On-demand Direct Design of Polymeric Thermal Actuator by Machine Learning Algorithm

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Abstract The design optimization of thermal-driven actuators is a challenging task because the performance depends on multiple materials parameters, structural parameters, and working conditions. In this work, we adopted large scale finite element simulation together with machine learning algorithm to fulfill the on-demand design of thermal actuators. Finite element analysis was used to simulate the performance of thermal actuator with two-layer structure, which generated large amount of dataset by considering the variation of parameters including the moduli, thermal expansion coefficient, sample thickness and length, and temperature. Support vector regression (SVR) was adopted to establish the relationship between multiple input parameters and the resulting contact pressure. Thereafter, a simple interior point algorithm was used to achieve the on-demand design based on the SVR model. The contact pressures of thermal actuator constructed from the optimized parameters deviated less than 15% of the target values.

Keywords Polymer composites; Thermal actuator; Finite element analysis; Support vector regression

INTRODUCTION

Stimuli-responsive actuating materials have great potential in the fields of soft robotics,[1–3] artificial muscles,[4] drug delivery,[5] and so on. Hydrogel and carbon nanotube/polymer composites are two typical actuator materials.[6,7] They have obvious advantages including large deformation while light weight, vulnerable stimulation and flexibility. Different ways of stimuli have been suggested, such as light,[6] thermal,[5] and electrical field[8] based on different materials.

Recently, polymer materials with different coefficients of thermal expansion (CTE) have been widely studied as model thermal-driven actuators.[9,10] Most of them have double-layered structure with controllable bending deformation in response to heat.[11,12] The deformation and thereby the force or pressure the actuator generates are affected by multiple parameters including material properties, geometry of structures as well as working environment like temperature. The optimization of thermal actuator is a challenging task. Exploration of the whole space of different parameters is difficult to implement experimentally. Therefore, simulations have been adopted for structural and topology optimization.[13,14] However, because of the large number of parameters, direct search in parameter space[14] or simple optimization method is not efficient to find the best solution for the specific target in the design and application of thermal-driven actuators.

Machine learning method has been successfully applied in material development.[15–16] Based on large amount of data from material parameters, structural parameters, processing parameters, and dependent material properties, it could discover hidden and rich relationship among them. Neural networks are one of the popular methods because of powerful functions that could establish arbitrary nonlinear relationship between input features and targeted variables. Other machine learning algorithms such as support vector machine (SVM) also attract attention of researchers, since the better performance is acquired in small data. The universal approximation of neural networks has proved that a feed-forward network with a single hidden layer containing a finite number of neurons can approximate functions of arbitrary complexity with arbitrary precision.[17] Wang et al.[18] proved the universal approximation of SVM with radial basis function (RBF) kernel to arbitrary functions on a compact set and deduced it to the approximation of discrete function. Besides, the RBF function based least-squares SVM is effective in nonlinear function estimation and has generalization ability.

In the present study, firstly, an ideal model of thermal actuator was presented. We used finite element analysis (FEA) method to simulate the process of thermal responsive actuator being bent to contact with objects by thermal expansion and create large dataset for data mining. In this process, hyperelastic model (the Mooney-Rivlin two parameters model)
was chosen to describe the behavior of material elastic deformation. Secondly, machine learning algorithm, the support vector regression (SVR), was used to predict the contact pressure of thermal actuator and analyze the sensitivity of structural, material, and processing parameters. Finally, on-demand direct design was implemented by an optimization algorithm together with the established SVR model.

**METHODS**

**Finite Element Analysis (FEA)**

In this work, we consider a thermal actuator of two-layer structure, which is composed by two thermal materials with different thermal expansion coefficients. A linear elastic “wall” is added below them. The bilayer structure of the actuator is shown in Fig. 1. Upon heating, the two-layer thermal actuator will bend because of the different thermal expansion coefficients of two layers. If the upper layer has higher thermal expansion coefficient, the actuator will bend downwards to the plate during heating once the left end of the thermal actuator and lower plate were fixed. The performance of thermal actuator is evaluated by the contact pressure on the wall instead of simple bending deformation.

We adopted finite element analysis (FEA) to predict the behavior of the thermal actuator. It is implemented by combining solid mechanics and heat transfer for the coupled thermal expansion and contact problems. Two layers of the thermal actuator are modeled by the hyperelastic two-parameter Mooney-Rivlin model, where the strain energy density $W_S$ is expressed as

$$W_S = C_{10} (I_1 - 3) + C_{01} (I_2 - 3)$$

where $C_{10}$ and $C_{01}$ are two material constants, and $I_1$ and $I_2$ are the two invariants of the elastic right Cauchy Green deformation tensor.

