Deformation Perception of Germanium Based on Finite Element Force-Electric Coupling Field Simulation

Heng Liang

School of Physics and Astronomy, Sun Yat-sen University, Zhuhai 519000, China
liangh78@mail2.sysu.edu.cn

Abstract. This study delves into the deformation perception of germanium through finite element force-electric coupling field simulation within the evolving domain of modern materials science and engineering. As germanium is pivotal in electronics and optoelectronics due to its distinct mechanical and electrical properties, understanding its behavior under mechanical and electrical stimuli is crucial for developing advanced sensors, actuators, and smart materials. Utilizing COMSOL Multiphysics software, this research simulates the deformation of germanium under varied mechanical forces and a constant electric field. The primary method employed is the coupled-field simulation (CFS), enhancing our comprehension of the interactions between mechanical loads and electric fields within solids. Additionally, this investigation incorporates a multilayer perceptron (MLP) to predict germanium's deformation extent based on changes in potential distribution, thereby demonstrating the synergy between finite element simulation and machine learning. The findings reveal that the MLP model can successfully predict the deformation extent, thereby underscoring the utility of integrating machine learning with traditional simulation techniques. This research not only advances our understanding of germanium's mechanical and electrical behavior but also showcases the potential of machine learning in enhancing material sensing capabilities, which could propel the development of innovative materials and devices with superior sensory and actuation functions.

Keywords: Germanium, Coupling Field Simulation, Multilayer Perception.

1 Introduction

The study of solid deformation under the influence of external forces and electric fields is a fundamental aspect of material science and engineering, with significant implications for the design and development of various technological applications. In particular, the ability to accurately characterize and predict the response of materials to mechanical and electrical stimuli is crucial for the advancement of sensors, actuators, and smart materials [1]. Among the various materials of interest, germanium (Ge) stands out due to its unique combination of mechanical and electrical properties, making it a promising candidate for applications in electronics, optoelectronics, and beyond [2].

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The interaction between mechanical forces and electric fields in solids can lead to complex deformation behaviors and changes in electrical properties. Rodzevich et al. reviewed the approach of fabricating and handling materials under the weak constant electric field, which involved discussing force-electric interaction for materials [3]. Apart from that, the application of mechanical loads such as bending, elongation, and rotation can induce changes in the voltage distribution within a material, which in turn can affect its electrical conductivity, permittivity, and other key parameters. Understanding these interactions is essential for the development of materials and devices that can leverage these effects for practical applications.

Finite element simulation has emerged as a powerful tool for studying the coupled mechanical and electrical behavior of materials [4]. By employing a force-electric coupling field simulation (CFS) approach, researchers can model the intricate interactions between mechanical loads and electric fields in solids, providing detailed insights into the resulting deformation and changes in electrical properties. In this study, COMSOL Multiphysics software is utilized to simulate the deformation of germanium under a constant electric field and various mechanical forces. Lin et al. utilized COMSOL Multiphysics to simulate the temperature and stress distribution between the pantograph and the contact line in a variety of physical conditions [5]. This study aims to investigate how different degrees of force loading, especially elongation, affect electric potential distribution on the surface of the material.

In addition to understanding the fundamental interactions between mechanical and electrical properties, there is a growing interest in leveraging machine learning techniques to interpret and classify the responses of materials to different stimuli. Multilayer perceptron (MLP), one of the artificial neural network algorithms [6], is capable of enabling the development of intelligent materials and devices that can perceive and respond to various mechanical stimuli in a controlled and predictable manner [7]. This study explores the use of MLP to predict the degree of deformation of a germanium cuboid based on observed changes in electric potential distribution.

Overall, this study aims to help understand the coupled mechanical and electrical behavior of germanium and other similar materials, and to demonstrate the potential of machine learning techniques in sensing different degrees of solid deformation. By combining finite element simulation with machine learning, this study hopes to broaden the way for new advances in materials science and engineering, thereby developing innovative materials and devices with enhanced sensing and driving capabilities.

2 Methods

2.1 Geometry Model Construction

In this study, a simple geometric model of germanium is constructed by COMSOL Multiphysics to apply to CFS and explore the excellent properties of germanium.

