User Implemented Nitinol Material Model in ANSYS

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Abstract

Nitinol is an acronym for NIckel TItanium Naval Ordinance Laboratory since the alloy was originally developed at the Naval Lab. It is used to describe a family of materials, which contain a nearly equal mixture of nickel and titanium. Nitinol alloys are attractive to the medical device industry because they are biocompatible and when processed correctly, are at their optimum superelastic behavior at body temperature.

Nitinol exhibits a different stress-strain curve for loading and unloading that cannot be modeled with existing material models in ANSYS. This paper describes the implementation of a unique user material model in ANSYS that simulates the nitinol superelastic behavior. Example analyses are provided demonstrating the application of this material model for medical implant devices called stents.

Introduction

Metallic materials that exhibit elasticity over large levels of strain are being used in commercial products in a variety of industries. The increased flexibility obtained in these products by undergoing large elastic strain can improve their performance. For example, Nitinol stents have the advantage that they can be self-deployed, relying on the super elasticity of the material to expand the stent against the artery walls after angioplasty. The superelasticity eliminates the need for balloon expansion and guarantees residual forces between the stent and artery wall. Eyeglass frames constructed from Nitinol will withstand extreme bending that would break conventional frames. Long-stroke deployment actuators are another application for shape memory alloys since they do not suffer from end-of-deployment shocks seen in conventional systems. These are used in a variety of electronic applications such as switches, controls, breakers, etc.

If there is going to be a continued conversion of products to Nitinol, the product structural stability must be evaluated. Detailed stress analyses are required to evaluate the ultimate strength and fatigue lifes. This data is needed to improve the designs of these products and obtain government regulatory approval.

Often Nitinol is used as a replacement to stainless steel components. A comparison of nominal properties between Nitinol and Stainless Steel is provided in the following table:

Property	NiTi	Stainless Steel
Recovered Elongation	8%	0.8%
Biocompatibility*	Excellent	Fair
Effective Modulus**	~ 48 GPa	193 GPa
Torqueability	Excellent	Poor
Density	6.45 g/cm^3	8.03 g/cm^3
Magnetic	No	Yes
Ultimate Tensile Strength (UTS)	~ 1,240 MPa	~ 760 MPa

The superelasticity, which results in an order of magnitude increase in recoverable strain, is one of the most attractive assets of Nitinol. Finite element modeling has been used for many years as a predictive tool for capturing the stress and strain response of metallic structures. Isotropic and Kinematic plasticity laws have allowed analyst to predict the response of steels well beyond their initial yield point. Material laws have also been able to capture the hysteretic behavior using material laws such as the rate-independent nonlinear kinematic hardening model proposed by Chaboche [1, 2] to simulate the ratcheting response under cyclic loading. These material laws however cannot capture the unique loading and unloading response of Nitinol. In order to simulate the unique cyclic structural response of Nitinol products, a new material model is required.

Analytical material models currently used to evaluate the response of metallic parts in ANSYS are inadequate to characterize the unique hysteretic behavior of Shape Memory Alloys such as Nitinol. In traditional plasticity laws, the unloading behavior of the material follows the elastic modulus slope. With Nitinol the behavior follows a hysteresis where the unloading curve follows neither the non-linear loading nor elastic modulus unloading curves. The material model described in this paper provides a unique ability using ANSYS to characterize the response of Shape memory alloys.

Shape Memory Alloy Unique Behavior

Conventional isotropic material models and hyperelastic material models have been used in the past to approximate the material behavior of Nitinol. These material laws can adequately model the material response of Nitinol provided the material undergoes monotonic loading. These material laws cannot however capture the unique unloading behavior of Nitinol. The hyperelastic model unloading follows back down the loading stress-strain response, while the isotropic hardening law assumes unloading on the original modulus until twice the current yield point is reached. Neither of these conditions exists with Nitinol.

