Design and optimization of carbon nanotube/polymer actuator by using finite element analysis*

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In recent years, actuators based on carbon nanotube (CNT) or graphene demonstrate great potential applications in the fields of artificial muscles, smart switches, robotics, and so on. The electrothermal and photothermal bending actuators based on CNT/graphene and polymer composites show large bending actuations, which are superior to traditional thermal-driven actuators. However, the influence of material parameters (thickness, temperature change, etc.) on the actuation performance needs to be further studied, because it is a critical point to the design and fabrication of high-performance actuators. In this work, finite element analysis (FEA) is employed to simulate the actuation performance of CNT/polymer actuator, which has a bilayer structure. The main focus of this work is to design and to optimize material parameters by using computational method. FEA simulation results show that each layer thickness of actuator has an important influence on the actuation deformation. A maximum curvature of 2.7 cm^{-1} is obtained by simulation, which is much larger than most of the actuator curvature reported in previous experiments. What is more, larger temperature change and larger difference of coefficient of thermal expansion (CTE) between two layers will result in larger bending actuation. This study is expected to provide valuable theoretical reference for the design and realization of CNT-based thermal actuator with ultra-large actuation performance.

Keywords: actuator, carbon nanotubes, nanocomposites, finite element analysis

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1. Introduction

Smart actuating materials are able to convert different types of energy into mechanical energy.[1–3] Among different types of actuators, thermal-driven actuators have been widely studied and used in microelectromechanical systems (MEMS). However, traditional thermal-driven actuators are based on metal (or semiconductor) and their oxides.[4,5] The relative small coefficient of thermal expansion (CTE) results in small actuation performances. What is more, the rigid characteristic of traditional thermal-driven actuators is not suitable for using as artificial muscles. Recently, researchers have studied new types of flexible thermal-driven actuators based on carbon nanotube (CNT)/graphene and polymer composites, including electrothermal and photothermal actuators.[6–14] Most of them are bending actuators, which employ two layers of materials having different CTEs and forming a bilayer structure. When the actuator is heated, the internal stress of two layers caused by great CTE mismatch makes the actuator bend to the side which has a smaller CTE. The electrothermal actuators can be driven by low driving voltages and perform large bending actuations,[6–12] while the photothermal actuators are remotely controllable and wavelength-selective.[13,14]

Among these studies, only a few have mentioned the influence of film thickness on the actuation performance. Zhang *et al.* proposed a photothermal actuator based on single-walled CNT and polycarbonate and found that the maximum deflection of actuator increases with CNT film thickness.[13] Hu *et al.* developed a graphene/polydimethylsiloxane (PDMS) actuator.[8] They found that in order to get a high actuation performance, the thickness of PDMS layer should be neither too thin nor too thick. Later on, Hu *et al.* demonstrated a photothermal actuator, which was fabricated by reduced graphene oxide (RGO)-CNT/PDMS composite.[14] The curvature of the actuator was also related to the thickness of RGO-CNT layer and PDMS layer. However, the influence of material thickness on the actuation performance was not fully studied as only thickness of one layer was altered with a few data points, while the thickness of the other layer was fixed. Besides experiment studies, there were merely several research studies using finite element analysis (FEA) to explain experimental results.[9,15] The influence of other parameters (Young's modulus, temperature change, CTE difference, etc.) on final actuator deformation should be further studied in detail.

In this work, we study the actuation performance of a

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thermal-driven actuator based on CNT and PDMS by modeling and simulation. The main focus of this study is to investigate the influence of different parameters on actuation performance. This study will help to understand the mechanism of film deformation and quantify the influence of each parameter on actuation performance, which exceeds the experimental limitations.

2. Modeling and calculation

FEA is a powerful tool to understand the characters of macroscopic structural materials, thus it has been widely introduced into analyzing thin film deformation and stress.[16,17] Compared with analytical modeling that cannot deal with nonuniform microstructure, FEA could achieve the numerical results for complicated systems and thus provide insight into their microscopic or submicroscopic mechanism.

The core of FEA is to obtain the nodal displacement of the system by solving a group of linear and nonlinear equations and the system behavior could be accurately simulated:

$$F = kq. \tag{1}$$

Here F denotes external force, k denotes nodal displacement and q is the stiffness matrix which represents the material properties and geometry of the system.

