PARAMETER OPTIMIZATION FOR LAMINATED MULTIFERROIC COMPOSITES

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Ключевые слова: магнитоэлектрический эффект, магнитострикция, пьезоэлектричество, тонкие слои, оптимизация.

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Оптимизация параметров слоистых композиционных мультиферроиков

Аннотация: Рассматривается максимизация магнитоэлектрического коэффициента по напряжению в слоистом магнитострикционно-пьезоэлектрическом композите путём оптимизации физических параметров магнитострикционного материала. Получено, что в диапазоне параметров используемых магнитострикционных материалов имеется комбинация значений, которая придаёт магнитоэлектрическому коэффициенту более высокое значение, чем отдельные материалы. В расчётах были рассмотрены применяемые на практике известные магнитострикционные материалы.

Abstract: Maximization of voltage coefficient of a multiferroic laminated composite is considered via optimization of physical parameters of magnetostrictive material. It is obtained, that in the range of parameters of magnestrictive materials in use there is a combination of values, which gives to the voltage coefficient a higher value than separate materials. Practically well-known magnetostrictive materials were considered in the calculations.

Introduction

Multiferroic magnetoelectric (ME) structures, at the same time exhibiting ferromagnetism and ferroelectricity, have recently motivated increasing number of research activities for their scientific interest and drawn significant interests due to their potential applications in many multifunctional devices, such as transducers, passive magnetic field sensors, electric-write magnetic-read memory devices, microwave filters, energy harvest devices, actuators, etc. [1,3]. Natural multiferroic single-phase compounds are rare, and their ME responses are either relatively weak or occurs at temperatures too low for practical applications. In contrast, multiferroic composites, which incorporate both ferroelectric and ferri-ferromagnetic phases, typically yield giant ME coupling response above room temperature, which makes them ready for technical applications.
The historical perspective of the multiferroic ME composite materials appeared in 1972. In such composites the ME effect is generated as a product property of a magnetostrictive and a piezoelectric material. Multiferroic materials [4, 6] with coexistence of at least two ferroic orders (ferroelectric, ferromagnetic, or ferroelastic) have drawn growing interest due to their potential for applications as multifunctional devices. In multiferroic materials, the coupling interaction between the different order parameters could produce new effects, such as ME effect [7,10]. Magnetoelectricity has been observed as an intrinsic effect in some natural material systems at low temperature, which have been under intensive study

recently [11,18], motivated by potential applications in information storage, spintronics, and multiple-state memories. Research progress in single-phase multiferroic ME materials have been summarized and reviewed in a series of conference proceedings on ME interaction phenomena in crystals [7,10] and especially in recent review articles [5,8,17,]. The magnetoelectric response is the appearance of an electric polarization ***P*** upon applying a magnetic field ***H*** (i.e., the direct ME effect, designated as ME_H effect: ***P*** = ***(H)*** and/or the appearance of a magnetization ***M*** upon applying an electric field ***E*** (i.e., the converse ME effect, or MEE: ***M = (E)***. An electric polarization is induced by a weak ac magnetic field oscillating in the presence of a dc bias field, and/or a magnetization polarization appears upon applying an electric field.

Of interest, motivated by on-chip integration in microelectronic devices, nanostructured composites of ferroelectric and magnetic oxides have recently been deposited in a film-on substrate geometry. The coupling interaction between nanosized ferroelectric and magnetic oxides is also responsible for the ME effect in the nanostructures as was the case in those bulk composite materials.