Figure 1 illustrates the loading and unloading material behavior seen in Shape Memory material models when used in their superelastic state. At low levels of stress, the material exists in an austenite phase. Upon further loading, the material undergoes a stress-induced transformation from the austenite phase to a martensite phase. The material behaves as linear elastic in both austenite and martensite phases, however, the modulus of elasticity in the two phases is different. During the stress induced transformation from austenite to martensite there is very little change in stress, but a large increase in strain. Beyond the transitions region the martensite phase ultimately results in permanent unrecoverable set in the material. Unloading for cases that do not reach the transformation state follow the elastic modulus. For cases in the transition region, you will see a hysteresis type behavior. If stresses reach above the yield limit of the material, permanent set is seen, but the unloading curve is still highly nonlinear.

The superelastic behavior of nitinol is used in the design of stents. The transformation temperatures are set to be slightly below body temperature. The superelastic effect is caused by the stress-induced formation of some martensite above its normal temperature. Because it has been formed above its normal temperature, the martensite reverts immediately to undeformed austenite when the stress is removed. This process provides the elasticity in these alloys for strains up to about 8%.

User Materials in ANSYS

Starting in Version 5.6 as an undocumented feature and documented in later releases [3], ANSYS has included a much-improved interface for specifying user customized material models via the `USERMAT` subroutine. This user-defined subroutine allows users to define the stress-strain constitutive behavior of unique materials. In the past, material models had to be either input as a user plasticity (`USERPL`) or creep law (`USERCR`) or through a user element (`UE`*x*`101-UE`*x*`105`). Defining materials through the `USERMAT` allows for the flexibility of a unique material law to be defined for all types of elements including links, beams, shells, and solids. Developing material models will never be a trivial task, but the new tools in ANSYS allow for the implementation of this general material model. Implementation of a material model requires the compiling of the material law subroutine using the consistent version of FORTRAN that ANSYS was compiled with so that consistent linking can be achieved. This new executable can then be provided to users of the `USERMAT` without the need of providing them with the source code of the subroutine.

`USERMAT` is an ANSYS user programmable feature for use with the 18*x* family of elements including 3D links, 3D beams, 3D shells and both 2D and 3D solids. The subroutine is used to define the material stress-strain relation and can be used in any mechanical ANSYS analysis. The subroutine is called at every material integration point for every Newton-Raphson iteration. ANSYS passes in stresses, strains and state variables at the beginning of each time increment along with the current strain increment. `USERMAT` then updates the stresses and state variables to the values at the end of the time increment and provides the material Jacobian matrix.

Data passed into the `USERMAT` subroutine also includes information about the element type, load step, substep, number of direct components of stress and strain, etc. Mechanical strains and strain increments are passed into the subroutine with the thermal strains removed. Also passed into the subroutine are the coordinates of the material integration points and the incremental rotation matrix. The deformation gradient is included at the beginning of the step as well as its current status.

Input and output arguments passed in and out of the subroutine include the true stress and the state variables which are used to track items like the transformation strains, strain invariants and martensite volume fraction. The state variables are used to track the position and direction along the stress-strain curve. Quantities that are output by `USERMAT` include the symmetric material Jacobian matrix and a flag which controls time stepping bisection used to improve convergence.

Material property data read in to generate the stress strain curve for the `USERMAT` model is passed into ANSYS through the `TB,USER` and `TB,STATE` command options. Figure 1 illustrates the material properties required to characterize the Nitinol response.

Demonstration of Material Model Implementation

Nitinol Constitutive Model

The development of the model implemented in this paper is based on the framework of generalized plasticity theory [4]. Taking an additive decomposition of the total strain into a purely linear elastic part, ε^{el} plus a transformation component, ε^{tr} we have,

$$\varepsilon = \varepsilon^{el} + \varepsilon^{tr}.$$

The stress to linear elastic strain relationship is given by

$$\sigma = E(\xi_M)(\varepsilon^{el} - \varepsilon^{tr}),$$

where $E(\xi_M)$ is the modulus and is a function of the Martensite volume fraction,

$$\xi_M = \begin{cases} 0, & \text{fully Austenite} \\ 1, & \text{fully Martensite} \end{cases}.$$

The Martensite volume fraction is tracked throughout the analysis and is stored as a state variable.

