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Computational and Experimental Analyses of Martensitic Transformation Propagation in Shape Memory Alloys

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Abstract. This study investigates the creation of heterogeneous martensitic transformation field in shape memory alloy structures with geometrical nonuniformity through experiments and finite element computational analysis. Geometrically graded superelastic NiTi thin plates with series and parallel design configurations with respect to the loading direction have been created. The nonuniform transformation evolutions within these structures are presented by thermal images captured by an infrared camera during tensile experimentation. It is found that the transformation propagation is along the loading direction in a sample with the series design configuration unlike that in a sample with the parallel design configuration. Also, the geometrically graded structures exhibit stress gradient over stress-induced transformation. The transformation propagation and the deformation behaviour of these structures are presented by numerical modelling which is in good agreement with experimental data.

Keywords: Martensitic transformation; Shape memory alloy; NiTi; Functionally graded material.

1. Introduction

Shape memory alloys (SMAs) are a group of materials which can return to their original shapes after being largely deformed [1]. Near-equiatomic NiTi is the most widely used SMA owing to its excellent shape memory properties and good fabricability. One unique feature of this alloy is pseudoelasticity (or superelasticity), which refers to the ability of the alloy to accommodate relatively large deformation (typically 6~8% tensile strain) during loading and return to the initial undeformed configuration upon unloading [2]. As a result of this

outstanding behaviour, superelastic NiTi have been increasingly used in various engineering fields, such as in structural engineering and biomedical engineering [3].

It is known that NiTi alloy exhibits Lüders-type deformation via stress-induced martensitic transformation between austenite (A) and martensite (M) phases [4]. This A→M transformation occurs over a flat stress plateau with an almost nil stress window over the transformation strain, which is undesirable for stress-controlled actuation applications. For such applications, it is required to have a reasonably wide stress window for the stress-induced transformation within NiTi alloy. To achieve this goal, one approach is to create functional gradient throughout the structure [5].

In functionally graded structures, the material properties vary along one or more directions. These variations originate from gradients in such factors as microstructure, composition, and geometry [6]. In NiTi, the material gradient can be acquired in microstructure by variation in heat treatment [7-9] or in composition by variation in Ni/Ti ratio [10-12]. In addition, by variation in the geometry of NiTi structure, the alloy experiences a nonuniform stress field upon loading, thus progressive martensitic transformation within the structure is achieved [13-15].

The property gradient can be created based on either a series design configuration or a parallel design configuration with respect to the loading direction. In the former configuration, the property gradient is maintained along the loading axis, thus the martensitic transformation and the resultant deformation are expected to occur sequentially along this axis [16]. In the latter configuration, the property gradient is created perpendicular to the loading axis, which yields in transformation propagation vertical (or oblique) to the loading direction. Consequently, the local deformations mainly add to the global deformation in a parallel manner [17].

In previous studies, we have investigated geometrically graded SMA structures with gradients along the loading direction (i.e., the series design configuration) and established closed-form solutions for stress-strain relationship during all deformation stages. The developed analytical model was then used to predict the macroscopic deformation behaviour of such 1D [15] and 2D [14, 16] NiTi structures. Also, geometrically graded NiTi 2D structures with the parallel design configuration have been investigated through tensile

experimentation [13, 17]. In the present study, thermal fields of superelastic NiTi structures with uniform and nonuniform geometries during stress-induced transformation are obtained by a high-resolution infrared camera and the martensitic transformation propagation is investigated for different types of geometries. Also, the transformation propagation and the deformation behaviour of these structures are presented by numerical modelling based on finite element method.

2. Experimental setup and materials

Fig. 1(a) shows the experimental setup used for this study. Instron 5982 machine under displacement-control condition was used for tensile loading. The samples were loaded at the strain rate of $\sim 10^{-3}$ /sec relative to the maximum length of the sample. The testing temperature was 296 K. The temperature field (thermal images) of samples during tensile deformation was acquired using an infrared camera (Nippon Avionics, Model R500EX), which had a resolution of 1280×960 pixels.

