# The micro-macroscale correlation of NiTi mechanical behavior: a finite element analysis

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## Abstract

One material that has found particular favor for use in biomedical endovascular stents is the near equi-atomic NiTi alloy, Nitinol. One remarkable trait exhibited by this superelastic material is the improvement of its fatigue performance with increasing mean strain [1, 2]. Clarification into this phenomenon still remains incomplete in literature. This study proposes a microstructural explanation for this unique macroscopic behavior; it is hypothesized stress-induced martensite (SIM) will stabilize with increasing strain which, in turn, leads to the observed increase in fatigue life. Finite Element Analysis (FEA) is employed to investigate the behavior of a 'v-strut' stent subcomponent under various strain levels. The volume fraction of SIM is analyzed to identify its potential influence on macroscopic response and, ultimately, fatigue behavior. In addition, a computational investigation is performed on the effect of crystallographic texture on macroscopic response. Granular transformational behavior is analyzed using FEA models with realistic and idealized grain structures, specifically evaluating the effect of individual grain orientations on the stress-induced martensite transformation (SIMT).
*Keywords: Nitinol, microstructure, superelasticity, fatigue.*

## 1 Introduction

### 1.1 Medical use of Nitinol

Nitinol possesses a unique combination of properties, which renders it suitable in a broad range of engineering applications. In particular, characteristics such as superelasticity, biocompatibility, flexibility, and compatibility with magnetic

 
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resonance imaging (MRI) procedures make it particularly appealing in the biomedical industry for use as self-expanding endovascular stents [3]. Such devices have proven effective in the treatment of atherosclerosis in a variety of vessels and arteries. However, fracture rates of up to 65.4% in such stents used in the superior femoral artery have been reported in clinical studies [4]. Due to physiological movement from the cardiac systolic-diastolic cycle, in addition to the muscular movement associated with the anatomy in which they are placed, such failures can be attributed to cumulative fatigue damage. Accurate characterization of the fatigue behavior of such stents is therefore essential for their prolonged safe use in human arteries.

### 1.2 Superelasticity

Superelasticity is the term given to the first-order phase transformation, from a parent austenite to a daughter martensite phase, which underpins Nitinol's unique performance. Nitinol's phase transformation can be induced by a change in temperature or stress; via an application of load, or upon cooling below the martensite-start temperature ($M_s$). Austenitic Nitinol is a hard, stiff material whereas martensitic Nitinol is a softer, more ductile material with a lower yield stress [5]. These vast differences in material properties can be explained by their different microstructural crystallographic structures; austenite has an ordered cubic B2 structure while martensite has a more complex twinned monoclinic B19' structure.

In a crystallographic context, the stress-induced martensite transformation (SIMT) occurs by rearrangement of atomic planes via Bain strain and lattice invariant shear. The twin boundaries in martensite readily shift such that the twins are predominantly oriented in one preferential direction; this process is known as de-twinning. By this microstructural process, the material can withstand approximately 6% strain without permanent deformation. This ability to accommodate such significant strains is highly desirable in stent device design for stent deliverability, durability and conformance. The SIMT has no associated breaking of atomic bonds, therefore, no macroscopic change is associated with the transformation; this can be explained by the self-accommodating nature of twinned martensite variants. Upon removal of the stress the superelastic strain recovers at a lower stress level than at which it is induced, i.e. along a hysteresis curve (Figure 1).

### 1.3 Microstructural texture

As described, Nitinol derives its unique mechanical behavior from the coordinated atomic movements manifesting in a phase transformations from cubic austenite to monoclinic martensite. Therefore, any significant alignment of the atomic planes resulting from crystallographic texture in the polycrystalline material can have a marked influence on the mechanical response. It has been experimentally shown that the crystallographic texture has a significant effect on crack trajectories in NiTi tube specimens subjected to uni-axial cyclic loading [8]. In addition, significant variations in mechanical behavior have been

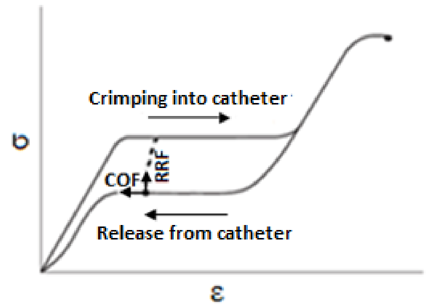


Figure 1: Superelastic stress–strain curve portraying the stent's chronic outward force (COF) on blood vessel in retaining it open from a stressed configuration, and radial resistive force (RRF) in resisting stent collapse (adapted from [3]).

