The Fabrication of a New Actuator Based on the Flexoelectric Effect

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Abstract: This paper presents a novel methodology towards the design, analysis, and the fabrication process involved in developing a cost effective method to create a piezoelectric actuator by means of the flexoelectric effect. This effect is used to align nano-particles within a closed medium such as a vacuum during semiconductor fabrication. The above analysis will in turn be utilized to gain a better understanding of the working principles behind various geometric shapes prior to the fabrication of the actuator. By using various shapes for the actuating electrode, we may gain a better understanding of the field strength capability, and thus increased control over the actuator itself.

Keywords: Flexoelectric effect, NEMS actuator

1. Introduction

The development and fabrication of eco-friendly piezoelectric composites has attracted major interest in recent years. There are several methods to fabricate such composites. Our main effort and emphasis of research in this area is to derive the composites directly from the synthesis of lead-free piezoceramics, for example, (K,Na) NbO_3-$LiTaO_3$ and (K,Na)-NbO_3-$LiTaO_3$-$LiSbO_3$ systems developed by Saito et al.[4]. However, there is an alternative way to indirectly fabricate these composites by exploiting flexoelectric effects [5]. It has been observed in industry and research that the former direct method is complicated, expensive, and its synthesis process cannot be easily controlled. The further development of reliable non-lead piezoceramic with high performance based on these methods may be questionable. Therefore, it is worth considering the aforementioned indirect method.

For any crystal material, Newman‟s principle can be explained as follows: “The symmetry of any physical property of a crystal must include the symmetry elements of the point group of the crystal”. It is expected that this principle also applies with equal validity to texture materials whose point group symmetry properties are described by Curie groups. The idea of the aforementioned method is to fabricate a piezoelectric composite, in which one or several of its components are non-piezoelectric texture materials that posses a specific macroscopic geometric shape and render the generation of a ∞m oriented conical symmetric structure. As a result, the composite as an ensemble, would have piezoelectric responses as required by the Curie group symmetry, even when all components are Centro-symmetric materials.

The connectivity patterns, working mechanisms, and corresponding properties of the general kind of flexoelectric type piezoelectric composites differ from those of conventional piezoelectric or pyroelectric composites. The flexoelectric properties are largely dependent on the magnitude of the applied field gradients as well as the active degree of their flexoelectric performance which is enhanced when the size of its geometric shape is reduced. The introduced field gradient will steepen as the corresponding composite dimension decreases. Such an expectation has been confirmed by recent papers on the fabrication of millimeter scale and micrometer-scale flexoelectric piezoelectric composites [2,6].

However, fabricating an active flexoelectric phase of such a composite, with a specific geometric shape at micrometer scale is not a trivial matter [2]. Here, we propose a new method which is not directly related to the composite itself, but rather deals with an asymmetric configuration of electrodes deposited on the boundary surfaces of the composite. Our method could significantly simplify the fabrication of flexoelectric piezoelectric composites.

In this study, based on simulation results, a flexoelectric actuator will be fabricated by deposition of electrodes on the surface of the $BaSrTiO_3$ thin layer. Variation in the electric field gradient will also be utilized in order to create a new type of actuator designed to arrange the nanotubes using the flexoelectric effect.

Based on Ref. paper [6], the flexoelectric effect was investigated in $Ba_{0.67}Sr_{0.33}TiO_3$ (BST) ceramic at temperature about 25°C Curie point. $\mu_{11} = 115x10^{-6}$ C/m and $\varepsilon_r = 16000$. The proportional relationship between μ_{11} and ε_r is given by Figure 12 in Ref. 8 and confirms Tagantsev‟s theoretical prediction that electric susceptibility plays an important role in the enhanced direct flexoelectric effect.

This paper mainly deals with the converse flexoelectric effect under the non-homogeneous electric fields introduced by the specific boundary shape in a BST model with varying electrodes. The basic physical equations of the flexoelectric effect and the qualitative analysis of the flexoelectric actuator using COMSOL Multiphysics will be discussed in the following sections.

2. Flexoelectric polarization

2.1 Theory

The first phenomenological model to describe the coupling relationship between the induced electric polarization and an applied inhomogeneous strain is given by Kogan (1964), which states

$$P_i = \mu_{ijkl} \nabla_l S_{jk}$$

Where, P_i is the induced polarization, ∇_l represents the gradient, μ_{ijkl} represents the flexoelectric coefficient, and S_{jk} is the applied strain. Here Kogan suggested using gradient terms in order to represent the inhomogeneous components of the applied strain field within the linear range, which significantly simplifies the mathematical expressions of the effects. Similarly, the converse coupling relationship between the induced elastic stress and an applied electric field can be expressed as follows

