

Mechanistic simulation of thermomechanical behaviour of thermoelastic martensitic transformations in polycrystalline shape memory alloys

Y. Liu¹, D. Favier² and L. Orgeas²

¹*School of Mechanical Engineering, University of Western Australia, Crawley WA 6009, Australia*

²*Laboratoire Sols-Solides-Structures, UMR CNRS 5521, UJF –INPG, BP. 53, 38041 Grenoble Cedex, France*

Abstract. This paper proposes a mechanistic model to simulate the thermal and mechanical behaviour of shape memory alloys. The model is based on the thermodynamic concept of chemical, elastic and frictional energies for thermoelastic martensitic transformations and plasticity concept of grain interior and grain boundary phases. In a thermoelastic martensitic transformation system, a thermally induced transformation and a mechanically induced (stress-induced) transformation require different operating mechanisms from a mechanistic viewpoint. For a thermally induced transformation, the driving force arises from within the matrix and internal stresses are created as a result of frictional movement. For a mechanically induced transformation, the driving force is provided externally and the frictional movement occurs when the stress exceeds a critical value. This paper proposes a unified mechanistic model taking into account this difference. The model is able to describe, in a schematic and qualitative manner, the behaviour of a thermoelastic martensitic transformation system in both thermally induced and mechanically induced processes, including full and partial thermal transformation cycles, stress-induced martensitic transformation, pseudoelastic deformation and ferroelastic deformation via martensite variant reorientation. Such a model allows the discussion of several aspects concerning the thermal and mechanical behaviour of thermoelastic martensitic transformations, such as the non-linear pseudoelasticity, deformation-induced two-way memory effect, strain dependence of mechanical hysteresis and minor loop behaviour of deformation.

Key words. martensitic transformation, martensite stabilisation, shape memory effect, NiTi, spring-dashpot model

1. INTRODUCTION

Shape memory alloys, owing to their thermoelastic martensitic transformations, exhibit a range of unique thermomechanical behaviour, including shape memory effect, two-way memory effect, pseudoelasticity associated with stress-induced phase transformations, and ferroelasticity associated with martensite variant reorientations. The process of a thermoelastic martensitic transformation, in fact, is a combination of a phase transformation and a mechanical deformation. This unique combination renders the transformation special thermodynamic characteristics. It has been established in thermodynamic theories that the process of a thermoelastic martensitic transformation is governed by a free energy balance including reversible elastic energy and irreversible frictional energy contributions [1, 2].

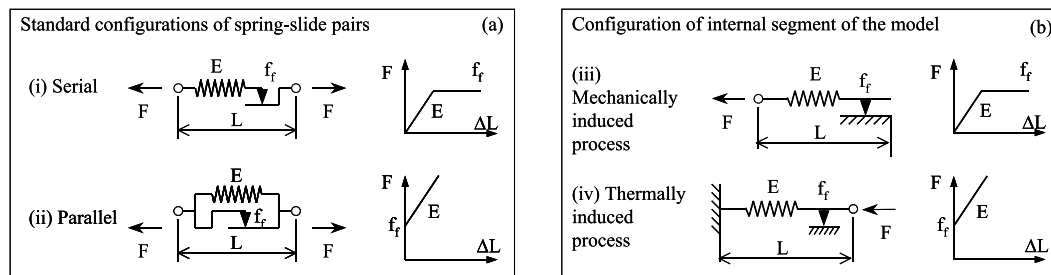


Figure 1. (a) Standard serial and parallel configurations and their mechanical characteristics of spring-slider pairs; (b) Spring-slider configuration of the model and its performances when activated from the left (external loading) and from the right (internal loading).

As a result, the transformation exhibits typical hysteretic loops during a transformation cycle, induced thermally or mechanically.

Such behaviour, from a mechanistic point of view, can always be simulated by simple mechanistic models. Such one-dimensional models have been extensively used in the development of plasticity and viscoelasticity theories [3]. Based on the analysis of such mechanical models, three-dimensional theories are then proposed as a generalisation. Such mechanistic models have proven to be very useful in illustrating, at least qualitatively, the roles played by various factors embedded in complex thermal and mechanical behaviour of specific materials [4]. Mechanistic models describing plastic behaviour involve springs reflecting elasticity of the crystallographic network and slides depicting mechanisms like slip. Simple serial and parallel configurations of spring-slider pairs are shown in Figure 1(a) together with their force-displacement characteristics, with (i) for the serial connection and (ii) for the parallel connection. Similar mechanistic expressions are also made for viscoelasticity using springs and dashpots.