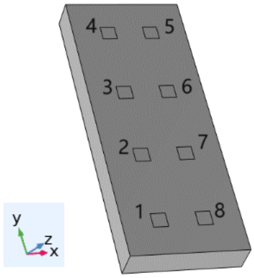


Fig. 1. The geometry model of germanium used for CFS (Photo credited: Original)

Fig. 1 shows a germanium cuboid constructed by COMSOL Multiphysics in this paper, with a size of 0.4m×1.0m×0.1m. The upper surface of the cuboid is equidistantly distributed with 8 electrode sheets with a side length of 0.05 m (thickness is negligible), labeled with serial numbers from 1 to 8 respectively, which forms a sensing array.

The parameters of germanium used in this paper are shown in Table 1.

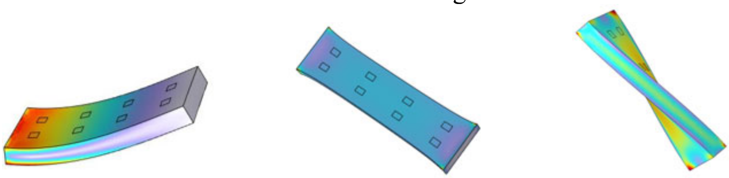
Table 1. Material parameters (germanium) [8]

Density	5.32×10^{3} kg·m^{-3}
Young's modulus	1.22×10^{6} Pa
Poisson's ratio	0.28
Conductivity	2×10^{3} S/m
Relative permittivity	16.2

2.2 Coupling Field Simulation

Simulation of Force. To show the application of finite element analysis in multi-physical field coupling, three classical modes of deformation caused by the force load are simulated: bending, elongation, and rotation.

The three modes of deformation are shown in Fig. 2.



(a) Bending (b) Elongation (c) Rotation

Fig. 2. The distribution of stress in three modes of deformation (Photo credited: Original)

In bending, the germanium cuboid is fixed on one face vertical to the y-axis, and the other face vertical to the y-axis is subjected to a certain force along the positive direction of the z-axis, which makes the germanium cuboid bend to a certain extent.

In elongation, one surface of the germanium cuboid vertical to the y-axis is fixed, while forcing the other face opposite it to move a certain distance along the y-axis, thus causing the germanium cuboid to stretch and deform around the y-axis.

In rotation, the surface perpendicular to the y-axis of a germanium cuboid is fixed, while forcing the opposite surface to rotate counterclockwise around the y-axis by a certain angle, thereby distorting and deforming the germanium cuboid around the y-axis.

Simulation of Electric Field. The electrodes on the cubic surface of germanium act as current sources to generate steady current, thus forming a steady electric current field (EC field) on the surface of germanium. In Fig. 3, electrode 1 and electrode 6 are selected, with the former applying positive current and the latter applying negative current.

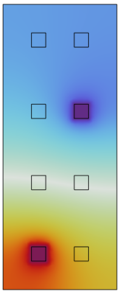


Fig. 3. The potential distribution of simulated EC field (Photo credited: Original)

Simulation of Force-Electric Coupling. As bending, elongation, and rotation cause different types of deformation of the germanium cuboid, one pair of the eight electrodes on the deformed germanium cuboid are selected to apply positive and negative currents respectively, to realize the force-electric coupling.

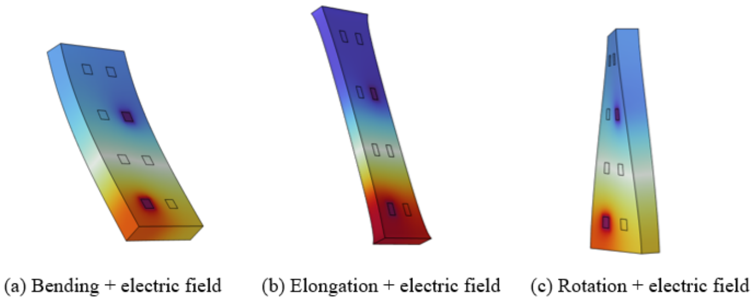


Fig. 4. The potential distribution in three modes of deformation under EC field (Photo credited: Original)

Fig. 4 shows that force-electric coupling is achieved by bending, stretching, and twisting the germanium cuboid while electrodes 1 and 6 respectively release currents of equal magnitude and opposite directions to form an EC field.

