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Numerical modeling of magnetoelectric effect in a novel composite structure

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Abstract

The magnetoelectric coupling effect in a bilayered magnetostrictive/piezoelectric composite structure consisting of a $Tb_{0.3}Dy_{0.7}Fe_{1.9}$ layer bonded with a $Pb(Zr_{0.52}Ti_{0.48})O_3$ layer is numerically simulated using the finite-element method. The numerical algorithm is based on a synchronization of the mechanical coupling and resonance between the two layers along the bonding interface. The magnetoelectric effect calculated as a function of the dimension of the two components, respectively, allows us to conclude that a significant enhancement of the magnetoelectric effect by optimizing the thickness of the two layers respectively is possible.

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Keywords: Magnetoelectric effect; Magnetostrictive; Piezoelectric; Bilayered composite

1. Introduction

Magnetoelectric (ME) effect is a two-field cross effect by which an electric voltage signal would be generated once a ME system is subjected to a magnetic field, or a magnetization is activated when an electric field is applied to this system [1–3]. This effect can be employed in quite a lot of potential applications [4,5]. There have been a number of oxide compounds which exhibit ME effect, but the effect they exhibit is commonly weak at room temperature, and the use of these materials for device applications has never been successful, to the authors' knowledge. The multi-phase magnetoelectric composites where the magnetostrictive and piezoelectric components are mixed together, in either granular form or multi-layered form, developed in last several years, have been found to exhibit much larger ME effect than ME compounds [6–14].

The generation of ME yield in these composites is based on the product effect which is available in neither of the two components: when a magnetic field is applied to the system, the magnetostrictive component (MSCP) is strained, which is transferred via the two-phase interface to the neighboring piezoelectric component (PECP). The electric field generated in PECP is ascribed to the piezoelectric effect. The ME effect is reversible and the reversal sequence is true too. Along this line, a number of two-phase composites were fabricated for achieving a big ME yield [6]. Multi-layered $CoFe_2O_4/Pb(Zr_{0.52}Ti_{0.48})O_3$ (PZT) composites were prepared and a ME yield coefficient $\alpha_E \sim 75$ mV/cm Oe was recorded [7], here the ME yield coefficient or ME coupling coefficient α_E is defined as the electric field output activated per Oe magnetic field. A ME yield coefficient as large as ~1.5 V/cm Oe was obtained for a multi-layered nickel-ferrite/PZT composite [8]. By replacing ferrites with giant magnetostrictive material $Tb_{0.3}Dy_{0.7}Fe_{1.9}$ (Terfenol-D), a giant ME yield coefficient $\alpha_E \sim 5.9$ V/cm Oe was measured in a sandwiched structure [9]. Therefore, one is allowed to argue that the layered ME composite may represent one of the most promising materials for the predicted applications.

Nevertheless, it is understood that both magnetostrictive and piezoelectric behaviors are anisotropic and thus the

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product effect must be anisotropic and strongly dependent of the alignment of the two layers. Therefore, the orientation relationship between the two components represents one of the dominant parameters affecting the ME effect. And more, the dimension of the two components has to be chosen carefully in order to generate the maximal ME yield since the efficiency of strain-transfer from MSCP to PECP or in reversal, driven under an alternative electric or magnetic source, is determined by the structure dimension. Our numerical modeling indicated that the ME effect can be improved significantly by optimizing the component dimension based on the mechanical coupling mechanism and resonance synchronization [10]. While an experimental optimization of the component dimension by searching for the resonance synchronization of the two components would be tedious and inefficient, a numerical technique should be adopted for such an optimization.

In this article, we would like to perform a numerical modeling on the ME effect of a bilayered ME composite consisting of a MSCP bonded with a PECP, focusing on the dimension optimization in terms of the maximal ME yield. The two components chosen for modeling are Terfenol-D and PZT, for they exhibit large magnetostriction and piezoelectricity, respectively. It is found that the simulated ME yield is significantly dependent on the thickness of the two components, although the length and width play an important role too.