The thermal strain ($\varepsilon_{th}$) depends on the coefficient of thermal expansion (CTE, $\alpha$), the temperature ($T$), and the strain-free reference temperature ($T_{ref}$) as,

$$\varepsilon_{th} = \alpha (T - T_{ref})$$

The penalty method was used to calculate the contact pressure. This algorithm inserts a stiff spring between the contacting boundaries. The penalty factor is interpreted as the stiffness of spring. A high value of the factor fulfills the contact conditions more accurately, and it was set to be $10^5$ in this work. For calculation of contact pressure, details of implementation can be found in literature\(^{[19]}\).

**Support Vector Regression (SVR)**

The support vector machine (SVM) is a widely used algorithm in machine learning as it may give significant accuracy with less computation power. The SVM is a supervised learning method with several advantages as compared to other machine learning algorithms, including better results for small scale of samples and the ability of mapping inputs into high dimensional feature spaces by kernel functions, which helps to solve problems with strong nonlinearity and high dimensionality. Herein, a regression-based support vector machine method\(^{[20]}\) was used. Support vector regression (SVR) is the application of SVM in regression learning, which aims to identify a function to fit the training dataset at most $\varepsilon$ derivation from the experimental values for the introduced error $\varepsilon$. Considering the experimental errors, a soft margin was introduced by using slack variables, whose contribution to the optimizing target function was controlled by a penalty factor, $C$. To solve nonlinear problems, RBF or Gaussian kernel function (with parameter $\gamma$) was adopted. Accuracy of support vector regression is dependent on the selection of two factors. The parameters $C$ and $\gamma$ were set as 1 and 2, respectively, which can give satisfactory results in this work.

**Prepared Dataset**

Herein, the influence of structural parameters ($D_1, D_2, L$), material parameters ($\alpha, C_{10}, C_{01}$), and processing parameters ($T$) on the contact pressure will be studied. The range of length ($L$) was set from 0.015 m to 0.02 m and the range of thickness ($D_1, D_2$) was set from 0.1 mm to 0.5 mm. For material parameters, only those for the thermal material 1 was adjusted. The coefficient of thermal expansion varied from $6 \times 10^{-6}$ K$^{-1}$ to $3 \times 10^{-4}$ K$^{-1}$ for the thermal material 1. For the Mooney-Rivlin constitutive model, $C_{10}$ was set from 0.5 MPa to 1.0 MPa and $C_{01}$ was set from 0 to 0.5 MPa. The material parameters were chosen to cover wider range of possible materials, including different rubbers, polyurethanes and hydrogels materials\(^{[21–23]}\). For processing parameters, the temperature was changed from 340 K to 390 K. Detailed parameters are given in Table 1. Symbol “$*$” represents temperature. Material parameters of thermal material 2 were kept constant, i.e., the CTE was $6 \times 10^{-6}$ K$^{-1}$, and two parameters of Mooney-Rivlin model $C_{10}$ and $C_{01}$ were 1.0 and 0.9 MPa, respectively.

Based on the design of parameters space, a large amount

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*Fig. 1* Bilayer structure of thermal actuator and bending upon heating. The distance $S$ between the thermal actuator and the wall is set to be 5 mm. The fixed constraint is applied on the left end of the thermal actuator, and the contact constraint is applied on other boundaries of thermal actuator and the top surface of wall. 

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of data on the bending and contact behavior can be obtained by automatic model generation, mesh generation, and FEA simulation using MATLAB and COMSOL Multiphysics. There are 90911 samples in all, nearly 30% of which result in contact pressure by simulation. The dataset was divided in 3 subsets randomly, which include training samples (70%), validating samples (20%), and testing samples (10%). This process was implemented by the scikit-learn module in Python.

RESULTS AND DISCUSSION

Simulation Result of Thermal Actuator

Fig. 2 shows a series of simulation results at constant material parameters and structural parameters but varying temperature. In Fig. 2(a), the bilayer structure just contacted the “wall” and the critical contact pressure was 42 Pa. In Fig. 2(b), the contact pressure was 1270 Pa at 390 K and the structure slightly curved. With the increase of temperature, it not only contacted but also curved heavily and the contact pressure was 7640 Pa, as shown in Fig. 2(c). Severe deformation may appear at higher temperature without contact between the thermal actuator and the wall, as shown in Fig. 2(d).

