1-1-2015

Thermal modeling and coefficient identification of shape memory polymer nanocomposites structure

He Shen

University of Central Florida

August Mark

University of Central Florida

Kenneth Thompson

University of Central Florida

Yunjun Xu

University of Central Florida

Fei Liang

*University of Central Florida*Find similar works at: <https://stars.library.ucf.edu/facultybib2010>University of Central Florida Libraries <http://library.ucf.edu>

See next page for additional authors

This Article is brought to you for free and open access by the Faculty Bibliography at STARS. It has been accepted for inclusion in Faculty Bibliography 2010s by an authorized administrator of STARS. For more information, please contact STARS@ucf.edu.

Recommended Citation

Shen, He; Mark, August; Thompson, Kenneth; Xu, Yunjun; Liang, Fei; Gou, Jihua; and Mabbott, Bob, "Thermal modeling and coefficient identification of shape memory polymer nanocomposites structure" (2015). *Faculty Bibliography 2010s*. 6798.
<https://stars.library.ucf.edu/facultybib2010/6798>

Authors

He Shen, August Mark, Kenneth Thompson, Yunjun Xu, Fei Liang, Jihua Gou, and Bob Mabbott

Thermal modeling and coefficient identification of shape memory polymer nanocomposites structure

Cite as: Appl. Phys. Lett. **106**, 081907 (2015); <https://doi.org/10.1063/1.4913804>

Submitted: 08 December 2014 . Accepted: 16 February 2015 . Published Online: 25 February 2015

He Shen, August Mark, Kenneth Thompson, Yunjun Xu, Fei Liang, Jihua Gou, and Bob Mabbott

View Online

Export Citation

CrossMark

ARTICLES YOU MAY BE INTERESTED IN

[Recovery torque modeling of carbon fiber reinforced shape memory polymer nanocomposites](#)
Applied Physics Letters **103**, 201903 (2013); <https://doi.org/10.1063/1.4829937>

[Artificial muscles made of chiral two-way shape memory polymer fibers](#)
Applied Physics Letters **109**, 183701 (2016); <https://doi.org/10.1063/1.4966231>

[An investigation of a thermally steerable electroactive polymer/shape memory polymer hybrid actuator](#)
Applied Physics Letters **108**, 062901 (2016); <https://doi.org/10.1063/1.4941802>

Applied Physics Reviews
Now accepting original research

2017 Journal
Impact Factor:
12.894

Thermal modeling and coefficient identification of shape memory polymer nanocomposites structure

He Shen,¹ August Mark,¹ Kenneth Thompson,¹ Yunjun Xu,^{1,a)} Fei Liang,² Jihua Gou,² and Bob Mabbott³

¹*Dynamics and Controls Laboratory, Department of Mechanical and Aerospace Engineering, University of Central Florida, Orlando, Florida 32816, USA*

²*Composite Materials and Structures Laboratory, Department of Mechanical and Aerospace Engineering, University of Central Florida, Orlando, Florida 32816, USA*

³*HB Polymer Company, Sarasota, Florida 34243, USA*

(Received 8 December 2014; accepted 16 February 2015; published online 25 February 2015)

An increasing amount of research has been conducted on developing new shape memory polymer nanocomposite structures. Estimating thermal properties of these types of structures is a crucial step towards their successful application. In this paper, a finite element based thermal model is proposed, of which the coefficients are identified using a nonlinear programming method in a nested loop. The model and identification results are validated in three material samples. © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4913804>]

Shape memory polymers (SMPs) are polymeric smart materials that can recover to their permanent shapes under various stimuli.^{1–5} Among these stimulation methods, electric actuation using resistive heat has recently received much attention.^{1,6} However, this method can introduce non-uniform thermal loading in manufactured SMP nanocomposite structures (SMPNSs) resulting in over-heating in certain areas.⁷ Meanwhile, the thermal properties of SMPNSs for new applications are often not provided or cannot be readily measured. To date, many different approaches have been used to quantify thermal properties. Laser reflectance thermometry is used to measure the thermal conductivity in thin films,⁸ thermal diffusivity in polymer matrix composites can be obtained through a laser flash apparatus,⁹ while differential scanning calorimetry can measure the glass transition temperature in SMPs.¹⁰ Micro-electrode structures can also be used to measure the thermal conductivity in thin films with precisely designed assistive micro-electron structures.¹¹ However, the above mentioned methods require expensive equipment and/or multiple testing devices to measure multiple thermal properties. Thus, a low cost approach to predict simultaneously multiple thermal properties is necessary for rapidly designing and customizing SMPNSs for applications.