Some mechanistic models aimed at describing the behaviour of shape memory alloys have been reported in the literature [5–9]. Some of the models have been the basis of three-dimensional constitutive equations [7]. Most of the models focus on the hysteretic behaviour of the transformations, with no distinction between thermally induced and mechanically induced processes. Regarded as a mechanistic system, however, thermoelastic martensitic transformations impose a dilemma. From a mechanistic viewpoint, a thermally induced transformation and a mechanically induced (stress-induced) transformation require different operating mechanisms. For a thermally induced transformation, the driving force arises from within the matrix and internal stresses are created as a result of frictional movement. For a mechanically induced transformation, the driving force is provided externally and the frictional movement occurs when the stress exceeds a critical value. Largely due to this difference, existing models based on the spring-slide concept are mostly suited for either thermally induced transformations or mechanically induced transformations. In this paper a unified mechanistic model is proposed. The model is able to describe, in a schematic and qualitative manner, the behaviour of a thermoelastic martensitic transformation system in both thermally induced and mechanically induced processes, including full and partial thermal transformation cycles, stress-induced martensitic transformation, pseudoelastic deformation and ferroelastic deformation via martensite variant reorientation. Such a model allows the discussion of several aspects concerning the thermal and mechanical behaviour of thermoelastic martensitic transformations, such as the deformation-induced two-way memory effect [10], strain dependence of mechanical hysteresis and minor loop behaviour of deformation [11, 12].

2. THE PHYSICAL PHENOMENA IMPLIED IN THE BEHAVIOUR OF SHAPE MEMORY ALLOYS

It is known that thermally induced martensite forms in self-accommodating structures [13, 14]. Martensite induced by stress is generally regarded to form into single variants of most favoured orientations relative the external stress in each grain. However, such a transformation-deformation process is practically impossible in a polycrystalline matrix without internal plastic deformation to co-ordinate for the mismatch in orientation among the favoured variants in neighbouring grains [10, 15, 16]. This implies that, in addition to frictional resistance to transformation phase boundary movement, which is universal for both thermally induced and mechanically induced transformations, there also exists a mechanical resistance to global deformation in a polycrystalline matrix [17]. The effect, or the existence, of this resistance can be explained as following. In the absence of this resistance, it would be expected that only an infinitesimal external force be required to trigger a stress-induced martensitic transformation in a polycrystalline specimen at a temperature just above M_s , when the chemical resistance to the transformation is practically zero (taking into account of the frictional resistance to phase boundary movement). This, obviously, has never been observed. In fact, experimental evidences have shown that a finite external stress is always required to induce a martensitic transformation for polycrystalline NiTi at M_s [18, 19]. Based on this understanding, from a mechanical viewpoint, a polycrystalline aggregate can be modelled as shown in Figure 2, in which a network of finite volume is created to represent the “grain boundaries” or “grain boundary affected regions”. This is similar to the simulation of “grain boundary phase” and “grain interior phase” in the discussion of plasticity for polycrystalline materials [20, 21]. The interior of the cells (grains) represents the transforming body, which is capable of multiple-variant shape distortion, and the arrows indicate the orientations of the favoured variants in each grain with respect to one unmarked external stress. The grain boundary regions impose resistance to global shape change and thus experience plastic deformation during stress-induced martensitic transformation and martensite reorientation deformation processes. It needs to be clarified that the width of the “grain boundary affected regions” (GBAR) is dependent on the nature of the deformation. For plastic deformation, the width is compatible to the need to accommodate dislocation activities and thus is generally significant only for ultrafine-grained and nanocrystalline structures. For deformation via stress-induced martensitic transformation or martensite reorientation, where the lattice distortion is large (up to 9%) and the physical size of martensite variant domains is large, the width is also expected to be large. This also naturally extends to that the width of the GBARs for an isotropic matrix, where deformation mismatch between grains is large, is greater than that in preferentially textured structures where grains deform coordinatively in the same direction. Thus, during a thermally induced transformation where no global deformation is produced, the boundary regions are ineffective (virtually of zero width) and the transformation operates within the interior of the cells (grains). During a stress-induced process, via either a phase transformation or variant reorientation, both the boundary regions and the interior are active. It may also be postulated that during mechanical cycling, via either stress-induced martensitic transformation (pseudoelastic cycling) or martensite reorientation (ferroelastic cycling), the critical stresses decrease in subsequent cycles relative to those in the first transformation cycle, due to reduction of the effective width of the GBARs. It ought to be pointed out that, in similar mechanistic models reported in the literature, the effects of GBARs and the differences in this aspect between thermally induced and mechanically induced transformation processes have largely been neglected.