In this work, the actuator based on CNT and PDMS composite is simulated by using commercial FEA software ANSYS. The bilayer structure of actuator is shown in Fig. 1(a). The upper layer is a CNT-PDMS composite layer, in which the CNTs are super-aligned nanotubes and have an orientation along x axis. The lower layer is pure PDMS layer.[6] Because the system has an xy-mirror symmetry and a yz-mirror symmetry, the part in the cuboid marked with red-dotted lines is chosen as the model for simulation to minimize the computer time. The dimensions of the simulated model are 15 mm × 3 mm (length × width). The related material parameters used in simulation are summarized in Table 1.

Table 1. Material parameters used for simulation. CTE is coefficient of thermal expansion in unit of K^{-1}, E is Young's modulus, C_{10} and C_{01} are constants, D is incompressibility parameter in Mooney–Rivilin model.

Material	CTE/ppm·K^{-1}	E/MPa	C_{10}/MPa	C_{01}/MPa	D/MPa^{-1}
CNT-PDMS composite	6	1031	1.0	0.9	0.0001
Pure PDMS	300	0.85	0.5	0.0	0.0001

From Table 1, we can see that the introduction of CNT significantly reduces the CTE of CNT-PDMS composite (∼ 6 ppm·K^{-1}), compared to pure PDMS (300 ppm·K^{-1}).[6] Due to excellent mechanical characteristic of super-aligned CNTs, the Young's modulus of CNT-PDMS composite (1031 MPa) is much larger than that of pure PDMS (0.85 MPa).[18] In Mooney–Rivilin model, C_{10} and C_{01} are constants.[19] D is the incompressibility parameter and is set to be 0.0001.

When the actuator is heated, the expansion of PDMS layer will be larger than that of CNT-PDMS layer with same temperature increase, since the CTE of PDMS is much larger than that of CNT-PDMS composite. The interface between two layers is constrained. Thus the whole actuator will generate large internal stress and bend towards the side of CNT-PDMS layer. The illustration of the bending actuation mechanism is shown in Fig. 1(b). When the heating is stopped, the temperature of the actuator decreases and the actuator returns to its initial flat state.

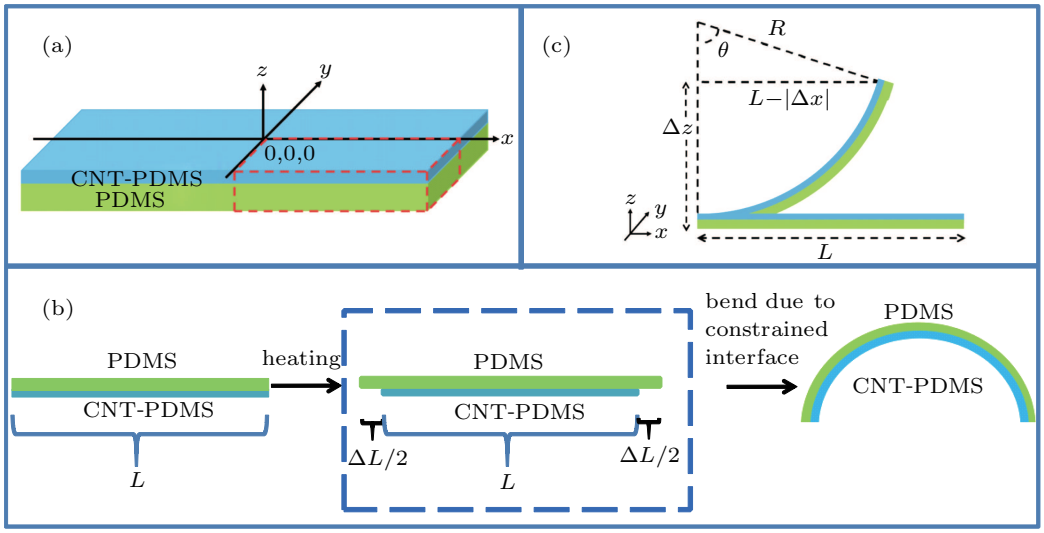


Fig. 1. (color online) (a) Bilayer structure of CNT-PDMS/PDMS actuator without deformation. The line on the y axis is constrained, which is on the bottom surface. The part in the cuboid marked with red-dotted lines is the model used in the FEA simulation. (b) Illustration of the actuator bending mechanism. (c) Illustration of model at initial state and at bending state. L is defined as the length input for model. Δx and Δz are the free-end displacements of model from initial flat state to final bending state along x and z directions, respectively. θ is the bending angle of the model. R is the radius of the bending arc.

