Predictions of electromotive force of magnetic shape memory alloy (MSMA) using constitutive model and generalized regression neural network

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Received 19 October 2022, revised 21 December 2022
Accepted for publication 12 January 2023
Published 24 January 2023

Abstract

Ferromagnetic shape memory alloys (MSMAs), such as Ni-Mn-Ga single crystals, can exhibit the shape memory effect due to an applied magnetic field at room temperature. Under a variable magnetic field and a constant bias stress loading, MSMAs have been used for actuation applications. Under variable stress and a constant bias field, MSMAs can be used in power harvesting or sensing devices, e.g., in structural health monitoring applications. This behavior is primarily a result of the approximately tetragonal unit cell whose magnetic easy axis is approximately aligned with the short axis of the unit cell within the Ni-Mn-Ga single crystals. Under an applied field, the magnetic easy axis tends to align with the external field. Similarly, under an applied compressive force, the short side of the unit cell tends to align with the direction of the force. This work introduced a new feature to the existing macro-scale magneto-mechanical model for Ni-Mn-Ga single crystal. This model includes the fact that the magnetic easy axis in the two variants is not exactly perpendicular as observed by D’silva et al (2020 Shape Mem. Superelasticity 6 67–88). This offset helps explain some of the power harvesting capabilities of MSMAs. Model predictions are compared to experimental data collected on a Ni-Mn-Ga single crystal. The experiments include both stress-controlled loading with constant bias magnetic field load (which mimics power harvesting or sensing) and field-controlled loading with constant bias compressive stress (which mimics actuation). Each type of test was performed at several different load levels, and the applied field was measured without the MSMA specimen present so that demagnetization does not affect the experimentally measured field as suggested by Eberle et al (2019 Smart Mater. Struct. 28 025022). Results show decent agreement between model predictions and experimental data. Although the model predicts experimental results decently, it does not capture all the features of the experimental data. In order to capture all the experimental features, finally, a generalized regression neural network (GRNN) was trained using the experimental data (stress, strain, magnetic field, & emf) so that it can make a reasonably better prediction.
Supplementary material for this article is available online

Keywords: MSMA, smart materials, power harvesters, materials modeling, neural network, machine learning

(Some figures may appear in colour only in the online journal)

1. Introduction

Magnetic shape memory alloys (MSMAs) are a type of smart material that exhibits a magnetic field and stress-induced shape memory effect at room temperature. The most common alloy in this class is NiMnGa, which is the material used in this work. The twin variants in NiMnGa alloys reorient at low-stress levels, which changes the material’s magnetization. This phenomenon makes MSMAs suitable for power harvesting and sensing applications [1]. Also, the twin variants reorient under the applied field. This, along with the relatively fast response (∼1 kHz) of MSMAs, makes these materials suitable for actuation [2] and micropump applications [3].

The microstructure of the material shown in figure 1 can explain the unique behavior. The magnetic easy axis is approximately aligned with the short side of the unit cell (figure 1 left). When compressive stress is applied to the material, the short side of the unit cell tends to align with the direction of the stress (figure 1, top, right). Once fully aligned, this configuration is called the stress-preferred variant. The magnetization vector $\mathbf{M}$ begins to align with the direction of the external field when magnetic field $\mathbf{H}$ is applied (figure 1 right, bottom). Once fully aligned, this configuration is known as the field-preferred variant. As can be seen in figure 1, transitions between stress-preferred and field-preferred variants or vice versa cause a change in the magnetization vector inside the material and the bulk magnetic field around it which can be harvested into useful voltage in conjunction with the proper setup [4]. For proper implementation of MSMA as a sensor, energy harvester, and actuator, a generalized constitutive model is required that can predict the behavior of MSMA subject to general magneto-mechanical loading. Several constitutive models for the macroscale behavior of MSMAs have been proposed, including but not limited to, those by Kiefer and Lagoudas [5], Wang and Steinmann [6], LaMaster et al [7], and others. But no model has been shown to satisfy all the laws of thermodynamics and accurately capture the magnetization and applied field ($\mathbf{M}$ vs. $\mathbf{H}$) curves as well as the stress–strain and field-strain response under a wide array of loading conditions. Nelson et al [4] attempted to predict the electromotive force (emf) generated by MSMA under particular loading by using LaMaster’s model [7]. However, there was a noticeable difference between predicted peak-to-peak emf and experimental peak-to-peak emf. Further, D’Silva et al [8] observed that the field-preferred and stress-preferred variants are not exactly perpendicular to each other. This offset from the perpendicular has not been included in any models. For the first time, this offset angle was considered in constitutive modeling for better emf prediction which was one of the novelties of this study. Furthermore, in order to predict mechanical behavior, besides using constitutive modeling, machine learning-based modeling is getting popular [9–13]. Machine learning-based modeling, specifically neural networks can predict nonlinear behavior very well. Previously, several authors [1, 4, 14] performed various experiments to find the capability of producing a voltage output of MSMA under specific configurations and loading scenarios. The experimental curve they obtained was nonlinear (peak emf vs. angle) and periodic (emf vs. time) in nature. To predict this experimental nonlinear curve, a machine learning algorithm was enforced which was another novelty of this work.

