_0^a \leq M_0 \leq M_0^b)$, of finding a region in the polycrystal with transformation temperatures in the range, $M_0^a \leq M_0 \leq M_0^b$. Thus

$$Pr(M_0^a \leq M_0 \leq M_0^b) \equiv \frac{V(M_0^a \leq M_0 \leq M_0^b)}{V}. \qquad (7)$$

If $M_0^a = -\infty$ and $M_0^b = M_0$, we adopt the following notation

$$P(M_0) = Pr(-\infty \leq \tilde{M}_0 \leq M_0) \qquad (8)$$

where $P(+\infty) = 1$. With the definition given by (8), we rewrite (7) as

$$P(M_0) = \frac{V(-\infty \leq \tilde{M}_0 \leq M_0)}{V} \equiv c(M_0) \qquad (9)$$

where the function $c(M_0)$ is the volume fraction of that part of the polycrystal containing transformation temperatures in the range $-\infty \leq \tilde{M}_0 \leq M_0$. If the probability distribution function, $P(M_0)$, is differentiable, then we can also define a probability density function

$$p(M_0) = \frac{\mathrm{d}P(M_0)}{\mathrm{d}M_0} \qquad (10)$$

where the definition

$$\int_{-\infty}^{+\infty} p(M_0)\, \mathrm{d}M_0 = 1 \qquad (11)$$

holds. The probability density distribution, $p(M_0)$, will have to be determined from a set of experimental data; the procedure will be elucidated in section 4. In the sequel, we shall have to deal with finding volume averages of a generic quantity, θ_c, defined at the level of a cluster (could be a scalar or a tensorial quantity). Its volume average at a given temperature T during the $A \to M$ transformation can be given in terms of $p(M_0)$ as

$$\theta = \frac{1}{V} \int_V \theta_c\, \mathrm{d}V = \int_V \theta_c\, \mathrm{d}c = \int_{-\infty}^{+\infty} \theta_c\, p(M_0)\, \mathrm{d}M_0 \quad (12)$$

where the latter follows from (9) and (10). For the reverse $M \to A$ transformation, the distribution in the stress-free austenitic transformation temperatures will be denoted as $g(A_0)$. While not essential, if we assume that the difference between A_0 and M_0 is identical for all clusters, then denoting the difference $A_0 - M_0 = \Delta T_{MA}$, the distribution in the stress-free austenitic temperatures is given as

$$g(A_0) = p(A_0 - \Delta T_{MA}). \qquad (13)$$

The distribution in the austenitic stress-free temperatures given by (13) can be thought of as being obtained from $p(M_0)$ by a 'rigid body' shifted by the amount ΔT_{MA} along the temperature axis. The volume average of a generic quantity θ_c during the $M \to A$ transformation can be given in terms of $g(A_0)$ as

$$\theta = \frac{1}{V} \int_V \theta_c\, \mathrm{d}V = \int_V \theta_c\, \mathrm{d}c = \int_{-\infty}^{+\infty} \theta_c\, g(A_0)\, \mathrm{d}A_0. \quad (14)$$

In the next section, we use the thermodynamic model of Boyd and Lagoudas (1996) to characterize the evolution of the first-order transformation in a cluster and then invoke a simple averaging process over all clusters constituting the polycrystal to get the overall response of the latter.

3. The thermodynamic model for the cluster and the homogenized response of the polycrystal

The thermomechanical transformation of the polycrystal under dead loading will occur owing to the phase transformation in the individual clusters. After establishing the thermomechanical transformation of each cluster, a micromechanical averaging process needs to be invoked in order to get the overall response. Since the transformation in a generic cluster will be controlled by the stress and temperature in it, a micromechanical scheme is needed to establish the stress concentration factors relating the stresses in the cluster to the average macroscopic stress, σ, and the 'thermal' concentration factors that relate the temperature in the cluster to the average temperature of the polycrystal, T; in general, then, a thermomechanical micromechanics-based problem needs to be solved. While this is certainly possible in principle, it is difficult and tedious. We shall make the simplifying assumption of

uniform stress and temperature throughout the polycrystal. With such an assumption, we give the thermodynamic model for the cluster first. This is followed by a simple averaging process to get the polycrystal response. Since we restrict the theory to dead loading, we shall assume that the macroscopic stress, σ, of the polycrystal does not change; thus we take $\dot{\sigma} = 0$.

3.1. The thermodynamic model for the cluster

The thermodynamic model of Boyd and Lagoudas (1996) is invoked to quantify the phase transformation in a cluster with stress-free transformation temperatures, M_0 and A_0. Among the quantities pertaining to a cluster, those with a subscript c change from cluster to cluster; those quantities without the subscript are taken to be identical in all clusters. It is assumed that the current martensitic volume fraction of a generic cluster is $\dot{\xi}_c$ where $\dot{\xi}_c$ may differ from one cluster to another, according to our convention of using the subscript c. If the constituent austenitic and martensitic parts of the cluster possess an isotropic moduli, L_A and L_M, respectively, an assumption of uniform stress, σ, in the cluster (and assumed to be identical in all clusters) yields a Voigt bound for the effective moduli, $L_c = [L_A^{-1} + \xi_c(L_M^{-1} - L_A^{-1})]^{-1}$, of the cluster; this assumption was shown to be reasonable in the estimate of the elastic moduli by Boyd and Lagoudas (1994). For simplicity we continue to make the same assumption in the current problem where inelastic strains are involved. In line with the uniform stress assumption, if the temperature, T, is assumed uniform in all clusters, the thermal expansion tensor for the cluster follows from the rule of mixtures applied to the isotropic thermal expansion tensors, α_A and α_M, respectively, of austenite and martensite. Thus, for the cluster, $\alpha_c = \alpha_A + \xi_c(\alpha_M - \alpha_A)$. The total strain rate, $\dot{\epsilon}_c$, in a cluster in the absence of transformation or during transformation follows from Boyd and Lagoudas (1994). In the absence of transformation, the strain rate is

$$\dot{\epsilon}_c = \alpha_c \dot{T} \qquad \text{for } \dot{\xi}_c = 0. \qquad (15)$$

During a first-order phase transition (when $\dot{T} = 0$), the strain rate becomes

$$\dot{\epsilon}_c = [\Delta L^{-1} \sigma + \Delta\alpha \Delta T + \lambda_c] \dot{\xi}_c \qquad \text{for } \dot{\xi}_c \neq 0 \quad (16)$$

where $\Delta L^{-1} = L_M^{-1} - L_A^{-1}$, $\Delta\alpha = \alpha_M - \alpha_A$, $\Delta T = T - T_0$, with T_0 being a reference temperature and the assumption of a dead load, $\dot{\sigma} = 0$, has been used. We have also assumed a flow rule for the inelastic strain rate, $\dot{\epsilon}_c^t$, in the local region as

$$\dot{\epsilon}_c^t = \lambda_c \dot{\xi}_c. \qquad (17)$$

The tensor λ_c provides the 'direction' in which the irreversible strains develop and needs to be specified. Note that the choice for λ_c will be made such that it renders $\mathrm{tr}(\dot{\epsilon}_c^t) = 0$; this assumption was made by Boyd and Lagoudas (1996) to reflect the fact that the phase transformation in polycrystalline SMAs is primarily a shear process. We shall make the assumption that even in a cluster, with its constituent grains, the phase transformation will occur in a manner so as to render the inelastic strain

traceless (i.e. have a vanishing hydrostatic component). Based on such an assumption, during the $A \rightarrow M$ transformation, we prescribe

$$\boldsymbol{\lambda}_c = \frac{3}{2} H \frac{1}{\sigma_e} \boldsymbol{\sigma}' \qquad \text{for } \dot{\xi}_c > 0 \qquad (18)$$

where $\sigma_e = \left[\frac{3}{2}(\boldsymbol{\sigma}' : \boldsymbol{\sigma}')\right]^{1/2}$. In the above equation, H is a parameter which will have to be determined from a thermal transformation in the presence of an uniaxial dead loading of the polycrystal. In the absence of stress, the transformation is assumed to be self-accommodating (no overall shape change for the cluster). Thus

$$\boldsymbol{\lambda}_c = 0 \qquad \text{for } \boldsymbol{\sigma} = 0. \qquad (19)$$