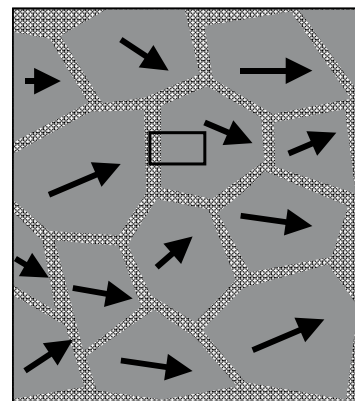


Figure 2. Schematic illustration of polycrystalline aggregate of grains of preferential variants of various orientations.

3. THE MECHANISTIC MODEL

In principle, a hysteretic thermoelastic transformation process can always be described by using certain arrangement of elastic springs and frictional slides. Figure 3 depicts a mechanical model describing the thermomechanical behaviour of one austenitic single crystal transforming into one single martensite variant. This elementary model is similar to that used by Lu et al [5]. Element A represents a finite unit that transforms to one martensite variant upon cooling. This unit is accompanied by a frictional slide (element B) and by a spring (element C). The frictional slide accounts for the internal resistance to transformation or reorientation boundary movement. The slide has a limited sliding distance determined by the lattice distortion of the transformation. The spring expresses the elastic aspect of the transformation. Assembly A-B-C expresses a transformation unit. The plasticity of the martensite is expressed by frictional slide F. Function box F_{ch} expresses the chemical (thermal) driving force for the transformation, which is temperature-dependent. This force is defined as a linear function of temperature, to conform to the Clausius-Clapeyron relation:

$$\begin{aligned} \text{For } A \rightarrow (M+) \text{ or } (M+) \rightarrow A: & \quad F_{ch} = -k(T - T_0), \\ \text{For } A \rightarrow (M-) \text{ or } (M-) \rightarrow A: & \quad F_{ch} = k(T - T_0), \end{aligned} \quad (1)$$

where $T_0 = \Delta H / \Delta S$, the equilibrium temperature between the two transforming phases, and k is the Clausius-Clapeyron coefficient (i.e. a stress-temperature converter). This force is ineffective ($F_{ch} = 0$) for deformation in single-phase state, e.g., martensite reorientation or plastic deformation of austenite.

The challenge in achieving a valid arrangement to describe the thermal and mechanical behaviour of a thermoelastic martensitic transformation in a polycrystalline specimen, however, rests with the intrinsic differences between a thermally activated process and a mechanically activated (stress-induced) process. For a thermally induced transformation, the driving force arises from within the matrix and internal stresses are created as a result of frictional movement. For a mechanically induced transformation, the driving force is provided externally and the frictional movement occurs when the stress field exceeds a critical value. Based on the physical phenomena implied in the behaviour of shape memory polycrystalline alloys presented above and with respect to the local environment indicated by the rectangle in Figure 2, a twin-variant mechanistic model is developed to model the behaviour of a polycrystalline shape memory alloy, as shown in Figure 4.

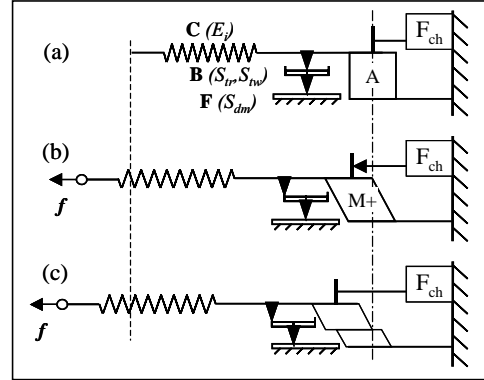


Figure 3. Single variant mechanistic model based on spring-slide concept: (a) austenite, (b) martensitic transformation and (c) plastically deformation of martensite.