Electrical Perception of Mechanical Deformation (Elongation). When an EC field is distributed on the surface of a germanium cuboid, the types and degree of deformation mode and the degree of deformation will affect the distribution of the electric potential. In other words, the electric potential distribution on the surface of the cuboid can be regarded as the response of the EC field to the deformation caused by the force load.

The potential differences between two by two in electrodes 1 to 8 (a total of 49 data points) are taken as the response of the 8-electrode sensing array (shown in Fig. 1) to the cuboid deformation in the form of potential distribution, in which way the 8-electrode sensing array can realize the perception of the deformation type as well as the degree of deformation in one certain deformation type.

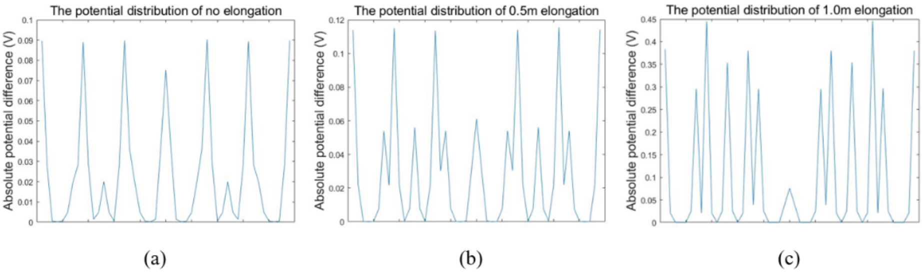


Fig. 5 The potential distribution of simulated EC field (Photo credited: Original)

In Fig. 5, one face of the germanium cuboid is fixed, and the other face is forced to elongate 0 meters, 0.5 meters, and 1.0 meters respectively along the negative direction of the y-axis. The potential distribution on the surface of the cuboid reflects these three elongation lengths, which is the perception of mechanical deformation by the EC field.

2.3 Implementation of MLP Algorithm

Theoretical Basis. Multilayer perceptron (MLP) is a feed-forward artificial neural network, which simulates complex nonlinear relationships through multiple levels of structure. The MLP is made up of an input layer, a hidden layer, and an output layer, and each of them possesses several neurons. These neurons communicate with each other through weighted connections and use nonlinear activation functions to process information. In MLP, data begins from the input layer propagates through multiple layers, and arrives at the output layer with the eventual result. Through the backpropagation algorithm, MLP enables the variation in weights and biases in the network to reduce the error of output. This training process is repeated to ensure the network performance reaches an acceptable level [9]. A theoretical example of an MLP network is shown in Fig. 6.

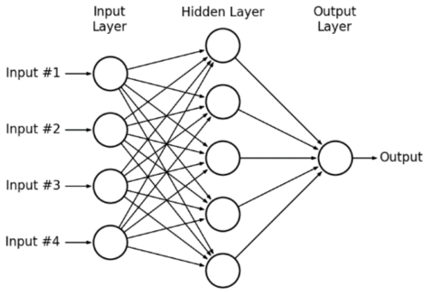


Fig. 6. One theoretical example of MLP network [10]

In this study, MLP was used as a powerful tool for regression to establish a complex relationship between potential distribution and solid deformation, which is capable of capturing and learning the nonlinear characteristics of input data through its multi-layer structure.

Fig. 7 depicts the process of perceiving elongation degree in the germanium cuboid with MLP.

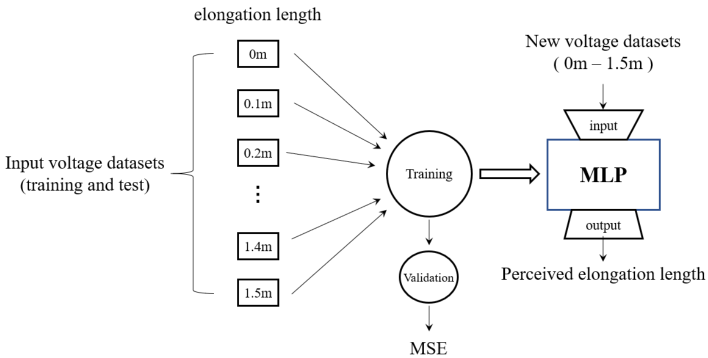


Fig. 7. Process of deformation perceiving with MLP in EC field (Photo credited: Original)

Data Preparation. In this study, the potential difference distribution of germanium cuboids with different elongation lengths is used as the data set for training the MLP model. The data set contains the potential difference distribution of the elongation length from 0m to 1.5m, and each interval is 0.1m. A total of 15 sets of distribution data are included.