If $\boldsymbol{\epsilon}_c^{t,p}$ is the inelastic strain accumulated in the cluster before the onset of the $M \rightarrow A$ transformation,

$$\boldsymbol{\lambda}_c = H \frac{1}{\epsilon_{c,e}^{t,p}} \boldsymbol{\epsilon}_c^{t,p} \qquad \text{for } \dot{\xi}_c < 0 \qquad (20)$$

where $\epsilon_{c,e}^{t,p} = \left[\frac{2}{3}(\boldsymbol{\epsilon}_c^{t,p} : \boldsymbol{\epsilon}_c^{t,p})\right]^{1/2}$. In the context of dead loading, if $\boldsymbol{\sigma}_p$ was the stress required to generate the inelastic strain $\boldsymbol{\epsilon}_c^{t,p}$ in the cluster before the onset of the $M \rightarrow A$ transformation, it can be shown that equation (20) reduces to

$$\boldsymbol{\lambda}_c = \frac{3}{2} H \frac{1}{\sigma_{p,e}} \boldsymbol{\sigma}'_p \qquad \text{for } \dot{\xi}_c < 0. \qquad (21)$$

The key issue now is to determine ξ_c during a thermal transformation under dead loading. This follows from the formulation of a dissipation potential. The derivation needs to start with the description of the Gibbs free energies of the austenitic and martensitic portions of the cluster. We identify a Gibbs free energy per unit mass (or alternatively, the specific Gibbs free energy) for the region (or cluster) of the polycrystal (with stress-free temperatures M_0 and A_0) as G_c. It is defined as (Boyd and Lagoudas, 1996)

$$G_c = G_A + \xi_c[G_M - G_A] + G_c^{mix} \qquad (22)$$

where G_A and G_M are the specific free energies of the austenitic and martensitic phases in the cluster of the polycrystal whereas G_c^{mix} is the specific free energy of mixing of the two phases. These are given as

$$G_\beta = -\frac{1}{2\rho}(\boldsymbol{\sigma} : L_\beta^{-1}\boldsymbol{\sigma}) - \frac{1}{\rho}(\boldsymbol{\alpha}_\beta : \boldsymbol{\sigma})\Delta T$$
$$+ C_\beta \left[\Delta T - T \ln\left(\frac{T}{T_0}\right)\right] - S_\beta \Delta T + G_{\beta,0}$$
$$(\beta = A, M). \qquad (23)$$

We have made the assumption that the mass densities of both phases are identically equal to ρ. The parameter C_β is the specific heat, S_β and $G_{\beta,0}$ are the specific entropy and the specific free energy, respectively, at the reference state (this occurs at $\boldsymbol{\sigma} = 0$ and $\Delta T = 0$), for phase β. The free energy for mixing is defined as

$$G_c^{mix} = \frac{1}{2}b_c^1\xi_c^2 + \frac{1}{2}(\boldsymbol{\epsilon}_c^t : B_c^2\boldsymbol{\epsilon}_c^t) + (\boldsymbol{b}_c^3 : \boldsymbol{\epsilon}_c^t)\xi_c \qquad (24)$$

where b_c^1 is a scalar parameter, B_c^2 and $\boldsymbol{b}_c^3$ are fourth- and second-order tensors respectively. The values of these quantities can be found from thermodynamic restrictions and experimental data.

The microstructural rearrangements owing to the phase transformation lead to entropy production. If the local entropy production rate is, $\dot{\eta}_c$, the second law requires

$$T\dot{\eta}_c \geq 0 \qquad (25)$$

where

$$T\dot{\eta}_c = (\boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}_c) - \rho\dot{\psi}_c - \rho S_c\dot{T}. \qquad (26)$$

The $\dot{\boldsymbol{\epsilon}}_c$ is the total strain rate in the considered region of the polycrystal, $\dot{\psi}_c$ is the specific Helmholtz free energy rate and $S_c = -\partial G_c/\partial T$. Therefore

$$S_c = \frac{1}{\rho}(\boldsymbol{\alpha}_c : \boldsymbol{\sigma}) + C_c \ln\left(\frac{T}{T_0}\right) + S_c^0 \qquad (27)$$

where $C_c = C_A + \xi_c\Delta C$, $\Delta C = C_M - C_A$, $S_c^0 = S_A + \xi_c\Delta S$ and $\Delta S = S_M - S_A$. Knowing that for a first-order transition, $\dot{T} = 0$, (25) becomes

$$(\boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}_c) - \rho\dot{\psi}_c \geq 0. \qquad (28)$$

The Helmholtz free energy rate, $\dot{\psi}_c$, is related to the Gibbs free energy rate through a Legendre transformation, $\dot{\psi}_c = \dot{G}_c + \rho^{-1}(\boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}_c^{te})$, where the thermoelastic strain rate in the cluster is $\dot{\boldsymbol{\epsilon}}_c^{te} = \dot{\boldsymbol{\epsilon}}_c - \dot{\boldsymbol{\epsilon}}_c^t$. Algebraic manipulation of (28) leads to

$$\Pi_c\dot{\xi}_c \geq 0 \qquad (29)$$

where

$$\Pi_c = [(\boldsymbol{\sigma} - \rho\boldsymbol{\mu}_c^t) : \boldsymbol{\lambda}_c] - \rho\mu_c. \qquad (30)$$

The parameters in (30) are defined as

$$\boldsymbol{\mu}_c^t = \nabla_{\boldsymbol{\epsilon}_c^t} G_c \qquad \text{and} \qquad \mu_c = \nabla_{\xi_c} G_c \qquad (31)$$

where the former in component form, can be written as $\mu_{c_{ij}}^t = \partial G_c/\partial\epsilon_{c_{ij}}^t$. The explicit expression for Π_c can be derived from (22)–(24), by which (30) reduces to

$$\Pi_c = [(\boldsymbol{\sigma} - \rho B_c^2\boldsymbol{\epsilon}_c^t - \rho\xi_c\boldsymbol{b}_c^3) : \boldsymbol{\lambda}_c] + \frac{1}{2}\boldsymbol{\sigma} : \Delta L^{-1}\boldsymbol{\sigma}$$
$$+ (\Delta\boldsymbol{\alpha} : \boldsymbol{\sigma})\Delta T - \rho\Delta C\left[\Delta T - T\ln\left(\frac{T}{T_0}\right)\right]$$
$$+ \rho\Delta S T - \rho\Delta G_0 - \rho b_c^1\xi_c - \rho(\boldsymbol{b}_c^3 : \boldsymbol{\epsilon}_c^t) \qquad (32)$$

where $\Delta G_0 = G_{M,0} - G_{A,0}$. It has been shown by Boyd and Lagoudas (1996) that at the onset of phase transformation and during the course of it, $\Pi_c = Y_c$, a constant threshold value similar to classical plasticity. This parameter will be found from experimental data. Therefore during the course of transformation

$$\dot{\Pi}_c = 0. \qquad (33)$$

Assuming $\dot{T} = 0$ during the transformation in the considered cluster and $\dot{\boldsymbol{\sigma}} = 0$, (33) reduces to

$$\nabla_{\xi_c}\Pi_c + (\nabla_{\boldsymbol{\epsilon}_c^t}\Pi_c : \boldsymbol{\lambda}_c) = 0 \qquad \text{when } \dot{\xi}_c \neq 0 \qquad (34)$$

which, using (30) and (31), becomes

$$b_c^1 + [B_c^2\boldsymbol{\lambda}_c + 2\boldsymbol{b}_c^3] : \boldsymbol{\lambda}_c = 0. \qquad (35)$$

This condition was first derived by Boyd and Lagoudas (1996) who proposed a thermodynamic theory for SMAs with 'start' and 'finish' temperatures. They derived the above condition for the first-order transition for the overall polycrystal.