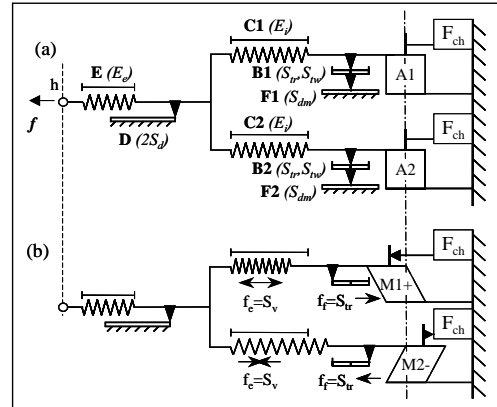


Figure 4: Twin-variant mechanistic model based on spring-slide concept: (a) austenite; (b) thermally formed self-accommodating martensite, at just before the completion of the transformation.

In this model two identical transformation units are connected in parallel to form the transformation segment. Outside the transformation segment there is another slide (element **D**) and another spring (element **E**). The external spring expresses the elasticity of the aggregate. The external slide expresses the frictional resistance to global shape change imposed by the boundary regions, or plasticity of the aggregate experienced during stress-induced martensitic transformation or variant reorientation deformation processes. It ought to be pointed out that this plasticity is in addition to the plasticity of the martensite, as defined in the strict sense of dislocation movement and dislocation production of martensite, which is expressed by the slides **F**. It is deemed that the friction on slides **F** is greater than the friction on either slide **B** or slide **D**, to allow stress-induced martensitic transformation (within the vicinity of M_s temperature) or martensite reorientation without plastic deformation. The characteristic frictions of the slides and stiffness of the springs are indicated in parentheses for each element in the figure. Slide **B** is given two friction values, S_{tr} and S_{tw} , corresponding to the friction for phase boundary movement during phase transformation and that for variant boundary movement during reorientation, respectively. It is clear by these definitions that slide **B** is operative for martensite reorientation in single crystals, slide **B** and slide **D** are effective for martensite reorientation in a polycrystalline matrix, and slides **B**, **D** and **F** are operative for plastic deformation of oriented martensite in both single crystal and polycrystalline matrices. The frictions on all three slides are subjected to strain hardening when plastic deformation occurs. It needs to be pointed out that having surrendered its elastic and frictional aspects to the internal spring and the internal slide and its plasticity to slide **F**, element **A** becomes symbolic of the transforming unit preserving only its geometric attributes. This model conforms to the two distinctive requirements for thermally induced and mechanically induced transformation processes in one unity. Extract of the internal segment for the transforming units of the model and its behaviour are shown in Figure 1(b), with (iii) showing the unit operating in the mode of mechanically induced transformation and (iv) showing the unit operating in the mode of thermally induced transformation.

For a thermally induced transformation, the driving force is from within the transforming units. Upon cooling, the two units form into variants in opposite directions to express the self-accommodating structure of the variants, as shown in Figure 4(b). In the presentation, slides **F1** and **F2** are omitted for simplicity. These two slides are only operative for plastic deformation of austenite or oriented martensite. It is seen that each variant produces a local deformation corresponding to the lattice distortion of the martensite. The local deformations of the two variants are cancelled in the self-accommodating structure, giving a net zero displacement at location **h**, which corresponds to the perimeter of the grain, or the grain boundary. During the transformation a frictional force, $f_f=S_{tr}$, is experienced by each unit, where S_{tr} is the frictional resistance to the displacive movement of transformation boundaries. At the same time, an elastic force, $f_e=S_v$, is gradually accumulated during the growth of martensite variants (the original length of the springs are marked atop the springs as reference to indicate the states of the elastic forces). It also needs to be clarified that, in the real case, the majority of the lattice distortion of the transformation is accommodated in the self-accommodation structure and only a small portion of it contribute to the establishment of long range internal elastic stresses beyond the immediate vicinity of transformation boundaries. This translates in the model characteristics a much-softened stiffness for the internal springs, as relative to the modulus of elasticity of the matrix.

