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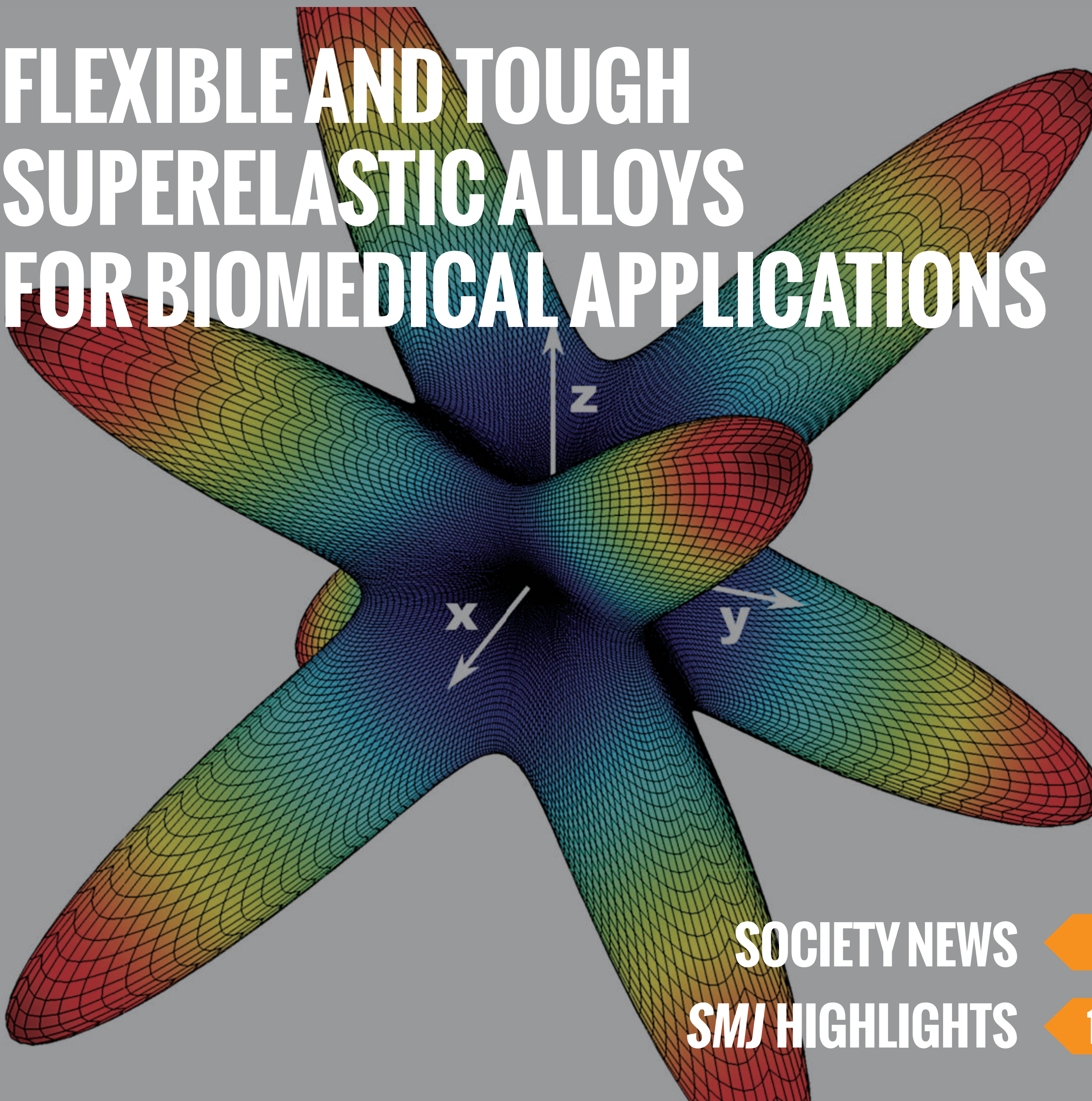
FLEXIBLE AND TOUGH SUPERELASTIC ALLOYS FOR BIOMEDICAL APPLICATIONS



QUANTIFYING AND PROPAGATING UNCERTAINTY IN SUPERELASTICITY SIMULATION INPUTS

Digital image correlation data and Bayesian inference used together facilitate rigorous quantification of the uncertainty in material input parameters for finite element simulations of superelastic deformation.

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Computer simulations using methods such as finite element analysis (FEA) play an important role in the design of implantable medical devices that are manufactured from superelastic materials like nickel-titanium (NiTi) shape memory alloys (SMA). The simulations are typically performed in a specific context of use, for example, durability assessment of a device under a particular anatomical boundary condition. A topic of emerging importance to NiTi simulation is the assessment and reporting of the credibility of a computational model for its context of use[1,2]. This credibility assessment generates evidence supporting the use of a computational model for decision making. Moreover, higher model credibility enables medical device manufacturers to use modeling for higher risk and higher impact contexts of use. As part of credibility activities, quantification and propagation of the uncertainty in material parameter inputs increases overall model credibility by providing conservative bounds on the uncertainty in model predictions.