During a thermomechanical transformation, heat is absorbed or released. The amount is determined by applying the first law of thermodynamics. If $\dot{u}_c$ and $\dot{Q}_c$ are the average specific internal energy rate and specific heat input rate at a cluster, respectively, the first law of thermodynamics dictates

$$\dot{u}_c = \rho^{-1}(\boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}_c) + \dot{Q}_c \qquad (36)$$

where

$$\rho u_c = \rho G_c + (\boldsymbol{\sigma} : \boldsymbol{\epsilon}_c^{te}) + \rho T S_c^0. \qquad (37)$$

Equations (36)–(37) can be used to derive the specific heat rate in terms of the temperature rate (when $\dot{\xi}_c = 0$) and the martensitic volume fraction rate during transformation (when $\dot{T} = 0$). The former results in the familiar heat conduction equation

$$\rho \dot{Q}_c^{NT} = \rho C_c \dot{T} \qquad \text{for } \dot{\xi}_c = 0, \ \dot{T} \neq 0 \qquad (38)$$

where $\dot{Q}_c^{NT}$ is indicated with a superscript NT to indicate that it is the heat exchange rate in a non-transforming cluster. During transformation, the heat exchange rate is indicated as $\dot{Q}_c^T$, and is given as

$$\rho \dot{Q}_c^T = [\rho T (\nabla_{\xi_c} S_c + \nabla_{\epsilon_c^t} S_c : \boldsymbol{\lambda}_c) - \Pi_c] \dot{\xi}_c$$
$$\text{for } \dot{\xi}_c \neq 0, \ \dot{T} = 0. \qquad (39)$$

With S_c given by (27), (39) reduces to

$$\rho \dot{Q}_c^T = \left[\Delta \boldsymbol{\alpha} : \boldsymbol{\sigma} T + \rho \Delta C T \ln\left(\frac{T}{T_0}\right) + \rho \Delta S T - \Pi_c\right] \dot{\xi}_c. \qquad (40)$$

An alternative form of (40) can be written using (32), and is given by

$$\rho \dot{Q}_c^T = [-(\boldsymbol{\sigma} - \rho B_c^2 \boldsymbol{\epsilon}_c^t - \rho \xi_c \boldsymbol{b}_c^3) : \boldsymbol{\lambda}_c - \tfrac{1}{2}\boldsymbol{\sigma} : \Delta L^{-1} \boldsymbol{\sigma}$$
$$+ \rho \Delta C \Delta T + \rho \Delta G_0 + \rho b_c^1 \xi_c + \rho (\boldsymbol{b}_c^3 : \boldsymbol{\epsilon}_c^t)] \dot{\xi}_c. \qquad (41)$$

Considering the special case of isotropic hardening, we assume $B_c^2 = 0$ and also $\boldsymbol{b}_c^3 = b_c^3 \boldsymbol{I}$. Since $\text{tr}(\boldsymbol{\lambda}_c = 0)$, $\boldsymbol{b}_c^3 : \boldsymbol{\lambda}_c = 0$, with which (35) reduces to $b_c^1 = 0$. The simplified relation in the context of isotropic hardening for the combination of stress and temperature causing the transformation in a cluster follows from (32) for $\Pi_C = Y_c$, and is given by

$$Y_c = \boldsymbol{\sigma} : \boldsymbol{\lambda}_c + \tfrac{1}{2}\boldsymbol{\sigma} : \Delta L^{-1} \boldsymbol{\sigma} + (\Delta \boldsymbol{\alpha} : \boldsymbol{\sigma})\Delta T$$
$$- \rho \Delta C \left[\Delta T - T \ln\left(\frac{T}{T_0}\right)\right] + \rho \Delta S T - \rho \Delta G_0. \qquad (42)$$

(41) has a particularly simple form

$$\rho \dot{Q}_c^T = [-\boldsymbol{\sigma} : \boldsymbol{\lambda}_c - \tfrac{1}{2}\boldsymbol{\sigma} : \Delta L^{-1} \boldsymbol{\sigma} + \rho \Delta C \Delta T + \rho \Delta G_0] \dot{\xi}_c. \qquad (43)$$

Equation (43) thus gives the relation between the heat rate controlling the evolution rate of the martensite volume fraction in the cluster.

The total energy per unit volume of the cluster needed to undergo a change in its martensitic volume fraction by

an amount $\Delta \xi_c$ is denoted as ρQ_c^T and is obtained by integrating (43). Noting that $\boldsymbol{\lambda}_c$ does not change when $\dot{\xi}_c \neq 0$ (see (18) and (21)), (32) reduces to

$$\rho Q_c^T = [-\boldsymbol{\sigma} : \boldsymbol{\lambda}_c - \tfrac{1}{2}\boldsymbol{\sigma} : \Delta L^{-1} \boldsymbol{\sigma} + \rho \Delta C \Delta T + \rho \Delta G_0] \Delta \xi_c. \qquad (44)$$

3.2. The homogenized response of the polycrystal

The homogenized response of the polycrystal at a given temperature T follows from those of its constituent clusters. During the phase transformation, the evolution rate of the martensitic volume fraction of the polycrystal, $\dot{\xi}$, follows from those of the individual clusters. Thus

$$\dot{\xi} = \frac{1}{V} \int_V \dot{\xi}_c \, dV \qquad (45)$$

and using (12) for the $A \to M$ transformation, we have

$$\dot{\xi} = \int_{-\infty}^{+\infty} \dot{\xi}_c \, p(M_0) \, dM_0. \qquad (46)$$

The total average strain rate of the polycrystal follows from the volume average of the strain rates of the constituent clusters. It is

$$\dot{\boldsymbol{\epsilon}} = \int_{-\infty}^{+\infty} \dot{\boldsymbol{\epsilon}}_c \, p(M_0) \, dM_0 \qquad (47)$$

where the inelastic strain rate in a generic cluster follows from either (16) or (15). The rate at which the polycrystal exchanges latent heat with the environment during the transformation is given by

$$\dot{H}_f = \int_{-\infty}^{+\infty} \rho \dot{Q}_c^T \, p(M_0) \, dM_0 \qquad (48)$$

where $\dot{Q}_c^T$ follows from (41). Identical equations can be written for the $M \to A$ transformation, with the volume average given by (14). In the sequel, we shall usually give the averages with respect to only the $A \to M$ transformation, as those for the $M \to A$ transformation will follow similarly.

3.3. Uniaxial loading of the polycrystal

For the important case of uniaxial loading of the polycrystal, the above equations simplify considerably. We reproduce some of the key equations in the context of uniaxial loading.

It is assumed that the only non-zero component of the stress is denoted as σ at a given temperature, T, and this stress acts uniformly throughout the polycrystal. The corresponding component of the strain in a generic cluster is denoted as ϵ_c whereas the corresponding component of the overall polycrystalline strain is denoted as ϵ. We now give the simplified equations for the cluster and then give those for the polycrystal.

3.3.1. A generic cluster. The uniaxial inelastic strain rate for the cluster follows from (17) as

$$\dot{\epsilon}_c^t = \lambda_c \dot{\xi}_c \tag{49}$$

where λ_c in the context of uniaxial loading takes a particularly simple form (for $\sigma \neq 0$). It follows from (18) and (21), both cases identically reducing to

$$\lambda_c = H \qquad \text{for } \dot{\xi}_c \neq 0. \tag{50}$$

The inelastic strain rate follows from (16) and (15) as

$$\dot{\epsilon}_c = [(E_M^{-1} - E_A^{-1})\sigma + (\alpha_M - \alpha_A)\Delta T + H]\dot{\xi}_c$$
$$\text{for } \dot{\xi}_c \neq 0, \ \dot{T} = 0 \tag{51}$$

and

$$\dot{\epsilon}_c = \alpha_c \dot{T} \qquad \text{for } \dot{\xi}_c = 0, \ \dot{T} \neq 0 \tag{52}$$

respectively. The combination of uniaxial stress and temperature at which transformation occurs in a cluster follows from (42) as

$$Y_c = \sigma H + \tfrac{1}{2}(E_M^{-1} - E_A^{-1})\sigma^2 + (\alpha_M - \alpha_A)\sigma \Delta T$$
$$- \rho \Delta C \left[\Delta T - T \ln\left(\frac{T}{T_0}\right) \right] + \rho \Delta S T - \rho \Delta G_0. \tag{53}$$

The heat rate follows from either (38) for a non-transforming region or from (43) for a transforming region as

$$\rho \dot{Q}_c^T = \left[-\sigma H - \tfrac{1}{2}(E_M^{-1} - E_A^{-1})\sigma^2 + \rho \Delta C \Delta T + \rho \Delta G_0 \right] \dot{\xi}_c$$
$$\text{for } \dot{\xi}_c \neq 0, \ \dot{T} = 0. \tag{54}$$

3.3.2. The polycrystal. The total strain rate for the polycrystal during the $A \to M$ transformation follows as

$$\dot{\epsilon} = \int_{-\infty}^{+\infty} \dot{\epsilon}_c \, p(M_0) \, \mathrm{d}M_0 \tag{55}$$

where $\dot{\epsilon}_c$ is either of equation (51) or (52).