$$X_{ij} = \mu_{ijkl} \frac{\partial E_k}{\partial x_l} + D$$

Where, X_{ij} is the induced stress; E_k is the applied electric field, x_l is the directional vector of the external electric field gradient, and D is the nonlinear higher order response term. If the material is in the elastic region, then the equation becomes

$$X_{ij} = C_{ijkl} S_{kl}$$

where, C_{ijkl} is the elastic constant, and S_{kl} is the induced strain. For an isotropic material, the above equation can be simplified for an axial gradient system in matrix notation

$$S_1^f = \frac{\mu_{11}}{C_{11}} \frac{\partial E_1}{\partial x_1}$$

where, S_1^f represents the elastic strain in direction 1 induced by flexoelectricity. Since we know that μ_{ijkl} is a fourth rank tensor, the Kogan model can be defined as the direct flexoelectric effect. This was later generalized to solid crystalline dielectrics by Tagantsev [7]. In his theoretical investigation he explains that piezoelectricity is different from the flexoelectric effect, and also derived a relationship between the flexoelectric coefficient μ_{ijkl}, which is proportional to the material dielectric susceptibility of a solid dielectric material. This relationship is given as

$$\mu_{ijkl} = X_{ij} \gamma_{kl} \left(\frac{e}{a} \right)$$

where X_{ij} is the susceptibility of the bulk dielectric material under mean field approximation, γ_{kl} is an inhomogeneous susceptibility coefficient tensor, „e‟ represents the electron charge, and „a‟ is the atomic dimension of the unit cell of dielectric.

Fousek et al. proposed a method to fabricate some unique 0-3 piezoelectric composites, in which none of their actual components are piezoelectric [5]. The physical basis of this method is Newman‟s principle in texture materials.

Fu and Cross proposed the existence of type-I and type-II flexoelectric effects in solid dielectrics [1].

3. Flexoelectric Actuator using COMSOL

3.1 Selection of Electrode Shape

The electrode size used in the simulation of the flexoelectric actuator plays an important role in deciding the direction and the control of the actuation. Initially, two non uniform electrode designs were considered for the simulation. First one with a square shaped top electrode and a second one with a circular shaped top electrode.

The simulation was carried out in COMSOL Multiphysics under Electromagnetic module. Electrostatics is chosen due to the dielectric nature of the material. DC current is only used for the initial excitation of the BST model and also for the initial simulation, hence making the above module suitable for our current work.

3.1.1 FEM MODEL

The geometry and boundary condition used in the initial BST FEM model is a three dimensional rectangular thin film with a base dimension of 100 µm in length, 100 µm in width, extruded by 50 µm in height. The upper surface of the electrode is coated with silver metal paste with a thickness of 1 µm and it is placed in the exact center of the BST. The lower surface is fully covered with silver electrode 1 µm in thickness, thus forming a non uniform electrode. In the electromagnetic module of COMSOL Multiphysics, the sub domain properties of the BST are defined with a relative permittivity of 16,000 at 25°C. This high permittivity at room temperature is suitable for the actuator applications. For this study, electrodes are chosen with relative permittivity of 10. The boundary of the top electrode is modeled with an electric potential of 100 V while the lower electrode is defined as a ground boundary condition. Additionally, the outer boundaries are selected with zero charge boundary conditions. The entire actuator model is placed in the vacuum chamber with a relative permittivity of 1.

This module solves the Laplace equation for potential to derive the electric field in a dielectric material. For the flexoelectric effect, there is a linear coupling relationship between applied inhomogeneous electric field and the induced strain deformation, i.e., its converse effect, in a solid dielectric material.

3.1.2 DISCUSSION

Both the square electrode and circular electrode are taken in such a way to form an equal area by modifying a_1 between the upper and lower electrode.

$$Area\ ratio = \frac{a_1}{b_1} = \frac{Area\ of\ upper\ electrode}{Area\ of\ lower\ electrode}$$

The BST model for nine area ratios are considered and analyzed for both the square and circular electrode in order to determine the effective gradient of the electric field for a given area ratio. Figure 1 shows the electrodes on the upper and lower surfaces for an area ratio of 0.4 and the results are displayed with arrows indicating the electric field gradient in the middle region. The electric field is within an average range of 10^6 V/m and the gradient of the electric field is in the range of 10^{11} V/m^2.