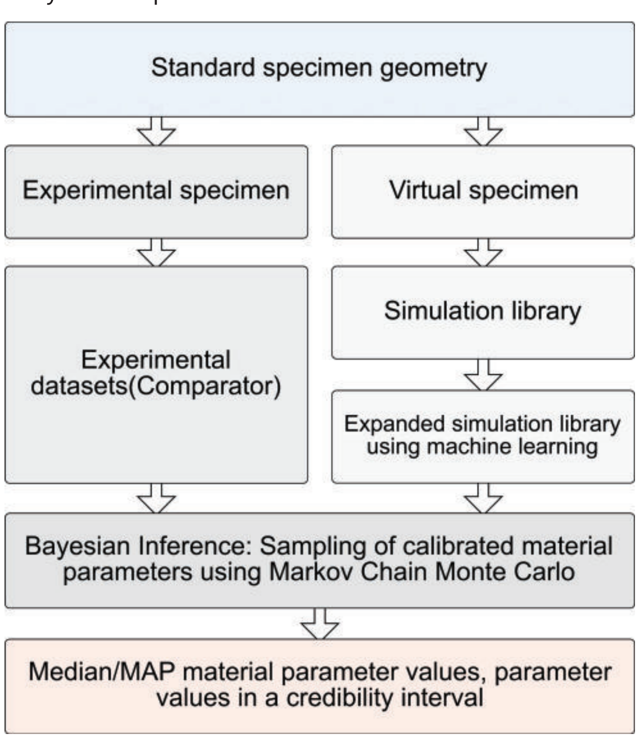

Fig. 1 — A flowchart summarizing the material property determination method. MAP stands for *maximum a posteriori.* Reproduced from Paranjape et al.[3].

A recent work by the authors implemented a method to determine the material parameter inputs and their uncertainty for a computational model of the superelastic deformation of NiTi[3]. The material property determination is colloquially referred to as model calibration. This method for superelastic model calibration is unique in that it has uncertainty quantification built in, it uses full-field surface strain data together with global load data as inputs, and it is able to furnish both tensile and compressive plateau stress material properties from a single test.

CALIBRATION FRAMEWORK

A flowchart summarizing the material property determination method is shown in Fig. 1. The method essentially has three components: (1) a standard tensile test specimen geometry and a test protocol to obtain the surface strain fields in the test specimen using digital image correlation (DIC); (2) a library of simulations of the tensile test specimen loading protocol using a range of material parameter input values; and (3) a data-processing method using Bayesian Inference (BI) to minimize a cost function based on the local strain and global load measured experimentally and simulated in the simulation library.

The calibration scheme is demonstrated on a Ti-50.8 at.%Ni superelastic NiTi sheet material and the superelastic constitutive model implemented in the Abaqus finite element framework[4]. The typical stress-strain response for the

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NiTi material is shown in Fig. 2a and the six material property inputs for the superelastic model in Abaqus—austenite and martensite loading slopes (E_A and E_M), tensile plateau stresses (σ_{UPS} and σ_{LPS}), compressive plateau stress (σ_{CPS}), and transformation strain (ε_t)—are annotated in the stress-strain curve. A standard diamond specimen geometry is used. When a diamond specimen is loaded in the deformation sequence shown in Fig. 2b, its struts are subject to bending, and the specimen thus exhibits both tensile and compressive strains as reflected in the shear strains shown in Fig. 2c. The surface strains are experimentally measured using a single-camera DIC setup.

A computational model of the diamond geometry shown in Fig. 2a is built in Abaqus, and the superelastic constitutive material model and the loading path shown in Fig. 2b are applied. A simulation library is constructed by instantiating the model 544 times with varied material parameter inputs. Specifically, the six material parameters are varied such that they span the typical range of values observed in commercially relevant NiTi. From each simulation result, a quantity of interest (QoI) is defined based on: (1) the local strain values at points 1 to 4 shown in Fig. 2c and (2) the global load values in the loading direction at 22 equidistant points on the loading path A-B-C shown in Fig. 2b. A regression model is fitted using the support vector machine (SVM) machine learning (ML) method that takes a set of six material parameters as inputs and furnishes the QoI values. Given an experimental dataset consisting of QoIs listed above and the trained SVM model that estimates the simulated QoIs, the optimum material parameters are determined using the BI method, which is a statistical method of determining probability of a hypothesis based on available data. The numerical determination of the Abaqus material parameter probability distributions is performed using Markov Chain Monte Carlo (MCMC) sampling[5]. In summary, given an experimental dataset consisting of local surface strain and global load data from a tensile test and a simulation library built from a model of the experimental protocol, the method furnishes the probability distributions for the six key material parameters for the superelastic constitutive model in Abaqus. The uncertainty in the determined material properties can be quantified from the width of the probability distribution and is expressed in terms of credibility intervals.