Ti-50.8at%Ni sheets of 0.2 mm in thickness were used to fabricate uniform and geometrically graded NiTi samples by means of electrical discharge machining. Fig. 1(b) shows the actual deformation behaviour of the alloy under tensile loading. Here, a uniform strip of NiTi material was tested. The sample had a gauge section of 2×30 mm. The forward A $\rightarrow$ M and reverse M $\rightarrow$ A transformation stresses were measured to be ~ 330 MPa and ~ 100 MPa, respectively.

In this article, the nominal stress is defined as the load over the initial maximum cross-sectional area of the sample. Also, the nominal strain is defined as the elongation over the initial maximum length of the sample. For a sample with the series design configuration, the width aspect ratio is defined as $\alpha = w_1/w_2$, where w_1 and w_2 are the minimum and the maximum plate widths, respectively as noted in Fig. 3(a). For a sample with the parallel design configuration, the length aspect ratio is defined as $\alpha = L_1/L_2$, where L_1 and L_2 are the minimum and the maximum edge lengths, respectively, as noted in Fig. 4(a) for a continuous (plate) structure and Fig. 5(a) for a discrete (multiple-strip) structure. For both design configurations, $\alpha = 1$ indicates a geometrically uniform sample, which exhibits the original material behaviour.

Fig. 1. Experimental procedure; (a) experimental setup (for a parallel design configuration), (b): experimental measurement and FEA prediction of the deformation behaviour of a uniform NiTi alloy under tension at 296 K.

3. Computational framework

Various constitutive modelling and simulation studies have been reported in the literature on the thermomechanical behaviour of SMAs. In some more recent studies, the proposed constitutive models are implemented in computational codes, developed by numerical methods such as finite element analysis (FEA). The computational tools make it possible to describe the behaviour of SMAs with complex geometries or under complex thermomechanical (and transformation) conditions [18-20].

Here, we used Abaqus software with a built-in UMAT subroutine based on Auricchio et al.'s constitutive model [21]. In this model, the total deformation is calculated as the summation of elastic, plastic, and transformation deformations. The plastic deformation is developed when

the recoverable pseudoelastic limit of the material is exceeded. To obtain realistic outcome by considering all components of normal and shear stresses, a 3D geometry with C3D20R elements has been employed for all FEA computations. To simulate the transformation evolution and the deformation behaviour of the geometrically graded NiTi structures, the code has been initially trained with the actual global deformation behaviour of NiTi alloy under tensile loading as shown in Fig. 1(b). It is seen that the FEA code can suitably predict the whole range of deformation of NiTi under tension. The local stress and strain fields of different types of geometrically graded NiTi structures are presented in Ref. [22], which is the supplement of this paper.

4. Results and discussion

4.1. Uniform design configuration

Fig. 2 shows the transformation and deformation behaviours of a NiTi sample with uniform geometry ($\alpha = 1$) under tensile loading. Fig. 2(a) shows the thermal images of this sample during tensile loading up to 7% as acquired by an infrared camera. Fig. 2(b) shows the deformation behaviour of this sample. As observed, the forward transformation initiates at $\sim 0.85\%$ of strain by exhibiting the first martensite band. A few more bands appear as the sample is stretched to 2% nominal strain. Beyond 3% nominal strain, the transformation and deformation progress almost uniformly throughout the structure. Globally, the sample exhibits a flat stress plateau with almost nil stress-strain slope over $A \leftrightarrow M$ transformations. The recorded video of the thermal field evolution within this sample during one loading cycle is presented in Ref. [22].

Fig. 2. Transformation and deformation behaviours of NiTi with uniform geometry; (a): temperature fields acquired by an infrared camera, (b): tensile deformation behaviour.

