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In Silico Finite Element Approach on Mechanical Behavior in Superelastic Nitinol

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Abstract. Over the recent years, Nitinol (Ni-Ti) shape memory alloys have gained popularity in the medical, aerospace and energy sectors, due to their superelasticity, shape memory effect, low stiffness, good biocompatibility and corrosion resistance. Compared to steels and other common metallic materials, it is difficult to model the mechanical behavior of Ni-Ti due to the inherent functional properties caused by the diffusion-less solid-state phase transformations. With the help of Laser Powder Bed Fusion (L-PBF) process, these transformational characteristics can be controlled. This will ultimately lead to controlling the mechanical and thermal properties for specific applications. In this work, Finite Element Analysis (FEA) was conducted to replicate the actual mechanical phenomenon occurring in Nitinol. Models were generated for simulating the superelastic and plastic behaviors, and were validated against actual experimental data. The ability to model the complex mechanical response of Nitinol will enable exploration into the sensitivity of material response to phase volumes, material composition, and strain rate. Robust models of these phenomenal also provide the potential for tailoring in-silico the microstructure required for specified desired macroscopic material properties.

Introduction

Compared to most intermetallics, Ni-Ti has high ductility which makes it suitable for various engineering applications. It also has low anisotropy and small grain size compared to other alloys [1-3]. By altering the composition, microstructure and processing conditions, Ni-Ti can be processed with specific functional properties that can be utilized for bespoke applications.

The shape memory effect in Ni-Ti originates from the solid-state phase transformations that occur during the deformation and/or thermal cycling [4]. When Ni-Ti with a martensitic phase is deformed, the crystal structure of the phase transforms to a detwinned martensite phase. When the temperature of the material is then raised above the transformation temperatures (TTs), the phase changes from martensite (B19' monoclinic crystal structure) to austenite (B2 BCC structure) regaining the pre-trained shape. When the material is then cooled to room temperature, the phase reverts back to a twinned martensite state. It has been found that a higher Ti content results in higher transformation temperatures enabling this shape memory effect. A higher Ni content on the other hand can be set to lower the transformation temperatures sufficiently below room temperature such that the austenite phase is present, enabling the superelastic (pseudoelastic) property. The superelasticity in Ni-Ti can recover high strains of 10-15%, before it deforms plastically [5, 6]. At room temperature, the superelastic Ni-Ti will be in austenite phase. When stress is applied beyond the start of martensitic phase transformation, distortion of the crystal lattice occurs. This is associated with low hardening, and the lattice transforms completely into martensite. The crystalline phase of detwinned martensite occurs at lower temperatures and higher stresses, whereas the crystallization of austenite occurs at higher temperatures and lower stresses [7]. As seen in Fig. 1, when the material is deformed at constant (room) temperature, initially it follows the Hooke's law with the stiffness (E_A) as that of the austenite phase. As the stress levels cross a certain value (σ_s^{AM}) a solid-state diffusion-less phase transformation from austenite to martensite will occur, gradually forming a fully stress-induced martensite phase. A coordinated motion of a large number of atoms relative to their neighbors, causes this diffusion-less displaced transition. A new crystal structure is formed from parent phase without any change in the composition [8]. When stress levels are further increased beyond σ_f^M, Hooke's law is again followed with the stiffness of the martensite phase. After reaching the maximum elastic strain limit, yielding occurs creating a residual strain. If the material is unloaded within the elastic strain limit (stress corresponding to σ_s^{MA}), martensite phase reverts to austenite (stress, σ_f^A). Both phase transformations are associated with latent heat release or absorption (during reverse loading) [9, 10]. This concept has inspired the use of Ni-Ti in heat pump and heat recovery applications, for which high heat transfer rates can be realized by creating Ni-Ti geometries with high surface areas.