observed between rolled and transverse directions of cold-drawn NiTi sheets [6, 7]; this can be attributed to the hindrance of deformed martensite structures and defects in the specimen leading to differing dominant detwinning and reorientation modes and dislocation densities. This, in turn, may result in discrete areas of the microstructure no longer being able to transform back into austenite (stabilized SIM); on a microstructural scale the stress fields of the dislocations are high enough to prevent unloading, even if the material is macroscopically without load. Thus, the material locally behaves as a standard metallic material accumulating plasticity during cyclic mechanical loading. Clarification into the effect of this process with regard to fatigue performance, however, still remains unexplored in literature.

Initial processing techniques used to form Nitinol specimens have also been investigated to determine the correlation between differing product forms and resulting microstructures. Results confirm that the crystallographic texture in Nitinol can be significantly different depending on product form selected. Specifically, thin-section flattened tube materials (0.2–0.4mm) Nitinol specimens showed higher fatigue thresholds of $\Delta K_{th} > 2.5$ MPa√m, as compared to values of $\Delta K_{th} < 2$ MPa√m in thick-section bar material (9–10mm) [9]. It was observed that crystallographic texture anisotropies are present when specimens were compressed in different crystallographic directions [10]; varying recovery strains and strength levels were displayed. Namely, the compression strength of polycrystalline NiTi is stronger when tested in the longitudinal direction, which has a [111] texture, as compared with NiTi material that was tested in the transverse direction with a [110] crystallographic texture. These results confirm there are underlying microstructural mechanisms taking place with varying textures and this, in turn, can lead to profound effects on the overall macroscopic material behavior.

### 1.4 Fatigue of Nitinol

For the past four decades, researchers have been eagerly attempting to fully understand the unique behavior of this remarkable superelastic material. Melton and Mercier [11] were the first to extensively study the S/N fatigue behavior of Nitinol. While these initial studies provide tremendous insight into baseline fatigue properties, much of their work was under stress control conditions, which are difficult to adapt to strain life; that being relevant for stent fatigue analyzes. This difficulty can be attributed to the near constant stress plateau associated with the phase transformation upon loading and unloading (Figure 1). In addition, Nitinol research utilizing *in situ* loading in conjunction with microscopy is seldom found in literature; yet these experiments can offer a rich understanding of Nitinol's fundamental material response as they address both microstructural and macro-mechanical response simultaneously.

Nevertheless, standard and thermal cameras have been successfully employed to capture the macro-transformation thermal signatures of Nitinol upon loading [12, 13]. With evidence of the latent heat release, which occurs during the first-order transformation, the thermal camera supports the hypothesis that SIMT is occurring. Similarly, high-speed and infra-red cameras have been used to observe the complete transformation process, from nucleation to growth and to the eventual vanishing of SIM, in a tube specimen under displacement-controlled uni-axial tension [14]. A similar evaluation of Nitinol's surface in strain-free, strained and unloaded states was carried out using scanning electron microscopy (SEM) [15]. In all cases mentioned however, attention is simply focused on a single macroscopic deformation domain; no further investigation for possible effects of microstructural deformation evolution on the transformation process is performed.

In a study by Brinson [16] the microstructural and macroscopic transformation behavior of polycrystalline NiTi specimens was investigated under low level cyclic loading. In this study, focus is again placed on the macroscopic behavior of the material rather than delving into the underlying microscopic phenomena taking place. However, one key result is presented which offers a correlation between the microscopic and macroscopic behaviors; localized plastic deformation is observed in the NiTi specimen after as few as 10 cycles (potentially being caused by the presence of stabilized SIM). The plastic deformation is observed to appear with cycling in the vicinity of the forming martensitic plates (Figure 2). Due to the increased localized deformation, it is

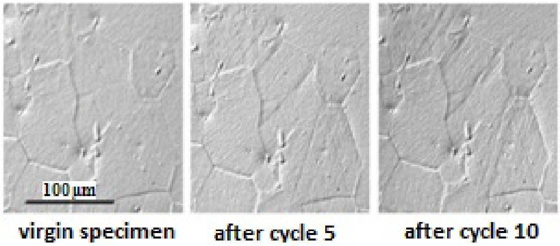


Figure 2: Accumulation of localized plastic deformation within the grains upon loading cycling for 0, 5 and 10 cycles. Specimen fully unloaded following each cycle [16].

observed that additional variants are formed at each cycle, providing a microscopic explanation for the macroscopically observed strain hardening.