4. THERMOMECHANICAL BEHAVIOUR OF THE MODEL

4.1. Thermal transformation

Figure 5(a) shows the behaviour of the model operating in thermal transformation mode. The envelope loop shows the full transformation cycle. The lines within show the possible paths of partial cycles, in any combination following clockwise flow. The model suggests that the temperature hysteresis is independent of the fraction of transformation. Reflecting critical driving force, F , in terms of temperature

according to:

$$T = T_0 - \frac{1}{k}F \quad (2)$$

conditions at the critical points of the complete transformation cycle can be identified as:

$$T_{(1)} = T_0 - \frac{1}{k}S_{tr}, \quad T_{(2)} = T_0 - \frac{1}{k}(S_{tr} + S_v), \quad T_{(3)} = T_0 + \frac{1}{k}(S_{tr} - S_v), \quad \text{and } T_{(4)} = T_0 + \frac{1}{k}S_{tr} \quad (3)$$

The thermal hysteresis of the transformation cycle is:

$$\eta_{th} = T_{(4)} - T_{(1)} = \frac{2}{k}S_{tr} \quad (4)$$

Actual thermal transformation behaviour, as measured by DSC, of a Ti-50.2at%Ni alloy is shown in Figure 5(b) [22], where the results are shown as integrated curves of transformation heat effect. The measurements were carried out in partial transformation cycles, either on cooling or on heating, as well as in a full transformation cycle. For a partial cooling transformation measurement, the interruption of the cooling midst of the transformation distorted the thermal peak; thus only the heating branch of the partial cycle, where the shape of the (reverse) transformation peak is intact, is integrated for heat determination. Similarly, for partial heating transformations, only the cooling branches are integrated for heat measurements. Therefore, the partial transformation cycles shown in Figure 5(b) appear only as half cycles. It is evident that temperature hysteresis of thermally induced transformations is independent of the fraction of the transformation.

4.2. Deformation via martensite reorientation

Figure 6(a) shows the force (per variant)-displacement behaviour of the model in deformation via variant reorientation of thermally formed self-accommodating martensite. The slopes of the sections of loading and unloading curves are determined by the spring constants (per variant) as:

$$E_1 = \frac{1}{2}E_e ; E_2 = \frac{E_e E_i}{E_e + 2E_i} \text{ and } E_3 = C E_3^0 = C \frac{E_e E_1}{2(E_e + E_i)} \quad (5)$$

As evident, E_1 corresponds to the stiffness of the system when only the external spring is in action. E_2 corresponds to the stiffness when both the external and the two internal springs are in action. E_3^0 corresponds to the stiffness of the system when the external spring and one of the two internal springs are active. The section marked with E_3 corresponds to the reorientation of variant M2 shown in Figure 4(b). E_3 is the apparent stiffness of the system during variant reorientation. As explained earlier, in practice the majority of the transformation lattice distortion is accommodated inelastically in the self-accommodation structure of the variants and only a small fraction of the distortion is accommodated as elastic strain that causes internal elastic stresses. To account for this, E_3^0 is converted to E_3 via a coefficient C , which expresses the ‘‘effective’’ fraction of the lattice distortion that contributes to creating internal stresses and is, thus, less than unity. The critical forces (per variant) are indicated in the figure. The plastic deformation, which is shown in dashed line with strain hardening, is not simulated by the model. It is seen that the loading and unloading curves are non-linear, resulting in a hysteresis. The hysteresis of the unloading-reloading loops increases with increasing total strain. The dashed line following the trace (a-b-c) marks the elbow on the reloading curve. The dashed trace (d-e-f-g) marks the knee of the unloading curve. Figure 6(b) shows the experimentally measured stress-strain curves of a polycrystalline Ti-50.2at%Ni alloy deformed in tension in martensitic state via variant reorientation. Due to the occurrence of the localised deformation (Lüders-like deformation) during martensite reorientation, unloading-reloading curves from the stress plateau region exhibited negligible hysteresis. For sections of deformation beyond the end of the stress plateau, it is clear that the unloading-reloading hysteresis increases with increasing pre-deformation, consistent with the behaviour of the model.