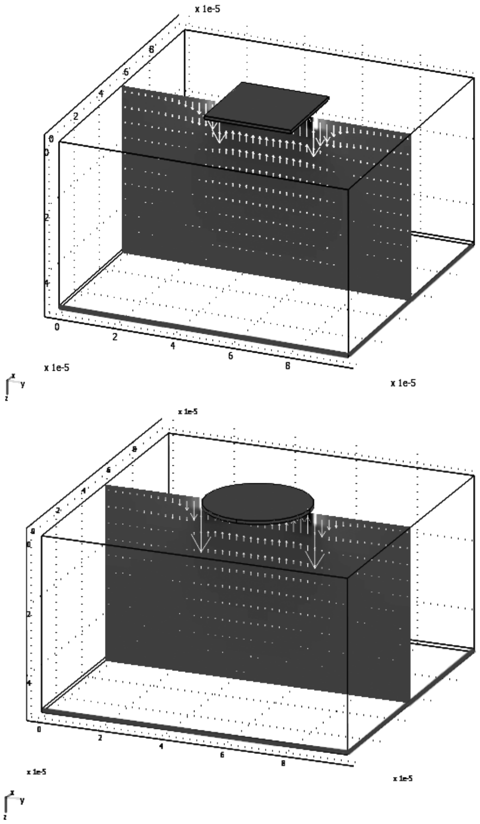

Figure 1. Two non-uniform electrodes across the upper and lower surfaces of the flexoelectric actuator showing slice plot and arrows indicating the electric field gradient (~10^{11} V/m^2) [generated using COMSOL]

Figure 2 shows the plot result, for the effective d_{33} ratio with increasing area ratios for both square and circular electrodes. Generally, the top electrode tends to move along with the BST top surface with the application of an electric field.

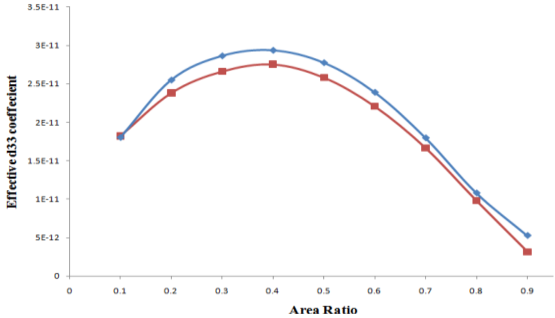

Figure 2. Effective strain displacement co-efficient for each area ratio of the square (blue) and circular (red) electrodes, which shows a maximum at 0.4 area ratio for the square electrode

The square electrode with an area ratio 0.4 shows the highest strain d_{33} value for the BST material when compared with the circular electrode on the top. Also it shows that as the area ratio increases, the d_{33} tends to almost unity.

4. AC Actuator in 2-D

A 2-D model of the flexoelectric actuator layer is modeled in COMSOL with two electrodes, A and B, on the top surface; the lower surface is fully coated with electrode and nanotubes are placed on the surface marked C.

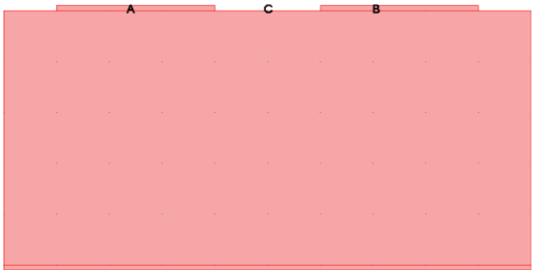

Figure 3. 2-D model describing electrodes A and B ; proposed position for nanotube alignment C

As shown in Figure 3, A and B are equally sized electrodes of an active flexoelectric layer. The model is simulated with a frequency of 1 kHz. If we apply AC voltages of low frequencies

$$V_A=V_0\cos(\omega_t+\Phi_A) \quad \text{and} \quad V_B=V_0\cos(\omega_t+\Phi_B)$$

where, V_A and V_B are the instantaneous voltages of electrodes A and B respectively. If we manage to choose appropriate values of the phase angles Φ_A and Φ_B, we can control the movement of the position of C via the converse flexoelectric effect. This is due to the fact that the electric field gradient at C can be controlled by manipulating the values of Φ_A and Φ_B. Such a device can be used to design a unique NEMS actuator. An analysis of actuator performance requires information of electric field gradient around an electrode. If the electric field gradient achieved by the BST film is greater than the single electrode, there is a possibility of clamp effect associated with the actuator. Therefore, accurate determination of gradient of the electric field or the polarization pattern of the dielectric is important for the evaluation of the flexoelectric actuator.

4.1 FEM Model

The electrode on the top surface of BST with an area ratio of 0.4 has been chosen because of its high effective strain gradient. As seen previously, the two silver coated square electrodes can be used for the application of varying electric fields and the lower electrode as ground.

In this 2D model, the BST flexoelectric layer is 100 µm in length and 50 µm in height. The entire bottom surface is covered with electrode, and the top surface with the electrode length of 30 µm forming symmetry, with electrodes set apart by a distance of 20 µm. This configuration allows for the placing of nanotubes (note that all the three electrodes are drawn to a height of 1 µm). The BST layer is placed in a vacuum chamber with a relative permittivity of 1. In this model, nanotubes were not taken into account, but the deformation due to electric field induced strain can be used to predict the movement of nanotubes on the top surface of the thin flexoelectric layer. The analysis is conducted in the 2-D COMSOL AC/DC Module. A time harmonic analysis was performed in order to obtain a particular frequency.