Single Element Test Case

During the development of a new material model, a one element problem is usually sufficient to test the initial implementation of the constitute model. The Nitinol material model undergoes large strain behavior that can be tested by performing a displacement controlled solution simulating a uniaxial stress and strain state. By comparing the input with the computed stress and strain state, checking of the correct implementation of the material model is obtained.

Figure 2 illustrates the one element model used in the testing of the Nitinol material model. Symmetry boundary conditions were used on all faces to create a uniaxial stress state. Checking of the stress state in all directions was used to indicate proper implementation. Figure 3 illustrates a history plot of the material model input vs. the calculated stress vs. strain response. Note that a number of runs are superimposed where different levels of hysteretic behavior are modeled. Strain levels of 2% - 7% are included in both loading and unloading curves. The hysteretic behavior is clearly seen in these curves. The data extracted from the time history postprocessor matches within acceptable error the material properties input into ANSYS. By using a single element model, testing of highly nonlinear analyses can be performed in seconds. Although this analysis does not guarantee an acceptable model has been achieved, it is the first step in the verification process.

Example Stent Simulation

An example application where this material model is used is in the simulation of implanted stent devices. The following analysis procedure is used to characterize the response of Nitinol Stents. The loading procedure consists of the typical steps performed in the design of nitinol stents:

1) The Laser-cut polished stress free geometry is the starting point of the analyses. Often this is provided to the engineer in the form of a 2D drawing, where a geometry transformation is necessary to generate a 3D model of the smallest repeatable segment. Figure 4 illustrates the results of extruding the given 2D geometry into a flat 3D meshed repeatable segment of the device followed by a coordinate transformation from Cartesian to Cylindrical to create the 3D model.
2) The initial analyses simulate the expansion of the stent which is typically performed using a series of mandrels and may include intermediate annealing steps along the way. For FEA analysis, we can use an isotropic hardening material law to characterize this step of the behavior since the stent will ultimately be annealed after full expansion.
3) After expansion, the stent is annealed using the `UPCOORD` capability in ANSYS (Figure 4), which returns the stent to a stress free state.
4) The stent is next compressed onto the delivery device, which is typically at a similar diameter to the original tubing. A "rigid" cylinder contact surface is used for this stage of the analysis process. (Figure 5)
5) Releasing the stent from the delivery device simulates deployment. In the finite element model enlarging the "rigid" cylinder to the vessel diameter can simulate this deployment.

Conclusion

The development of a Nitinol material model provides an analysis tool for characterizing Nitinol devices under their true stress and strain history. By having a more accurate material model, more accurate simulations can be performed. This finite element simulation can be used to:

1. Perform Design Verification of existing or new designs
2. Perform Design Optimization to design a better device.
3. Failure Investigation

The Nitinol material model in ANSYS allows the analyst to take advantage of the flexibility of the full suite of ANSYS capabilities in conjunction with predicting a more accurate analysis, with the end result being a closer prediction to the real structure.

References

1. Chaboche, J.L., "Equations for Cyclic Plasticity and Cyclic Viscoplasticity", *International Journal of Plasticity*, Vol. 7, pp. 247-302 (1989).
2. Chaboche, J.L., "On Some Modifications of Kinematic Hardening to Improve the Description of Ratcheting Effects", *International Journal of Plasticity*, Vol. 7, pp. 661-678 (1991).

3. Lin, G., “ANSYS USER Material Subroutine USERMAT Standard Package”, ANSYS Inc., Canonsburg, PA (1999).
4. Jia, H., Lalande, F. and Rogers, C., “Review of Constitutive Modeling of Shape Memory Alloys”, Center for Intelligent Material Systems and Structures, Virginia, USA.