4. Numerical and experimental results

4.1. Determination of material parameters

The various material parameters needed for the general theory will be obtained from a thermal transformation under uniaxial dead load. The parameters occuring in equations (49)–(55) are listed below in the order that they are discussed subsequently. These are

$$E_A, E_M, \alpha_A, \alpha_M, \rho C_A, \rho C_M, \rho \Delta G_0, p(M_0), \rho \Delta S, Y_c, H. \tag{56}$$

The first two parameters, E_A and E_M, can be found from the slope of a stress–strain curve of a purely austenitic polycrystal and the slope of the elastic part of the stress–strain curve of a purely martensitic polycrystal, respectively. The coefficients of thermal expansion, α_A and α_M, are measured from specimen length changes owing to a change in temperature of an austenitic SMA and a martensitic SMA.

The next four parameters can be found by correlating the heat exchange rate for the polycrystal predicted by the theory with that of the measured heat exchange rate of a SMA polycrystalline sample used in a differential scanning calorimetric (DSC) measurement as it is cooled at a constant temperature rate from an elevated temperature and caused to undergo the $A \to M$ transformation. Denoting the total heat exchange rate from the SMA sample with volume V and mass density ρ as $\dot{Q}_v$, the specific heat rate then follows as

$$\dot{Q} = \frac{\dot{Q}_v}{\rho V}. \tag{57}$$

We derive $\dot{Q}$ for a thermal $A \to M$ transformation in an initially austenitic stress-free SMA polycrystal next. Consider a purely thermal transformation of an initially austenitic, stress-free SMA polycrystal ($\xi_c = 0$ everywhere) to martensite, caused by a decrease in the temperature. At a given temperature T, all clusters with stress-free martensitic transformation temperature, M_0, in the range $T \leq M_0 \leq \infty$ would have completely transformed to martensite. The change, $\Delta \xi_c$, in the martensitic volume fraction in a generic cluster is

$$\Delta \xi_c = \begin{cases} 1 & T \leq M_0 \leq \infty \\ 0 & M_0 < T. \end{cases} \tag{58}$$

The total martensitic volume fraction of the polycrystal at the temperature T follows from the volume average of $\Delta \xi_c$, given in (58). This volume average is written using (12) as

$$\xi = \int_T^{\infty} p(M_0) \, \mathrm{d}M_0. \tag{59}$$

The rate of change of the overall martensitic volume fraction with temperature T then follows from the above equation as

$$\frac{\partial \xi}{\partial T} = -p(T). \tag{60}$$

The total latent heat per unit volume of a generic cluster with transformation temperature in the range $T \leq M_0 \leq \infty$ and which has transformed from pure austenite to martensite follows from (44) with $\sigma = 0$, $\Delta \xi_c = 1$ as

$$\rho Q_c^T = \begin{cases} \rho[\Delta C \Delta M_0 + \Delta G_0] & T \leq M_0 \leq \infty \\ 0 & M_0 < T \end{cases} \tag{61}$$

where $\Delta M_0 = M_0 - T_0$. The total latent heat per unit volume of the polycrystal exchanged when the temperature during the $A \to M$ transformation has been reduced to T follows from the volume average of (61) as
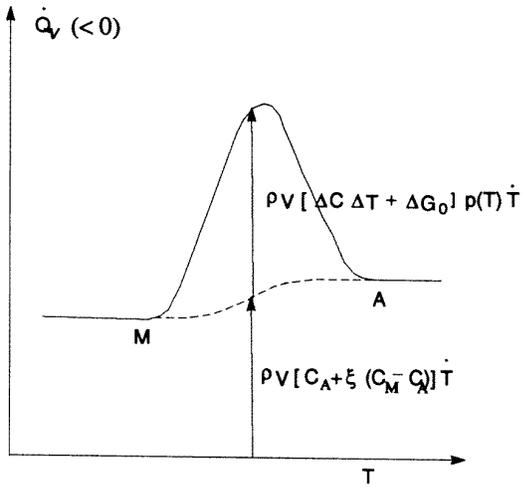
$$\rho Q^T = \int_T^{\infty} \rho[\Delta C \Delta M_0 + \Delta G_0] p(M_0) \, \mathrm{d}M_0. \tag{62}$$

The rate of change of the total latent heat per unit volume of the polycrystal with temperature is

$$\rho \frac{\partial Q^T}{\partial T} = -\rho[\Delta C \Delta T + \Delta G_0] p(T). \tag{63}$$

If $\dot{T}$ is the rate of change of temperature with time at the temperature T, the evolution rate of ξ and ρQ^T with time are written respectively as

$$\dot{\xi} = \frac{\partial \xi}{\partial T} \dot{T} = -p(T)\dot{T} \tag{64}$$

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Figure 4. A schematic of the heat exchange rate, $\dot{Q}_v$, of a SMA polycrystal when $C_M \neq C_A$, during a $A \to M$ transformation.

and

$$\rho \dot{Q}^T = \rho \frac{\partial Q^T}{\partial T} \dot{T} = -\rho [\Delta C \Delta T + \Delta G_0] p(T) \dot{T} \quad (65)$$

where the latter terms in (64) and (65) follow from (59) and (63), respectively. The total latent heat per unit volume following completion of the $A \to M$ transformation is defined as

$$H_f = \int_{-\infty}^{+\infty} \rho \dot{Q}^T \, dt = \rho \int_{-\infty}^{+\infty} [\Delta C \Delta T + \Delta G_0] p(T) \dot{T} \, dt \tag{66}$$

where the time t is in the range $0 \leq t \leq \infty$ corresponding to the temperature range, $-\infty \leq T \leq \infty$. As the polycrystal has been cooled from an elevated temperature to the current value, T, a certain amount of heat had to be extracted from the specimen to cause the temperature change. The corresponding total heat rate needed to change the temperature of the polycrystal follows from the volume average of (38) alongwith (58). Noting that for $\xi_c = 0$, $C_c = C_A$ and for $\xi_c = 1$, $C_c = C_M$, the total heat rate needed to cause the temperature change is

$$\rho \dot{Q}^{NT} = \rho C_A \dot{T} \left[1 - \int_T^\infty p(M_0) \, dM_0 \right]$$
$$+ \rho C_M \dot{T} \left[\int_T^\infty p(M_0) \, dM_0 \right]$$
$$= \rho [C_A + \xi (C_M - C_A)] \dot{T}. \tag{67}$$

The total heat exchange rate is

$$\rho \dot{Q} = \rho \dot{Q}^T + \rho \dot{Q}^{NT} \tag{68}$$

which reduces to the following expression using (65) and (66)

$$\rho \dot{Q} = -\rho [\Delta C \Delta T + \Delta G_0] p(T) \dot{T} + \rho [C_A + \xi (C_M - C_A)] \dot{T}. \tag{69}$$

The above expression with equation (57) gives

$$\dot{Q}_v = -\rho V [\Delta C \Delta T + \Delta G_0] p(T) \dot{T} + \rho V [C_A + \xi (C_M - C_A)] \dot{T}. \tag{70}$$