To investigate the bending actuation of the actuator, bending curvature is employed to quantify the actuation performance. An illustration of the model at initial flat state and at bending state is shown in Fig. 1(c). At the initial state, the model is flat and its length is represented as L, which is half length of the CNT-PDMS/PDMS actuator. At the bending state, the free-end displacement of the model along x and z directions are denoted as Δx and Δz respectively. Thus the bending angle θ of the model shown in Fig. 1(c) could be calculated by using Eq. (2).

$$\theta = 2 \times \tan^{-1}\left(\frac{\Delta z}{L - |\Delta x|}\right). \tag{2}$$

Thus, the curvature of the actuator (the same as the curvature of model) could be given by:

$$1/R = \theta/L, \tag{3}$$

where R is the radius of the bending arc.

3. Results and discussion

In this work, the key factors which have influence on the actuation performance of the actuator are studied in detail, including thickness of each layer, temperature change, and CTE difference between two layers, and so on. This could help to understand the actuation mechanism and to optimize CNT-PDMS/PDMS actuator design with large bending.

First, in order to be compared with experiment result, we input structural data of CNT-PDMS/PDMS actuator used in previous experiment into the model: length = 15 mm, width = 3 mm, initial temperature $T_0 = 26$ °C, final temperature $T = 98$ °C. The CTEs and Young's moduli of two material layers are listed in Table 1. The simulation result shows that the curvature of actuator is 0.14 cm^{-1}, which is comparable with the curvature observed in a previous experiment (0.22 cm^{-1}).[6]

Then, the thickness dependence of actuation performance is studied. The thickness of CNT-PDMS layer and PDMS layer are set as variables. Then basic parameters are also input into the model as length = 15 mm, width = 3 mm, initial temperature $T_0 = 22$ °C, and final temperature $T = 199$ °C. The maximum temperature is set to be 199 °C, because differential scanning calorimetry (DSC) analysis showed that the thermal decomposition temperature of PDMS was measured to be as high as larger than 200 °C.[20] The CTEs and Young's moduli of two material layers are listed in the Table 1.

Figures 2(a) and 2(b) are three-dimensional (3D) pictures, showing the bending curvature of actuator with thickness variation. Figure 2(a) is the front view of 3D picture, while Fig. 2(b) is the back view. The curvature of the actuator is intensively influenced by both thicknesses of CNT-PDMS layer and PDMS layer. When the PDMS layer is very thin, the bending curvature of the actuator sharply increases with the thickness increase of PDMS layer, until it reaches a peak value. Afterwards, the curvature relatively slowly decreases with the increases of PDMS thickness. Such curvature change tendency could be explained as follows. Assuming the PDMS layer is very thin, it does not have the strength to bend the CNT-PDMS layer. If the PDMS layer is extremely thin, which is approaching zero, then the whole actuator is similar to a monolayer structure of CNT-PDMS. There will be no actuation deformation after heating. Conversely, assuming the PDMS layer is extremely thick, which is approaching infinite,