In the present work, a general constitutive model was proposed that accounted for some of the limitations of LaMaster’s model [7] in predicting emf. The modified model was able to predict the $\mathbf{M}$ vs. $\mathbf{H}$ curves correctly and give a decent prediction of the stress–strain and field-strain curves under various load conditions by using the manufacturer-given anisotropy constant. The offset angle from perpendicular to the variants is also included in the model. After that, the model is used to predict emf. Finally, a generalized regression neural network (GRNN) [15] based model is used to predict the emf. The predictions of emf from both models are compared.

2. Constitutive modeling

Among the many potential applications of MSMA, power harvesting is one of the most promising ones. MSMAs are becoming popular in energy harvesting applications. Their high fatigue life of around $10^9$ cycles [16], ease of design, particularly compared to piezo and magnetostrictive material [17], and the range of operational frequencies, 2–100 Hz [17]. In power harvesting applications, an MSMA specimen is exposed to variable mechanical stress in combination with a constant external magnetic field. During mechanical loading, the internal magnetization vector of the MSMA changes. This facilitates power generation in a pickup coil that surrounded the MSMA specimen (see figure 2). In the configuration shown in figure 2, the MSMA specimen is kept under a constant lateral magnetic field $H_2$ (0.3–0.8 Tesla) with a varying compressive load of $\sigma_1$ between 0 and 5 MPa to generate emf. Previously Gueil et al [1] found that a small constant axial magnetic field $H_1$ (0.03–0.1 T) dramatically increased the emf output of the power harvesting system shown in figure 2. In order to design and optimize such power harvesting devices, a model is required to predict emf under the loading conditions shown in figure 2.
In order to give physical grounding to this work, the predictions of emf will be based on the model by LaMaster et al [7]. This model is based on sufficient conditions to satisfy the laws of thermodynamics and has been shown to be able to predict stress–strain experiments and some field-strain experiments reasonably well. However, an offset angle observed experimentally by D’Silva et al [8] is introduced to the model. Light microscopy on the MSMA surface reveals that the field-preferred and stress-preferred variants are not exactly perpendicular to each other (see figure 3). The offset from the perpendicular between the two variants will be called $\beta$. The value of $\beta$ can be arbitrarily positive or negative depending on how the specimen is oriented as shown in figure 4. By performing the stress-controlled test, Nelson et al [4] experimentally showed that the orientations shown in figures 4(a) and (b) produced similar emf as well as figures 4(c) and (d) produced similar emf. Figures 4(a)–(d) presume that $\beta$ is positive and negative, respectively. This offset angle may explain the different responses of the material with different orientations of the specimen as represented by Nelson et al [4].

2.1. Model derivation

The model is homogenized [18], which means that the model does not capture specific features of the microstructure but rather captures the average behavior of the material at a point. In this case, it is also assumed that the load on the MSMA is uniform, and thus, all points in the material are in the same sense. The model captures the average behavior through three
internal variables which are each associated with its microstructure: magnetization vector rotation ($\dot{\theta}$), the volume fraction of the magnetic domain ($\alpha_i$), and the volume fraction of variants reorientation ($\xi_i$). The model assumes that the MSMA consist of only two possible variants (figure 5) $\xi_1$ and $\xi_2$, which as volume fraction must sum to 1:

$$\xi_1 + \xi_2 = 1,$$

and are subject to the constraint:

$$0 < \xi_i < 1,$$

where $i = 1, 2$. The other two internal variables shown in figure 5, $\alpha_i$ and $\theta_i$ are independent of each other and bound by the following range:

$$0 < \theta_i < \frac{\pi}{2}$$

Obeying the rules of thermodynamics and considering mechanical and magnetic energy sources, the Gibbs free energy takes the following form:

$$g(\sigma, H^{opp}, \xi, \alpha, \theta) = \frac{1}{2\rho} \sigma : S\sigma - \frac{\mu_0}{\rho} M.H$$

$$+ g^m + \frac{1}{\rho} f^\alpha + \frac{1}{\rho} f^\beta.$$  

where $\sigma$ is stress, $S$ is the compliance tensor, $M$ is the magnetization vector, $H$ is the magnetic field, $g^m$ is the anisotropy energy, and $f^\alpha$, $f^\beta$ are assumed hardening functions. These hardening functions capture how the evolution of the internal variables affects energy storage in the material. These terms aim to capture micro-structural interactions in a phenomenological sense. In this model, the values of $f^\alpha$ and $f^\beta$ are assumed to be zero. The $f^g$ term is used to help predict changes seen in the stress–strain and field-strain curves during reorientation.

The strain $\varepsilon$ in MSMA can be expressed as:

$$\varepsilon = \varepsilon^e + \varepsilon^r,$$

where $\varepsilon^e$ is the elastic strain tensor and $\varepsilon^r$ is the reorientation strain tensor.

The reorientation strain tensor $\varepsilon^r$ can be written as:

$$\varepsilon^r = \begin{bmatrix} \xi_1 & 0 \\ 0 & \xi_2 \end{bmatrix} \varepsilon^{r, \text{max}},$$

where $\varepsilon^{r, \text{max}}$ is the maximum achievable reorientation strain obtained from the experimental data.

The bounds on $\alpha_i$ are because it is also a volume fraction. The bounds on $\theta_i$ are based on physical constrain shown in figure 5. When $\theta_i = 0$ there is no rotation, and when $\theta_i = \frac{\pi}{2}$ the magnetization vector has fully rotated towards the hard axis in that variant.

With the offset angle $\beta$ added, the rotation of the internal magnetization vector of one of the variants will be changed, as the no-field applied position of the internal magnetization vector changes. Figure 5, shows a schematic of the Cartesian component of the magnetization vector, which can be written as a form shown in equation (5) where $M_i$ is the magnetization saturation value given by the manufacturer:

$$M = M_i \begin{bmatrix} \xi_2 \sin(\theta_2) + \xi_1 (\alpha_1 - 1) \cos(\theta_1 - \beta) + \xi_1 \alpha_1 \cos(\theta_1 + \beta) \\ \xi_1 \alpha_1 \sin(\theta_1 + \beta) + \xi_1 (1 - \alpha_1) \sin(\theta_1 - \beta) + \xi_2 (2 \alpha_2 - 1) \cos(\theta_2) \end{bmatrix}.$$  

The compliance tensor $S$ can be expressed as:

$$S = S^{\xi_1} \xi_1 + S^{\xi_2} \xi_2,$$

where $S^{\xi_1}$ and $S^{\xi_2}$ are the compliance tensors for variants 1 and 2, respectively.

Following [19, 20], and neglecting the higher order term, the anisotropy energy $g^m$ [21] can be written as:

$$g^m = \xi_1 K_1 \sin^2 \theta_1 + \xi_2 K_1 \sin^2 \theta_2,$$

where $K_1$ is the anisotropy coefficient which is the measurement of the magnetization vectors’ resistance to rotation.

The internal magnetic field is assumed as follows:

$$\textbf{H} = \textbf{H}^{opp} - \textbf{D} \textbf{M},$$

where $\textbf{H}$ is the internal magnetic field experienced by the MSMA specimen, $\textbf{H}^{opp}$ is the external magnetic field applied on the specimen, $\textbf{D}$ is the demagnetization tensor [22].