Since the polycrystal is being cooled, heat will be lost by the SMA. This continues to be the case as it goes through the exothermic $A \to M$ transformation. Hence $\dot{Q}_v$ will be negative, as indicated in figure 4. The reverse is true for the $M \to A$ transformation. It is seen that at a low temperature when the polycrystal is in a martensitic phase (below the point M), $\xi = 1$ and $p(T) \approx 0$. Therefore, it follows from (70) that

$$C_M = \dot{Q}_v / (\rho V \dot{T}). \tag{71}$$

Thus, C_M can be found once the quantities on the right-hand side of the above equation are measured. Similarly, at a high temperature when the polycrystal is all austenitic (beyond the point A), $\xi = 0$ and $p(T) \approx 0$, (70) reduces to

$$C_A = \dot{Q}_v / (\rho V \dot{T}). \tag{72}$$

In between the high- and low-temperature conditions, the material undergoes a phase transformation, with the measured heat exchange rate given by $\dot{Q}_v$ in (70). The unknown parameters in the expression on the right are ΔG_0 and the distribution $p(T)$, with ξ given by (59). In general, it is necessary to choose a functional form for the distribution, $p(M_0)$. This distribution will have certain parameters. Those parameters along with ΔG_0 need to be found by matching the theoretically measured $\dot{Q}_v$ by (70) and experimentally measured values of the same quanity. This can be done, in principle, by using established numerical procedures on system identification. However, the problem is considerably simplified if it is assumed that $C_M = C_A$ (Boyd and Lagoudas 1996), which is frequently the case for Ni–Ti SMAs. This implies $\Delta C = 0$. In that case, (70) reduces to

$$\dot{Q}_v = -\rho V \Delta G_0 p(T) \dot{T} + \rho V C_A \dot{T} \tag{73}$$

or

$$\dot{Q}_v - \rho V C_A \dot{T} = -\rho V \Delta G_0 p(T) \dot{T}. \tag{74}$$

For this special case, the line joining the points M and A is parallel to the horizontal axis. The latent heat per unit volume reduces from (66) to

$$H_f = \rho \int_{-\infty}^{+\infty} \Delta G_0 p(T) \, dT = -\frac{1}{V} \int_{-\infty}^{+\infty} \frac{1}{\dot{T}}$$
$$\times [\dot{Q}_v - \rho V C_A \dot{T}] \, dT \tag{75}$$

where the integral on the right-hand side is the area between the full curve and dashed curve (for the case, $C_M = C_A$). The derived expression in (75) reduces to (1) when $\dot{T}$ is constant. Since in a DSC measurement, $\dot{T}$ is held constant and by the definition, $\int_{-\infty}^{+\infty} p(T) \, dT = 1$ (see (11)), (75) becomes

$$\rho \Delta G_0 = -\frac{1}{\dot{T} V} \int_{-\infty}^{+\infty} [\dot{Q}_v - \rho V C_A \dot{T}] \, dT. \tag{76}$$

Once $\rho \Delta G_0$ is found from (76), the distribution, $p(T)$, follows from (74) as

$$p(T) = -\frac{1}{\rho V \Delta G_0 \dot{T}} (\dot{Q}_v - \rho V C_A \dot{T}). \tag{77}$$

The next parameter to be determined is $\rho\Delta S$ which can be found by computing $\partial\sigma/\partial T$ from (53) at the reference state, $\sigma = 0$ and $T = T_0$. At a given σ and T, $\partial\sigma/\partial T$ from (53) is

$$\frac{\partial\sigma}{\partial T} = -\frac{(\alpha_M - \alpha_A)\sigma + \rho\Delta C \ln(T/T_0) + \rho\Delta S}{H + (E_M^{-1} - E_A^{-1})\sigma + (\alpha_M - \alpha_A)\Delta T} \quad (78)$$

where it is seen that $\partial\sigma/\partial T$ is not constant (as it depends on σ and T) unlike the original assumption made, $\partial\sigma/\partial T = D_M$ (the slope of the martensitic transformation lines in figure 2(b)). In reality, the deviation of $\partial\sigma/\partial T$ from linearity will be small when $\alpha_M \approx \alpha_A$, $\Delta C \approx 0$ and $H \gg (E_M^{-1} - E_A^{-1})\sigma + (\alpha_M - \alpha_A)\Delta T$, a situation not uncommon in Ni–Ti SMAs, for example. For the general case however, we shall assume that the theory satisfies the identity $\partial\sigma/\partial T = D_M$ only at the reference state. At that state with $\sigma = 0$ and $T = T_0$ (or $\Delta T = 0$), (78) reduces to

$$\frac{\partial\sigma}{\partial T} = -\frac{\rho\Delta S}{H} = D_M \quad (79)$$

by which

$$\rho\Delta S = -HD_M. \quad (80)$$

The procedure to determine the parameter H will be given at the end of this section. The parameter D_M can be found from constant load thermal transformations at two different stress levels. We shall return to this point in the last section.

The last parameter Y_c for a cluster (with martensitic transformation temperature M_0) will follow from (53) (with $\sigma = 0$) as

$$Y_c = -\rho\Delta C\left[\Delta M_0 - M_0\ln\left(\frac{M_0}{T_0}\right)\right] + \rho\Delta S M_0 - \rho\Delta G_0. \quad (81)$$

Using the parameters found above in (80) and (81), the relation between σ and T at which the transformation occurs in a cluster with stress-free transformation temperature, M_0 is given as

$$\sigma H + \tfrac{1}{2}(E_M^{-1} - E_A^{-1})\sigma^2 + (\alpha_M - \alpha_A)\Delta T$$
$$-\rho\Delta C\left[\Delta T - T\ln\left(\frac{T}{T_0}\right) - \Delta M_0 + M_0\ln\left(\frac{M_0}{T_0}\right)\right]$$
$$-HD_M(T - M_0) = 0. \quad (82)$$

The above equation has a particularly simple form if we assume $\Delta C = 0$ and $H \gg \tfrac{1}{2}(E_M^{-1} - E_A^{-1})\sigma + (\alpha_M - \alpha_A)\Delta T$. It reduces to

$$M = M_0 + \frac{\sigma}{D_M} \quad (83)$$

where M is the modified martensitic transformation temperature of a generic cluster. Equation (83) is a 1D analog of (5) once we identify $D_M^c = D_M$. It is seen from (83) that the stress-free transformation temperature, M_0, for all clusters are modified by the same amount σ/D_M. Thus when $\sigma \neq 0$, the statistical distribution, $p(M_0)$, in the stress-free case can be restated as $p(M - \sigma/D_M)$; the original distribution $p(M_0)$ thus undergoes a 'rigid body' shift along the temperature axis, by an amount σ/D_M. An identical relation follows for $D_A^c = D_A$ with

$$A = A_0 + \frac{\sigma}{D_A} \quad (84)$$

with the modified distribution being $g(A - \sigma/D_A)$.