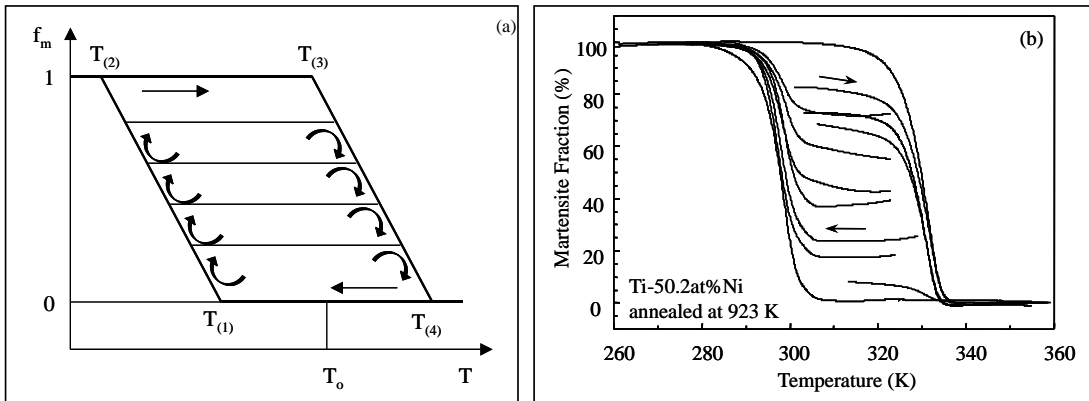


Figure 5. Thermal transformation behaviour, full and partial transformation loops: (a) the model; (b) transformation behaviour of fully annealed polycrystalline Ti-50.0at%Ni.

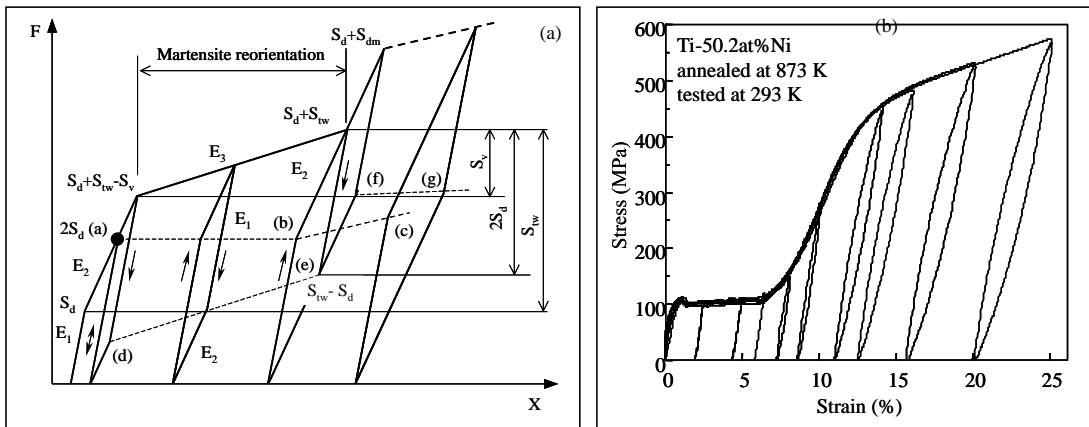


Figure 6. Deformation of thermally formed self-accommodating martensite via martensite reorientation - unloading and reloading behaviour: (a) the model; (b) deformation behaviour of polycrystalline Ti-50.2at%Ni.

Figure 7(a) shows ferroelastic deformation loops via martensite reorientation. The critical stresses and the force-displacement gradients of various sections of the ferroelastic cycle are indicated in the figure. The section between the origin and the point at $(S_d+S_{tw}-S_v)$ corresponds to the initial loading of the self-accommodating thermal martensite, as in the case shown in Figure 6(a). The section following that corresponds to the reorientation of the thermal martensite. The dashed line between (a) and (b) marks the knee point of the unloading curve from the initial reorientation deformation. The dashed horizontal line at (a) marks the knee point of the unloading curve from the full ferroelastic cycle. A reciprocal dashed line is at the symmetric position (point (e)) in the third quadrant for the same event. The dashed line between (c) and (d) marks the onset of martensite reorientation upon reverse loading. With these criteria, deformation behaviour within the envelope of the full ferroelastic loop can be completely mapped out.

Figure 7(b) shows an experimental measurement of the ferroelastic behaviour of a polycrystalline Ti-50.15Ni alloy deformed in shear. It is seen that the model resembles well the experimental observation, notably:

- (i) The initial deformation curve appearing below the full ferroelastic cycle within the first quadrant;
- (ii) The unloading and reloading curves being non-linear in the regime prior to variant reorientation movement;
- (iii) Minor ferroelastic cycles having smaller stress hysteresis than that of the full cycle.