As an exciting step forward such studies begin to correlate micromechanical behavior with the overall macroscopic material response of Nitinol, however further work in this research field is still required. The aim of the work presented in this paper was to establish a correlation between microscopic behavior, in particular the volume fraction of SIM, and the overall macroscopic material response employing Finite Element Analysis. In addition, using Finite Element models incorporating a granular structure, identification of possible effects of crystallographic texture on the SIMT was also investigated.

# 2 Material characterization

## 2.1 Material imagining

To create a realistic Finite Element Analysis (FEA) model of polycrystalline superelastic Nitinol, microstructural geometries of suitable specimens were required. Nitinol wire samples underwent a recrystallization anneal (750$^{o}$C for 1hr) and the transformational behavior was subsequently analyzed using the bend-free recovery test; the austenite finish temperature ($A_f$) was found to be 1.5±0.5$^{o}$C. Specimens were then set in an epoxy resin for ease for handling. Specimens were manually polished to a finish of 0.06μm and chemically etched using a $1HF{:}4HNO_3{:}5H_2O$ solution. Finally, specimens were viewed under the optical microscope; grain distribution and average grain size were specifically identified (Figure 3(a)). Utilizing the obtained micrographs, realistic FEA models were created which incorporated the complex microstructural nature of the superelastic austenitic material (Figure 3(b)); these models will be discussed further in Section 3.2.

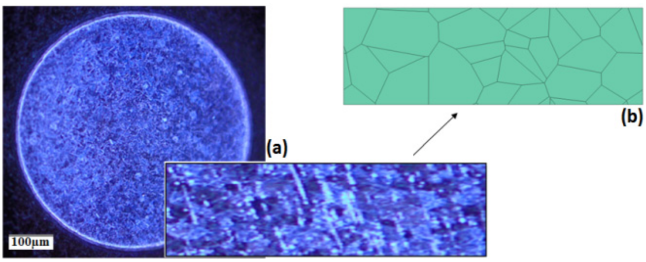


Figure 3: (a) Experimental micrograph and, (b) Finite Element representation of the microstructure of superelastic austenite wire.

## 2.2 Test specimens

Nitinol ‘v-strut’ specimens were custom fabricated for this study. The ‘v-strut’ is representative of a single strut of a Nitinol self-expanding stent; in this way the mechanical behavior of the individual stent components can be identified and analyzed clearly. The manufacturing and processing techniques used on the specimens are consistent with those preformed on commercially available endovascular stents. The specimen's $A_f$ temperature was found to be 11.2±2$^o$C using the bend-free recovery method, thus confirming its suitability for use as a self-expanding stent as it will exhibit superelastic behavior at human body temperature. To accurately characterize Nitinol's asymmetric behavior for input into a user defined UMAT/Nitinol, uni-axial tensile and compressive experimental testing were performed on linear support struts (Figure 4); as will be discussed further in Section 2.2.1 and Section 2.2.2. Excess materials at both ends of the specimens, along with the support struts, were included in the design to provide precise alignment, structural stability and secure gripping during testing.

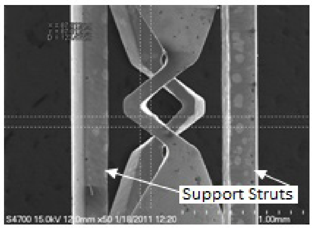


Figure 4: SEM of 'v-strut' specimen used, showing vertical support struts.