The elastic coupling interaction between the magnetostrictive phase and piezoelectric phase leads to giant ME response of these ME composite materials. For example, a Metglas/lead zirconate titanate fiber laminate has been found to exhibit the highest ME coefficient, and in the vicinity of resonance, its ME voltage coefficient as high as 102 V/cm Oe orders has been achieved, which exceeds the ME response of single-phase compounds by many orders of magnitude. Alternatively and with greater design flexibility, multiferroic ME composites [19] made by combining piezoelectric and magnetic substances together have drawn significant interest in recent years due to their multifunctionality, in which the coupling interaction between piezoelectric and magnetic substances could produce a large ME response [20] (e.g., several orders of magnitude higher than that in those single phase ME materials so far available) at room temperature. The ME effect in composite materials is known as a product tensor property [19,21], which results from the cross interaction between different orderings of the two phases in the composite. Neither the piezoelectric nor magnetic phase has the ME effect, but composites of these two phases have remarkable ME effect. Thus the ME effect is a result of the product of the magnetostrictive effect (magnetic/mechanical effect) in the magnetic phase and the piezoelectric effect (mechanical/electrical effect) in the piezoelectric one.

Magnetostrictive-piezoelectric bilayer structures offer certain advantages over bulk composites [22], because they can be polarized much easier and exhibit practically no leakage currents as the magnetostrictive phase is insulated by the high-resistivity piezoelectric layer. Thereby the value of ME effect in such samples is greater than in bulk composites and they are of great interest in promising novel devices based on ME interaction. The theory of the ME effect in bulk composites based on the effective parameters method at the low frequency region was presented in works [23,27] and in the region of electromechanical resonance first was developed in works [28,31]. But the method of effective parameters can be used when the characteristic size of the structure units of the composite is much smaller than the acoustic wavelength. In this case, the composite can be regarded as a homogeneous medium. Consideration of the ME effect in layered structures based on the simultaneous solution of the equations of motion and constitutive relations for the magnetostrictive and piezoelectric phases were previously presented in [32,39]. Therein, an expression for the ME voltage coefficient was derived, taking into account the boundary conditions on the interface. Thus, the consideration of the interlayer bonding material was taken into account formally by an interface coupling coefficient [32, 35] or by an assumption of perfect interfacial bonding and equal oscillation amplitude over the thickness of both magnetostrictive and piezoelectric phases [36]. The ME effect in bilayer magnetostrictive-piezoelectric structure taking into account the changes of the amplitude in oscillations over the thickness of the sample was presented in [37,38]. But in these works also the model of the perfect bonding between magnetostrictive and piezoelectric layers was used. Recently, the ME effect was investigated in laminated composite structure coupled by a bonding material and the ME voltage coefficient was derived considering the interlayer bonding material in work [39]. But in this work, the amplitude change of the oscillations over the thickness of the sample (in direction perpendicular to the interface) was not assumed.

Material parameters play a very important role in problems of coupled fields: electro-magneto-elasticity, thermo-elasticity, etc. The independent fields (for instance, electric, magnetic and elastic) are interacting through coupling constants, which characterize the strength of interaction. Higher the coupling coefficient, more significant is the interaction between fields. The coupling coefficient depends only on the material of continuum and differs for different materials. Nevertheless, due to significant progress in material processing, it is possible to create materials with desired (practically arbitrary) coupling coefficient. It is a challenging feature, allowing to process materials according to needs of a particular process, in which they are involved in. For material optimization in thermo-elasticity we refer to [40,41], in magneto-electro-elasticity we refer to [42,43] and references therein. For general and instance considerations see [44,46].

The aim of the paper is twofold: optimize the voltage coefficient over a given set of parameters and by varying the independent material parameters. In the first case, physical parameters of several known materials form the mentioned set, while in the second case, variation is given to independent parameters and parameters for phenomenological materials are derived.

2. Optimization procedure

In the low-frequency region, the magnetoelectric voltage coefficient is nearly independent of frequency. The low-frequency value of the coefficient can be written in the following form [37]:

$$< \alpha_E^{low} >= \frac{{}^pY\,{}^pd_{xx,z}\,{}^mq_{xx,z}}{{}^p\varepsilon_{zz}\left(1-K_p{}^2\left(\dfrac{{}^mY\,{}^mt}{{}^mY\,{}^mt+{}^pY\,{}^pt}\right)\right)}\cdot\frac{{}^mY\,{}^mt}{{}^mY\,{}^mt+{}^pY\,{}^pt}\cdot\frac{{}^pt}{{}^mt+{}^pt} \tag{1}$$