Because we considered 7 parameters here, it is impossible to effect of all these parameters on the contact pressure simultaneously. Therefore, some simple tendencies are demonstrated in Figs. 3–5. In Fig. 3, the contact pressure is plotted against the coefficient of thermal expansion at different temperatures under constant structural parameters and Mooney-Rivlin model parameters. It is clear that the contact pressure is zero when CTE is small enough, illustrating no contact of the thermal actuator with the target plate. The critical CTE that produces the contact pressure gradually decreases as the temperature increases, indicating larger deformation at higher temperature. The contact pressure generally increases with the increase of thermal expansion coefficient and the temperature, which indicates that controlling the CTE of thermal actuator would be an efficient approach to manipulate the contact pressure. The fluctuation of data in the graph is due to the different contact states, as shown in Fig. 2.

Fig. 4 shows the influence of coefficient of thermal expansion on the contact pressure at different sample thicknesses with $D_1 = D_2$. The tendency is obviously different from the change of temperature in Fig. 3. As the thickness increases, the critical thermal expansion coefficient that produces the contact pressure also gradually increases, indicating that the thicker thermal actuators are more difficult to deform. When the thermal expansion coefficient is small, thinner thermal actuator will generate larger contact pressure, while thicker thermal actuator will generate larger contact pressure when CTE is large. Moreover, it is seen that the contact pressure quickly reaches a plateau at small thickness when the CTE increases. It implies complicated multiple factors in determination of the contact pressure.

Fig. 5 shows the effect of parameters of Mooney-Rivlin model, where the initial Young’s modulus $M = 6(C_{10} + C_{01})$ was used to represent the change of material parameters. Generally, the higher the modulus, the larger the contact pressure at the same coefficient of thermal expansion.

![Fig. 2](https://example.com/fig2.png)

**Fig. 2** Stress distribution at four different temperatures: (a) 315 K, (b) 390 K, (c) 409 K, (d) 500 K. Other parameters $D_1 = D_2 = 0.1$ mm, $L = 0.015$ m, $\alpha = 3 \times 10^{-4}$ K$^{-1}$, $C_{10} = 0.8$ MPa, $C_{01} = 0$ MPa.
However, such trend fails in certain range of CTE, which also implies complicated relationship between the material parameters, structural parameters, and the contact pressure.

Figs. 6 and 7 show clearer influence of the material parameters, structural parameters, and process parameters on the contact pressure. In Fig. 6(a), the mean contact pressure in the case of different thicknesses but constant length is shown, where the error bar denotes the variance of contact pressure in the range of thickness. It is very clear that the larger the thermal expansion coefficient and the higher the initial shear modulus of the material, the larger the contact pressure. It is also demonstrated that as the coefficient of thermal expansion decreases, the contact pressure gradually approaches zero. Moreover, the influence of CTE on contact pressure is bigger than that of modulus. According to the size of error bar, the variance of contact pressure is larger at higher CTE and initial modulus, indicating that the influence of structural parameters is also significant in this region. In Fig. 6(b), the mean contact pressure is shown in the case of different temperatures but with constant structural parameters. There are some local minima in the mean contact pressure surface, implying very complicated dependence. Large error bars at high CTE indicate strong influence of temperature.

In Fig. 7, the mean contact pressure under different thicknesses but same length and initial modulus is plotted against the CTE and temperature. There is no doubt that as the coefficient of thermal expansion and temperature increase, the
mean contact pressure gradually increases. Compared to the data in Fig. 6, the length of error bar in Fig. 7 is much smaller, which indicates that CTE and temperature might be the most important parameters to control the contact pressure.

**Machine Learning**

It has been shown above that the inputs (material parameters, structural parameters, and process parameters) have complicated influence on the contact pressure. Machine learning method was adopted to establish the connections. Support vector regression (SVR) algorithm was used. In order to directly illustrate if there was over-fitting or under-fitting in the regression, the learning process is as follows: (1) randomly chosen 10% of the training data was used for training by the SVR algorithm, (2) randomly chosen 20% of the dataset was used for cross validation, (3) calculate the accuracy of the training data and cross-validation data, (4) repeat steps 1–3 by increasing the training dataset by 10% in each repeat until the training dataset size is 100%. Score is used to evaluate the accuracy of this model, which is defined as \(1 - \frac{u}{v}\), where \(u\) is the residual sum of squares between actual values and prediction values, and \(v\) is the total sum of square of actual values. Higher score means better accuracy. The scores of training and cross-validation are shown in Fig. 8. As the training data set increases, accuracy of the cross-validation data also increases, and gradually approaches that of the training data. The scores of both cross-validation data and the training data converge to ~0.99 at sufficiently large training examples. The small bias and small variance in learning curve indicate that a suitable regression has been achieved with low possibility of under-fitting or over-fitting.