This paper presents an indirect method of estimating thermal properties for electrically actuated SMPNSs. An approximate thermal model is derived based on a finite element approach, in which the element size is determined by the pixel size of a thermal imager. Both conduction and convection are considered. Nonlinear programming in a nested loop is used to identify the thermal coefficients and glass transition temperature.

Figure 1 shows the SMPNS schematic. It is composed of an SMP matrix with a thin layer of carbon nanopaper (CNP) and a layer of distributed carbon fibers (CFs) meant to improve electrical conductivity and mechanical strength, respectively. The carbon nanofibers (CNFs) in the CNP,

from Applied Sciences, measure 100 nm in diameter and 20–200 μm in length, and have a non-bulk density of 1.9 g/ml at 25 °C.

Table I lists the thermal conductivity, specific heat, volume and mass percentages of SMP resin, CNF paper, and carbon fiber for three samples. The sizes of the samples (length, width, and thickness) are (77.8, 32.0, and 2.30) mm (78.4, 31.8, and 2.30) mm, and (80.6, 36.4, and 2.22) mm, respectively.

A finite element model is used to describe the heat transfer between the point of interest and its surroundings. In Fig. 2, we limit our region of interest to a single element P_0 surrounded by four adjacent elements P_i , $i = 1, 2, \dots, 4$. The element size can range between one or several pixels in thermal images. Conduction occurs between the element of interest and the four adjacent elements. Convection occurs between the upper and lower surfaces of the SMPNS and the ambient atmosphere. Energy is supplied to the SMPNS through electrical resistive heat. Radiation from the SMPNS to the surroundings is relatively small and omitted here.

Conduction between element P_0 and the adjacent elements is given by Fourier's Law¹⁶ as

$$\dot{Q}_1 = C_1(A_C/\Delta L) \sum_{i=1}^4 [T(t) - T_i(t)], \quad (1)$$

where C_1 , A_C , ΔL , T , and T_i , $i = 1, \dots, 4$ are the thermal conductivity coefficient, cross section area, length of element P_0 , temperature of element P_0 , and temperatures of adjacent

FIG. 1. The structure of SMPNS.

^{a)}Author to whom correspondence should be addressed. Electronic mail: yunjun.xu@ucf.edu

TABLE I. Properties of composites in samples.^{2,12–15}

	SMP resin	CNF paper	CF
Conductivity (W/m·K)	0.12	2000	15
Specific heat (J/g·K)	2.5–3.3	0.93	0.8
Sample 1 vol. %	69.37%	2.80%	27.83%
(mass %)	(48.39)	(5.22)	(46.39)
Sample 2 vol. %	70.31%	1.87%	27.83%
(mass %)	(50.65)	(3.45)	(45.90)
Sample 3 vol. %	67.62%	3.54%	28.82%
(mass %)	(37.92)	(7.51)	(54.58)

elements, respectively. From Refs. 2 and 12, the thermal conductivity coefficient varies by less than 10% with respect to temperature. Thus, we assume C_1 to be constant in the approximate model.

The convection to surrounding atmosphere follows the model discussed in Ref. 16 as:

$$\begin{aligned}\dot{Q}_2 &= \dot{Q}_{2,top} + \dot{Q}_{2,bot} \\ &= \frac{C_2 A_s}{L^{1/4}} \left[0.54(T - T_\infty)^{5/4} + 0.27(T + \Delta T - T_\infty)^{5/4} \right],\end{aligned}\quad (2)$$

where A_s , L , T_∞ , ΔT , and C_2 are the surface area of element P_0 , sample characteristic length, ambient temperature, temperature difference between the top and bottom surfaces, and remaining unknown terms used to calculate the coefficients of convection h for both surfaces. The dimensionless numbers 0.54 and 0.27 are the constants associated with free convection for hot surfaces facing upward and downward.¹⁶ While C_2 depends on the ambient and thermal boundary layer temperatures and ΔT varies over time, the change in both parameters is not significant, and they are assumed constant for the approximate model.