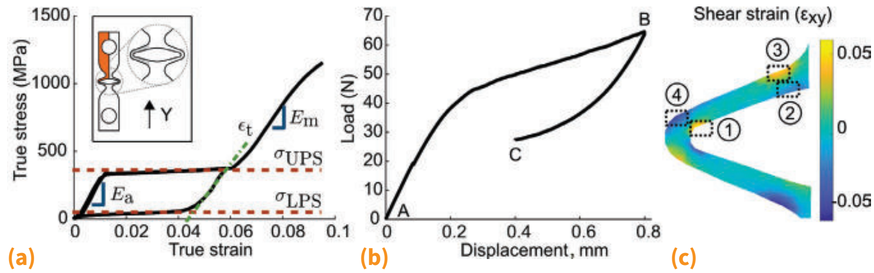

Fig. 2 — A summary of the test protocol: (a) diamond specimen geometry and a schematic of the superelastic stress-strain response; Y is the sheet rolling direction; (b) schematic of the loading sequence used in the test protocol; and (c) surface strain map of diamond at peak load measured using DIC. Adapted from Paranjape et al.[3].

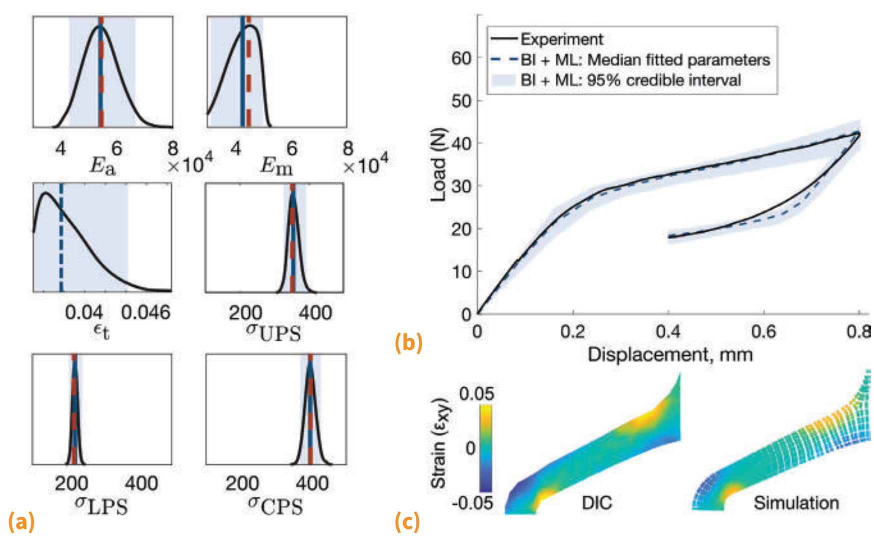

Fig. 3 — Sample results of the calibration method. (a) Probability distribution of determined material parameters. (b) Comparison of experimental load-displacement data and simulation results from the determined parameters. (c) A comparison of experimental and simulation data for surface shear strain. Adapted from Paranjape et al.[3].

CALIBRATION RESULTS USING GLOBAL LOAD AND LOCAL STRAIN DATA

Sample results for material parameter determination using the BI method are shown in Fig. 3. The probability distributions for the six material parameters are given in Fig. 3a, where the median parameters (dashed lines) and the 95% credibility intervals (gray highlights) are annotated. A comparison of the simulated load-displacement curve obtained from the median material parameters and the experimental input data is provided in Fig. 3b. A comparison between the simulated surface strain distribution in the diamond specimen model using the median material parameters and the DIC measurement of the surface strains at peak load is shown in Fig. 3c. The qualitative agreement between the simulated curve from the calibrated model and the experimental input is reasonable. Quantitatively, the error between the simulation and the experiment is 17.3% when calculated in terms of the mean absolute percent error (MAPE).