Using equations (7) and (8) in equation (6), the Clausius-Duhem inequality can be written as:

$$\left( \sigma_{11} \varepsilon_{r, \text{max}}^{\varepsilon} - \frac{\partial g}{\partial \xi_1} \right) \dot{\xi}_1 + \left( \sigma_{22} \varepsilon_{r, \text{max}}^{\varepsilon} - \frac{\partial g}{\partial \xi_2} \right) \dot{\xi}_2$$

$$- \frac{\partial g}{\partial \theta_1} \dot{\theta}_1 - \frac{\partial g}{\partial \theta_2} \dot{\theta}_2 - \rho \frac{\partial g}{\partial \alpha_1} \dot{\alpha}_1 - \rho \frac{\partial g}{\partial \alpha_2} \dot{\alpha}_2 \geq 0.$$  

Introducing $\pi$ as the driving force for change of each internal variable, equation (12) can be written as:

$$\pi^{\xi_1} \dot{\xi}_1 + \pi^{\xi_2} \dot{\xi}_2 + \pi^{\alpha_1} \dot{\alpha}_1 + \pi^{\alpha_2} \dot{\alpha}_2 \geq 0,$$

$$0 < \alpha_i < 1.$$
where the π terms are defined as:

\[ \pi^{\xi_i} = \left( \sigma_{11} \varepsilon^{r,\max} - \frac{\partial g}{\partial \xi_1} \right), \]

\[ \pi^{\xi_i} = \left( \sigma_{22} \varepsilon^{r,\max} - \frac{\partial g}{\partial \xi_2} \right), \]

\[ \pi^{\theta_i} = -\frac{\partial g}{\partial \theta_1}, \]

\[ \pi^{\alpha_i} = -\frac{\partial g}{\partial \alpha_1}, \]

where \( Y \) is a positive constant and calibrated from experimental data.

### 2.2. Model calibration

The model needs to be calibrated with the experimental data to find the hardening constants \( C_1, C_2 \), and the positive constant of the Kuhn-Tucker condition \( Y \). Following [7], the simplified loading condition is used for calibration. For calibration, the specimen is brought into a fully elongated state by applying a lateral field. Then the lateral field is removed, and the specimen is gradually compressed to 4.5 MPa no field applied. As there is no magnetic field, the magnetic domain \( \alpha_i \) is 0.5, and there is no variant rotation, i.e. \( \theta_i = 0 \). Using these values in equation (20) and considering \( \xi_i > 0 \), as the specimen is transitioning from variant 2 to variant 1, the following equation is obtained:

\[ Y + 2C_1 \xi_i^6 + 2C_2 \xi_i^4 = \varepsilon^{r,\max} \sigma_{11i} + \sigma_{11i}^2 (S_{\xi_i} - S_{\xi_i}), \]

where \( i = 1, 2, 3; \sigma_{11i}, \) and \( \xi_i \) are the compressive stress and variant volume fraction of the \( i \)th point on the experimental stress--strain curve with zero field shown in figure 6(a).

The variant volume fraction \( (\xi_i) \) shown in equation (21) can be found from the experimental data, using the equations (7)–(9), as:

\[ \xi_i = \frac{\varepsilon_{11i} - S_{\xi_i}}{S_{\xi_i} - S_{\xi_i}} \sigma_{11i} \varepsilon^{r,\max}. \]

The compliance tensor \( S_{\xi_i} \) is calculated by taking the inverse of the modulus of elasticity, measured directly from the experimental stress--strain curve. Two different moduli of elasticity are found; one is in variant 2 (fully elongated state), and the other is in variant 1 (fully compressed state) from the two distinct elastic regions in figure 6(a). Specifically, the two points in each elastic region (see figure 6(a), black dots) are used to calculate the slope, which gives the modulus of elasticity. The maximum reorientation \( \varepsilon^{r,\max} \) is calculated from the experimental data by using the following equations:

\[ \varepsilon^{r,\max} = \varepsilon_{\min} - \frac{\sigma_{\min}}{E_1}, \]

where \( \varepsilon_{\min} \) is the maximum negative strain of the data set, \( \sigma_{\min} \) is the maximum compressive stress of the experimental data, and \( E_1 \) is the modulus of elasticity of the variant 1. The origins of this equation are shown in figure 7. Finally, all the parameters of equation (21) are known except \( C_1, C_2 \) & \( Y \). These constants can be calculated by solving a system of three linear equations, which is obtained by taking three points on the calibration curve (see figure 6(a), red dots). These calibrated constants are listed in table 2.