Before training the MLP model, the voltage distribution data corresponding to different degrees of deformation is prepared.

To improve the generalization ability of the MLP model built in this study and avoid the gradient disappearance or explosion, it is necessary to normalize the data used for model training. In this study, Z-score normalization is used to convert the data into a distribution, in which the mean is 0 and the standard deviation is 1.

$$Z = \frac{X - \mu}{\sigma} \tag{1}$$

Equation (1) illustrates how the Z-score normalization is done, where X is the raw score (data), μ is the mean value of the data, and Z is the Z-score.

In addition, to evaluate the generalization ability of the model and avoid the overfitting problem in the training process, the data set is divided into 3 sets: training sets, validation sets, and test sets. In this study, normalized feature data were randomly divided into training sets and test sets to directly participate in the training, with a proportion of 70 % and 30 %, respectively.

Model Construction and Training. It can be seen from Fig. 8 how the MLP neural network is constructed in this study.

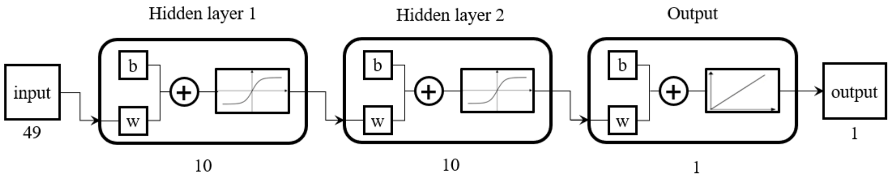


Fig. 8. Feed-forward neural network in MLP (Photo credited: Original)

This neural network contains 49 neurons in the input layer, corresponding to the input 1×49 voltage distribution data. The hidden layer 1 is made up of 10 neurons, with corresponding weights (w) and biases (b). This layer incepts the input data and begins extracting features. The hidden layer 2 also contains 10 neurons, which continue the feature extraction and transformation process. The output layer has a neuron that outputs the prediction results of the network. For the regression task, this value is continuous and represents the network's response to the input data. In the two hidden layers, the activation function is an S-type function, and the output layer uses a rectification linear unit (ReLU) [11] (shown by specific icons in Fig. 8). Finally, the final output value of the network is obtained, which is the perceived elongation length in this study.

After the model is constructed, 15 sets of data from 0m to 1.5m elongation length are input into the model for training. The purpose of training is to make the model perceive the elongation length according to the voltage distribution corresponding to any elongation length in the input 0 to 1.5m.

The whole model training process uses the Levenberg-Marquardt optimization algorithm.

Model Validation. In this study, the validation of the model is performed by calculating the mean squared error (MSE) on the test set. MSE is a commonly used validation index in regression problems [12]:

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n} (Y_i - \widehat{Y}_i) \tag{2}$$

In equation (2), Y_i is the actual value and $\hat{Y}_i$ is the predicted value.

In addition, the regression relationships of the training set, test set, and validation set are checked.

3 Result and Discussion

3.1 Voltage Distribution

As shown in Fig. 9, all 15 sets of voltage distribution that were used to train the MLP are exported, including the voltage distribution corresponding to the elongation of 0 to 1.5m.

