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The effect of crystallographic texture on stress-induced martensitic transformation in NiTi: A computational analysis

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ABSTRACT

NiTi's superelasticity is exploited in a number of biomedical devices, in particular self-expanding endovascular stents. These stents are often laser-cut from textured micro-tubing; texture is the distribution of crystallographic grain orientations in a polycrystalline material which has been experimentally shown to have a marked influence on mechanical properties. This study offers a computational examination into the effect of texture on the stress-induced martensite transformation (SIMT) in a micro-dogbone NiTi specimen subject to tensile loading. Finite Element Analysis (FEA) is employed to simulate the transformational behaviour of the specimen on a micro-scale level. To represent a realistic grain structure in the FEA model, grains present in a 200 μm × 290 μm test site located at the centre edge of the specimen were identified using Scanning Electron Microscopy (SEM). Grains are assumed to have homogenous behaviour with properties varying according to their crystallographic orientation to the loading direction. Required material properties were extracted from uniaxial stress–strain curves of single crystals for each crystallographic orientation for input into the in-built UMAT/Nitinol. The orientation of each grain in the test site was identified using Electron Back-Scatter Diffraction (EBSD) techniques. In this way, a quantitative explanation is offered to the effect of crystallographic texture on SIMT. Finally, the evolution of grains in the specimen, during the transformation process, was experimentally investigated by means of an *in-situ* SEM tensile test.

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1. Introduction

1.1. *Medical use of NiTi*

NiTi possesses a unique combination of properties which renders it suitable in a broad range of engineering applications. In particular, it has proven appealing in the biomedical industry for use in the construction of self-expanding endovascular stents (O'Brien and Bruzzi, 2011). Such devices have proven effective in the treatment of atherosclerosis in a variety of vessels and arteries. However, 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, fracture rates of up to 65.4% in such stents have been reported in

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clinical studies (Allie et al., 2004). Such failures have been attributed to cumulative fatigue damage. Accurate characterisation of NiTi fundamental fatigue behaviour, in particular the local microstructural effects on global mechanical response, is therefore essential for their prolonged safe use in human arteries.

1.2. Superelasticity

NiTi's phase transformation, from a parent austenite to a daughter martensitic phase, can be induced by a change in temperature or stress whereby martensite forms upon cooling below the characteristic martensite start temperature, M_s, or via the application of an external stress. Austenitic NiTi (ordered cubic B2 structure) is a hard, stiff material whereas martensitic NiTi (complex-twinned monoclinic B19' structure) is a softer, more ductile material with a lower yield stress (Van Humbeeck and Stalmans, 1998). In a crystallographic context, the stress-induced martensite transformation (SIMT) occurs by rearrangement of atomic planes via Bain strain and lattice invariant shear (Bhattacharya, 2003). The twin boundaries in martensite readily shift such that the twins are predominantly oriented in one preferential direction termed 'de-twinning'. By this microstructural process, NiTi can withstand approximately 6–8% strain without permanent deformation. This ability to accommodate such significant strains is highly desirable in stent device design for stent deliverability, durability, and conformance. 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.

1.3. Microstructural texture

As described above, NiTi derives its unique mechanical behaviour from the coordinated atomic movements manifesting in a phase transformation from cubic austenite to monoclinic martensite. Therefore, any significant alignment of the atomic planes resulting from crystallographic texture can have a marked influence on the mechanical response. It has been experimentally shown that crystallographic texture has an effect on crack trajectories in NiTi tube specimens subjected to uniaxial cyclic loading (Robertson et al., 2004). In addition, substantial variations in mechanical behaviour have been observed between rolled and transverse directions of cold-drawn NiTi sheets which can been attributed to the hindrance of deformed martensite structures and defects in the specimen leading to differing dominant de-twinning and reorientation modes (Liu et al., 1998). Despite the clear dependence of mechanical properties on crystallographic texture, standard practice used in the computational design of biomedical stent devices assumes the material behaves as a continuum. Therefore, this study aims to highlight the effect of crystallographic texture on stress-induced martensite transformation (SIMT), and ultimately on the overall macroscopic behaviour, in a superelastic micro-dogbone NiTi specimen in order to highlight concerns with the current design practice.

1.4. Modelling methodology

In the last four decades, constitutive modelling of superelastic materials has been an active research topic. The three main modelling methodologies used can be categorised as micro, micro–macro or macro scaled based approaches. Description of micro-scale features is the main focus of micro models. A micro-scale constitutive model was proposed for martensitic reorientation and detwinning in superelastic materials by Thamburaja (2005). This model was further developed by Pan et al. (2007) to be capable of quantitatively predicting the experimental response of an initially textured and martensitic polycrystalline NiTi rod under a variety of uniaxial and multiaxial stress states. Such models have proven useful in developing a further understanding of fundamental phenomena occurring at the microscopic level however, they are not easily applicable on the relatively larger biomedical device scale within numerical methods such as the Finite Element Analysis (FEA). A micro–macro thermomechanical model was proposed by Siredey et al., (1999) to capture granular transformational behaviour in polycrystalline superelastic materials using the average martensite fraction, in each domain containing marensite plates, as an internal variable. Fischer et al. (1997) suggested that the phase transformation in a micro-region is related to a critical value of the Gibbs free energy and obtained a description for the phase transformation in polycrystalline superelastic materials by statistical methods. Such micro–macro studies combine micromechanics and macroscopic continuum mechanics to derive constitutive laws. However, due to the time-consuming computations associated with such approaches, they have proven inappropriate for typical engineering applications.

Macroscale approaches use averaged material behaviour extracted from experimental tension-compression testing and, in general, are suitable to be used within numerical methods such as FEA. A constitutive model based on an internal variable formalism and the framework of generalised plasticity was proposed by Aurricchio and Taylor (1997). This model was used in the formulation of an in-built UMAT/Nitinol found in the commercially available FEA platform ABAQUS™. The generalised plasticity theory decomposes strain into two parts, a purely linear elastic strain component and a transformational strain component. A rule of mixtures is employed by the UMAT to implement the change in linear elasticity from the parent austenite phase to the stress-induced daughter martensite phase. The constitutive model assumes any change in externally applied stress levels results in a reorientation of the twinned martensite phase with negligible additional effort. Changes in temperature produces a shift in the stress levels at which the transformations takes place; this shift in temperature is linear. It has been observed experimentally that less stress is required to produce the transformation in tension rather than in compression. This is modelled using a linear Drucker-Prager-like approach in the UMAT for the transformation potential. Employing this UMAT/Nitinol, the basic features of NiTi can be reproduced in an efficient manner and is therefore often used to aid in the initial stages of design of biomedical stent devices.

In recent years, microscale constitutive models aim to describe the anisotropic behaviour of individual grains with the computational efficiency of a macroscale approach. Donnelly (2012) combined the relevant elements of crystal