Parameter Identification for Nitinol Shape Memory Alloy Modelling via Stress-Strain Curve Optimization

Bhanu Pratap Reddy[a], Pranshu Rajput[b], Venkateswaran Perumal[a],

[a]STRYKER GLOBAL TECHNOLOGY CENTER, Bengaluru, Karnataka, 560048, India
[b]STRYKER GLOBAL TECHNOLOGY CENTER, Gurugram, Haryana, 122101, India

Abstract

Accurate identification of constitutive model parameters is critical for predictive finite element analysis (FEA) of shape memory alloys (SMAs) such as Nitinol in applications such as medical devices and adaptive structures. Conventional parameter calibration which iteratively tunes model inputs to fit experimental stress–strain data is often computationally expensive, labor-intensive, and highly sensitive to data noise. In this work, we present a fully automated machine learning–based framework for parameter identification, capable of generating material model inputs for both Abaqus and Ansys directly from any given superelastic stress–strain curve. The proposed workflow integrates automated cleaning and segmentation of raw stress–strain datasets into loading and unloading cycles, extraction of key transformation features such as elastic moduli, transformation stresses, and transformation strains. Experimental and synthetic datasets were generated and used to train a supervised ML model capable of mapping curve features directly to the underlying parameters. Once trained, the model was evaluated against experimental test data achieving high accuracy while reducing calibration time by orders of magnitude. The framework offers a scalable and rapid alternative for SMA parameter identification, with potential applications in real-time quality control, adaptive design, and digital twins. Future work will extend the methodology to multiple constitutive models and other material systems.

1 Introduction

Shape memory alloys (SMAs) exhibit unique mechanical behaviors such as super elasticity and the shape memory effect, making them valuable in biomedical devices, actuators, and aerospace structures. Among SMAs, Nitinol (NiTi) is the most widely used due to its high recoverable strain, corrosion resistance, and biocompatibility. Predictive numerical modeling of Nitinol relies on accurate determination of constitutive model parameters, including transformation stresses, elastic moduli, and transformation strain.

Conventional parameter identification methods typically involve iterative finite element simulations or curve-fitting procedures, where predicted stress–strain curves are compared to experimental data until the error is minimized. While effective, these methods are computationally intensive, require expert supervision, and can be sensitive to experimental noise, particularly for hysteretic responses.

Machine learning (ML) offers a promising alternative for solving such inverse problems in material science. By learning the mapping between mechanical response curves and the underlying parameters, ML models can bypass the need for iterative optimization. Prior studies have demonstrated ML's potential for parameter identification in metals, polymers, and composites, but few have addressed the direct prediction of SMA parameters from raw experimental data.

In this work, we propose a supervised ML framework for direct parameter identification of Nitinol from stress–strain curves. Experimental and synthetic datasets, generated using a selected SMA constitutive model, are used to train regression models that capture the relationship between curve features and material parameters. The framework is validated against both synthetic and experimental curves, demonstrating its accuracy, robustness, and significant computational efficiency. The approach is designed for scalability, enabling future integration of multiple constitutive models and extension to other material systems.

2 Materials and Methods

2.1 Materials

The calibration workflow focuses on a widely used Nickel-Titanium (NiTi) shape memory alloy (SMA) known for its pronounced superelastic behaviour. Superelastic NiTi alloys undergo reversible martensitic phase transformations under mechanical loading at temperatures above their austenite finish temperature. This enables the material to accommodate large recoverable strains (up to 6-8%) while exhibiting a distinct plateau in the stress-strain response. Experimental data for calibration were obtained from uniaxial tension tests conducted in the superelastic regime, ensuring pronounced loading and unloading plateaus and characteristic hysteresis. All tests used standardized specimens and followed established protocols for SMA characterization.

2.2 SMA Superelastic Material Model

To numerically capture the stress–strain response of superelastic SMAs, we employ a phenomenological constitutive model that simulates the stress-induced martensitic transformation and reverse transformation in the alloy. Key features of the model include:

- **Austenite and Martensite Phases**: The material is assumed to exist in either austenite or martensite, or as a mixture (during transformation), each with distinct elastic moduli.
- **Transformation Start and Finish Stresses**: Forward transformation (A→M) initiates and completes at well-defined stresses/strains, similarly for reverse (M→A) transformation.
- **Transformation Strain**: The model incorporates a maximum transformation strain, representing the recoverable deformation associated with phase change.
- **Hysteresis and Plateau Regions**: The model mathematically reproduces the pronounced plateaus and hysteresis loop observed experimentally.