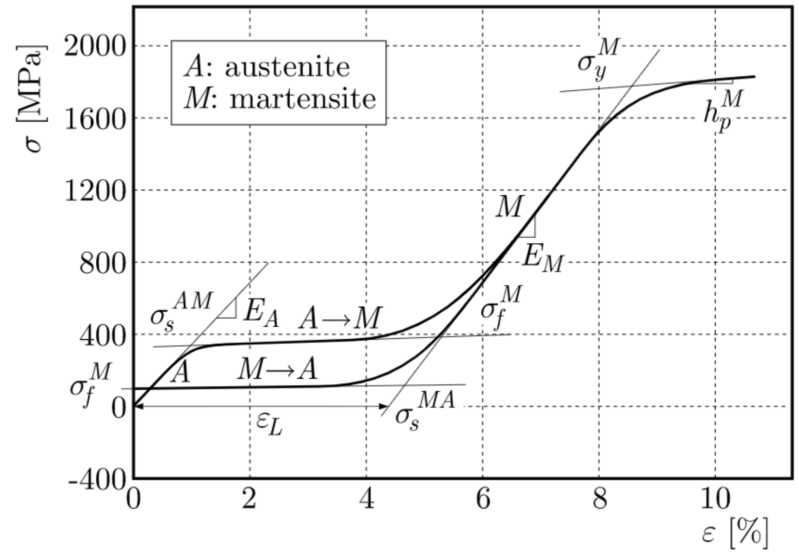

Fig. 1. Schematic illustration showing the nomenclature used during phase transformations and mechanical loading; σ_y^M – martensitic yield strength; h_p^M – plastic hardening modulus [11].

Nitinol is difficult to fabricate and process using traditional techniques, because of high chemical reactivity of titanium at high temperatures (formation of oxides), high inflammability of Ti powder when heated in air, and very low machinability (high hardness). Additive manufacturing (AM) techniques such as Laser Powder Bed Fusion (L-PBF) can create highly complex geometries in inert atmosphere with pre-designed porosity, homogeneous composition, and desirable transformation properties as compared to the traditional techniques. The process can also achieve structures with high density and near net shape, requiring very little or no post-processing. With L-PBF, we can also control the phase composition [4].

In this work, an in-silico finite element (FE) model is realized to simulate the mechanical behavior of superelastic Nitinol. The model is validated using experimental data from a previous research data. The mechanical/transformational behavior can also aid in calculating how much thermal energy is absorbed/released during the phase transformations.

Background

The mechanical behavior of Nitinol can be considered as three: elastic deformation, martensitic phase transformation, and plastic deformation. In elastic deformation, local atomic arrangements are continuously varied (reversible) proportionally to the change in applied stress. Whereas, the twinning and martensitic transformation can be considered as discontinuous and diffusion-less reversible changes of local arrangement of atoms propagating through the crystal as twin plane interfaces and habit planes, when stress/temperature is varied. Habit planes are well-defined interfaces or contact plane between the martensite and austenite phases; does not suffer any distortion. Here, the discontinuous finite strains formed are fully recoverable under thermomechanical loads [12].

Plastic deformation proceeds either as movement of slip dislocations, or irreversible twinning. The material is permanently deformed without inducing any change to the crystal lattice. It must be noted that, slip dislocations and twinning occurs locally at moving lattice defects such as habit plane interfaces and twin interfaces [12]. Due to the requirement for compatibility of large finite strains of martensitic variants created by the transformation or twinning, plastic strains, irrecoverable lattice defects, and internal stresses can be introduced into the Nitinol microstructure, specifically at elevated temperatures. Plasticity after forward martensitic transformation stabilizes the martensite phase and hinders the reverse transformation [12, 13].

It is often difficult to determine whether the martensitic transformation and plastic deformation propagate independently, or mutually coupled. The main concern is whether the strain compatibility is attainable only by transformation strains, and/or the plastic deformation plays a role in it. If this is the case, then the martensitic transformation and plasticity can be coupled intrinsically. During the reverse phase transformation, in order to achieve compatibility, martensite twinning and plastic slip in austenite often works combined. The residual plastic strain in austenite suppresses the twinning, and the slip is facilitated. Consequently, a stronger contribution of the plastic slip is expected to work for compatibility at the interfaces, depending on the residual strain levels [12].