4.2. Series design configuration

Fig. 3 shows the transformation and deformation behaviours under tension of geometrically graded NiTi structures with the series design configurations. The loading direction is along the x -axis. The width aspect ratio is $\alpha = 2/3$. The gauge length L is 30 mm and the maximum width w_2 is 6 mm. Fig. 3(a) shows the evolution of the martensitic transformation as predicted by FEA. The stress-induced transformation starts at the top end with the minimum width w_1 , where the stress was maximum. Then, the A→M transformation progressively propagates toward the bottom end with the maximum width w_2 by the increase of the nominal strain from 0.75% to 7%. As evident, the direction of the martensitic transformation propagation is along the loading direction, i.e. the x -axis. It is noted that the martensite fraction has values below 0 (negative) and above 1.0. This is a mathematical artefact of how the martensite fraction is defined in the FEA code. The martensite fraction (f_m) is defined as the local strain relative to the strain length of the stress plateau on the stress-strain curve shown in Fig. 1(b), i.e., $f_m = 0$ when the local strain equals that at the onset of the stress plateau and $f_m = 1$ when the local strain equals that at the end of the stress plateau. Therefore, $f_m > 1$ corresponds to the strained martensite beyond the stress plateau and $f_m < 0$ corresponds to the austenite phase prior to the stress plateau. Obviously, the f_m values outside the 0~1.0 range are mathematical artefacts of the modelling. Fig. 3(b) shows the thermal fields of this sample during tensile loading as acquired by an infrared camera. As observed, the forward transformation initiates from the top end at ~0.75% nominal strain and

the direction of transformation propagation is along the loading axis. This experimental observation is in good agreement with the FEA prediction presented in Fig. 3(a). The temperature variation along longitudinal direction at progressive loading levels and the recorded video of the thermal field evolution within this sample during one loading cycle are presented in Ref. [22]. Figs. 3(c) and 3(d) show the deformation behaviour of the above geometrically graded NiTi sample during one complete loading cycle based on FEA and the experiment, respectively. As evident, the sample exhibits a stress gradient over the stress-induced transformation, providing an expanded stress window of ~120 MPa in contrast to the original material behaviour shown in Fig. 2(b). This improves the controllability of such a shape memory component in actuation application.

Fig. 3. Transformation and deformation behaviours of a geometrically graded NiTi structure with series design configuration; (a): martensite fractions predicted by FEA, (b): temperature fields acquired by an infrared camera, (c) deformation behaviour based on FEA, (d): deformation behaviour based on experiment.

4.3. Parallel design configuration

4.3.1. Continuous structure

In this section, NiTi plates are used with a gripping mechanism shown in Fig. 1(a). The tapered gripper at the top end of the sample creates a continuous geometrically graded NiTi structure with parallel design configuration.

Fig. 4 shows the transformation and deformation behaviours of such a structure. The loading direction is along the x -axis. The length aspect ratio is $\alpha = 2/3$. The width w and the maximum gauge length L_2 are 6 mm and 30 mm, respectively. Fig. 4(a) shows the evolution of martensitic transformation as predicted by FEA. It is seen that the stress-induced transformation initiates at the tapered corner on the left side of the sample with the minimum

length L_1 and high stress concentration. Then, the A→M transformation progressively propagates toward the right side with the maximum length L_2 , in an oblique direction with respect to the loading axis, by the increase of the nominal strain from 0.75% to 7%. Fig. 4(b) shows the thermal fields of this sample during tensile loading as recorded by an infrared camera. As observed, the forward transformation initiates from the top left corner and propagates toward the right side of the sample. This experimental observation validates the FEA results presented in Fig. 4(a). Figs. 4(c) and 4(d) show the deformation behaviour of the above sample during one complete loading cycle based on FEA and the experiment, respectively. As evident, the sample exhibits two distinctive stages of deformation over stress-induced transformation: a stress plateau similar to the original material behaviour shown in Fig. 2(b) and a stress gradient over a wide stress window (~ 370 MPa).

Fig. 4. Transformation and deformation behaviours of a geometrically graded NiTi plate with parallel design configuration; (a): martensite fractions predicted by FEA, (b): temperature fields acquired by an infrared camera, (c) deformation behaviour based on FEA, (d): deformation behaviour based on experiment.

4.3.2. Discrete structure

In this section, NiTi multiple-strip structures are used with a gripping mechanism shown in Fig. 1(a). The tapered gripper at one end creates a variation in gauge lengths of the strips resulting in a discrete geometrically graded NiTi structure with parallel design configuration.

Fig. 5 shows the transformation and deformation behaviours of a three-strip structure. The loading direction is along the x -axis. The length aspect ratio is $\alpha = 2/3$. The width of each strip is 2 mm. The maximum gauge length L_2 is 30 mm. Fig. 5(a) shows the evolution of martensitic transformation as predicted by FEA. It is seen that the A $\rightarrow$ M transformation initiates at the shortest strip with length L_1 , where the strain and the stress are the maximum.