4.2 Boundary Conditions

The flexoelectric actuator top electrode acts as a source which is designated with a potential of V_A or positive charge. It is applied with a constant phase angle Φ_A of zero degrees. The adjacent electrode V_B has a varying phase angle Φ_B, which ranges from 15 to 360 degrees. The lower electrode covers the entire base and acts as a ground or negative charge. The remaining sides in and around the electrodes are designated as electric insulation boundary conditions. Note that no magnetic field effect has been taken into account. The subdomain and electrode settings remain the same as in the previous simulation.

4.2.1 Results and Discussion

The entire simulation is conducted under a frequency of 1 kHz which is used in calculating the natural frequency ω. After the application of electric field, based on the applied phase shift angle, the BST thin layer can actuate or come to a neutral position. The actuation of the electrode is determined by the polarization of the material. If the applied AC voltage forms a destructive interference pattern as in Figure 4 for angle shift in B as $\Phi_B = 180°$, then the electrode approaches an equilibrium position during actuation.

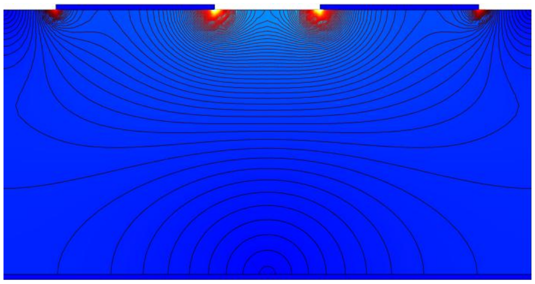

Figure 4. Electric field contour line for destructive interference for a phase shift angle [$\Phi_B = 180°$]

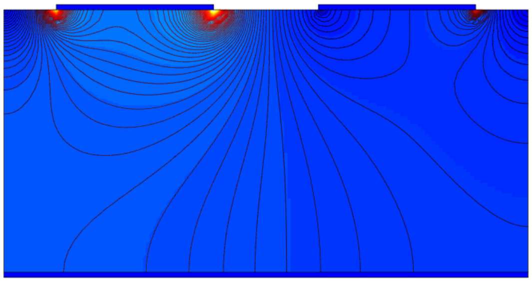

Figure 5. The electric field contour line for constructive interference with a phase shift angle [$\Phi_A = 45°$] and the surface (dark and light blue) indicated electric field gradient in Y

Similarly if the value of $\Phi_B = 45°$, the polarization occurs and lifts the zone below the A electrode while holding the zone below the B electrode with clamping effect for a brief period of time. In this manner, the nanotube can be aligned at an angle or perpendicular to the axis by controlling the phase angle alone which is evident from the graph below

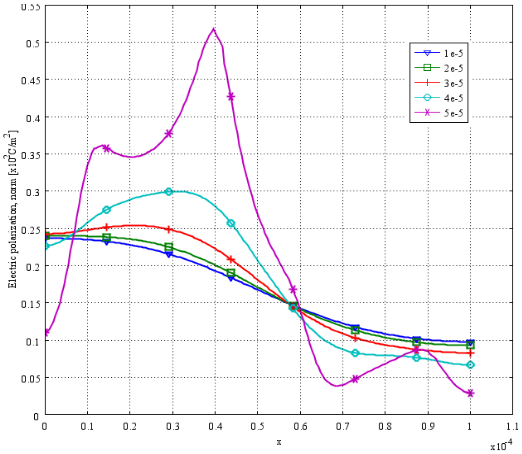

Figure 6. Electric polarization of the dielectric crystal with high polarization at one end for a phase shift of 45°

The gradient of the electric field in flexoelectric composites depends on the applied electric field and its frequency. Thus, by manipulating and choosing two component phases with mismatched electric dielectric properties, matched mechanical elastic properties are obtained. This deviates from the norm as explained in Ref. [1]. The electric field gradient will occur in the flexoelectric phase when a uniform electric field is applied. Note that no strain gradient will appear in the flexoelectric phase when a uniform elastic stress is applied. Therefore, this composite may only have the converse piezoelectric effect and its direct piezoelectric effect will be missing.

5. Conclusion

We propose a new method of fabrication for converse flexoelectric-piezoelectric composites, which is not directly related to the geometric shape of their active flexoelectric phases, but rather to the asymmetric configuration of the electrodes deposited on their boundary surfaces. We have shown that our method not only can significantly simplify the fabrication of flexoelectric piezoelectric composites but can also be used to design some unique, high sensitive piezoelectric actuators/sensors for application in NEMS.

6. References

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