Numerical methods including finite element analysis (FEA) methods, allow to analyze complex problems comprising of intricate geometries, interactions, nonlinearities, and dynamic conditions. Phenomenological constitutive models use macroscopic energy functions to obtain the responses. These functions depend on internal state variables. The evolution is simulated via the second law of thermodynamics. These models seek solutions to boundary value problems on the structural level through energy minimization, similar to classical plasticity models [14].

In this study, the Auricchio model [6] implemented in Ansys® FEA platform will be utilized for superelasticity and shape memory analysis. The rate independent 3D model assumes a single-variant martensite; utilizes an exponential hardening law, and accounts for martensitic transformations and martensitic reorientation. The model also indicates the dependency of elastic modulus on martensite-phase volume fraction (MVF). The Auricchio model can be divided into three segments:

1. 1D and 3D constitutive model to reproduce superelasticity
2. Time-discrete isothermal model
3. Algorithmic implementation with a finite element (FE) framework

The constitutive model includes the three phase transformation mechanics:

- Transformation of austenite to single-variant martensite ($A \rightarrow S$)
- Transformation of single-variant martensite to austenite ($S \rightarrow A$)
- Reorientation of single-variant martensite ($S \rightarrow S$)

The constitutive model is utilized in this current study, and uniaxial loading-unloading history is also considered in the time-discrete model, to open the possibility of computing a closed-form solution for evaluating accuracy of FE scheme. Most recent study by [15] proposed a model containing two limit functions, to define both the phase transformation domain and plastic domain for predicting cycling effects and accumulation of inelastic strains. This is based on the concept that the initiation and evolution of two distinct yield profiles can be used to fully capture the martensitic transformation and plastic slip yield simultaneously. Coupling these profiles can provide insight into the complete mechanical behavior of Ni-Ti.

Numerical Simulations

Compared to most metallic materials, Ni-Ti material is difficult to be modelled because of the complex mechanical behavior discussed in previous sections. In this study, FE modelling and simulation is performed using the package ANSYS® Workbench 2019. This software has an in-built Auricchio model for defining the shape memory material properties, and features custom material plasticity data implementation.

The superelasticity concept is focused for an easier understanding of the phase transformations. To keep the model simple, isothermal conditions (22°C) were assumed. Since the work focuses on stress-induced martensitic transformation, only the mechanical behavior is considered, and all thermal effects are ignored. The FEA work starts with performing a mesh convergence study, and then validating the created material model against a set of experimental data for superelasticity. Besides superelasticity, data from an experimental study has been used to check the plastic behavior of the model.

Three different material data has been used for the analysis works (Table 1). The density has been considered the same for the three materials as 6.45 g/cm3. For the macroscale study, a cube of geometry 5x5x5 mm has been used for the FEA, and uniaxial mechanical loading/unloading (tension or compression) at constant strain rate of 0.1/min is conducted. The bottom of the cube is completely fixed (completely constrained).

Table 1 Material data [11, 16] used in the FEA models for determining the stress-strain responses. ν: Poisson's ratio, ϵ_L: max. longitudinal strain

Material	E_A (GPa)	ν	σ_s^{AM}(MPa)	σ_f^{M}(MPa)	σ_s^{MA}(MPa)	σ_f^{A}(MPa)	ϵ_L
NT1	71.1	0.3	500	700	400	200	0.044
NT2	41	0.33	380	390	145	110	0.040

Mesh Convergence. Mesh convergence is performed to identify an appropriate mesh geometry that can be used in the model, to converge to an optimum solution. For this, material NT1 was used. The superelasticity model considered, traced almost similar curves for the different mesh sizes used (Fig. 2). Therefore, to distinguish the effect of mesh sizes, two factors were considered based on theoretical observations – non-convergent regions; and stress values at 4% strain.

Non-convergent regions. As seen in Fig. 2, larger mesh sizes show some anomaly at the start/end of phase transformations. These are the non-convergent regions in the solution. It was observed that mesh sizes from 0.5 mm and below did not show any non-convergent region.

Stress @ 4% strain. In Fig. 2, a noticeable difference in stresses can be seen around the strain value of 0.04 and above. Stress values at 0.04 strain for different mesh sizes are shown in Fig. 3. It can be seen that the stress values stabilize with low error value around a mesh size of 0.6 mm.