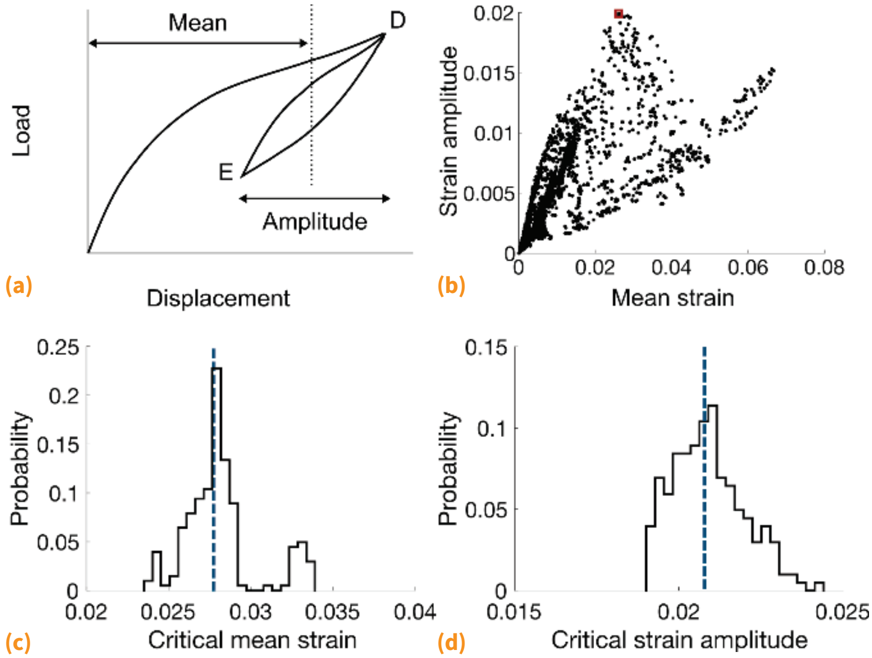

Fig. 4 — Propagation of uncertainty in material parameters to a simulation of cyclic loading: (a) cyclic loading path; (b) strain map obtained using a fatigue simulation; and (c, d) probability distribution of mean strain and strain amplitude respectively at the critical point obtained from a series of simulations. Adapted from Paranjape et al.[3].

The ratio of compressive plateau stress (σ_{CPS}) to the tensile plateau stress (σ_{UPS}) in the sample result above is approximately 1.0. This is a reasonable number for a typical NiTi sheet material that has a strong < 1 1 0 > texture component.

PROPAGATION OF MATERIAL PROPERTY UNCERTAINTY TO SIMULATIONS OF CYCLIC LOADING

Here, an example of propagating the uncertainty in the material parameters determined using the BI method is demonstrated using a simulation of NiTi fatigue loading. The material parameter probability distributions shown in the sample results above are used in a simulation of cyclic loading of the diamond-shaped NiTi specimen introduced in Fig. 1a. The cyclic loading path is shown in Fig. 4a and the extrema of the cyclic loading path are annotated by labels D and E. The commonly used fatigue indicator parameters for NiTi—mean strain and strain amplitude—are calculated using the tensor method[6]. A scatter plot of strain amplitude vs. mean strain obtained from a simulation is shown in Fig. 4b. Fatigue safety factors are typically estimated using the mean strain and strain amplitude at the critical point in the model. In this example, the critical point is taken as the point where the largest strain amplitude occurs. The critical point is shown by a red square in Fig. 4b. A series of simulations with material parameters in the 95% credible intervals of the material parameter distributions shown in the sample result above are carried out and probability distributions are constructed from the mean strain and the strain amplitude at the critical point in each simulation. These probability distributions are shown in Figs. 4c and d. The strain amplitude shows a range of approximately 0.007, which may translate to a large uncertainty in the fatigue safety factor calculated using these strain amplitude data.

CONCLUSIONS

In this article, the authors have developed and described the implementation of a method for determining the material parameter inputs to the superelastic constitutive model for nickel-titanium with their accompanying uncertainty. The inputs to the method are surface full-field strain data and global load data obtained from one or more tensile tests on an appropriate specimen and a simulation library that provides a dataset with various combinations of material parameter inputs and corresponding strain and load outputs. This method uses Bayesian Inference to obtain a probability distribution of the input parameters. The numerical implementation of the method uses Markov Chain Monte Carlo sampling accelerated by a machine learning method that augments the results obtained from the simulation library. There are four main benefits of this model calibration method:

i. The probability distribution of the material parameters determined using this method automatically furnishes a quantification of uncertainty in the parameters. The uncertainty can be communicated using measures such as credible intervals.

ii. The uncertainty in the material parameters can be propagated to subsequent simulations such as simulation of fatigue loading of NiTi samples.

iii. The diamond specimen geometry used in this method enables determination of tensile as well as compressive plateau stresses from a single test.

iv. The machine learning element of this method allows use of a relatively small simulation library compared to performing calibration without such library augmentation.

This is a versatile method in the sense that it can be applied to any constitutive model implemented in finite element solvers. The statistical methods such as Markov Chain Monte Carlo sampling used in this scheme are implemented in a wide variety of software tools such as Matlab and Python. While the overall accuracy of the simulation results primarily depends on the accuracy of the underlying constitutive model, methods such as these can help quantify, communicate, and propagate uncertainty in the simulation inputs. A wide adaption of methods such as these can help make the paradigm of using a risk-informed approach for incorporating computer simulation results in the design and performance evaluation of nickel-titanium-based implantable medical devices a standard practice.

Notes

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