2. Model and numerical procedure

The bilayered composite structure to be considered is schematically illustrated in Fig. 1, where the arrows show the directions of magnetization and electric poling in MSCP and PECP, respectively. It is argued that the voltage output of PECP can be large if the mechanical resonance of the two components keeps synchronizing. Therefore, the optimized state for the maximal ME yield is characterized by the identical resonance frequency between the two components, realized by adjusting their dimensions. The numerical modeling on the ME effect starts from the constitutive equations for the two components, respectively. In general, both MSCP and PECP should be treated as bi-anisotropic media [15,16]. However, the bi-anisotropic effect is quite small and can be neglected without losing the reliability and accuracy of simulation.

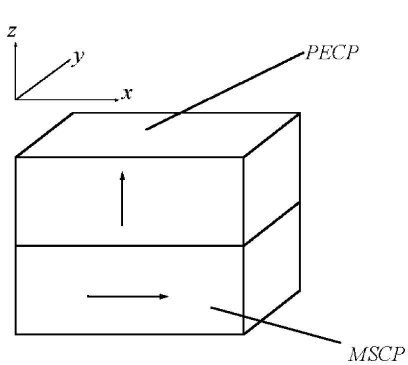

Fig. 1. A schematic drawing of the bilayered magnetoelectric composite structure.

The strain in MSCP is usually generated by a small ac-magnetic field signal imposed onto a big dc-magnetic field, because the magnetostriction is a nonlinear effect [11–13]. The constitutive coefficient can be derived from the secant modulus of the corresponding nonlinear stress (strain)–magnetic field relationship, i.e. a pseudo-linear piezomagnetic approximation. The constitutive equation for MSCP is written as [1]:

$$\sigma = C^H \varepsilon - \mathrm{d}H \tag{1}$$

$$B = d^T \varepsilon + \mu^\varepsilon H \tag{2}$$

where σ and ε denote the stress and strain of MSCP; B and H are the magnetic flux and magnetic field strength; C^H, d and μ^ε are the elastic stiffness constants at a fixed H, magnetoelastic coupling coefficient and magnetic permeability at constant strain, respectively. The constitutive equation for PECP is [1]:

$$\sigma = C^E \varepsilon - eE \tag{3}$$

$$D = e^T \varepsilon + \lambda^\varepsilon E \tag{4}$$

where σ and ε are the stress and strain in PECP; D and E denote the electric displacement and electric field; C^E, e and λ^ε are the elastic stiffness constants at a fixed E, piezoelectric coefficient and dielectric constants at constant strain, respectively.

The finite element analysis technique based on the ANSYS5.5/Multiphysics software package is employed to calculate the ME yield as a function of structure dimension. The dimension optimization is achieved by a harmonic analysis of the bilayered composite structure in terms of the maximal ME yield which implies a synchronization of the resonance frequency of the two components. In our calculation, a perfect bonding interface between MSCP and PECP is assumed [14]. The material parameters chosen for Terfenol-D and PZT were cited earlier [10]. The main procedure of the ANSYS5.5 calculation was described earlier [10] and here only a brief description is given.

(1) Meshing: the bonding of the two components is performed by the glue operation in the ANSYS algorithm. The dimension of components is given below. Through the pilot calculation, each component is divided into $10\,(L = \text{length}) \times 5\,(W = \text{width}) \times 3\,(T = \text{thickness})$, i.e. 150 elements.
(2) Boundary condition: referring to Figs. 1 and 2, six zero-strain points are set to restrict the rigid motion, i.e. three z-axis displacement restrictions are imposed at points A, B, and D, two x-axis displacement restrictions are set at points A and C, and one y-axis