The temperature change of P_0 is modeled as¹⁶

$$\dot{Q}_3 = C_3 m_E \dot{T}, \quad (3)$$

where C_3 is the specific heat and m_E is the mass of element P_0 . As shown in Refs. 2 and 12, the heat capacity of polymeric materials increases exponentially within $\pm 15^\circ\text{C}$ of the glass transition temperature, and is mostly constant outside this region. This behavior can be approximated by

$$C_3 = \begin{cases} C_{3,1} \exp[C_{3,2}(T - T_G)] + C_{3,4} & \text{if } T \leq T_G \\ C_{3,1} \{2 - \exp[C_{3,3}(T_G - T)]\} + C_{3,4} & \text{if } T > T_G. \end{cases} \quad (4)$$

FIG. 2. One test sample with element formulation.

The constants $C_{3,i}$, $i = 1, 2, 3, 4$ are to be identified. Equation (4) can generate specific heat profiles that approximately match the trend of those shown in Refs. 2 and 12 for temperatures up to 100°C . Assuming the heat generation over the SMPNS surface is uniform, the energy input to element P_0 is given by Ohm's Law¹⁷ as

$$\dot{Q}_G = (A_s/A)UI, \quad (5)$$

where A_s , A , U , and I are the surface area of element P_0 , top surface area of SMPNS, voltage, and current, respectively. Thermographic observations taken during experiments show that the heat generation is non-uniform and dependent on sample geometry. The temperature mismatch due to the assumption of uniform power generation can be compensated by the coefficients identified.

According to the law of conservation of energy

$$\dot{Q}_G = \dot{Q}_1 + \dot{Q}_2 + \dot{Q}_3, \quad (6)$$

in which the unknown coefficients $\mathbf{x}$, including C_1 , C_2 , $C_{3,i}$, $i = 1, 2, 3, 4$, ΔT , and T_G , are identified through two nonlinear constrained optimizations in a nested loop.

The inner loop optimization searches for a solution that can minimize the error between the predicted and measured temperature profiles for all the experiments. Nonlinear programming solvers can compute many local minima; therefore, an outer loop optimization is applied to control the bounds limiting the unknown coefficients. In this approach, the identified coefficients can be consistent among different experiments.

The inner loop finds the optimal $\mathbf{x}^j$ to match experiment j , $j = 1, \dots, N$, where N is the number of experiments being analyzed. The inner loop performance index for experiment j , J_{in}^j , is

$$J_{in}^j = \left(\sum_{k=1}^{N^j} |T_k^j - \hat{T}_k^j| \right) / N^j, \quad (7)$$

where N^j , T_k^j , and $\hat{T}_k^j$ are the number of time nodes, measured temperature at time node k , and the propagated temperature with identified $\mathbf{x}^j$.

$\mathbf{x}^j$ in the inner loop optimization is constrained by $\mathbf{x}_{LB} \leq \mathbf{x}^j \leq \mathbf{x}_{UB}$, and those bounds are optimized in the outer loop with the following performance index:

$$J_{out} = \sum_{l=1}^8 (\sigma_l / x_{\max,l}) + \sum_{j=1}^N P_j, \quad (8)$$

where σ_l and $x_{\max,l}$ are the standard deviation and maximum value of identified coefficient $\mathbf{x}_l$ across all N experiments. P_j is the penalty: $P_j = 1000J_{in}^j$ if J_{in}^j is above a user-defined threshold; otherwise, $P_j = 0$.

