Nonuniform transformation behaviour of NiTi in a discrete geometrical gradient design

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Abstract

Shape memory alloys exhibit unique thermomechanical properties, e.g., the shape memory effect and the pseudoelasticity. By proper geometrical gradient design, these alloys can be made to exhibit different and more intricate thermomechanical behaviour to enable innovative applications. This paper reports the design of geometrically gradient NiTi and characterisation of its complex and nonuniform transformation and deformation fields. The study investigated two designs, with one using multiple pseudoelastic NiTi strips of different lengths in parallel arrangement to create a discrete geometrical gradient in the direction perpendicular to the loading axis and the other a tapered plate to give a continuous length gradient in the lateral direction for comparison with the former. The geometrically gradient structures exhibited partial stress gradient during stress-induced transformation. A maximum stress window of 520 MPa was achieved, giving an expanded stress interval for shape memory actuation control. Finite element modelling was applied to characterise the deformation behaviour of such structures under tensile loading and to reveal the complex propagation of the stress-induced transformation in such structures.

Keywords: Shape memory alloy (SMA); NiTi; martensitic transformation; functionally graded material (FGM); geometrical gradient; pseudoelasticity.

1. Introduction

NiTi shape memory alloys (SMAs) exhibit unique thermomechanical properties, most notably the pseudoelasticity and the shape memory effect [1-3], owing to their thermoelastic martensitic transformations. In the case of the near-equiatomic NiTi, three stable crystal structures have been identified, including a B2 austenite, a B19' monoclinic martensite, and a trigonal R-phase [4-6]. Three martensitic phase transformations occur among the crystal structures, i.e., $B2 \leftrightarrow B19'$, $B2 \leftrightarrow R$, and $R \leftrightarrow B19'$, where B2 is always the parent phase to R

and B19', and R is a parent to B19'. The occurrence of the R-phase is prohibited when the near-equiatomic NiTi is fully annealed or solution treated [7]. These unique thermomechanical properties have been used in a wide range of applications, including sensors [8, 9], actuators [10, 11], and medical devices [12, 13]. Some of these applications are reactive and require no precision of movement. Some other applications, such as mirror actuators [14], guidewires [15], and spinal rods [16], require precision and controllability of movement.

In recent years, some new effort has been made to further expand and improve their application performances by designing and developing NiTi alloys of complex forms, such as architected NiTi [17-19], composite NiTi [20-22], and functionally graded NiTi materials [23-25]. The first approach is to design NiTi materials that combine the geometrical characteristics of engineering materials with the functional properties of NiTi to offer new and improved performances. Typical examples include NiTi textile and stents [26, 27], cellular and honeycomb designs [18, 19], and porous microstructures [17]. These materials exhibit shape memory behaviour and superelasticity in a light weight design. The design can offer much lowered and tailorable apparent Young's modulus, which is more desirable for biomedical applications to match the bone's Young's modulus, enhanced shape recovery, and faster thermal response due to the increased surface to volume ratio.

The second approach is to design hybrid NiTi materials. Earlier attempts have focused on using NiTi as a reinforcement in composites, in various forms such as fibre, ribbon, and particulate. These composites use the thermomechanical properties of NiTi to enhance the performances of the composites, for example for vibration and damping control [22, 28], enhanced damage resistance [21, 22], and to enable morphing or control of structures [21]. Recently, a new approach has been made to use NiTi to enable improved properties of other materials. One example is a NiTi-Nb nanowire composite, in which the NiTi matrix is used to induce ultra large elastic strains, thus high strengths, of the Nb nanowires embedded within the NiTi matrix [29-31].

The third approach is to create functionally graded (FG) NiTi to utilize and control the response of the shape memory component to the external stimuli. For stress-induced $B2 \leftrightarrow B19'$ martensitic transformation in NiTi, the alloy often undergoes Lüders-type deformation, which is described by a flat stress plateau with a nearly zero slope over a large

transformation strain of ~6% [32, 33]. This behaviour results in mechanical instability and poor control of the actuation displacement of the component by the application of load (or stress). This is a challenge for actuator design. One approach to solving this problem is to design functionally graded NiTi. These materials provide widened transformation stress (and temperature) windows, thus better controllability of the SMA element [24, 34]. In addition, FG NiTi can also exhibit new and unique properties, such as the “fishtail-like” behaviour of a compositionally graded NiTi thin strip [34, 35]. The functional gradient can be created by variation in composition [36-38], microstructure [39, 40], or geometry [41, 42].