### 2.2.1 Experimental set-up

As Nitinol's mechanical properties are highly temperature dependent, all investigations were carried out at 37$^o$C, i.e. body temperature, to accurately represent the material's behavior *in vivo*. This was achieved using the EnduraTEC ELF/3200 in conjunction with an environmental chamber with air-heating fan (Figure 5). The exothermic martensite transformation, and endothermic reverse transformation, has a considerable influence on the stress-strain response of Nitinol due to the release of latent heat due to the exothermic nature of the transformation process. Therefore, to ensure accuracy of data the test temperature was strictly monitored and controlled. Improved heat exchange

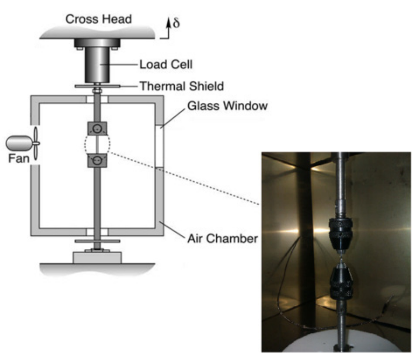


Figure 5: Experimental set-up using in this study for uni-axial tensile and compressive material testing procedures.

 
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results in more accurate and repeatable results. In addition, it allows higher strain rates to be used, due to the faster dissipation of heat from the sample, therefore reducing testing time.

### 2.2.2 Experimental results

To accurately characterize Nitinol's material behavior, uni-axial tensile and compressive experimental testing were performed on the support struts of the specimens (as discussed in Section 2.2). From the stress-strain curves (Figure 6(a)), key material properties are extracted for input into the user defined UMAT/Nitinol. Validation of the UMAT was completed through comparison of the simulated stress-strain response of a simple cubic FEA model to the experimental stress-strain data; ensuring the model was accurately predicting the complex superelastic material behavior of the specimen (Figure 7).

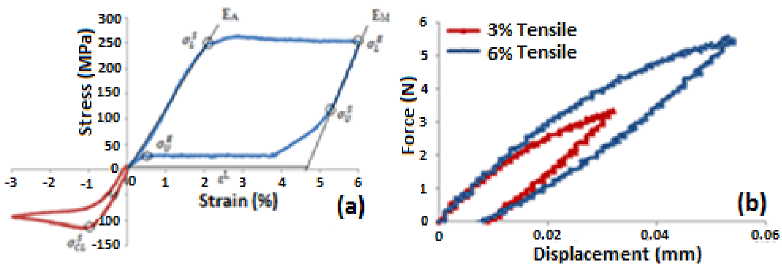


Figure 6: (a) Stress-strain behaviour of Nitinol to 3% compressive strain and 6% tensile, (b) Load-deflection curve for 'v-strut' specimens at 3% and 6% tensile strain.

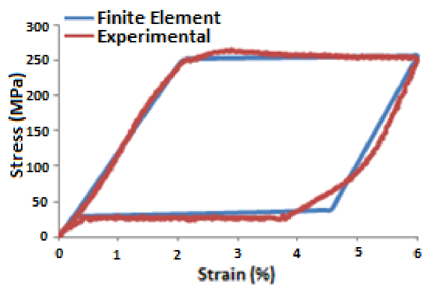


Figure 7: Validation of FEA model employing the UMAT/Nitinol.

# 3 Finite element model development

## 3.1 Correlation of SIMT to fatigue behavior

To investigate the effect of stress-induced martensite (SIM) on the fatigue behavior of a Nitinol stent device, a 3-dimensional homogenous FEA model of a 'v-strut' stent subcomponent was created. Employing a user defined material subroutine (UMAT/Nitinol), the model was capable of predicting Nitinol's complex transformational behavior on a macro-scale level. To accurately represent Nitinol's macroscopic material behavior in the FEA model, data from the uni-axial tensile and compressive experimental tests (as described in the Section 2.2.2) were inputted into the UMAT. Following validation (Figure 7), the influence of SIM on the overall macroscopic stress-strain behavior of the 'v-strut' specimens was established for various strain levels. Three strains spanning the experimentally established superelastic plateau of the specimen are targeted for analysis (namely, 2.5%, 4% and 6%) to investigate various physiologically relevant conditions experienced by a stent; variations of mean strain experienced by a stent *in vivo* are attributed to the vessel anatomy in which they are placed and extent of stent over-sizing.