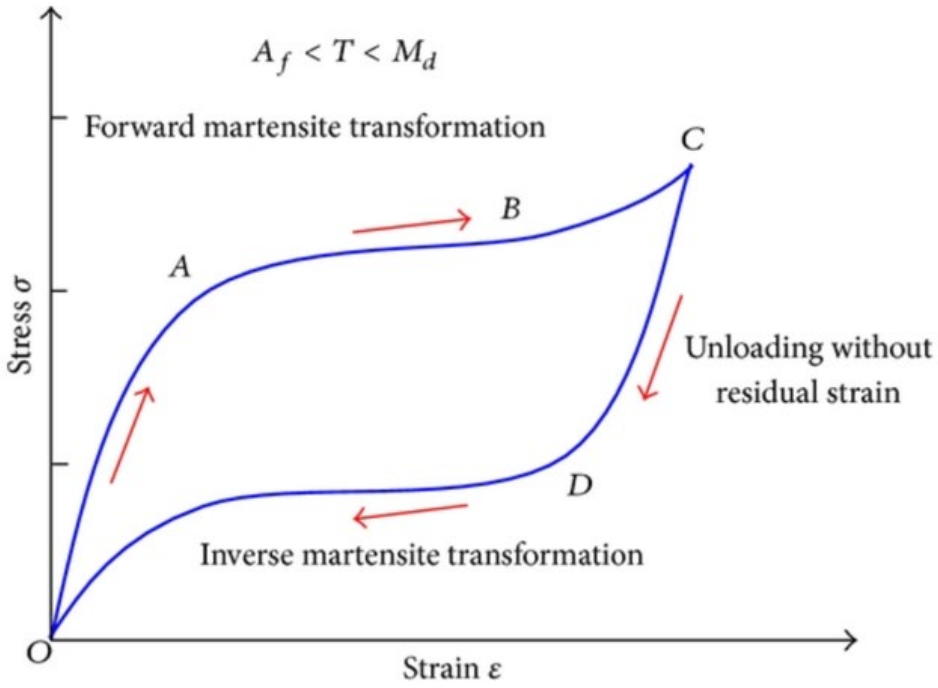

Figure 1. At stresses above the martensitic stress (A), austenite will transform to martensite and induce large macroscopic strains until no austenite remains (C). Upon unloading, martensite will revert to austenite beneath the austenitic stress, at which point strain will be recovered until the material is fully austenitic and little to no deformation remains. [1]

2.2.1 Material Parameters

Parameter	Symbol	Description
Sigma SAS	σ_s^{AS}	Starting stress value for forward phase transformation
Sigma FAS	σ_f^{AS}	Final stress value for forward phase transformation
Sigma SSA	σ_s^{SS}	Starting stress value for reverse phase transformation
Sigma FSA	σ_f^{SA}	Final stress value for reverse phase transformation
Epsilon	ϵ_L	Maximum residual strain
Austenite modulus	E_A	Elastic modulus of austenite
Martensite modulus	E_M	Elastic modulus of martensite

Table 1. Material model parameters for calibration

2.3 Methodology

The proposed framework comprises four primary stages: dataset generation, data preprocessing, machine learning model development, and validation.

2.3.1 Experimental and Synthetic Dataset Generation

Twenty uniaxial tensile stress–strain curves were obtained from experiments on superelastic Nitinol wires. These experimental datasets served as a reference for generating thirty additional synthetic stress–strain curves using a selected constitutive model. The synthetic data were generated over parameter ranges representative of the physically relevant behaviour observed in the experimental results, ensuring broad coverage of transformation stresses, elastic moduli, and transformation strains.

2.3.2 Data Preprocessing

Raw stress–strain data were subjected to smoothing and filtering to reduce noise, followed by resampling to a fixed number of data points to ensure consistent dimensionality across datasets. Each curve was segmented into distinct loading and unloading cycles. Key transformation features, such as plateau regions and elastic slopes, were extracted to enable feature-based learning approaches.

2.3.3 Machine Learning Model Development

A supervised regression framework was implemented to map processed curve data directly to constitutive model parameters. Feature-based regression models, including random forest and gradient boosting algorithms, were evaluated. Model hyperparameters were optimized via cross-validation using the synthetic dataset. Preliminary parameter fitting was used to establish baseline values for training and model comparison.