Figures

Figure 1 Superelasticity Hysteresis of Nitinol (hysteresis.jpg)

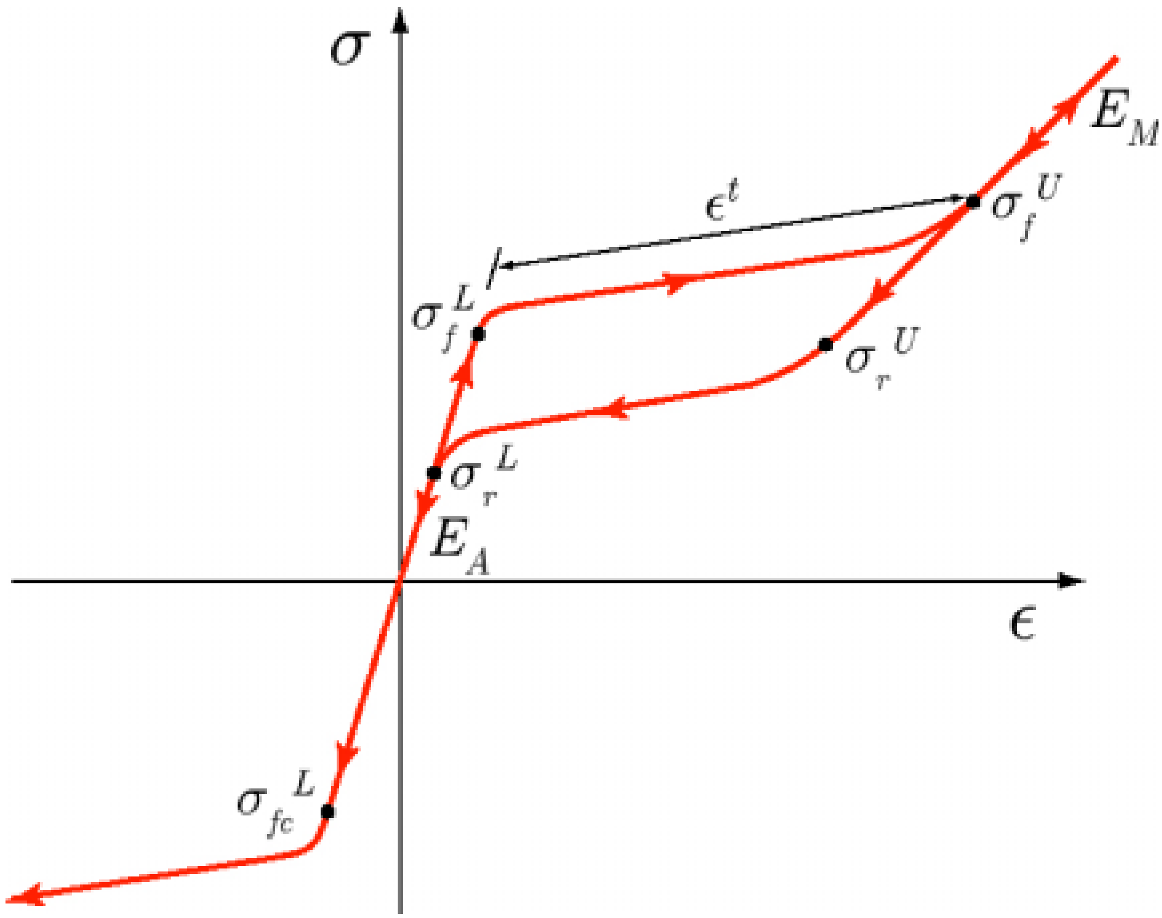

Figure 2 Single Element Test Model (oneLMN_schematic.png)