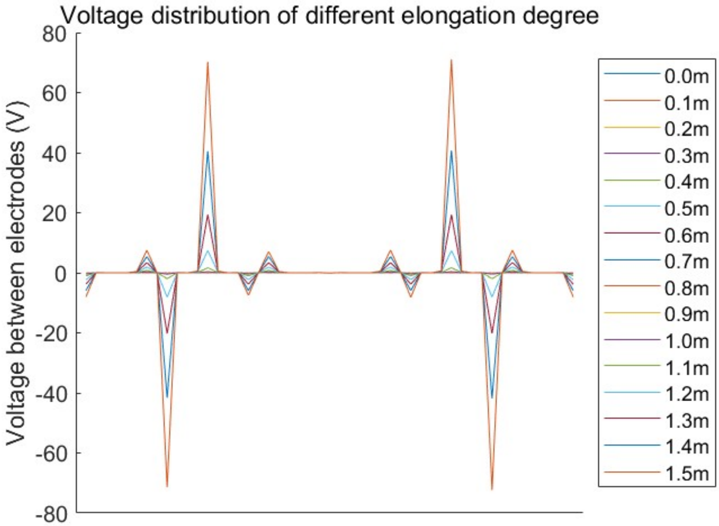


Fig. 9. Voltage data used in MLP training (Photo credited: Original)

Due to the equidistant and symmetrical arrangement of the sensing array composed of electrodes, the voltage distribution also exhibits a symmetrical and periodic arrangement.

In addition, the larger the elongation degree, the greater the voltage change caused by the change of the same elongation degree, indicating that the high elongation degree will make the sensing array more sensitive to the deformation of the germanium cuboid, and produce a more significant voltage distribution response.

3.2 Deformation Perception by MLP Model

Model Training Status. As can be seen from Fig. 10, after 5 epochs of training, the gradient of the loss function decreases rapidly to 3.07e-13, and the learning rate (Mu) in the Levenberg-Marquardt optimization algorithm also decreases steadily to 1e-8, indicating that the training process is stable and reaches the optimal state in the 5th epoch. Meanwhile, the model passes all the validation checks during the training process.

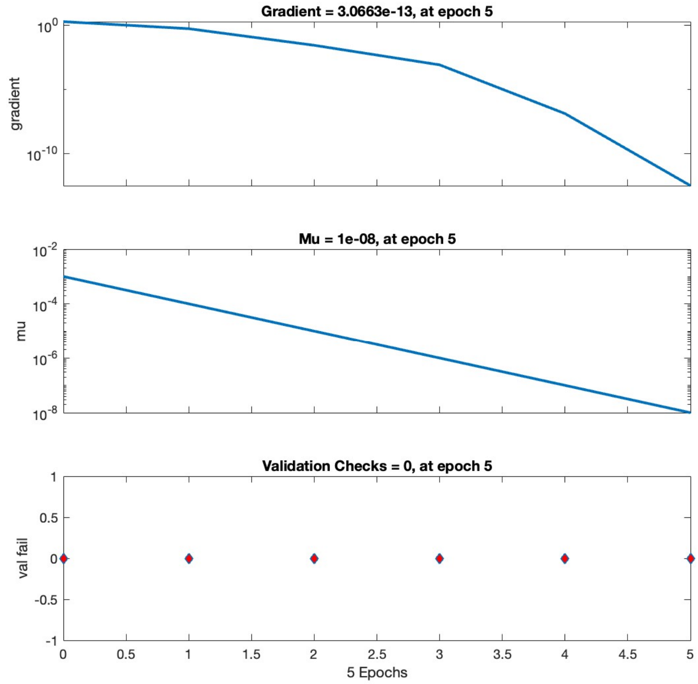


Fig. 10. Status plot of MLP training (Photo credited: Original)

Model Validation. Fig. 11 contains three curves, representing the MSE of the training set, the validation set, and the test set, respectively.

As the number of epochs increases, the MSE of the training set continues to decrease. This shows that the model is learning from the training data and is doing better and better in fitting the training data.

The MSE of the validation set decreases during the initial epochs of training, then stabilizes and begins to increase slightly. This is a common sign of overfitting [13], and the generalization ability of the unseen data is reduced.

The MSE of the test set is relatively stable during the training process and is very close to zero, which indicates that the model's performance on the test set is good.