Native vessels undergo diameter changes of approximately 0.16–0.34% when subjected to a typical 100mmHg pulse pressures in a healthy vessel [1], these changes being potentially lower in a stenosed vessel. This results in the endovascular stent experiencing strain amplitudes *in vivo*. The mean strain (mid-pulse), however, has the most significance when discussing the fatigue life of self-expanding Nitinol stents. Typical engineering materials will experience a decrease in fatigue life with increasing mean strain, however, Nitinol has been shown to exhibit improved fatigue performance in the region of approximately 1.5–6% mean strain [1, 2]. Therefore, employing FEA, the aim of this work is to investigate the macroscopic behavior of Nitinol 'v-strut' stent subcomponents at these various mean strains and evaluate the potential influence of SIMT on the observed macroscopic material response; through identification of the volume fraction of SIM at critical locations. The hypothesis presented in this paper states that, at sufficiently high mean strains, the resulting stress levels induce and stabilize the SIM and this is what gives rise to the increased fatigue performance.

#### 3.1.1 Simulated loading modes

The use of detailed FEA simulations allows evaluation of the stress-strain behavior of individual Nitinol stent components at various displacements; these being representative of various levels of physiologically relevant mean strains. Through systemic analysis, identification of the corresponding simulated displacements to induce the desired strains at critical locations in the FEA model (peak tensile strain on outer apex of 'v-strut') is achieved. It is also of significant importance, to ensure accuracy of results, that the chosen simulated loading modes represent physiological conditions experienced by the stent. As displayed in the contour plots in Figure 8, there is a considerable variation in the specimen response when loaded in compression (Figure 8(a)) or tension (Figure 8(b)). *In vivo*, a stent experiences compressive loading due to the pulsatile loading of the diastolic-systolic motion and thus compressive loading procedures are therefore performed in this study.

### 3.2 Effect of texture on fatigue behavior

To evaluate the effect of microstructural texture on Nitinol's macroscopic response, a 2-dimensional rectangular model was created using Voronoi Tessellation based on the obtained micrographs (Figure 3(b)). As the images had

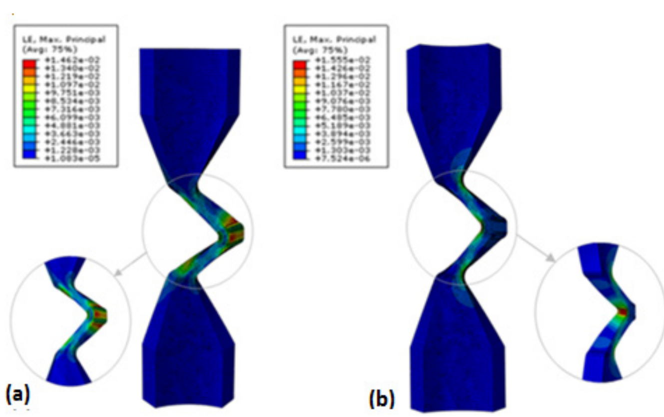


Figure 8: FEA models of ‘v-strut’ at 1.5% (a) compressive and (b) tensile strain.

an aspect ratio close to 1, it was determined the complex realistic models were properties were obtained from literature [17] for similarly processed NiTi not necessary; idealized hexagonal units were instead used in which each hexagonal unit represented an individual grain (Figure 9(b)). In this way, the constitutive behavior of Nitinol on a micro-scale was represented. Single crystal specimens (as those used in the material characterization of Section 2.1) and were assigned to the individual grains. The effects of individual grain orientation on SIMT were therefore investigated for randomly generated crystallographic textures.

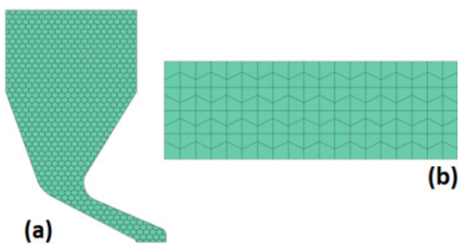


Figure 9: (a) 2-dimensional ‘v-strut and, (b) rectangular FEA models with idealized hexagonal grain structures used to investigate the effect of texture.

In order to investigate the influence of crystallographic texture on the behavior of a stent material, a similar 2-dimenstional ‘v-strut’ model with an idealized hexagonal grain structure was created (Figure 9(a)). It should be mentioned, common microstructures in Nitinol stents feature an ultrafine-grained microstructure in the order of 40–100 nm. In this study, however, larger grain geometries are employed; annealed NiTi single crystal properties are used in this study which would represent an average grain size of approximately 20µm [17]. Nonetheless, employing FEA, the effect of a randomly generated microstructure was represented in the complex ‘v-strut’ geometry. The overall macroscopic

 
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stress-strain behavior of the specimen was analyzed, in addition to identification and analyzes of critical locations of peak tensile stresses on the outer apex of the 'v-strut' model which may represent a potential fatigue failure initiation site.