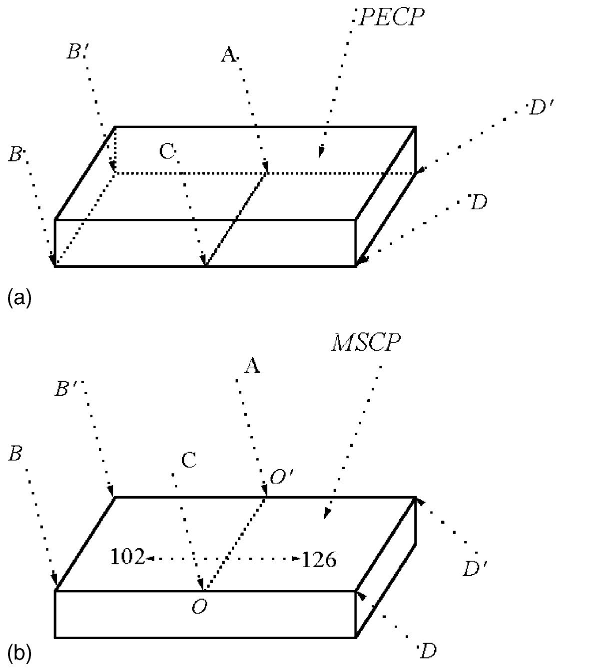

Fig. 2. A schematic illustration of MSCP and PECP components showing the boundary conditions and two symmetric points (102 and 126) with respect to central line O–O′.

displacement restriction is set at point C. The coordinates of these points are illustrated in Fig. 2, where points A and C are the two end points of the central line O–O′ on the top surface of MSCP. For MSCP, the magnetization and applied magnetic field are in the longitude direction and the left surface is then virtually grounded. The ac-signal is applied on the right surface of MSCP to simulate the ac-magnetic field. For PECP, the poling is along the transverse direction, so that the voltage degrees of freedom at the bottom surface are virtually grounded, and the top surface is an equi-potential surface.

(3) Covered range of frequency: 1–150 kHz.
(4) Effect of magnetic bias: a dc-magnetic bias benefits to the ME yield due to the nonlinear stress–magnetic field relation [11,17]. The bias will induce a variation of the magnetoelastic coupling coefficient and the stress in MSCP due to the magnetostrictive effect, then the PECP in the bilayers ME structure will be stressed also. Therefore, the ME structure in responding to the ac-magnetic field can be viewed as a pre-stressed system. Correspondingly, the magnetoelastic coupling coefficient given in the appendix should take the values of the pre-stressed system.

3. Results of numerical modeling

First of all, a harmonic analysis on MSCP upon an ac-magnetic field H is performed. It is understood that the as-induced strain distribution over the top surface of MSCP, $U_x(x,y,t)$, where t is time, behaves like a waveform in spatial and time scales. We evaluate the spatial magnitude of $U_x(x,y,t)$ as a function of frequency f, and the value of f corresponding to the maximal $U_x(x,y,t)$ is determined. Then, this waveform is coupled to the bottom surface of PECP, as shown in Fig. 2. On the other hand, the electric voltage V across PECP between the bottom and top surfaces as a function of f is evaluated from the numerical analysis on PECP, in order to obtain the frequency at which the maximal value of V is reached. Subsequently, the dimensions of the two components are adjusted so that both MSCP and PECP have the same resonance frequency. In our calculation, the cross-section of the two components is set as $L = 10$ mm and $W = 5$ mm, leaving the value of thickness T as the variable for optimization. The amplitude of the ac-magnetic field is set to 0.7 Oe.