In geometrically graded NiTi, the structure geometry can be graded either along the loading direction (in series configuration) [43] or perpendicular to the loading direction (in parallel configuration) [25]. The geometrical gradient causes the structure to experience a nonuniform stress field upon loading, thus progressive martensitic transformation within the structure [44, 45]. This concept can be applied to various forms of the alloy, including wires, sheets and plates, and rods [41, 42]. In previous studies, we have investigated geometrically graded NiTi with gradients along the tensile loading axis [41-43]. This article presents another design type with discrete geometrical gradient perpendicular to the loading direction by use of pseudoelastic NiTi strips.

2. Experimental analysis

Fig. 1 shows the general design concept of geometrically graded NiTi materials. Such materials can be created in series (see Fig. 1(a)) or parallel (see Fig. 1(b)) configurations with respect to the loading direction. The parallel design configuration can be achieved by using either a NiTi thin plate with its end(s) tapered, as seen in Fig. 1(b)-(I), or parallel arranged NiTi wires or strips of different lengths, as seen in Fig. 1(b)-(II). The former is referred to as the continuous gradient design and the latter the discrete gradient design.

Fig. 1. General design concepts of geometrically graded NiTi components.

In the present study, a Ti-50.8at%Ni sheet of 0.1 mm thickness was used to fabricate geometrically graded NiTi samples in parallel configuration. Two types of samples were fabricated as per design (b)-(I) and (b)-(II) shown in Fig. 1. For (b)-(II), strips of 1.5 mm in width were cut from the sheet by electrical discharge machining. The width of the tapered (b)-(I) samples was 7 mm. Different L_1/L_2 length aspect ratios were used for both designs. Tensile testing was carried out using an Instron 5982 machine under displacement-control mode at a strain rate of 2×10^{-4} /sec with respect to the maximum length (L_2). Fig. 2 shows the testing setup including the uniform and tapered grippers used for tensile experiments.

Fig. 2. Tensile experimentation setup with the details of grippers.

Fig. 3 shows the general material behaviour. Fig. 3(a) shows the tensile deformation behaviour of the alloy at 295 K, as tested using a uniform strip of 30 mm in gauge length. The material showed good pseudoelastic behaviour with a flat stress plateau at ~350 MPa over the forward A→M transformation and full transformation strain recovery upon reverse M→A transformation, where A and M denote austenite and martensite phases, respectively. Near full pseudoelastic recovery was measured with the stress-induced martensite deforming up to ~630 MPa (corresponds to ~0.077 of strain) beyond the stress plateau. The apparent yield point (σ_y) of the stress induced martensite was ~820 MPa and the ultimate tensile strength of the alloy was above 1130 MPa.

The crystal structure of the NiTi sample was analysed using an Empyrean X-ray diffractometer with Cu-K α radiation. Phase identification was carried out using HighScorePlus search-match software. Fig. 3(b) shows the XRD pattern of the alloy at the room temperature, which is fully indexed to the B2 austenite phase. The transformation behaviour of the NiTi alloy was measured using TA Q10 differential scanning calorimeter (DSC) in N₂ atmosphere. The cooling/heating rate used was 10 K/min. Fig. 3(c) shows a DSC measurement of the transformation behaviour. It reveals a two-step forward A→R→M and a one-step reverse M→A phase transformation, where R represent the trigonal phase of NiTi.

Fig. 3. Material behaviour of the NiTi alloy; (a): stress-strain behaviour at 295 K, (b): XRD pattern of the alloy, (c): transformation behaviour.

Fig. 4 shows the deformation behaviour of geometrically graded NiTi structures with parallel design configuration under uniaxial tensile loading. Here, the length aspect ratio is defined as $\alpha = L_1 / L_2$ ($\alpha \leq 1$), where L_1 and L_2 are the minimum and the maximum lengths corresponding to side (1) and side (2) of the structure, respectively, as shown in Fig. 1(b). $\alpha = 1$ corresponds to a sample with equal length across the width. Also, the nominal stress σ is defined as the load over the total cross-sectional area of the undeformed sample. The nominal strain ε is defined as the elongation over the initial maximum length of the sample L_2 .