Even though a mesh size of 0.6 mm was reasonable, 0.5 mm showed better convergence and low error % (Fig. 3). Lower mesh size gives better prediction; however, the computational time was almost twice when the mesh size was reduced from 0.5 mm to 0.4 mm. Therefore, a mesh size of 0.5 mm was selected for macro-scale analysis. While it not fully clear why the error is lower at 0.5 mm, this could be a discretization error from the mesh creation, numerical errors from integration or rounding errors from numerical calculation.

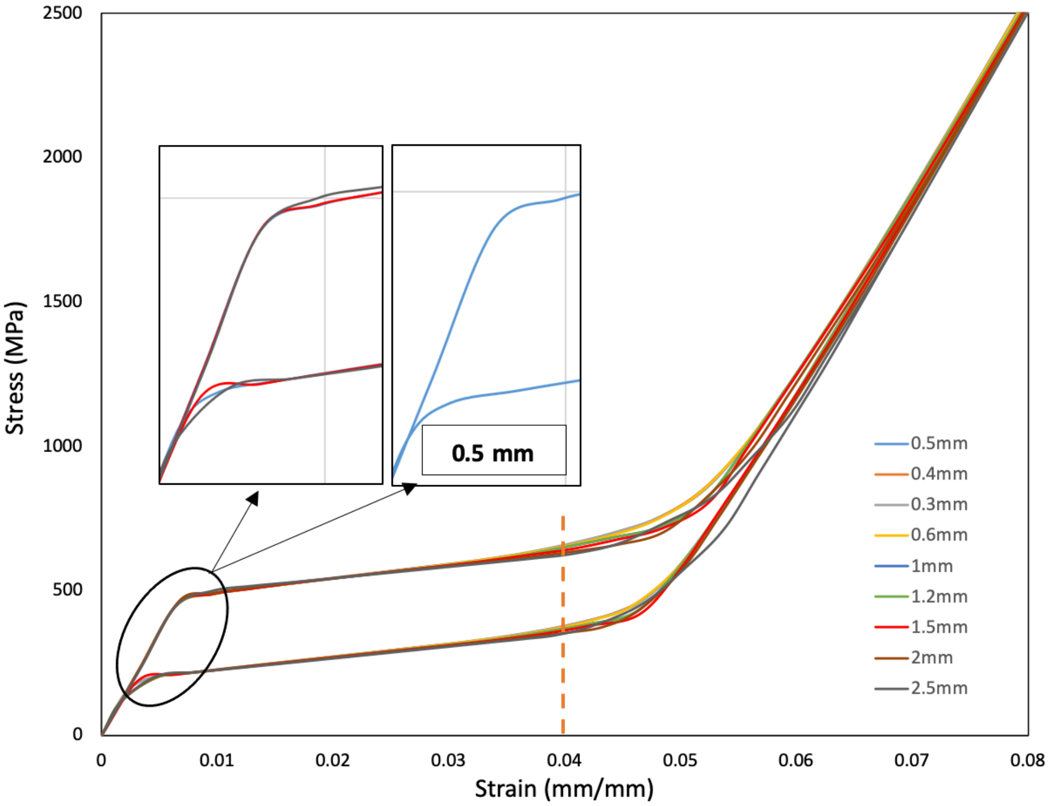

Fig. 2. Stress-strain graph for mesh convergence study.