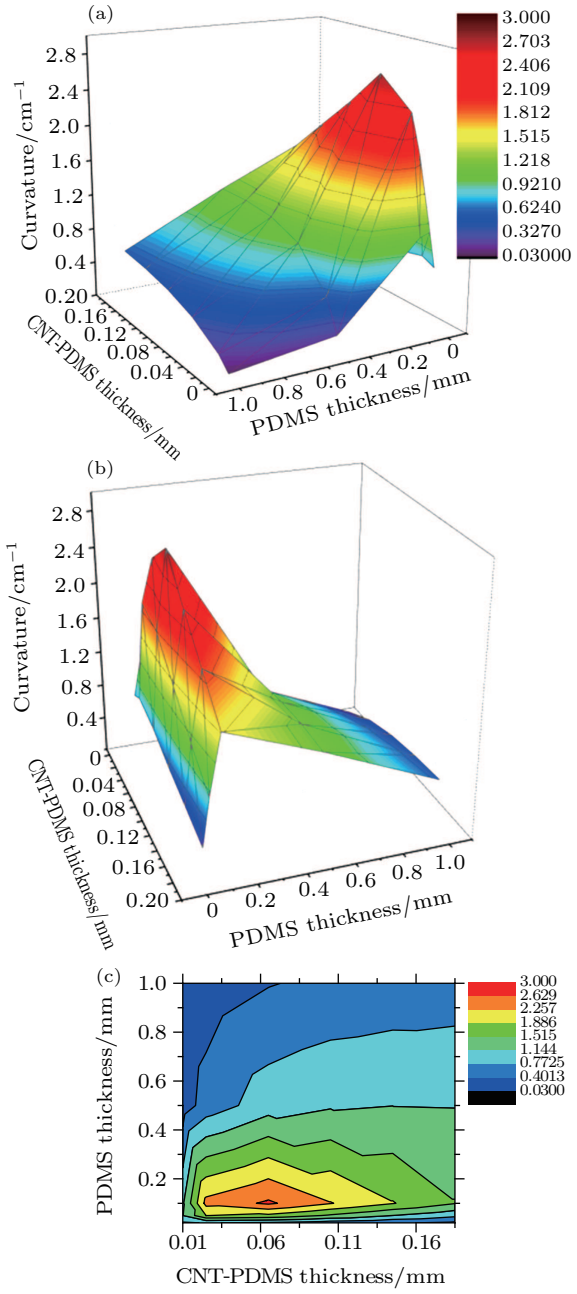


Fig. 2. (color online) 3D pictures showing thickness dependence of actuator curvature: (a) front view, (b) back view, (c) curvature contour map.

the actuator deformation will also tend to be zero. The reason is that although the actuator is still constructed by two layers of materials with different CTEs, the internal stress is not large enough to bend such a thick actuator. The above tendency of PDMS thickness dependence of bending curvature is also in accordance with experiment results of PDMS-based bilayer actuator.[8]

The tendency of CNT-PDMS thickness dependence of bending curvature is also demonstrated in Figs. 2(a) and 2(b) clearly, which has not been reported by previous related experiments. When the CNT-PDMS layer is thin, the bending curvature of the actuator increases significantly with the thickness increase of CNT-PDMS layer until it reaches a peak value. Afterwards, the bending curvature of actuator decreases gradually with the thickness increase of CNT-PDMS layer. The above results show that besides the thickness of PDMS layer, the thickness of CNT-PDMS layer also has a significant influence on the actuation performance of the actuator.

To get a holistic picture, a curvature contour map corresponding to Figs. 2(a) and 2(b) is shown in Fig. 2(c). It clearly indicates that there exists a relatively large curvature area for the actuator. Both the CNT-PDMS thickness and PDMS thickness should be optimized, in order to get a large deformation. When the CNT-PDMS thickness is around 0.06 mm and the PDMS thickness is around 0.10 mm, the calculated maximum curvature of 2.7 cm^{-1} could be achieved, which is much larger than most actuator curvatures reported by experiments.[6,8,10,11] Thus our theoretical results could shed light on the design and fabrication of actuators with ultra-large deformation for experiments.

The visual bending deformation of model simulated by ANSYS is shown in Figs. 3(a) and 3(b). According to the color scale, we could get the displacement of each model along z or x axis. The free-end of the model moves 8.12 mm along z direction (marked as Δz), while it moves 18.02 mm along negative direction of x axis (marked as Δx). By inputting these data into Eqs. (2) and (3), the related deformation curvature could be easily calculated. This also reveals that the bending actuation can be controlled precisely by tuning the thickness of PDMS layer or CNT-PDMS layer.