The harmonic analysis shows that for MSCP the maximal dynamic strain (displacement) wave $U_x(x,y,t)$ is observed at $f = 79$ kHz and this frequency does not depend on T_M, the thickness of MSCP. The spatial wavelength of $U_x(x,y,t)$ is compatible with the length L, which means that the spatial distribution of the dynamic strain is anti-symmetric with respect to the central line O–O′ (Fig. 2). Take points 102 and 126 on the top surface of MSCP as an example. The two points are symmetric about O–O′. The frequency dependence of $U_x(t)$ for the two points at a time when U_x reaches its maximal, as $T_M = 0.5$ and 1.0 mm, is calculated, and it is clearly shown that the displacements of the two points are identical in magnitude but opposite in phase. The displacement at $T_M = 0.5$ is almost two times that at $T_M = 1.0$ mm. In Fig. 3a–c are shown the maximal displacement contour of $U_x(x,y,t)$ of the top surface of MSCP at three different frequencies, where the numbers refer to the displacement. The whole component is divided into two regions separated by line O–O′. A mirror symmetry of the spatial displacement at any two points symmetric with respect to this line is shown. And more, when f is higher, the influence of the geometric boundary of MSCP becomes remarkable. One observes the strain reflection from the boundary at high frequency.

To simulate the piezoelectric yield of PECP, the strain distribution on the top surface of MSCP as the load applied to the bottom surface of PECP is employed. This assumes that the MSCP/PECP interface is perfectly bonded and no energy loss is generated. However, once the two components are bonded together, the elastic behaviors of MSCP would change a lot due to the change of boundary conditions. In spite of this bonding effect, one may argue that the anti-symmetric characteristic of the strain distribution with respect to line O–O′ remains true. Therefore, we assume that the displacements of the two edges B–B′ and D–D′ (shown in Fig. 2) are the same in magnitude but opposite in phase. A reasonable value of $U_x = 1.0$ μm at edge B–B′ or D–D′ is taken as the boundary condition. A pilot calculation shows that for a maximal strain (displacement) generated at $f = 79$ kHz, the thickness of PECP should be

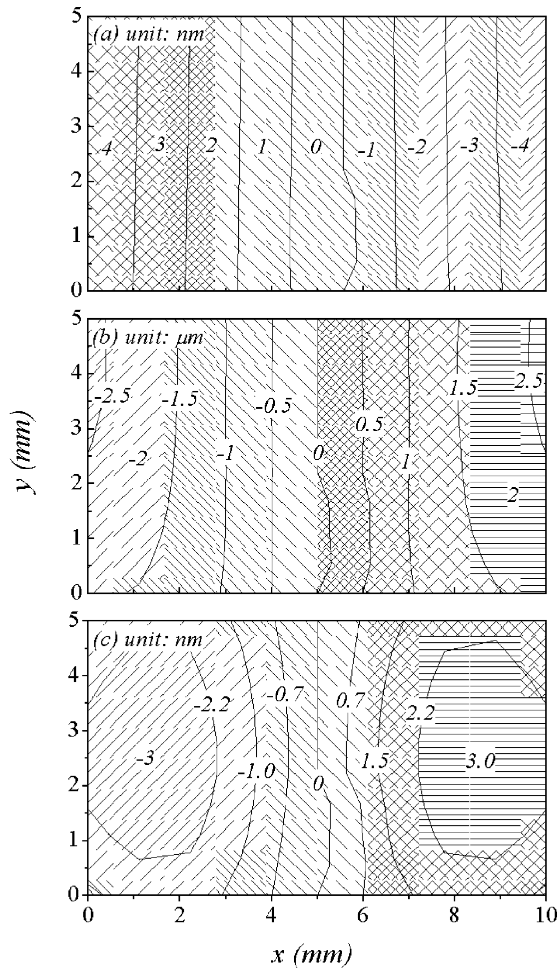

Fig. 3. In-plane contour of the maximal displacement U_x on the top surface of MSCP at three different frequencies: (a) $f = 10$ kHz, (b) $f = 79$ kHz and (c) $f = 120$ kHz.