## 4 Results and discussion

### 4.1 Correlation of SIMT to fatigue behaviour

The highly advantageous trait exhibited by Nitinol of increased fatigue performance with increasing mean strain still remains unexplained in literature, in particular in the correlation between microstructure and the observed macroscopic phenomenon. In this paper, it is hypothesized that the increased fatigue life is attributed to the phase transformation (SIMT) experienced by the superelastic material. The volume fraction of SIM is shown to increase with increasing strain at critical locations (Figure 10); namely at the regions of peak stresses under the compressive loading at the inner apex of the 'v-strut'. Under strain-controlled conditions, superior fatigue lives are shown in specimens that experience increased strain levels [1, 2]; it is therefore suggested there is a strong connection relating SIM, in particular at strain levels high enough to stabilize SIM, and the experimentally observed increased fatigue performance.

However, the most significant location for analysis is that of peak tensile strain (initiation site of fatigue failure). The volume fraction of SIM at this critical location is found to follow a similar trend to that of the experimentally established constant life diagram for Nitinol [1, 2]; see Figure 11. Furthermore,

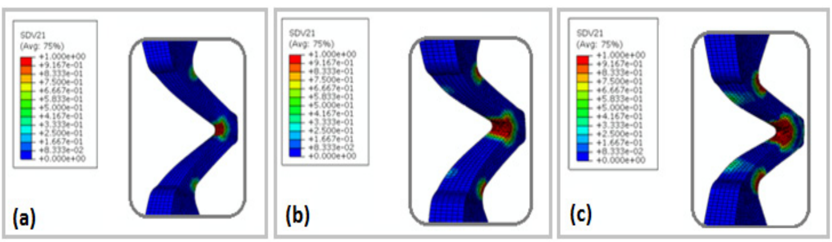


Figure 10: The volume fraction of SIM in 'v-strut' under (a) 2.5%, (b) 4% and (c) 6% compressive strain.

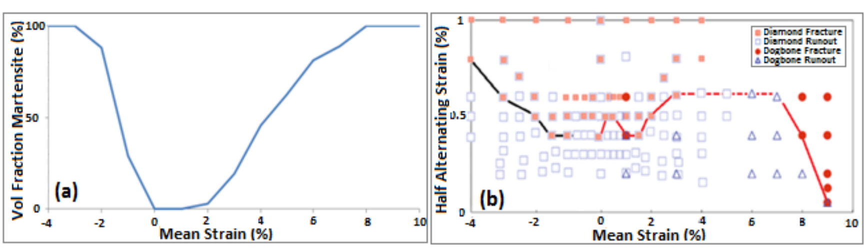


Figure 11: Comparing (a) the volume fraction of SIM present in the FEA model for various mean strains, and (b) the experimentally established constant life diagram for Nitinol [1, 2].

the observed on-set of increasing fatigue performance correlates with the onset of SIM at approximately 1.5% mean strain level which presents further evidence for the proposed hypothesis. It is proposed, at such strains the SIM is stabilized (through methods discussed in Section 1.3) and a strain hardening effect occurs, thus resulting in a strengthening effect on the Nitinol specimens. This, in conjunction with the self-accommodating nature of the twinned martensite, presents itself as a possible explanation to the observed increase in fatigue performance.

### 4.2 Effect of texture on fatigue behavior

This study successfully demonstrates the profound effect crystallographic texture (grain orientation distribution) has on overall macroscopic material response of Nitinol. In applying a load-unload procedure on the idealized hexagonal rectangular models described in Section 3.2, the effect of the randomly generated textures on the stress-strain response becomes apparent. It is found, grains orientated in (110) crystallographic direction inhibit, while grains in (111) orientations promote the SIMT [17]. This becomes particularly evident when comparing Figures 12(a) and (b); in including a higher volume of (111) orientated grains in model (b), it can be seen notably lower stress values are reached along the upper plateau due to the ease at which SIMT occurs.