Using the material parameters and constants listed in tables 1 and 2 and the derived model, the simulation is run, and the predicted calibration curve is shown in figure 6(b). As
expected, the calibration curve is well matched by the simulation and the simulation exactly matches the experiment at the red points used for calibration.

2.3. Introducing EMF to the model

From Faraday’s law of induction, the following equations can be used to calculate emf:

\[ E = -NA \frac{dB}{dt}, \quad (24) \]

\[ B = \mu_0 (H + M), \quad (25) \]

where \( E \) is emf, \( N \) is the number of turns in the coil, \( A \) is the cross-section area, \( \mu_0 \) is the magnetic permeability constant, and \( t \) is time.

Using equations (11), (24) and (25), emf can be simplified to:

\[ E = -N \mu_0 (1 - D_{11}) \frac{dM_1}{dt}, \quad (26) \]

where \( D_{11} \) is the 11 component of demagnetization tensor, and \( M_1 \) is the magnetization vector component in 1 direction shown in figure 2 obtained from the model. \( \frac{dM_1}{dt} \) can be calculated numerically by assuming:

\[ \frac{dM_1}{dt} \approx \frac{\Delta M_1}{\Delta t}, \quad (27) \]

where \( \Delta M_1 \) is the difference in magnetization between two consecutive time steps, and \( \Delta t \) is the time difference between those steps.
3. Experiments

The MSMA specimen under the experimental configuration shown in figure 2 was used to gather emf data from the coil. Several experiments were conducted by Nelson et al [4] and Guiel et al [1] to get voltage output from the MSMA specimen. Nelson et al [4] performed the stress-controlled test to be consistent with LaMaster’s model [7]. But instead of using the axial field, Nelson et al [4] tilted the lateral field at a certain angle. The tilted lateral field was not ideal because, in their setup, it was not possible to get a uniform magnetic field over the MSMA specimen. Moreover, more recent experimental results with a similar setup suggested that these experiments might have had significant variability of the stress and this input might not have been controlled as well as originally thought.

On the other hand, Guiel et al [1] performed the strain-controlled test, i.e. the Instron Machine was kept in position-controlled mode. In this setup, the maximum strain was measured experimentally before each cycle. But in this case, the specimen experienced higher compressive stress (∼8 MPa), which caused cracks in the specimen.

For several reasons, these experiments could not be directly compared with model predictions. First, the Guiel et al experiments were strain-controlled while the model is stress controlled. Next, the field was measured at the surface in these tests, which accordingly to Eberle et al [22] should not be used as the input applied field. Finally, the Guiel et al experiments, which were performed at 15 Hz frequency showed evidence that inertial effects were evident (i.e. the strain obtained from the tests at 15 Hz seemed different than the strain obtained from those tests done very slowly at 2 Hz).

Therefore, to be consistent with the model, additional stress-controlled experiments under the conditions shown in figure 2 were performed at a slower rate of 10 Hz in order to compare the results with the model. At this frequency level, the strain seems consistent with the strain obtained from the test of 2 Hz frequency. The power harvesting experimental data used to validate and test this model was acquired through stress-controlled tests that were performed with improved PID control parameters, correcting the errors encountered in the data reported by Nelson et al [4]. During these tests, the axial compressive stress was varied between 0 and 5 MPa at a frequency of 10 Hz, while the specimen is exposed to constant axial and lateral fields.

As shown by Guiel et al [1], the maximum emf can be obtained with a certain angle (\( \phi \)) of the resultant magnetic field with the horizontal axis (see figure 8). The angle \( \phi \) is calculated by using the following equation:

\[
\phi = \tan^{-1} \left( \frac{H_1}{H_2} \right).
\]  

(28)

The resultant field \( H_{res} \) is calculated as:

\[
H_{res} = \sqrt{H_1^2 + H_2^2}.
\]

(29)

The emf has been measured experimentally at several angles ranging from 0° to 7.2° while keeping the resultant field unchanged at 0.578 T. Using these angles and associated field values, simulations have been performed to calculate emf from the revised model.

