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Mechanistic simulation of martensite reorientation deformation of polycrystalline NiTi

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Abstract
This paper proposes a mechanistic spring–slider model for simulating the deformation behaviour of polycrystalline NiTi via martensite reorientation. The model is based on the thermodynamic concept of elastic and frictional energies for thermoelastic martensitic transformations and the plasticity concept of grain interior and grain boundary phases. This model is found to be able to describe, in a schematic and qualitative manner, the deformation behaviour of thermoelastic martensite via variant reorientation in polycrystalline matrices. Such a model allows the discussion of several aspects concerning the thermal and mechanical behaviour of thermoelastic martensitic transformations, such as the non-linear recovery, deformation-induced two-way memory effect, strain dependence of mechanical hysteresis and minor loop behaviour of deformation.

1. Introduction

Shape memory alloys, owing to their thermoelastic martensitic transformations, exhibit a range of novel thermomechanical properties, including the shape memory effect, the two-way memory effect, pseudoelasticity associated with stress-induced phase transformations and ferroelasticity associated with martensite variant reorientations. These unique thermal and mechanical properties have enabled a wide range of innovative applications of the alloys. Due to their technological importance, these alloys have attracted extensive research interest in the past few decades. One focus of the research is the simulation and modelling of the thermomechanical behaviour of these transformations. This paper presents a discussion of the simulation of ferroelastic deformation behaviour of polycrystalline NiTi using a mechanistic system.

Ferroelastic deformation via martensite reorientation of polycrystalline shape memory alloys exhibits typical elastohysteretic behaviour [1]. In principle, elastohysteretic behaviour can always be simulated using a certain arrangement of elastic springs and frictional sliders. Some models based on this concept have been proposed in the literature [2–5]. This paper proposes a new mechanistic model, which is an improvement on the previous models in taking into account the effect of grain boundaries and the intrinsic differences between a thermally induced and a mechanically induced transformation processes.

2. Deformation of polycrystalline matrix

It is known that thermally induced martensite forms in self-accommodating structures of multiple variants [6, 7]. It is generally thought that deformation in a martensitic state converts, via variant reorientation, the self-accommodating martensite into single variants of most favoured orientations relative to the external stress in each grain in a polycrystalline matrix. Considering that the favoured variants in neighbouring grains have different orientations, stemming from the orientation differences of the austenite grains, it is obvious that such a deformation mechanism alone cannot maintain the continuity of the matrix [8, 9]. This implies that

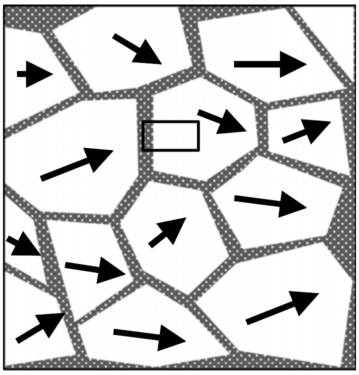

Figure 1. Schematic diagram of polycrystalline aggregate of grains of preferential variants of various orientations.

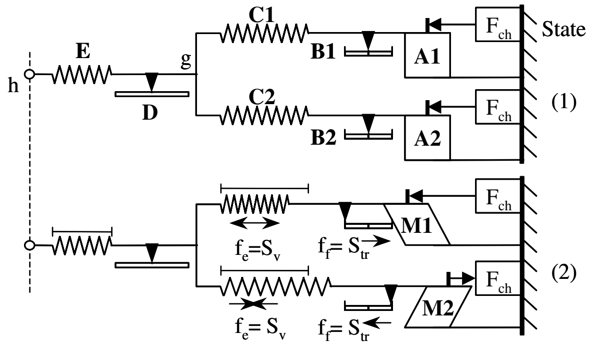

Figure 2. Twin-variant spring–slider mechanistic model of thermoelastic martensite in polycrystalline shape memory alloys, corresponding to the environment shown in the rectangle shown in figure 1; state (1): austenite; state (2): self-accommodating martensite.