Then, the transformation progressively propagates toward the longer strips by the increase of the nominal strain to 7%. It is inferred that the transformation propagation is along the y-axis, which is perpendicular to the loading direction. This behaviour is confirmed by the experimental data presented in Fig. 5(b) for the same sample. Figs. 5(c) and 5(d) show the deformation behaviour of the above sample during one complete loading cycle based on FEA and the experiment, respectively. As observed, the multiple-strip structure exhibits two distinctive stages of deformation over A→M transformation (i.e., stress plateau stage and stress gradient stage) similar to those of the plate sample analysed in Sec. 4.3.1. As understood from Fig. 5(d), all strips are in the course of A→M transformation during the stress plateau stage. At <5% nominal strain, the shortest strip finishes transformation and the stress gradient stage starts. At ~6% nominal strain, the transformation is also completed in the middle strip. At 7% nominal strain, the transformation is completed within the entire structure.

Fig. 5. Transformation and deformation behaviours of a geometrically graded NiTi multiple-strip structure with parallel design configuration; (a): martensite fractions predicted by FEA, (b): temperature fields acquired by an infrared camera, (c) deformation behaviour based on FEA, (d): deformation behaviour based on experiment.

It is noticed in Figs. 3~5 that the pseudoelastic return paths of the stress-induced martensite upon unloading are clearly different between the experiment and the simulation, whereas the forward transformation paths are largely in agreement. This is related to an intrinsic inadequacy of the shape memory alloy subroutine embedded in the Abaqus code for FEA. The constitutive model for the subroutine defines a fixed value for the stress hysteresis of the pseudoelasticity, thus is unable to take into account the effect of detwinning deformation and possibly plastic deformation that occur at beyond the stress plateau. In our geometrically graded sample, the zones of the sample having lower cross sections are clearly deformed well beyond the end of the stress plateau when zones of larger cross sections are completing their deformation within the stress plateau. The excessive detwinning and possibly plastic

deformation, which are known to lower the return path of pseudoelasticity, thus to widen the stress hysteresis, is the cause of this discrepancy. This also implies that the experimental observation reflects the true behaviour of the geometrically graded NiTi.

It is evident that in both series and parallel design configurations, the geometrical gradient expands the stress window over stress-induced martensitic transformation. It has been reported that the magnitude of stress window is mainly dependent on the aspect ratio of the geometrically graded structure. As the aspect ratio decreases, the magnitude of stress window increases, which results in better controllability of the shape memory component [5, 13]. When decreasing the aspect ratio, care needs to be taken to limit the total deformation to avoid plastic deformation in highly stressed areas of the sample and maintain full superelastic behaviour. Also, by comparing Fig. 3(d) and Fig. 4(d), it is inferred that the parallel design configuration provides wider stress window compared to the series design configuration with the same aspect ratio. However, the series design configuration provides a more continuous stress gradient over the whole range of martensitic transformation, which can be more desirable for actuation applications.

5. Conclusions

In this study, the martensitic transformation propagation of NiTi shape memory alloy structures with geometrical gradient and their deformation behaviour were investigated through experiments and finite element computation. The main findings are summarised as below:

- (1) Geometrically graded NiTi with parallel and series design configurations demonstrate partial and full stress gradients, respectively, over stress-induced martensitic transformation.
- (2) The transformation propagation is along the uniaxial loading direction in a sample with the series design configuration unlike that in a sample with the parallel design configuration.
- (3) The stress gradient over transformation stage provides expanded stress interval in a geometrically graded NiTi sample, which enhances the controllability of the shape memory component. The stress intervals of 120 MPa and 370 MPa were achieved, respectively, for the series and parallel design samples with the aspect ratio of 2/3.

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- Heterogeneous martensitic transformation fields in NiTi shape memory alloys were created
- Thermal fields in geometrically graded NiTi during transformation were obtained by infrared camera
- Geometrically graded NiTi structures exhibited stress gradient over martensitic transformation