The bounds on $\mathbf{x}_{LB}$ and $\mathbf{x}_{UB}$ must satisfy $D \leq \mathbf{x}_{UB} - \mathbf{x}_{LB} \leq E$, $\mathbf{x}_{UB} \leq \bar{\mathbf{x}}_{UB}$, and $\mathbf{x}_{LB} \geq \underline{\mathbf{x}}_{LB}$, in which D and E are the minimum and maximum separations between $\mathbf{x}_{LB}$ and $\mathbf{x}_{UB}$, while $\bar{\mathbf{x}}_{UB}$ and $\underline{\mathbf{x}}_{LB}$ are the upper and lower bounds placed on $\mathbf{x}_{LB}$ and $\mathbf{x}_{UB}$. These bounds are found from the known characteristics of SMPNS constituents, as shown in Table I. $\underline{\mathbf{x}}_{LB}$ and $\bar{\mathbf{x}}_{UB}$ for C_1 are chosen based on the Lewis and Nielson model.¹⁸ $\underline{\mathbf{x}}_{LB}$ and $\bar{\mathbf{x}}_{UB}$ for C_2 depend on the remaining coefficients from the free convection model

FIG. 3. Conduction coefficient C_1 : (1) sample 1, (2) sample 2, and (3) sample 3.

discussed in Ref. 16, which depend on the ambient temperature and the thermal boundary layer temperature. $\bar{x}_{LB}$ and $\bar{x}_{UB}$ for $C_{3,1}$ and $C_{3,4}$ are determined by assuming that the specific heat is proportional to the volume percentage of each composite material, and then adding a margin to each estimated value. $\bar{x}_{LB}$ and $\bar{x}_{UB}$ for $C_{3,2}$ and $C_{3,3}$ are chosen to match the specific heat profile, as shown in Refs. 2 and 12. $\bar{x}_{LB}$ and $\bar{x}_{UB}$ for ΔT are arbitrarily chosen to be -10°C and 0°C . T_G is known to be approximately 60°C , so margins of $\pm 1^\circ\text{C}$ are used.

The temperature and current are measured in real-time using a thermal imager and a current sensor. The MATLAB function `fmincon` is used as the optimization solver. It finds proper thermal coefficients to match the identified temperature profiles with the measured ones. Three samples were tested under voltage inputs from 16 V to 22 V with increments of 1 V. Under each voltage, five tests were carried out. Some obvious outliers are omitted.

In Figs. 3–5, the squares show the average of identified coefficients for C_1 , C_2 , and ΔT , and the error bars show the variation in these coefficients, which are shown to be small. Fig. 3 shows that the C_1 values are roughly $2.68 \text{ W}/(\text{m} \cdot \text{K})$, $0.95 \text{ W}/(\text{m} \cdot \text{K})$, and $2.0 \text{ W}/(\text{m} \cdot \text{K})$ for samples 1, 2, and 3, respectively. While we expect sample 3 to have a higher conduction compared to sample 1, given the increased CNF mass percentage, this discrepancy can be explained by the non-uniformity experienced in the carbon nanofibers. A sample with more nanofibers can be less conductive than a sample

FIG. 4. Convection coefficient C_2 : (1) sample 1, (2) sample 2, and (3) sample 3.

FIG. 5. Temperature difference between both surfaces ΔT : (1) sample 1, (2) sample 2, and (3) sample 3.

with longer and more aligned nanofibers. Fig. 4 shows that the C_2 values are approximately $3.0 \text{ W}/(\text{m}^{11/4} \cdot \text{K}^{5/4})$, $3.1 \text{ W}/(\text{m}^{11/4} \cdot \text{K}^{5/4})$, and $3.0 \text{ W}/(\text{m}^{11/4} \cdot \text{K}^{5/4})$ for samples 1, 2, and 3, respectively. All experiments were performed under the same ambient conditions, so this similarity is expected. Fig. 5 shows that the ΔT values for three samples are approximately -3.0°C , -2.9°C , and -3.7°C for samples 1, 2, and 3, respectively. This is expected, as the temperature difference is due to conduction through the SMP resin, and these samples have similar SMP contents. Fig. 6 shows the identified C_3 for the samples over temperature. It can be seen that the specific heats of samples 1 and 2 are very close, which are expected from the similar SMP resin and CF volume percentages. It can also be seen that the specific heats undergo the most change in the region of $\pm 15^\circ\text{C}$ of the T_G , which agrees with previously reported results.^{2,12} The decrease in specific heat of sample 3 can also be explained by the lower SMP mass percentage in sample 3 compared to samples 1 and 2. The measured temperature profiles and the predicted profiles using the identified thermal properties match well for all the experiments. In Fig. 7 (19V experiments for all three samples), example identification results show that the propagated temperature profiles match with the experimental data.