The last parameter H can be identified by either considering a $A \to M$ or a $M \to A$ transformation under dead load. We consider both, as these will be needed in the next section on the numerical and experimental results. Regarding the former, we find the total increment in uniaxial strain, $\Delta\epsilon$, of an initially austenitic polycrystal loaded with stress σ and made to undergo the $A \to M$ transformation by a decrease in the temperature. At a current temperature T, the total strain increment with reference to the initial state is denoted as $\Delta\epsilon$ and follows from (51) and (52). It is given as

$$\Delta\epsilon = \int_T^\infty [(E_M^{-1} - E_A^{-1})\sigma + (\alpha_M - \alpha_A)\Delta M + H]$$
$$\times p(M - \sigma/D_M)\,\mathrm{d}M + \int_T^\infty [\alpha_A + \xi(\alpha_M - \alpha_A)]\,\mathrm{d}\tilde{T} \quad (85)$$

where we have used the modified temperature, M, given in (83) and $\xi = \int_T^\infty p(M - \sigma/D_M)\,\mathrm{d}M$, in analogy to (59). The total change in the strain at the completion of the transformation occurs at $T \to -\infty$. Equation (85) simplifies considerably if it is assumed that $\alpha_M \approx \alpha_A$. In that case

$$\Delta\epsilon = [(E_M^{-1} - E_A^{-1})\sigma + H]\int_T^\infty p(M - \sigma/D_M)\,\mathrm{d}M$$
$$+ \int_T^\infty \alpha_A\,\mathrm{d}\tilde{T}. \quad (86)$$

In practice, the change in strain during the $A \to M$ transformation as the polycrystal is cooled from an elevated (but finite) temperature, T_h, to the current temperature T is of interest. It is given as

$$\Delta\epsilon = [(E_M^{-1} - E_A^{-1})\sigma + H]\int_T^{T_h} p(M - \sigma/D_M)\,\mathrm{d}M$$
$$+ \int_T^{T_h} \alpha_A\,\mathrm{d}\tilde{T}. \quad (87)$$

If the transformation is assumed to be practically complete at $T = T_l$ ($T_l < T_h$), then (87) reduces to

$$H = \Delta\epsilon - \alpha_A(T_h - T_l) - (E_M^{-1} - E_A^{-1})\sigma \quad (88)$$

where we have used $\int_{T_l}^{T_h} p(M - \sigma/D_M)\,\mathrm{d}M \approx 1$.

Similar equations can be derived for the $M \to A$ transformation. The total increment in strain of a fully martensitic polycrystal loaded with stress σ is

$$\Delta\epsilon = -\int_{-\infty}^T [(E_M^{-1} - E_A^{-1})\sigma + (\alpha_M - \alpha_A)\Delta A + H]$$
$$\times g(A - \sigma/D_A)\,\mathrm{d}A + \int_{-\infty}^T [\alpha_A + \xi(\alpha_M - \alpha_A)]\,\mathrm{d}\tilde{T} \quad (89)$$

where $\xi = 1 - \int_{-\infty}^T g(A - \sigma/D_A)\,\mathrm{d}A$. If $\alpha_A \approx \alpha_M$, the above equation reduces to

$$\Delta\epsilon = -\int_{-\infty}^T [(E_M^{-1} - E_A^{-1})\sigma + H]g(A - \sigma/D_A)\,\mathrm{d}A$$
$$+ \int_{-\infty}^T \alpha_A\,\mathrm{d}\tilde{T}. \quad (90)$$

In practice, if the change in strain during the $M \rightarrow A$ transformation by heating from a low temperature, T_l, to the current temperature T is of interest, it is given as

$$\Delta\epsilon = -\int_{T_l}^{T} [(E_M^{-1} - E_A^{-1})\sigma + H]g(A - \sigma/D_A)\,\mathrm{d}A$$

$$+ \int_{T_l}^{T} \alpha_A\,\mathrm{d}\tilde{T}. \tag{91}$$

If the transformation is practically complete at $T = T_h$, then (91) reduces to

$$H = \alpha_A(T_h - T_l) - (E_M^{-1} - E_A^{-1})\sigma - \Delta\epsilon \tag{92}$$

where we have used $\int_{T_l}^{T_h} g(A - \sigma/D_A)\,\mathrm{d}A \approx 1$.

4.2. The probability distribution function, $p(M_0)$

Before we turn to experimental results, we select the functional form of the distribution, $p(M_0)$. There are several functions at our disposal to model such a process. Some of the principal ones are the Gaussian, Poisson, beta distributions etc (Scheaffer and Mendenhall 1975) and Weibull and Normal distributions (Phoenix and Tierney 1983, Chou 1992). The naturally occuring defects in an annealed polycrystal (without any other special thermomechanical treatment) is expected to be adequately represented by a symmetric bell-shaped curve. Therefore, for the present problem, we select the normal distribution

$$p(M_0) = \frac{1}{s\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{M_0 - \bar{M}_0}{s}\right)^2 \right]$$

$$s > 0,\ -\infty \leq M_0 \leq +\infty \tag{93}$$

where $\bar{M}_0$ is the mean of the distribution and s is the standard deviation. While the choice of this function is not unique, it possesses the desirable feature that the range of M_0 is unbounded. In other words, there is no artificially imposed finite lower and upper limits for M_0, unlike the conventional assumptions of a M_s^0 and M_f^0 (as shown in figure 1). It is seen that with stress, σ, and the modified transformation temperatures M given by equation (83), it can be shown that (93) becomes

$$p(M - \sigma/D_M) = p(M_0). \tag{94}$$

The distribution in the austenitic temperatures follows accordingly. We now turn to a theoretical simulation of some experimental data for a purely thermal transformation first. This is followed by simulation/predictions for strain–temperature recovery under a dead load thermal transformation.

4.3. Comparison with experimental results

A DSC experiment was done to measure the heat release rate from a SMA polycrystal during a purely thermal transformation. This was first depicted in figure 1(a). The probability distribution function given by (93) is fitted through (74) which is written as

$$p(T) = -\frac{1}{\rho V \Delta G_0 \dot{T}}(\dot{Q}_v - \rho V C_A \dot{T}) \tag{95}$$
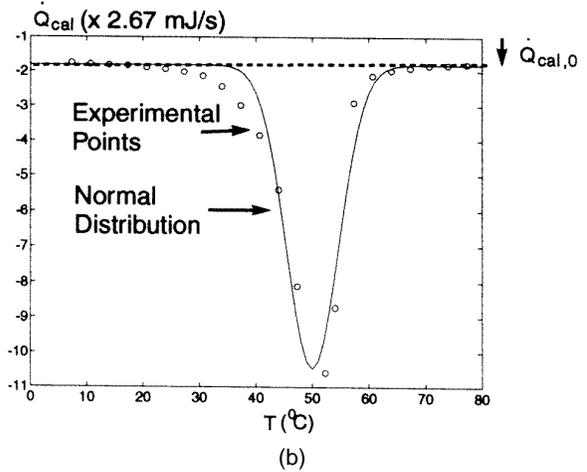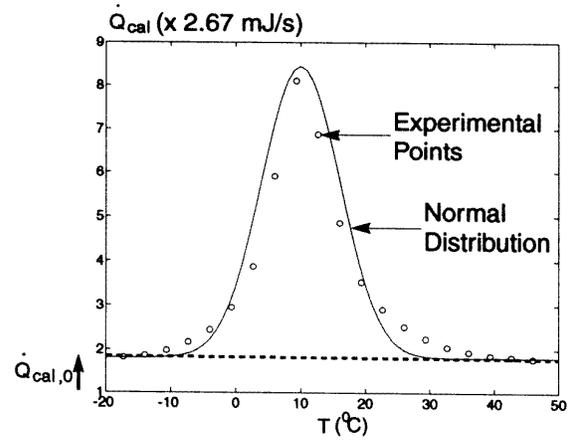
**Figure 5.** Theoretical simulation of a DSC measurement of a SMA polycrystal: (a) cooling and (b) heating.

and from (2)

$$p(T) - \frac{1}{\rho V \Delta G_0 \dot{T}}(\dot{Q}_{cal} - \dot{Q}_{cal,0}). \tag{96}$$

The value of $\rho V \Delta G_0 \dot{T}$ in (95) follows from the area between the curve defined by the circles and the horizontal dashed curve in figure 4. It is (from (2) and (76))

$$\rho \Delta G_0 = \frac{1}{\dot{T}V} \int_{-\infty}^{+\infty} (\dot{Q}_{cal} - \dot{Q}_{cal,0})\,\mathrm{d}T. \tag{97}$$