Fig. 4(a) presents the tensile deformation behaviour of three discrete (b)-(II) samples of different length aspect ratios ranging from $\alpha = 0.6$ to $\alpha = 1$. All the samples were strained up to $\varepsilon = 0.07$ nominal strain (relative to the maximum length L_2) before unloading. As observed, all the samples exhibited near pseudoelastic recovery upon unloading. The stress-strain curves of the geometrically graded samples ($\alpha \neq 1$) partially deviated from the original stress-strain behaviour of the NiTi alloy ($\alpha = 1$). This deviation increased as the aspect ratio decreased. The stress-strain curve over forward transformation consisted of two stages for the geometrically graded samples. Stage (I) is apparently the original stress plateau of the alloy. Stage (II) is a stress gradient with a positive slope. It is seen that both the stress and strain ranges of stage (II) increased with decreasing the aspect ratio. The stress window achieved for the sample with $\alpha = 0.6$ was ~ 400 MPa over 0.07 of nominal strain. Fig. 4(b) shows the cyclic deformation behaviour of a two-strip discrete NiTi sample with $\alpha = 0.75$. The sample

exhibited a stress gradient after 0.05 of nominal strain and provided a stress window of ~520 MPa over 0.08 of nominal strain, which was fully recovered upon unloading.

Fig. 4(c) shows the comparison of the deformation behaviour of three different designs of geometrically graded NiTi structures. Sample (i) is a continuous plate structure with a tapered end to form the geometrical gradient in the lateral direction. Sample (ii) is a two-strip discrete structure and sample (iii) is a three-strip discrete structure. All samples had the same aspect ratio of $\alpha = 0.65$. In comparison, sample (i) started stage (II) earlier and reached the higher level of stress at the end of loading to ~0.07 nominal strain. These differences were attributed to the stress concentration at the tapered edge corner of sample (i), which did not occur in the discrete strip samples. In this highly-stressed area, the material initiated and completed the phase transformation at a lower loading level compared to the strip samples. Also, at higher loading levels, the stress in this area may exceed the elastic limit and then the material may undergo plastic deformation. It is also noted that the stress-strain slope in sample (i) decreased at above 0.065 nominal strain, which indicated material yielding. This sample also showed a 0.004 residual strain after unloading, consistent with the expectation of local plastic deformation at the tapered corner. This is an obvious disadvantage of the tapered plate design relative to the discrete parallel-strip designs (samples (ii) and (iii)).

Fig. 4. Deformation behaviour of geometrically graded NiTi structures with parallel design configuration under uniaxial tensile loading; (a): different aspect ratios and the definition of deformation stages over forward transformation, (b): loading cycles for $\alpha = 0.75$, (c): comparison of continuous and discrete structures.

3. Numerical analysis

Finite element analysis (FEA) was carried out using ABAQUS 6.11-2 with built-in UMAT subroutine based on Auricchio et al.'s constitutive model [46, 47] for pseudoelastic behaviour of SMAs. The model takes into account the total strain as the sum of the elastic strain, the transformation strain, and the plastic strain. The plastic strain develops when the recoverable strain limit is exceeded. To simulate the mechanical behaviour of the NiTi samples, the UMAT subroutine was first trained with a loading-unloading uniaxial tensile test of the material. To achieve realistic results by considering all components of normal and shear stresses, a 3D geometry with C3D20R elements was considered for each calculation.

3.1. Global deformation behaviour

Fig. 5 shows the global deformation behaviour of the geometrically graded NiTi parallel-strip samples under uniaxial tensile loading as predicted by FEA. Fig. 5(a) shows a comparison of the global deformation behaviour based on the FEA prediction and the experimental data on a two-strip sample ($\alpha = 0.75$). The FEA modelling provided a good match with the experimental data. Fig. 5(b) shows the numerical stress-strain curves for three different samples: a geometrically uniform sample, a geometrically graded tapered plate sample ($\alpha = 0.65$) and a discrete geometrically graded parallel-strip sample ($\alpha = 0.65$) consisting of six strips of 1.5 mm width. It is seen that the stress-strain curve of the parallel-strip structure

deviated slightly from that of the tapered plate structure. Fig. 5(c) shows FEA predictions of the deformation behaviour of two-strip discrete NiTi samples of different aspect ratios. As evident, with the decrease of the aspect ratio, the strain length of stage (I) decreased and the maximum stress reached at a given strain (0.07 nominal strain in this case) increased. The average slope of the stress-strain curve in stage (II) increased with the decrease of the aspect ratio. These characteristics are similar to those observed experimentally (Fig. 4(a)).

Fig. 5. Global deformation behaviour of geometrically graded NiTi structures with parallel design configuration as predicted by FEA; (a): validation with experiment for discrete two-strip system, (b): comparison of the continuous plate and discrete parallel-strip systems with the uniform structure, (c): the effect of aspect ratio on deformation behaviour of two-strip structures.