Instead of measuring the thermal properties separately with different and expensive instruments, this paper presents an indirect method of estimating thermal properties for electrically actuated SMPNSs using the data measured via low cost, off-the-shelf devices (e.g., current sensor and thermal

FIG. 6. Specific heat C_3 vs. temperature: (1) sample 1, (2) sample 2, and (3) sample 3.

FIG. 7. Predicted (“line”) and measured (“dotted”) temperature profiles in a 19V case: (1) sample 1, (2) sample 2, and (3) sample 3.

imager). In the thermal model, convection and conduction are considered. Based on this model, a two-layer optimization is formulated and solved for the parameters. Three samples are tested. The temperature profiles predicted using those identified thermal coefficients match well with the measured ones. It is expected that the proposed method can significantly accelerate the design and application of SMPNSs.

Thanks are given to the HB Polymer, Inc., and the Florida High-Tech Corridor Program for financial support.

The authors would also like to thank John Sparkman for making several samples.

- ¹J. Gou, F. Liang, Y. Xu, and B. Mabbott, *Appl. Mech. Mater.* **423**, 97 (2013).
- ²B. Weidenfeller and M. Anhalt, *J. Thermoplast. Compos. Mater.* **27**, 895 (2014).
- ³A. Lendlein, H. Jiang, O. Junger, and R. Langer, *Nature* **434**, 879 (2005).
- ⁴K. Yu, Y. Liu, and J. Leng, *RSC Adv.* **4**, 2961 (2014).
- ⁵C. Zhang, H. Wei, Y. Liu, H. Tan, and Z. Guo, *High Perform. Polym.* **24**, 702 (2012).
- ⁶H. Shen, Y. Xu, F. Liang, J. Gou, and B. Mabbott, *Appl. Phys. Lett.* **103**, 201903 (2013).
- ⁷H. Lu, F. Lang, J. Gou, J. Leng, and S. Du, *Smart Mater. Struct.* **23**, 085034 (2014).
- ⁸K. Goodson, O. Käding, M. Rösler, and R. Zachai, *J. Appl. Phys.* **77**, 1385 (1995).
- ⁹B. Weidenfeller, M. Anhalt, and S. Kirchberg, *J. Appl. Phys.* **112**, 093513 (2012).
- ¹⁰J. Champagne, Ph.D. dissertation, Louisiana State University, 2013.
- ¹¹D. Chu, M. Touzelbaev, K. Goodson, S. Babin, and R. Pease, *J. Vac. Sci. Technol., B* **19**(6), 2874 (2001).
- ¹²M. Razzaq and L. Frommann, *Polym. Compos.* **28**, 287 (2007).
- ¹³J. Ullbrand, J. Cordoba, J. Tamayo-Ariztondo, M. Elizalde, M. Nygren, J. Molina-Aldareguia, and M. Oden, *Compos. Sci. Technol.* **70**, 2263 (2010).
- ¹⁴H. Lu, Y. Liu, J. Gou, J. Leng, and S. Du, *Int. J. Smart Nano Mater.* **1**, 2 (2010).
- ¹⁵V. Cecen, I. Tavman, M. Kok, and Y. Aydogdu, *Polym. Compos.* **30**, 1299 (2009).
- ¹⁶A. Bejan, *Heat Transfer* (Wiley, New York, 1993).
- ¹⁷J. Irwin, *A Brief Introduction to Circuit Analysis* (Wiley, New York, 2003).
- ¹⁸R. Pal, *Composites Part A* **39**, 718 (2008).