We now need to find the parameters $\bar{M}_0$ and s (for cooling) and $\bar{A}_0$ and s (for heating), pertaining to the distribution so that (95) is satisfied. Here, and subsequently, we shall assume that the distribution in the austenitic temperatures follow from a 'rigid' body shift of the distribution in the martensitic transformation temperatures, $p(M_0)$. Thus, with the form of (93) for the normal distribution, (13) becomes $g(A_0) = p(A_0)$. In reality, it will be possible to satisfy (95) only approximately. A reasonable simulation of the experimental data points in figure 5 by a normal distribution is obtained with parameters $\bar{M}_0 = 10\,°\mathrm{C}$, $s = 6$ (for cooling, figure 5(a)) and $\bar{A}_0 = 50\,°\mathrm{C}$, $s = 4.6$ (during heating, figure 5(b)).
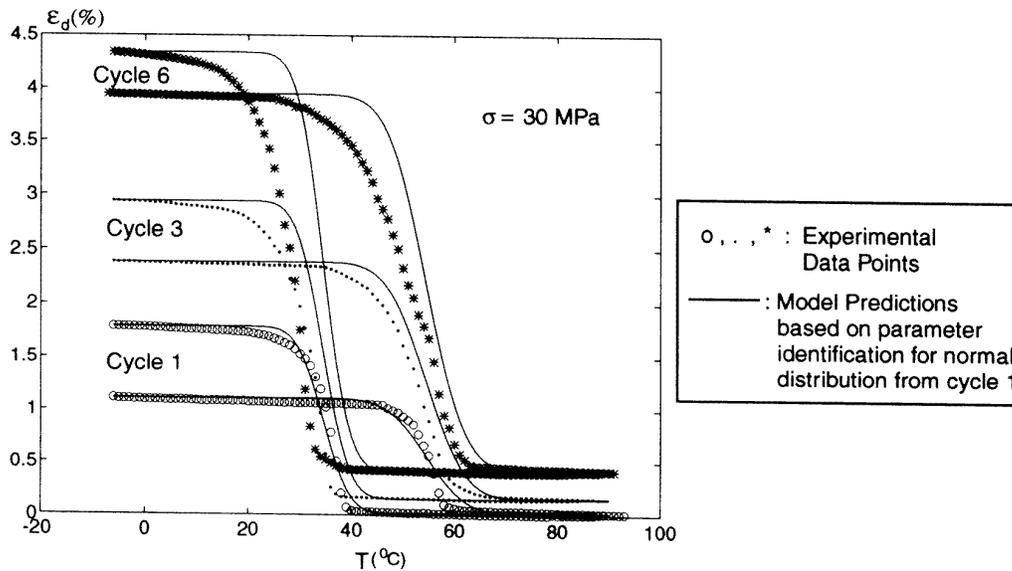
Figure 6. Cyclic thermally induced transformation under dead load of σ = 30 MPa: Comparison of theoretical simulation/prediction and experiment.
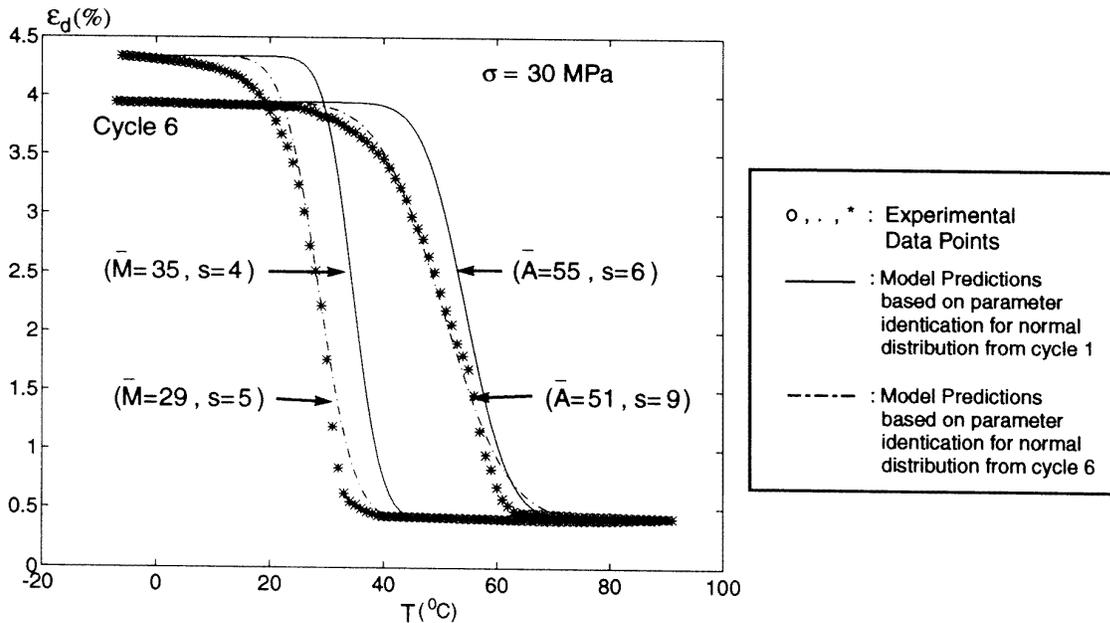
Figure 7. The sixth cycle of thermally induced transformation under dead load of σ = 30 MPa: Comparison of modified prediction and experiment.

We now report some ongoing experiments on the cyclic heating and cooling of an initially annealed SMA polycrystal under a dead load. The material tested is from a different batch from that for which the DSC measurements are displayed in figure 5. Hence, no attempt will be made to connect the DSC measurements with the dead load thermal transformation experiment. The latter was performed at the Active Materials Laboratory of Texas A&M University and is described briefly. The experimental setup was kept in a freezer at approximately $-20\,^{\circ}$C (experimental data points, when displayed, will be from $\approx -8\,^{\circ}$C to about $90\,^{\circ}$C, within which the transformation is observable), and at this

temperature, the originally annealed SMA wire was loaded to the stress of 30 MPa. This resulted in a substantial amount of permanent strain due to detwinning of the self-accomodating martensitic phase. While the stress was maintained at that level, the wire was heated with electrical current and made to undergo the complete martensitic to austenitic phase transformation; the inelastic strain was completely recovered during the first cycle. When the current was switched off, the wire cooled back to the low temperature of its environment and underwent the austenitic to martensitic phase transformation accompanied by the permanent strain due to detwinning. The inelastic strain at

the end of the cooling step was found to be more than that at the previous step. The second cycle, originally shown in figure 1(b), was somewhat different from the first. If the total strain at a given temperature T is ϵ, the depicted strain ϵ_d is taken as

$$\epsilon_d = \epsilon - E_A^{-1}\sigma - \alpha_A(T - T_l) \qquad (98)$$

where α_A, we recall, is the coefficient of thermal expansion of austenite. The change in the depicted strain, $\Delta\epsilon_d$, due to a change in temperature from T_1 to T_2 is related to the change in the total strain, $\Delta\epsilon$, through

$$\Delta\epsilon_d = \Delta\epsilon - \alpha_A(T_2 - T_1). \qquad (99)$$

It is seen that on heating the wire (at the end of the first cycle) from the point A at the low temperature T_l to the point B at the elevated temperature T_h, the strain changed from that at A, $\epsilon_{d,A}$, to that at B, $\epsilon_{d,B}$. Since between these points, it is clear that the $M \to A$ transformation is practically complete, it is expected that the inelastic strain owing to phase transformation would also have been recovered, resulting in $\epsilon_{d,B} = 0$. We interpret the residual strain at the point B as the plastic strain due to dislocation movement. Heating the wire back to the point C results in a strain, $\epsilon_{d,C}$, which is seen to be somewhat more than it had at the start of the second cycle (compare points A and C). The residual strain at the point B and the increase in the inelastic strain between cycles is indicative of the phenomenon of the two-way training of wires.

Since our focus is on the gradual transformation behavior and not on the two-way training of a SMA polycrystal, we shall implement the theoretical simulation/prediction separately for the heating and cooling curves.