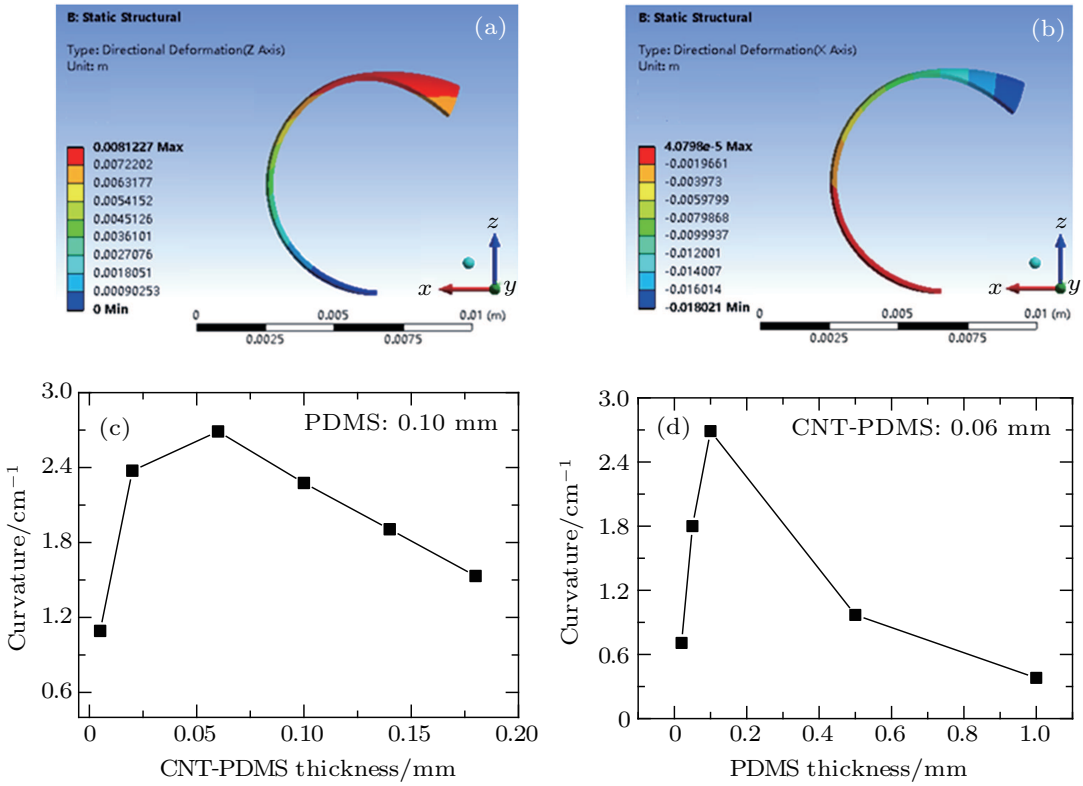


Fig. 3. (color online) Bending deformation of CNT-PDMS/PDMS model: (a) deformation analysis along z direction. (b) deformation analysis along x direction. (c) CNT-PDMS thickness dependence of curvature when the PDMS thickness is fixed as 0.10 mm. (d) PDMS thickness dependence of curvature when the CNT-PDMS thickness is fixed as 0.06 mm.

The thickness dependence of curvature around the peak value is further studied, as shown in Figs. 3(c) and 3(d). In Fig. 3(c), the thickness of the PDMS layer is fixed as 0.10 mm. The deformation curvature does not increase monotonously with the thickness increase of CNT-PDMS layer. It increases rapidly with the thickness increase of CNT-PDMS, when thickness of CNT-PDMS layer is less than 0.06 mm. Then it reaches a maximum curvature of 2.7 cm^{-1}, when the thickness of CNT-PDMS layer is around 0.06 mm. Afterwards the curvature decreases slowly with further increase of the CNT-

PDMS thickness. The curvature decreased from 2.7 cm^{-1} to 1.5 cm^{-1}, when the thickness of CNT-PDMS layer is increased from 0.06 mm to 0.16 mm.

The deformation curvature of the actuator shows a similar tendency, when the thickness of PDMS layer is changed and that of CNT-PDMS layer is fixed as 0.06 mm. The maximum curvature is achieved when PDMS thickness is 0.10 mm, as shown in Fig. 3(d). According to our simulation results, the optimized actuator with excellent actuation performance can be designed by tuning thickness of each layer in bilayer actuator structure.