2.3.4 Validation

Model performance was assessed on both unseen synthetic datasets and experimental curves excluded from the training phase. Evaluation metrics included the coefficient of determination (R^2), mean absolute error (MAE), and robustness under synthetic noise injection to emulate experimental uncertainty.

This methodology enables rapid and robust prediction of SMA model parameters from stress–strain data, removing the need for iterative forward simulations during calibration. The modular structure facilitates straightforward extension to other constitutive models and material systems.

3 Results and Discussion

In this study, constitutive material model parameters for superelastic shape memory alloys (SMAs), such as Nitinol, were successfully predicted using ML and subsequently optimized

using a least-squares error minimization approach. Figure 2 presents the idealized linear superelastic response, derived from predicted parameters, overlaid on the corresponding experimental stress–strain data. The linear model accurately captures the loading behaviour; however, it exhibits limitations in reproducing the nonlinear curvature observed during unloading, a discrepancy inherent to its linear formulation.

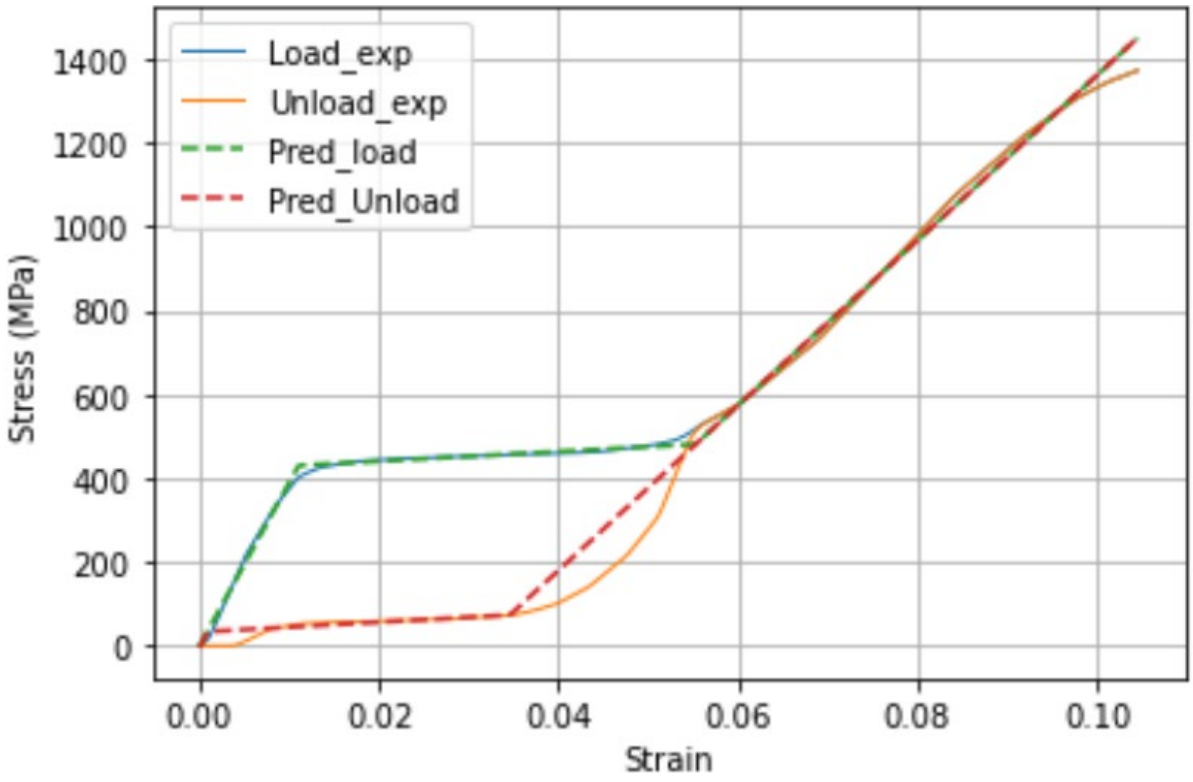

Figure 2. ML predicted superelastic parameters against experimental loading and unloading curve.

4 Conclusions

This work demonstrates the feasibility and advantages of a Python-driven, ML-accelerated calibration pipeline for SMA superelasticity. By decoupling parameter studies from commercial FEA tool constraints and employing flexible, open-source data science tools, the process is made faster, more transparent, and highly scalable for future smart materials research and engineering applications.

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