For the heating part of a cycle of heating and cooling, we find H from (92) and (99) with $T_2 = T_h$ and $T_1 = T_l$ (the other parameters in these two equations are given subsequently). For the cooling part, we find H from (88) and (99) with $T_2 = T_l$ and $T_1 = T_h$ (we take $T_l = -6\,°C$ and $T_h = 90\,°C$ respectively at $\sigma = 30$ MPa). The Young's modulus of austenite and martensite are taken as $E_A = 30$ GPa and $E_M = 13$ GPa. The coefficient of thermal expansion for the two phases are $\alpha_A = 11 \times 10^{-6}\,°C^{-1}$ and $\alpha_M = 6.6 \times 10^{-6}\,°C^{-1}$ will also be used. These parameters are obtained from Boyd and Lagoudas (1996). The prediction of the increment in the strain, $\Delta\epsilon_d$, will be found from (98) where $\Delta\epsilon$ follows from either (87) or (91) which are based on the assumption, $\alpha_M \approx \alpha_A$. Even though, in reality, $\alpha_A \approx 2\alpha_M$, the assumption of $\alpha_M \approx \alpha_A$ is still felt to be reasonable as increments in thermal strains are very small compared to inelastic strains of phase transformation. Recall that since the wire is under stress, the modified transformation temperatures, A and M, given by (83) and (84) are operative and hence $p(M)$ will follow from (94) (and likewise for $p(A)$). With such an assumption, the parameters of the normal distribution for the first cycle at $\sigma = 30$ MPa turn out to be $\bar{A} = 55\,°C$ and $s = 6$ (for heating) and $\bar{M} = 35\,°C$ and $s = 4$ (for cooling). The comparison between the simulation and the experiment is shown as Cycle 1 in figure 6 (compare the open circles of

the experimental data points and the associated continuous curve). With these values of the parameters, we predict the evolution of the strain at the third and the sixth cycle (with corresponding values of H), also shown in the same figure. It is seen that with increase in the number of cycles, the prediction deteriorates. This is probably due to the fact that with continued thermal cycling under stress, the inherent defect structure of the polycrystal undergoes changes owing to, in part, development of residual plastic strains and thus a distribution which models the defect structure in the first cycle may not continue to represent equally well the modified defect structure in subsequent cycles. In fact, we recompute the parameters of the normal distribution to improve upon the original prediction for the sixth cycle, shown in figure 7. It is seen that with new parameters, $\bar{A} = 51$, $s = 9$ (for heating) and $\bar{M} = 29$, $s = 5$ (for cooling), the prediction improves significantly. It is thus seen from figure 7 that during heating, the average austenitic transformation temperature, $\bar{A}$, decreases from its value in the first cycle by $4\,°C$ whereas the average martensitic transformation temperature, $\bar{M}$, decreases by $6\,°C$. It thus appears that the cyclic thermal response seems to favor the austenitic transformation to occur during heating (evidenced by the decrease in $\bar{A}$) whereas it makes it more difficult for the martensitic transformation to occur during cooling (evidenced by the decrease in $\bar{M}$). Regarding the change in the standard deviation, it is seen that it increased by $3\,°C$ for the austenitic transformation, whereas the increase for the martensitic transformation is $1\,°C$. The standard deviation could be taken as a measure of the extent by which the defects interact to cause the polycrystal to deviate from a first-order transition (transformation at a single temperature and not over a range). In that context, it is seen that the modified defect structure in the sixth cycle influences the austenitic transformation more than the martensitic one. We point out that these observations are strictly valid only for the Nitinol wire tested; whether that is a general trend for Nitinol has to be confirmed by additional experiments. In any case, the results of figure 7 indicate that the use of the parameters obtained from the first cycle should be used in the subsequent cycles with caution.

Finally, we give an estimate of the parameters D_M and D_A in (83) and (84). To find these parameters, the simulations are needed to be done at two stress levels. A change in the martensitic temperature follows from (83) as $\Delta M = \Delta\sigma/D_M$, where $\Delta\sigma$ is the difference between the two stress levels (and likewise for D_A). This implies that distributions at two different stress levels will share the same standard deviation but different means. Thus we turn to last figure—figure 8—which is a similar plot of strain–temperature data for the first thermal cycle of an initially annealed SMA wire (different from the wire tested at 30 MPa but from the same batch) under a dead load of $\sigma = 45$ MPa (at this stress, we take $T_l = -8\,°C$ and $T_h = 90\,°C$). We assume that the heating and cooling part of the cycle at $\sigma = 45$ MPA are obtained by a 'rigid body' shift of the distribution obtained for the first cycle at 30 MPa. Thus retaining the standard deviation of 6 and 4 for heating and cooling obtained from the transformations at 30 MPa for that at 45 MPa, we obtain the new means at
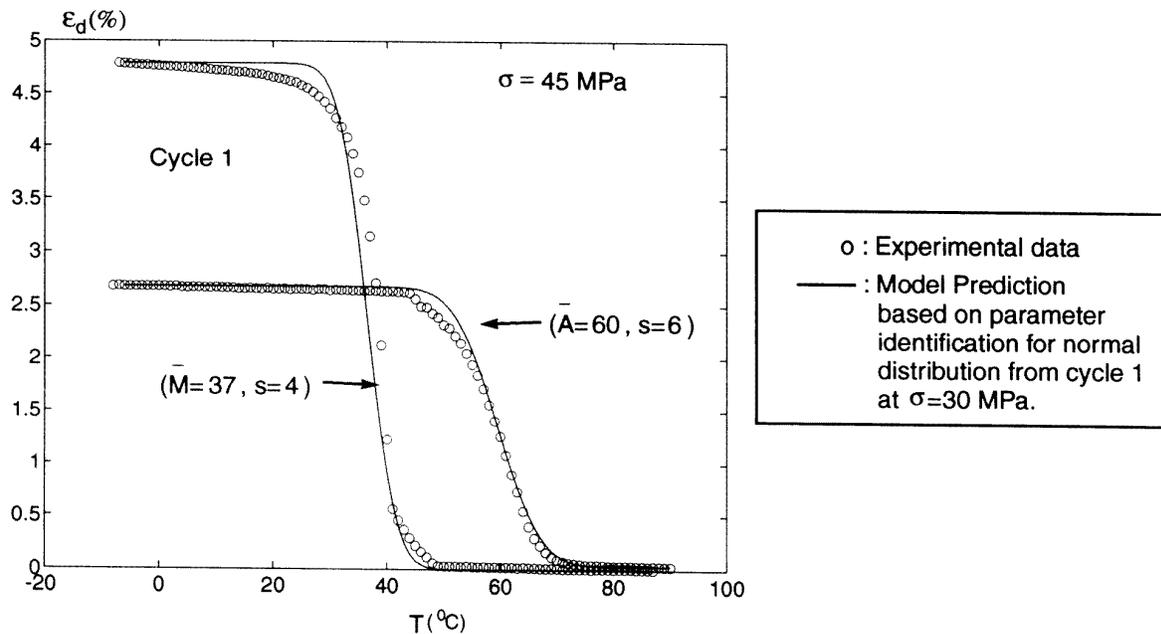
Figure 8. The first cycle of thermally induced transformation under dead load of σ = 45 MPa: Comparison of theoretical prediction and experiment.

45 MPa as $\bar{A} = 60$ (for heating) and $\bar{M} = 37$ (for cooling). It is seen from the comparison that the assumption of the 'rigid body' shift in the temperatures is indeed a good one for the wire tested. With the new mean values, we have $D_A = 3$ MPa $°C^{-1}$ and $D_M = 7.5$ MPa $°C^{-1}$.

5. Conclusions

We have addressed the issue of gradual thermally induced transformation in SMA polycrystals under dead load. It is assumed that a local region of the polycrystal, or a cluster of grains, undergos a first-order transition (transformation at a single temperature), but that owing to the presence of defects and internal stresses, the transformation temperature is taken to vary from one local region to another. The first-order transition of a generic cluster is modeled using the thermodynamic theory of Boyd and Lagoudas (1996) and a spatially uniform stress and temperature assumption leads to a tractable averaging process over all clusters to yield the overall response of the polycrystal. The concept of a statistical distribution in the transformation temperatures is introduced. A significant result of the proposed stochastic thermodynamic theory is that it does away with the necessity of having to artificially introduce 'start' and 'finish' temperatures to characterize the phase transformation in the polycrystal. The statistical distribution is correlated with calorimetric measurements of the latent heat of transformation in a SMA polycrystal and also with the strain recovery against temperature experimental results for untrained SMA wires. We intend to use the concept of the distribution in a future work on stress-induced phase transformation (with changing stresses in addition to changing temperature) of the SMA polycrystal.

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