The experimental setup for power harvesting is shown in figure 10. The lateral field (\( H_2 \)) was applied by using an electromagnet (3470 GMW) having a pole of 45 mm in diameter shown in figure 10. The axial field (\( H_1 \)) was applied using the two permanent magnets which were placed at the top and bottom of the specimen (figure 10). The magnitude of these magnetic fields was measured by using a Hall probe and the angle was calculated by using equation (28). The magnitude of the axial field (\( H_1 \)) is higher closer to the top and bottom of the specimen (i.e. closer to the magnets). To get an approximate uniform axial field over the entire length of the sample to use as model input, the weighted average of the magnitude of the field was calculated. The field was measured at multiple points of \( h_1, h_2, h_3, h_4 \) distance apart shown in figure 9. Using the figure 9, the weighted average of the axial field \( H_1 \) is calculated by using the following equation:

\[
H_{1\text{avg}} = \left\{h_1(H_1 + H_1) + h_2(H_1 + H_1) + h_3(H_1 + H_1) + h_4(H_1 + H_1)\right\} / \left\{2(h_1 + h_2 + h_3 + h_4)\right\}. \tag{30}
\]

The compressive stress was applied to the sample through the grip shown in figure 10 by using an 8874 Instron testing machine. The applied load oscillated at a frequency of 10 Hz with a maximum amplitude of 5 MPa. The machine was kept in load-controlled mode and the applied forces on the specimen were recorded via Instron Machine associated data acquisition software ‘Wavematrix 2’. The force applied to the specimen and the displacement of the top part of the sample was recorded automatically by the software controlling the machine. The strain could not be measured during the experiment with the available equipment because the coil surrounded the sample (see figure 10). The strain could be calculated, although not very accurately, from the position data collected. Before running the experiment, a white dot was placed on one of the sides of the specimen through which the lateral field was applied. When the dot was kept on the top left side of the specimen, this configuration was assumed as +\( \beta \), and when the

![Figure 8. Schematic of MSMA with magnetic field and angle.](image)
Figure 9. Schematic of the measurement of the axial magnetic field. Note that the field is measured over the length of the specimen covered by the coil (see figure 10).

Figure 10. Experimental setup for the power harvesting test. Axial field $H_1$ is applied on the specimen by using a permanent magnet and lateral field $H_2$ is applied by using an electromagnet. Different values of $\phi$ are obtained by varying $H_1$ & $H_2$. Note that $H_{tot}$ is always kept the same.

dot was held at the top right side of the specimen, the configuration was assumed as $-\beta$. Finally, during the load oscillation, the emf data was recorded using LabVIEW graphical programming environment and the raw data was processed by using the Microsoft Excel program.

4. Generalized regression neural network

GRNN which was proposed by Specht [15], was adapted from radial basis neural networks [23] so that it can be used for regression, prediction, and classifications (see figure 11).

GRNN represents an enhanced technique in the neural networks on the basis of non-parametric regression [24] which bounds every training sample to represent a mean to a radial basis neuron. Mathematically it can be expressed as:

$$Y(x) = \frac{\sum_{k=1}^{N} y_k K(x, x_k)}{\sum_{k=1}^{N} K(x, x_k)},$$

where $y_k$ is the activation weight for the pattern layer neuron at $k$, $K(x, x_k)$ is the Radial basis function kernel (RBFK) [25]. Here Gaussian kernel is used as RBFK which can be expressed as:

$$K(x, x_k) = e^{-d^2 / 2\sigma^2},$$

where $d_k$ is the squared euclidean distance between the training samples ($x_k$) and the input ($x$) which is expressed as:

$$d_k = (x - x_k)^T(x - x_k).$$

Equation (31) can be modified as [15]:

$$E(F, H_1, H_2) = \frac{\sum_{k=1}^{N} A^k e^{-d_k^2 / 2\sigma^2}}{\sum_{k=1}^{N} B^k e^{-d_k^2 / 2\sigma^2}},$$

where $E$ indicates the estimator of emf, $A^k$ & $B^k$ represent the coefficients for the cluster.

In this work, the GRNN is chosen for the prediction because of its advantages over other neural networks. In our study, the data set is small and GRNN is efficient working with less volume of data and it utilizes Gaussian functions which increase the prediction accuracy. Moreover, GRNN does not require any backpropagation to update the weights which makes it possible to avoid the limitation of backpropagation [26]. In figure 12 a feed-forward neural network is shown which can be used to estimate the emf $E$ from the measurement vector, force ($F$), and magnetic field ($H$).