The mechanical hysteresis of the full ferroelastic cycle is:

$$\eta_{MR} = 2S_d + 2S_{tw} \quad (6)$$

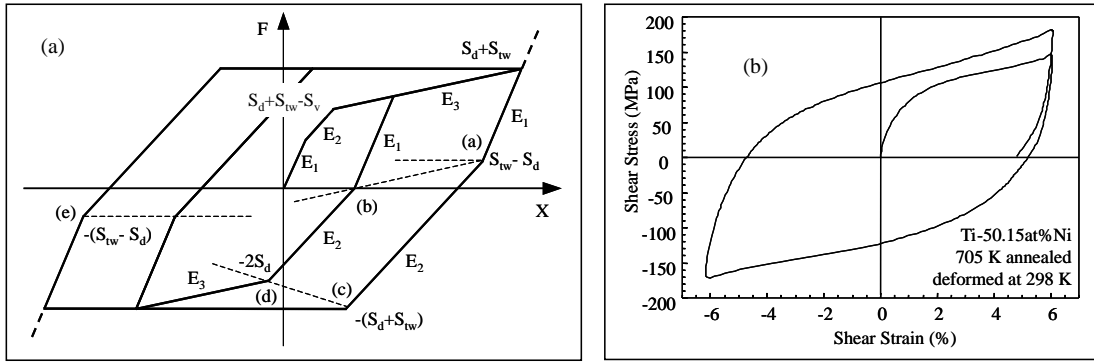


Figure 7. Ferroelastic deformation via martensite reorientation: (a) the model; (b) deformation behaviour of polycrystalline Ti-50.0at%Ni

4.3. Deformation via stress-induced martensitic transformation

Figure 8 shows the deformation behaviour of the model via stress-induced martensitic transformation at two different temperatures. The horizontal dashed line at (S_d+S_{tr}) marks the minimum stress required for stress-induced martensitic transformation at $(M_s < T < T_o)$. The horizontal dashed line at (S_d+2S_{tr}) marks the driving force required for stress-induced martensitic transformation at A_s (neglecting the difference between A_s and A_f), the critical temperature for the reverse transformation of thermally formed martensite. The dashed line at $(2S_d+2S_{tr})$ marks minimum stress required for pseudoelastic recovery, which occurs at $T = A_s^*$, the critical temperature for the reverse transformation of reoriented martensite. The deformation occurring at $T = T_1$ proceeded via stress-induced martensitic transformation. The deformation at $T = T_2$ occurred in pseudoelastic mode with simultaneous recovery at a stress of $(W(T_2) - S_d - S_{tr})$. The hysteresis of the pseudoelasticity is:

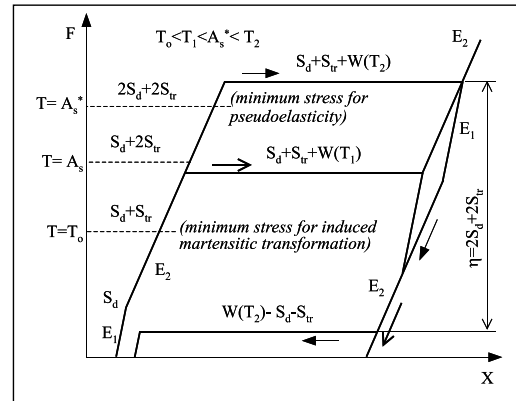


Figure 8: Deformation via stress-induced martensitic transformation.

$$\eta_{ps} = 2S_d + 2S_{tr} \quad (7)$$

It is seen that the hysteresis of pseudoelasticity is compatible to that of ferroelasticity (considering that both processes involve coherent boundary shear movement and assuming that S_{tw} is compatible to S_{tr}) and that the mechanical hysteresis of pseudoelasticity and ferroelasticity are greater than the thermal hysteresis of thermal transformation. It is also noted that the deformation via stress-induced martensitic transformation occurred over a stress plateau, in contrast to that for martensite reorientation.

5. CLOSING REMARKS

Several mechanistic models based on similar spring-slide concept have been proposed in the literature to simulate the thermomechanical behaviour of shape memory alloys. In principle, elastohysteretic phenomena can always be simulated using this concept. The model proposed in this paper is unique and improves existing similar models in two main aspects: (1) it considers the influences of grain boundaries, which is incapable of lattice distortion, which in turn is crystallographically reversible; and (2) recognises and accommodates the intrinsic differences between thermally induced and mechanically induced transformation (and reorientation) processes caused by the effects of the grain boundaries. Consequently, the model is able not only to describe the elastohysteretic behaviour of thermally and mechanically induced transformations, but also lends to direct comparisons between the various processes and the effect of deformation on the thermal transformation behaviour.

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