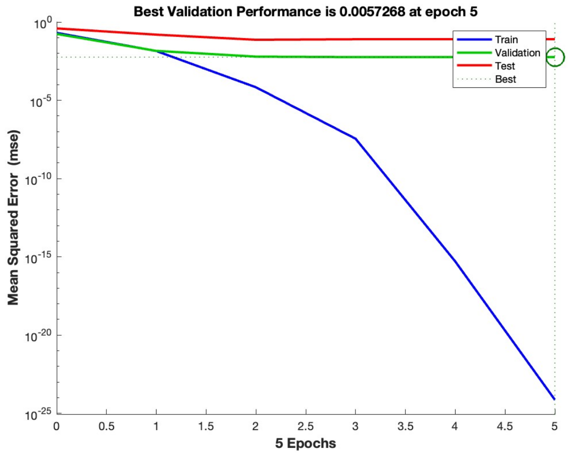


Fig. 11. MSE status of MLP (Photo credited: Original)

Fig. 12 shows the relationship between the perceived elongation degree and the actual elongation degree of the neural network model on different data sets.

The predicted values of the three data sets are quite close to the actual values, and from all the data, $R^2 = 0.97626$, which is very close to 1, indicating that the model has very good fitting and predictive ability.

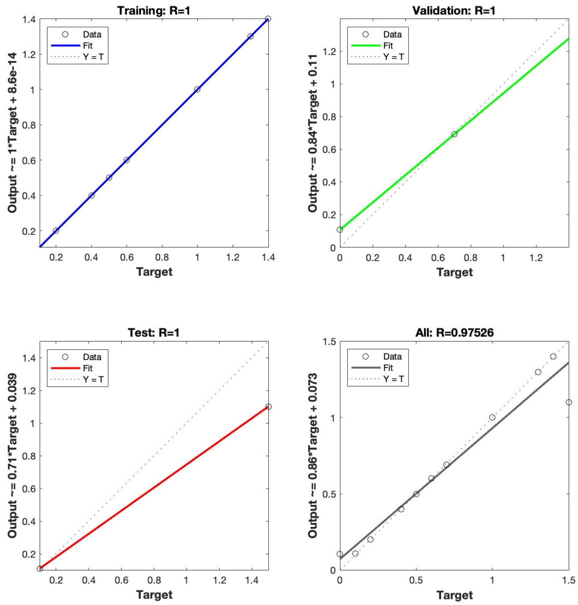


Fig. 12. Regression diagram of datasets in training (Photo credited: Original)

Application of the Model. Several sets of unseen data from 0m to 1.5m are input into the trained MLP model to realize the application of deformation perception.

Table 2. Elongation degree perception by MLP

Actual elongation degree (m)	Perceived elongation degree (m)	Relative error
0.2500	0.2879	15.12%
0.4500	0.4597	2.16%
0.6500	0.6321	2.75%
0.8500	0.8040	5.41%
1.0500	0.9763	7.02%
1.2500	1.1482	8.14%
1.4500	1.3204	8.94%

In Table 2, the relative error is large when the actual elongation degree is 0.25 m, which indicates that this MLP model performs poorly when processing data at the edge of the data distribution.

In addition to the data points with an elongation degree of 0.25 m, larger relative errors can be observed at larger elongation degrees. When the deformation degree of solid material is large, there is a complex nonlinear relationship between deformation and potential distribution. In the case of limited training data, the model is not able to fully accurately simulate this complex behavior.

4 Conclusion

In this study, the germanium deformation perception based on multi-layer perceptron (MLP) is discussed by finite element force-electric coupling field simulation. The deformation of germanium under a constant electric field and various mechanical forces was simulated by COMSOL Multiphysics software. The interaction between mechanical loads and electric fields in solids is simulated by the coupled field simulation (CFS) method, which provides insight into the changes in deformation and electrical properties caused by these interactions.

However, this study has many limitations. First, the simplification and assumption of the model may affect the generality and accuracy of the results. For example, the germanium cuboid model used in the experiment only considers several specific force loading conditions, and cannot fully simulate the more complex force and electric field environment in the real world. Secondly, although the model's performance on the test set is satisfactory, the data used to train this model is too small in this study, and there are problems of overfitting and insufficient generalization ability. There are accidental factors in the success of training, and the effect of deep learning is not realized.

Despite these limitations, this study demonstrates the potential of machine learning techniques in sensing different degrees of solid deformation and provides a valuable reference for the development of germanium materials and equipment with enhanced sensing and driving capabilities.

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