In figure 13, a simplified workflow chart of the machine learning-based modeling are shown. We had a total of four variables, axial force ($F$), axial magnetic field ($H_1$), lateral magnetic field ($H_2$), and emf, among these three, are independent variables and one is the dependent variable (emf). 75% of the total data was used for training the model and the rest 25% was used to test the model using the built-in 'test-train split' function of scikit-learn. All the values of the data set were scaled in-between 0 and 1 to increase the model efficiency. $k$-fold cross-validation is used in this model where the original sample is randomly separated into $k$ equal-sized subgroups. Among $k$ subgroups, a single group is picked as the validation data for testing the model, and the rest of the ($k-1$) subgroups are used as training data.
5. Results

The experimental results shown in figure 14 were obtained using the loading frequency of 10 Hz. The predicted curve follows the same trend as the experiment, suggesting that this model reasonably predicts the angle for maximum emf. For instance, the 0.578 T of the resultant magnetic field gave the peak emf at an angle of around 3 degrees which was well predicted by all the models (figure 14). In figure 15, emf is plotted against time using experimental emf and the emf predicted by a machine-learning-based model (GRNN). Unlike physics-based modeling, GRNN predicts the experimental curve very well, i.e. this model captures the experimental curve with an accuracy of 99.5%. In figures 17 and 18, predicted emf and variant reorientation ($\xi_i$) were shown for low and high-stress levels, respectively. The positive and negative $\beta$ orientations were considered for both cases. At low stress (figure 17), $+\beta$ orientation produced more peak-to-peak emf than $-\beta$ while the high stress (figure 18) showed the opposite behavior.

6. Discussion

The primary purpose of this study was to accurately predict the open circuit emf output of MSMA in power harvesting applications. Although model prediction is crucial to design and optimizing power harvesting devices, previously very few authors [4] tried to predict the emf using constitutive modeling. However, their approach was lacking some features for a decent model prediction. In our current approach, emf was predicted from the LaMaster et al [7], a modified model where an experimentally observed offset angle was added to the model proposed by LaMaster et al and GRNN model. All models were used to predict experimental emf data and the results are shown in figure 14. The experimental emf shown in figures 14
and 15 were obtained by performing a load control test with a magnetic field applied at various angles. Note that the models all assume that the applied field was uniform, but that was hard to achieve experimentally.

One of the significant contributions of this study is to add an offset angle to the model which helps to explain some of the power-harvesting capabilities of MSMAs. Using figure 16, the reason for getting different peak-to-peak emf from different orientations [4] of the MSMA can be hypothesized. There seem to be competing factors explaining how β affects emf output. On the one hand, figure 16(a) with β positive seems to make reorientation easier. As the ξ_v vs. time plot in figure 17 shows, there is more reorientation, and the slope is stiffer with +β than with −β because of the requirements of less energy to reorient. Thus, change in magnetization within a certain time period is more in figure 17(left) than figure 17(right). As the difference in magnetization is higher, the emf is also higher (equation (26)). On the other hand, in figure 16(b) there is more overall change in magnetization as the specimen changes from the stress-preferred state to the field-preferred state. Thus, when the full reorientation is obtained (see figure 18), −β gives more emf than +β. In this case, the stress and field level is very high, more than 8 MPa and 0.7 T, respectively. As the variants are fully reoriented, there is no additional reorientation of the case of +β and instead, the more change in magnetization in −β case leads to more emf with −β.

In this work, the experiments performed were stress-controlled, and the stress varies between 0 and 4.8 MPa. Therefore, full reorientation was not obtained. Thus, the ease of reorientation dominates, and as seen earlier, the +β configuration (see figure 16(a)) produces more emf than −β configuration (see figure 16(b)). The configuration which produces more emf experimentally than the other is assumed as +β configuration in figure 14. The idea that −β produces more emf with very large fields and stresses was not verified experimentally, however, it should be as part of future work. The hypotheses about the sign of β and the maximum emf suggest that two different types of energy harvesters are possible to design, one is for low-stress levels, and another one is for a high-stress level or strain-controlled. In either

Figure 14. Peak to peak emf vs. angle plots. The solid blue curve represents the experimental emf with positive β. The dashed red, black, and orange curves represent the model predicted emf with the modified model, LaMaster et al model [7], and GRNN model, respectively. The resultant magnetic field was 0.578 T.