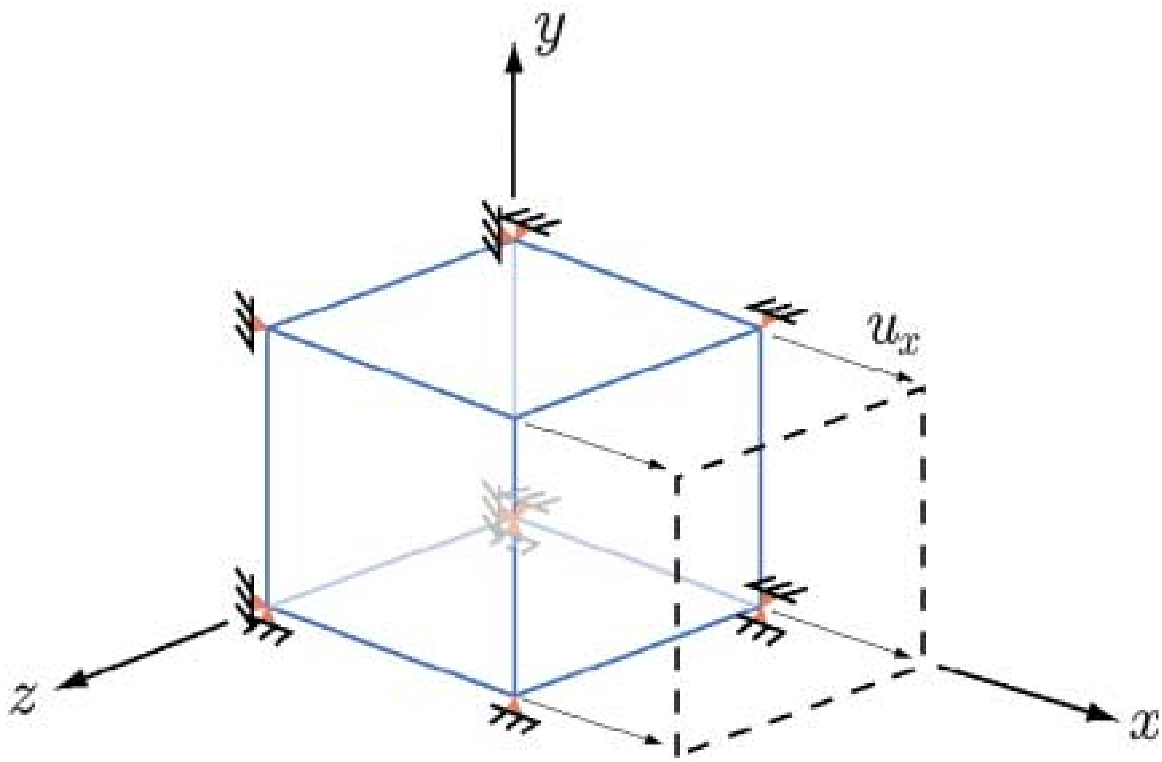

Figure 3 Single Element Uniaxial Stress-Strain Response (single_lmn_s-e.gif)