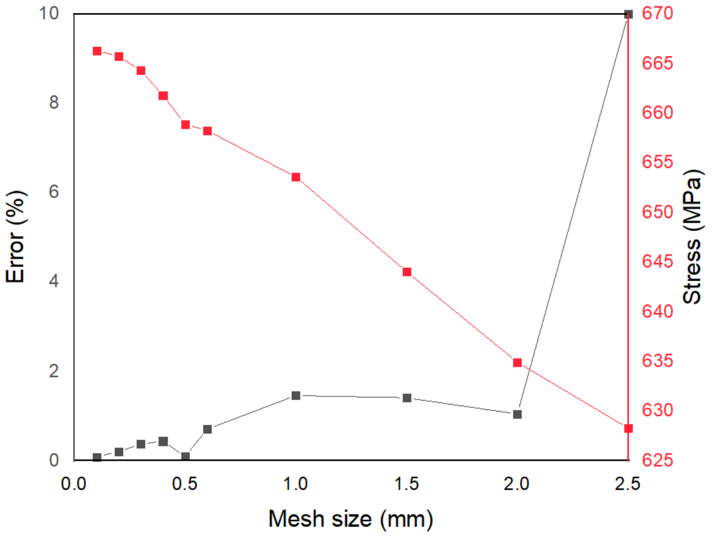

Fig. 3. Stress values (red) at 4% strain and respective error % (black) for different mesh sizes.

Model Validation. Initially, the in-built Auricchio superelasticity model [6], was validated against the experimental data by Jiang & Li [11] (ref. material NT2). After completing the plasticity and superelasticity behaviors separately, the output data were combined to represent the coupled mechanical behavior. This procedure of combining the output data can be justified based on Fig. 1, where it can be seen that the plastic region always lies after a complete martensitic transformation, inferring that the superelastic phenomenon is distinct (analogous to the elastic region in steel), until the strain limit for plastic deformation has reached. The plastic deformation was modelled to be triggered in the martensite phase (Fig. 4).

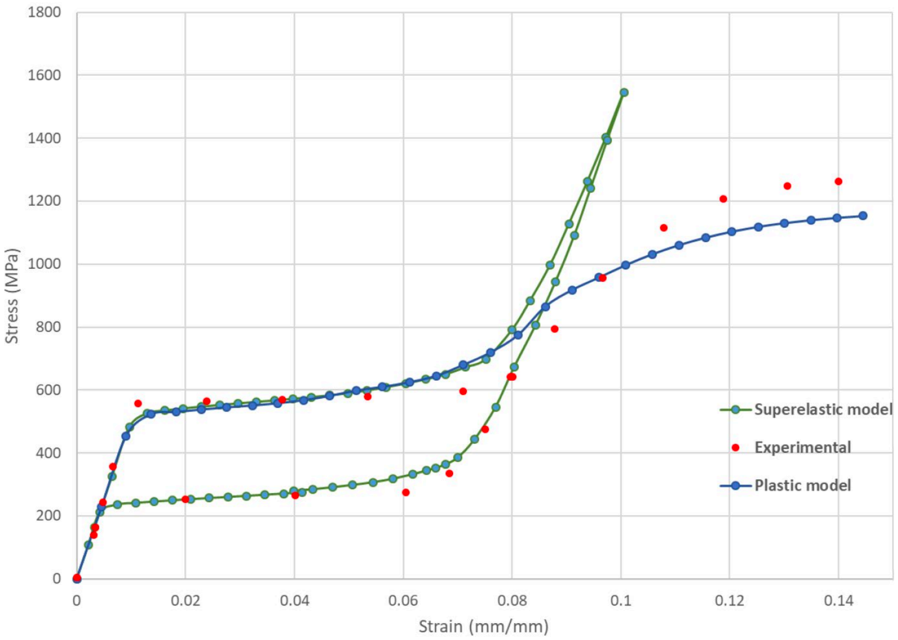

Fig. 4 Validation graph showing superelasticity and plasticity models separately.

Conclusions

An Auricchio material model was used to simulate the superelasticity in Ni-Ti alloys. The solid-state phase transformation from austenite to martensite was simulated and the plastic behavior was also coupled to this, realizing an actual real-life mechanical behavior of Ni-Ti. Even though the Auricchio model performed decently, the model was not built to simulate the stabilization effect during mechanical cycling. In real scenario, during the first cycle, the microstructure is modified and self-oriented, and a plastic deformation is usually observed [17]. This residual deformation will propagate until the mechanical curve stabilizes. Along with this, the model is not sufficiently sensitive to the martensite stiffness profile, hence it is not effective to explore the post-transition strain characteristics. This model was used only to observe the mechanical phenomenon (thermal effects unaccounted). Therefore, a more robust model which considers these factors is needed to fully understand the functional behavior of Nitinol.

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