Results for Pearson correlation analysis between input parameters are shown in Fig. 9 in the form of heat maps. The change of color shows how positively or negatively that the input parameters are correlated with each other. From Fig. 9, we can see that there is a weak correlation between all parameters. Therefore, dimensionality reduction of parameters is not necessary.

Fig. 10 shows the contact pressure as predicted using the SVR-based machine learning model versus the respective FEA simulations. The inset shows the relative error distribution of SVR model prediction, indicating that the average error for contact pressure is of the order of 0.5% or less. Therefore, the trained SVR model has the ability to perform on-demand property (i.e., the contact pressure) prediction with reasonably low errors.

The trained SVR model can also help to reveal which para-

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**Fig. 7** Influence of CTE and temperature on the mean contact pressure under different thicknesses.

**Fig. 8** Learning curve of SVR model.

**Fig. 9** Correlation of input parameters shown in the form of heat map.

**Fig. 10** Performance of SVR model predictions. The frequency of relative error is shown in the inset.
meter has the greatest impact on the contact pressure. To evaluate the role of each parameter, we adopted training accuracy and prediction accuracy of the existing model as standards. Here, the accuracy is equal to score from above. Each parameter was sequentially removed from input, and the training accuracy and prediction accuracy of the model after the parameter removing were then determined. Fig. 11 shows the change of accuracy of training and prediction after deleting different input parameters. It is seen that after removing the coefficient of thermal expansion, thickness of thermal material 1, and temperature, the accuracy of the model decreases greatly as compared with other parameters. Such results imply that the CTE, thickness, and temperature are key points for the performance of thermal actuator.

**On-demand Direct Design**

Although the whole range of parametric space could be covered by numeration, it is almost impossible in practice to search the suitable material, structures of thermal actuator, and operating conditions for a specified target contact pressure. We thus attempted to find an alternate efficient route to the on-demand direct design. We adopted the interior point method for the nonlinear function optimization, where the trained SVR model was used to generate the mapping between multiple inputs and the resulting contact pressure. The direct design can be used for any single specified parameter, or for any multiple parameters. In practice, the absolute difference between desired contact pressure and contact pressure predicted by the SVR model is used as the target function. Random initial values were produced as input for the SVR model.

Some examples are shown in Fig. 12. Actually, we can optimize the design with combination of structural parameters, material parameters, processing parameters, and/or all of

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**Fig. 11** Sensitivity analysis of all parameters.

**Fig. 12** Inverse optimization design for four conditions: (a) optimizing temperature with specified other parameters, (b) optimizing initial modulus and CTE with specified other parameters, (c) optimizing temperature and two thicknesses with specified other parameters, and (d) optimizing temperature, CTE, and two thicknesses with specified length and initial modulus.

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them. The target values of contact pressure were chosen as 500, 600, 700, 800, 1000, 1500, and 2000 Pa, which can be other specified values as well. After obtaining the optimized parameters, they were used as input for the FEA simulations, and the contact pressures from simulation were compared with the target values. In order to show the results clearly, we just plot the contact pressure with one of the parameters. In Fig. 12(a), temperature was optimized with all material parameters and structural parameters being constant. It is clear that the optimized contact pressure is very close to the target, and the contact pressure increases monotonically with temperature when all other parameters are fixed. The number of optimizing parameters increases to 2, 3, and 4 in Figs. 12(b), 12(c), and 12(d), respectively. In all cases, the contact pressures from the optimized parameters are close to the target, with the maximum relative error less than 15%. It is also manifested that the combination of machine learning and simple optimizing algorithm is sufficient to accomplish the on-demand direct design of the thermal actuator with specified target property, i.e. the contact pressure in this work.

CONCLUSIONS
We presented an optimization design method for polymeric thermal actuator, which combined the large-scale finite element analysis and machine learning method. Firstly, the thermal response process was analyzed by FEA simulation and large dataset was produced for data mining. Secondly, successful training by the SVR model had been obtained, which resulted in accurate prediction of the contact pressure. On this basis, sensitivity analysis was conducted to show that CTE, temperature, and thickness were key factors affecting the contact pressure. Finally, we adopted the nonlinear optimization algorithm to implement on-demand design with SVR model. The optimization design was facile with arbitrary input parameters. The relative errors between the target and the optimization results were less than 15%. This method provides a new route to on-demand design of polymeric materials with proper target properties.

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