internal plastic deformation is a necessary accompaniment for the reorientation deformation of multiple-variant martensite in polycrystalline materials, particularly in the vicinity of grain boundaries where deformations of the favoured variants in neighbouring grains need to be coordinated. On the basis of this understanding, from a mechanical viewpoint, a polycrystalline aggregate can be modelled as shown in figure 1, in which a network of finite volume is created to represent the 'grain boundary affected regions' (GBARs). This is similar to the simulation of the 'grain boundary phase' and 'grain interior phase' in the discussion of plasticity for polycrystalline materials [10]. The interior of the cells (grains) represents the transforming body, which is capable of multiple-variant lattice distortion, and the arrows indicate the orientation of the favoured variants in each grain with respect to one unmarked external stress. The GBARs, which are not capable of transformation lattice distortion, impose resistance to global shape change and thus experience plastic deformation during martensite reorientation deformation. It needs to be clarified that the width of GBAR is dependent on the nature of the deformation. For plastic deformation, the width is compatible with the need to accommodate dislocation activities and thus is generally significant only for ultrafine structures and nanocrystalline matrices. 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. With this model it is obvious that deformation via martensite reorientation in polycrystalline materials is subject to two sources of frictional resistance: (i) the friction for twin boundary movement and (ii) the resistance to global shape change.

3. The mechanistic model

As mentioned earlier, an elastohysteretic process can always be described by using a certain arrangement of elastic springs and frictional sliders. The challenge in achieving a valid arrangement for describing the thermal and mechanical behaviour of a thermoelastic martensitic transformation, however, rests with the intrinsic differences between a thermally activated process and a mechanically activated 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, typifying a parallel assembly of the basic spring–slider elements. For a mechanically induced transformation, the driving force is provided externally and the frictional movement occurs when the stress field exceeds a critical value, typifying a serial assembly of the spring–slider elements.

On the basis of the concept of the physical model presented above, taking into account the influence of GBARs and the differences between thermally activated and mechanically activated processes, a twin-variant mechanistic model has been proposed [11], as shown in figure 2. The model consists of six elements. Element A represents a finite unit that transforms to one martensite variant upon cooling. Slider B expresses the internal resistance to variant boundary movement for reorientation. The slider has a limited sliding distance determined by the lattice distortion of the transformation. Spring C expresses the elastic aspect of the transformation. Assembly A–B–C expresses a transformation unit. In this model two identical transformation units are connected in parallel to form the transformation segment. Outside the transformation segment are slider D and spring E. The external spring expresses the elasticity of the aggregate. The external slider expresses the frictional resistance to global shape change imposed by GBARs, or plasticity of the aggregate experienced during variant reorientation deformation. A function box, F_{ch}, is added to each transformation unit to express the chemical driving force for the transformation, which is a function of temperature. This model conforms to the two distinctive requirements for thermally induced and mechanically induced transformation processes in one unit.

For a thermally induced transformation on cooling, the two units of austenite, as shown in state (1), transform into martensite variants, driven by the chemical forces, in opposite directions to express the self-accommodating structure of the variants, as shown in state (2). 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 g, which corresponds to the perimeter of the grain. During the transformation a frictional force, $f_f = S_{tr}$, is experienced by each unit on its slider. At the