3.2. Local deformation behaviour

Fig. 6 shows the distribution of the normal stress component along the loading direction x of three samples, including a geometrically uniform sample, a geometrically graded continuous

and tapered plate sample ($\alpha = 0.65$), and a discrete six-strip sample ($\alpha = 0.65$). The strips are 1.5 mm in width. It is seen that the uniform sample exhibited largely uniform stress fields at all loading levels. The tapered plate sample exhibited highly nonuniform stress fields at all nominal strain levels. The highest stress appeared to occur at the tapered corner on side (1) of the sample, implying that the transformation and post-transformation plastic deformation both initiated from this corner and propagated toward other regions of the plate upon loading. In the parallel-strip sample, the stress fields were practically uniform along the length but clearly discrete and nonuniform across the transverse direction among the strips. The shortest strip experienced the maximum stress, thus the stress-induced martensitic transformation started from this strip first and propagated progressively to the longer strips with increasing the nominal strain. At $\varepsilon = 0.05$ nominal strain, the shorter strips on side (1), which experienced higher stresses, have completed A $\rightarrow$ M transformation and entered the martensite elastic deformation stage with an increasing stress whereas the longer strips remained in the transformation stage with uniform stress. At 0.07 nominal strain, the entire structures of all three samples, except a small area on side (2) of the tapered plate sample, have exited transformation as the local stresses reached above 400 MPa. Plastic deformation has occurred at highly-stressed areas where the stress is above 820 MPa, in particular at the taper edge corner on side (1) of the tapered plate sample.

Fig. 6. Local stress fields of the uniform and the continuous and discrete geometrically graded samples at different loading levels.

Fig. 7 shows the evolution of the volume fraction of martensite upon loading to $\varepsilon = 0.07$ for the three samples. The uniform plate sample exhibits a uniform distribution of martensite fraction within the sample except at its gripping areas, where stress variation exists. In the tapered plate sample, the martensitic transformation initiates at the tapered corner on side (1) and propagates toward side (2) in an oblique direction with respect to the loading axis. In the parallel-strip sample, the A $\rightarrow$ M transformation starts from the shortest strip on side (1) and propagates parallel in the transverse direction to the loading axis towards the longest strip on side (2). It is observed that at 0.04 nominal strain, ~47% of the structure is transformed to martensite in the tapered plate sample, whereas this value is ~17% in the discrete parallel-strip sample. As explained earlier, in the tapered plate sample, due to the stress concentration at the tapered edge corner on side (1), the transformation initiates and completes at a lower stress level compared to in the parallel-strip sample.

Fig. 7. The distribution of martensite volume fraction within the uniform and the continuous and discrete geometrically graded samples at different loading levels.

4. Conclusions

In this study, the unique stress-strain behaviour of stress-induced martensitic transformation

and the complex transformation field of geometrically graded NiTi structures were analysed through experiments and finite element computation. The main findings are summarised as below:

- (1) Geometrical gradient in parallel configuration can be achieved using either continuous tapered plate or discrete parallel strips. The geometrically gradient structures show two deformation stages over the forward stress-induced martensitic transformation, i.e., a flat stress plateau and a stress gradient with a positive slope. The gradient stress stage provides a stress window for improved actuation controllability. The magnitude of the stress window increases with the decrease of length aspect ratio of the geometrically gradient design, and reached 520 MPa for a discrete strip sample of length aspect ratio of 0.75.
- (2) The discrete parallel-strip design is more advantageous than the continuous tapered plate design by avoiding stress concentration, thus early plastic deformation, at the tapered corners during loading. In addition, the discrete parallel-strip design requires less manufacturing effort by simply using cut wires or strips of different lengths than the tapered plate design.
- (3) The geometrical gradient creates complex and nonuniform transformation field within the structure during uniaxial tensile loading. The direction of transformation propagation in the parallel-strip design is perpendicular to the loading direction whereas that in the tapered plate design is oblique with respect to the loading direction.

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Data availability

The raw data required to reproduce these findings will be available in the article. The processed data required to reproduce these findings will be available in the article.

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- Nonuniform transformation field was created in parallel geometrical gradient design
- Geometrically graded NiTi demonstrated partial stress gradient over transformation
- Widened transformation stress window for actuation application was created
- Transformation propagation in discrete design was perpendicular to the loading axis

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