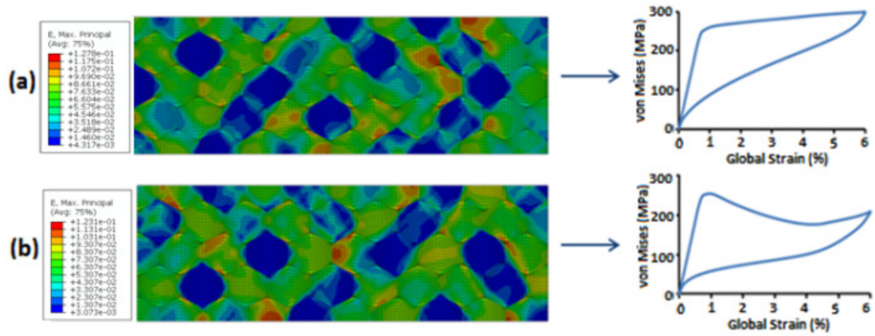


Figure 12: Maximum principal strains in idealized hexagonal model with two random texture deformed (a) and (b) to 6% global strain.

The difference in transformation behavior in the individual grains results in localized stress gradients over grain boundaries; these peak stresses become particularly important when discussing fatigue behavior. To further explore this, the influence of texture was investigated in the 'v-strut' stent subcomponent; a 2-dimenstional idealized hexagonal model was created for analysis (Figure 13). Due to the presence of (110) orientated grains at critical locations in the 'v-strut' geometry (Figure 13(a)), SIMT has been hindered and therefore localized peak strains have been induced. Consequently, the peak tensile stresses induced on the outer apex of the 'v-strut' become significant as fatigue failure initiation sites in the 'v-strut' stent subcomponent.

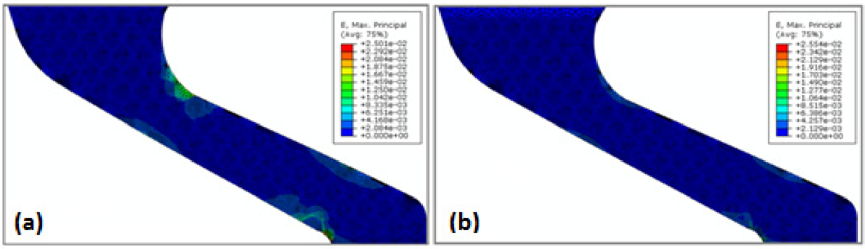


Figure 13: Maximum strains in 'v-strut' with two varying textures (a) and (b). Peak strains in texture (a) due to presence of (110) orientated grains.

As discussed in Section 3.2, the granular FEA models created in this study contain larger average grain sizes (20µm) than those typically found in Nitinol endovascular stent devices (40–100nm). Therefore models created in this work demonstrate a more severe impact of crystallographic texture on macroscopic material response; due to the larger sized grains. However, it can be stated, in understanding the impact of local microstructural effects on global mechanical response, it can lead to a much fuller understanding of the causes of deviation of the mechanical response from predictions and unforeseen fracture in Nitinol biomedical devices.

## 5 Concluding remarks

Finite Element Analysis (FEA) models capable of predicting the complex constitutive behavior of Nitinol were created to determine the influence of stress-induced martensite (SIM) on the fatigue behavior of Nitinol 'v-strut' stent subcomponents. Utilizing FEA, the volume fraction of SIM was established in the specimens for various levels of mean strain. As the strain levels in the specimen increase, the volume fraction of SIM present correspondingly increases. Furthermore, the percentage of SIM at critical locations of fatigue failure initiation follows a similar trend to that of the constant life diagram experimentally established for Nitinol [1, 2]. Therefore it can be suggested, there exists a strong correlation between SIM and the observed increase in fatigue performance due to possible combined effects of strain hardening (from stabilized SIM) and the self-accommodating nature of the twinned martensite itself.

This study also successfully demonstrates the profound effect texture has on stress-induced martensite transformation (SIMT); it was demonstrated that grains orientated in (110) crystallographic direction inhibit, while grains in (111) orientations promote the stress-induced martensite transformation progression [17]. This conflict between individual granular behavior has been shown to result in localized stress and strain gradients over grain boundaries which may previously have been neglected in simplistic homogenous FEA models disregarding influence of individual grain anisotropies. However, due to the mechanical property variation with texture, these induced peak tensile stresses become particularly important when discussing fatigue behavior in complex stent geometries and may present an explanation for unforeseen fatigue failures in stent devices.

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