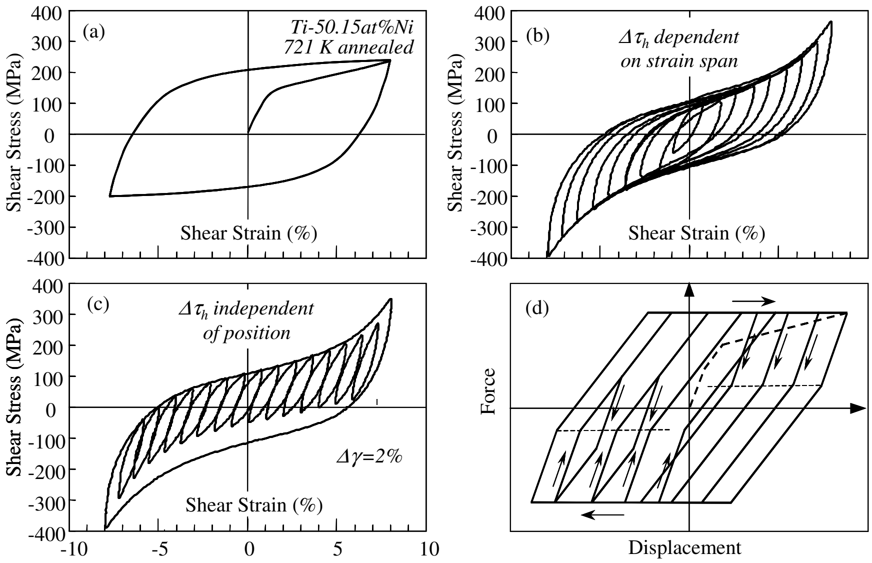

Figure 3. Comparison of ferroelastic behaviour of polycrystalline Ti–50.15 at.% Ni and the model: (a) initial deformation and the first full ferroelastic cycle; (b) subloops of various strain spans; (c) subloops of the same strain span; (d) ferroelastic behaviour of the model.

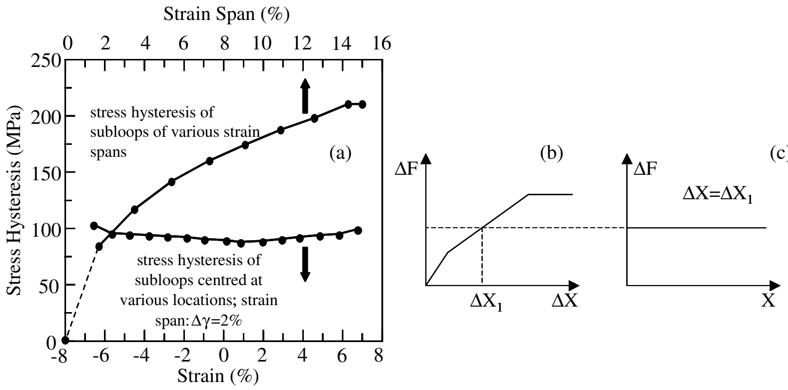

Figure 4. Stress hysteresis of ferroelastic deformation in shear via martensite reorientation: (a) experimental measurements on polycrystalline Ti–50.15 at.% Ni; (b) dependence of stress hysteresis on the strain span of subloops as predicted by the model; (c) independence of stress hysteresis of the position of the subloop as predicted by the model.

same time, an elastic force, $f_e = S_v$, is gradually accumulated during the growth of martensite variants.

4. Deformation of self-accommodating martensite

Martensite reorientation is achieved by applying a force at location h. Figure 3 shows the ferroelastic behaviour of a polycrystalline Ti–50.15 at.% Ni deformed in shear. Figure 3(a) shows the first ferroelastic loop. It is seen that the stress–strain curves of the initial reorientation deformation of the thermally formed self-accommodating martensite appeared within the envelope of the first full ferroelastic cycle. Figure 3(b) shows a set of minor ferroelastic loops symmetric about the centre, which are all confined within the envelope of the full loop, conforming to the notation of 'return point memory effect' [12]. Figure 3(c) shows minor loops of equal strain span of 2% at various positions of the full loop. It is seen that the shape of the minor loops is largely independent of the location. Figure 3(d) shows the force–displacement behaviour of the model deformed via reorientation of self-accommodating variants. It is seen that the model behaves in agreement with all characteristics observed experimentally.

Figure 4(a) shows the measurements of stress hysteresis of the ferroelastic loops shown in figures 3(b) and (c). It is seen that the stress hysteresis is dependent on the strain span of a minor loop but independent of the position of a minor loop on the full loop. Figures 4(b) and (c) show the prediction of the model of the stress hysteresis for centred minor ferroelastic loops as a function of the strain span and that for minor loops of a given strain span as a function of the position of the minor loop on the full loop, respectively. It is seen that the model agrees with experimental observations well.

5. Closing remarks

This mechanistic model is based on the thermodynamic concept of elastic and frictional free energy contributions and the plasticity concept of grain boundary and grain interior phases for deformation. The model is an improvement on similar models proposed in the literature in two respects: (1) it considers the effect of grain boundaries on mechanically induced transformation or martensite reorientation processes and (2) it provides force–displacement characteristics of both serial and parallel connections on the spring–slide elements in one unified structure, allowing the simulation of both thermally induced and mechanically induced transformation processes. This is of particular importance in the discussion of thermomechanical behaviour involving both thermal and mechanical aspects, such as deformation-induced martensite stabilization and a two-way memory effect.

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