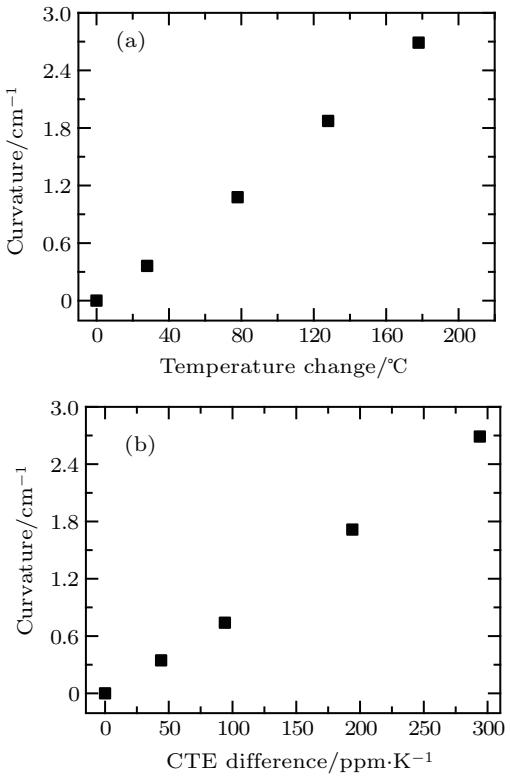


Fig. 4. (a) Temperature change dependence of deformation curvature. (b) The CTE difference dependence of deformation curvature.

Based on the above results, we further explored temperature change dependence of the deformation curvature of CNT-PDMS/PDMS actuator, as shown in Fig. 4(a). In this calculation, parameters below are used for simulation: CNT-PDMS thickness = 0.06 mm, PDMS thickness = 0.1 mm, length = 15 mm, width = 3 mm. The CTE and Young's moduli for two layers of materials are listed in Table 1. From Fig. 4(a), we can see that larger temperature change results in larger deformation curvature. The curvature is nearly proportional to the temperature change. The result also shows that the actuator bending is attributed to the thermal effect.

Furthermore, considering the thermal expansion property of materials, CTE is of great importance to future actuator design and material selection. Therefore, we studied the relationship between CTE difference of two layers and deformation curvature. The result is illustrated in Fig. 4(b). Here, the CTE of CNT-PDMS layer is fixed as 6 ppm·K^{-1}, while the CTE of the other layer is changed. The CTE change of the other layer can be realized by not using pure PDMS, but using other composite material. Other parameters are chosen as CNT-PDMS thickness = 0.06 mm, the other layer thickness = 0.1 mm, length = 15 mm, width = 3 mm, $T_0 = 22$ °C, and $T = 199$ °C. Young's modulus of the CNT-PDMS composite is listed in Table 1. Although the Young's modulus of the other layer may be altered a little by not using pure PDMS, the value of 0.85 MPa is still used as an approximation for calculation simplification.

The simulation results show that when the CTE difference of two layers is approaching zero, there will be no actuation performance and the deformation curvature is zero as well. Larger CTE difference will lead to a larger deformation curvature. This result inspires us to find materials with different CTEs. By combining material having very small positive CTE (or even negative CTE) with material having large positive CTE, a large CTE difference can be achieved and larger actuation performances can be expected.

4. Conclusions

In summary, the actuation performance of a bending actuator based on super-aligned CNT and PDMS composite is successfully simulated by using FEA. The simulation results show that each layer thickness of the bilayer actuator has an important influence on the actuation deformation. The thickness of CNT-PDMS layer and pure PDMS layer should be neither too large, nor too small. A maximum curvature of 2.7 cm^{-1} is obtained by simulation, which is larger than most actuator curvature reported in previous experiments. Moreover, larger temperature change and larger CTE difference between two layers will result in larger bending actuation. This study is assumed to offer valuable information for the design of CNT-based thermal actuator. By using optimized parameters obtained from this study, an actuator with ultra-large actuation is expected to be realized in further experiment.

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