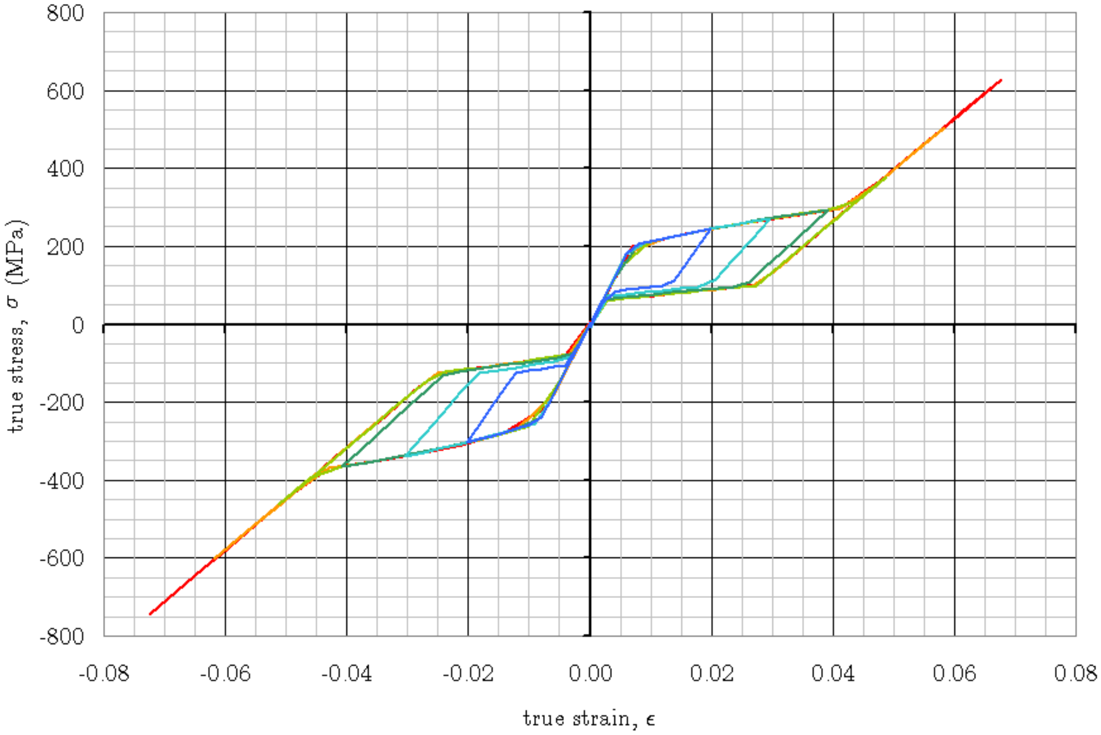

Figure 4 Stent Analysis Steps (process1.png)

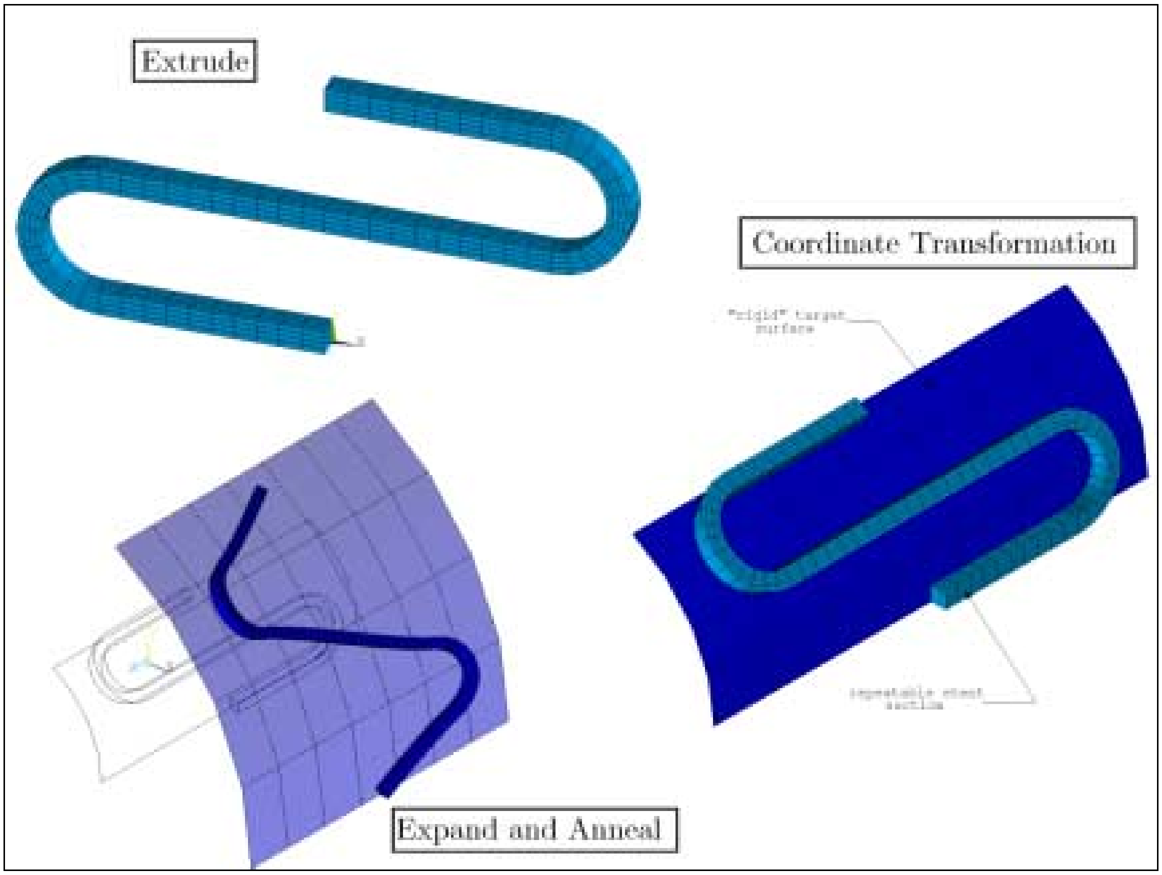

Figure 5 Stent Analysis Steps (process2.png)