Figure 15. Emf vs. time plots. The solid blue curve represents the experimental emf with positive β while the dashed orange curve represents the model predicted emf with the GRNN model. The lateral and axial magnetic fields were 0.575 and 0.057 T, respectively.
Figure 16. Schematic of MSMA with two different orientations, i.e. positive $\beta$ (a) and negative $\beta$ (b). Constant lateral ($H_2$) and axial ($H_1$) magnetic field are applied to the specimen. Varying axial compressive stress ($\sigma_{11}$) is also applied. $V_1$ and $V_2$ represent stress-preferred, and field-preferred variants, respectively.

Figure 17. Emf and variant volume fraction prediction with associate load condition from the model with offset angle added for both positive (left) and negative (right) $\beta$. Peak-to-peak voltages in (left) and (right) are 0.371 and 0.315 V, respectively. Note that full reorientation is not obtained here due to low axial stress (0–4.8 MPa) and resultant field (0.578 T) level. The axial field $H_1$ is 0.029 T.

case, figure 14 suggests that the peak-to-peak emf is maximum at an angle between $3^\circ$ and $7^\circ$ and these power harvesting devices of the type in figure 10 should have a small axial field to maximize emf output. However, as the angle depends on the magnitude of the axial and lateral field, it is necessary to pick suitable magnets for maximizing the emf output. Several
authors reported different optimal angles and the differences among these angles occurred due to the variation in the testing procedure and the magnitude of the resultant field and stress [1, 4, 14].

In figure 14 the predicted emf obtained from the modified model (red dashed line) falls closer to the experimental emf than the LaMaster et al model (black dashed line). This suggests that adding a new feature, i.e., offset angle to the model increases the model accuracy compared to the model prediction reported by another author [4]. Moreover, the added offset angle eliminated the constraint of getting zero emf at an angle of 0° (figure 14). However, there is still a significant difference between the experimental and the predicted results which suggests that some key features are still missing from the constitutive model. Model calibration can be the possible reason behind the inconsistency of poor prediction. All the constitutive models were calibrated at zero axial fields while the experiments were performed with the presence of different axial field values. This may be the possible reason for the deviation of the predicted trend extremely with increasing the angle (figure 14).

In order to overcome all the constrain of constitutive modeling, a GRNN model is implemented in this study to make accurate predictions. The GRNN model is extensively dependent on experimental data since the model learns from the data and finds the hidden co-relation. In our study, the GRNN model was able to predict the experimental curve with a high level of accuracy. Besides capturing peak-to-peak emf (figure 14), the GRNN model can predict emf as a function of time (figure 15) exceptionally well. However, there were some limitations to implementing the feasibility of machine learning-based modeling. The most common is the overfitting of the model which may occur due to the lack of enough experimental data. In this study, we had a limited amount of dataset, and we tried to overcome the overfitting by keeping the model as simple as possible, the offset angle (β) was not included in the GRNN model for that reason. In future studies, the model can be constrained by physic-driven features [27], trained with a robust dataset, and the offset angle may also be considered.

7. Conclusions
Since the constitutive models in this work were not particularly accurate enough at predicting emf, their use in design is limited, and significant future work is needed to find the missing features. Some future work is needed to test some of the hypotheses and understanding of the models in this work regarding the emf at the high-stress level. Further study is also recommended to find any other form of energy that may be included in Gibbs free energy to improve the prediction of variant reorientation. One such kind of energy is magnetic exchange energy which is the fundamental property of ferromagnetic materials that favors alignment of the magnetization vector spins along a common direction [28]. Although constitutive modeling does not produce good predictions, the GRNN model was successful to predict the behavior and these machine-learning
approaches can be useful in designing MSMA-based sensors and power harvesters.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

Acknowledgments

This work has been supported by the National Science Foundation under Grant Nos. 1101108 and 1561866. Any opinions, findings, conclusions, or recommendations expressed in this article are those of the author(s) and do not necessarily reflect the views of the National Science Foundation. The author would like to thank Glen D’Silva, for his constructive feedback and for helping to do the experiments. The author would also like to thank Professor Sybil Derrible for helping him to implement the machine learning algorithm.

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