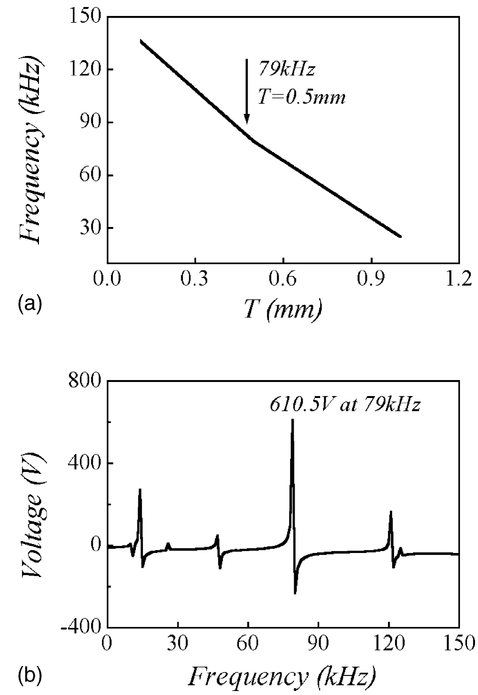

Fig. 4. (a) Resonance frequency f corresponding to the maximal voltage V, as a function of thickness of PECP, T_P, and (b) electric voltage V as a function of frequency when $T_P = 1.0$ mm.

0.5 mm, as shown in Fig. 4a. The frequency spectrum of the yielded voltage V for PSCP when its thickness $T_P = 0.5$ mm is shown in Fig. 4b, where the maximal voltage is 610.5 V at $f = 79$ kHz.

By fixing $T_P = 0.5$ mm for PECP, one calculates the dependence of the voltage V as a function of T_M for MSCP, where the maximal value of V is 25.3 V at $T_M = 0.9$ mm for MSCP. However, the corresponding frequency shifts to 67 from 79 kHz. A shift $\Delta f = 79–67$ kHz $= 12$ kHz is obtained. Subsequently, the cycle of optimization described above is repeated until that $\Delta f = 0$ is reached. Keeping $T_M = 0.9$ mm for MSCP, the harmonic analysis produces the dependence of maximal voltage as a function of T_P for PECP: $V = 56.4$ V at $T_P = 0.55$ mm but $f = 102$ kHz.

The above calculations show that the ME yield depends significantly on the dimension of both MSCP and PECP, and is also sensitive to the frequency of the applied magnetic field. One set of optimized dimension for the present bilayered composite is 10.0 mm × 5.0 mm × 0.9 mm for MSCP and 10.0 mm × 5.0 mm × 0.55 mm for PECP. The maximal ME yield from the PECP component is −56.4 V when it is driven under an ac-magnetic field of 102 kHz in frequency and 0.7 Oe in amplitude. As an experimental relevance, Ryu et al. [9] developed a bilayered structure whose cross section dimension differs a little from the present structure, and the optimized thickness data for the two components are close to the predicted values above: 1.0 mm for MSCP and 0.5 mm for PECP. Our simulated ME coupling coefficient $\alpha_E = 1465$ V/cm Oe, is however, much larger than the value measured experimentally [9]. Although there are quite a few of reasons which are responsible for this difference and really exist experimentally but not included in our calculation, the dimension of the bilayered structure deviating from the optimized one remains one of the major reasons, to the authors' argument.

4. Conclusion

In conclusion, we have performed a numerical modeling on the magnetoelectric coupling of a bilayered composite structure consisting of $Tb_{0.3}Dy_{0.7}Fe_{1.9}$ magnetostrictive plate and $Pb(Zr_{0.52}Ti_{0.48})O_3$ piezoelectric plate. We have shown that for this bilayered composite structure the magnetoelectric yield depends significantly on the dimensions of the two components, in particular the thickness. A magnetoelectric yield coefficient as high as 1465 V/cm Oe at a frequency of 102 kHz is predicted for a structure consisting of a 10.0 mm × 5.0 mm × 0.9 mm $Tb_{0.3}Dy_{0.7}Fe_{1.9}$ plate bonded with a 10.0 mm × 5.0 mm × 0.55 mm $Pb(Zr_{0.52}Ti_{0.48})O_3$ plate.

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