where upper-case index "m" is for magnetostrictive phase and "p" for piezoelectric; ${}^{m}Y$, ${}^{p}Y$ are the Young's moduli of the magnetostrictive and piezoelectric phases; ${}^{m}t$, ${}^{p}t$ are the thicknesses of the phases; ${}^{p}d_{xx,z}$ and ${}^{m}q_{xx,z}$ are the piezoelectric and piezomagnetic coefficients; ${}^{p}\varepsilon_{zz}$ is the tensor component of permittivity and ${K_p}^2 = \dfrac{{}^{p}Y({}^{p}d_{xx,z})^2}{{}^{p}\varepsilon_{zz}}$ the squared coefficient of electromechanical coupling.

The voltage coefficient α_E can be represented in a more convenient form:

$$\alpha_E = {}^{m,p}D \cdot \frac{{}^{m}q_{xx,z}\, {}^{p}Y\, {}^{m,p}A}{1 - {K_p}^2\left(1 - {}^{m,p}A\right)} \tag{2}$$

where

$${}^{m,p}A = \frac{1}{1 + {}^{m,p}B}, \quad {}^{m,p}B = \frac{\frac{1}{{}^{p}v^2}\, {}^{m,p}C - 1}{1 - \frac{{}^{m}\rho}{{}^{m}Y}\, {}^{m,p}C}, \quad {}^{m,p}C = \frac{{}^{m}Y\, {}^{m}t + {}^{p}Y\, {}^{p}t}{{}^{m}\rho\, {}^{m}t + {}^{p}\rho\, {}^{p}t}, \quad {}^{m,p}D = \frac{{}^{p}d_{xx,z}\, {}^{m}t}{{}^{p}\varepsilon_{zz}\left({}^{m}t + {}^{p}t\right)},$$

v is the longitudinal wave speed,

Since the aim is to optimize α_E with respect to material (physical) parameters of the magnetic, the variation of α_E with respect to material parameters with left superscript ^{m} is evaluated:

$$\delta\alpha_E = {}^{m,p}D \cdot \left[\begin{array}{l} \dfrac{{}^{p}Y\ {}^{m,p}A\ \delta\left({}^{m}q_{xx,z}\right) + {}^{m}q_{xx,z}\, {}^{m,p}A\delta\left({}^{m}Y\right)}{1 - {K_p}^2\left(1 - {}^{m,p}A\right)} - \\ -\dfrac{1}{{}^{m,p}A^2} \dfrac{{}^{m}q_{xx,z}\, {}^{p}Y\left(1 - {K_p}^2\right)}{1 - {K_p}^2\left(1 - {}^{m,p}A\right)} \left[{}^{m,p}E_1\delta\left({}^{m}Y\right) + {}^{m,p}E_2\delta\left({}^{m}\rho\right)\right] \end{array} \right]. \tag{3}$$

Here

$${}^{m,p}E_1 = \frac{{}^{m}t}{\left(1 - \frac{1}{{}^{m}v^2}\, {}^{m,p}C\right)\left(\frac{1}{{}^{p}v^2}\, {}^{m}\rho\, {}^{m}t + {}^{p}t\right)} - \frac{\frac{1}{{}^{p}v^2}\, {}^{m,p}C - 1}{\left(1 - \frac{1}{{}^{m}v^2}\, {}^{m,p}C\right)^2} \cdot \frac{{}^{m}\rho\, {}^{p}Y\, {}^{p}t}{{}^{m}Y^2\left({}^{m}\rho\, {}^{m}t + {}^{p}\rho\, {}^{p}t\right)},$$

$${}^{m,p}E_2 = -\frac{{}^{m}t\, {}^{p}Y\, {}^{m,p}Y}{{}^{p}\rho\left(1 - \frac{1}{{}^{m}v^2}\, {}^{m,p}C\right)\left({}^{m}\rho\, {}^{m}t + {}^{p}\rho\, {}^{p}t\right)} + \frac{1}{\left(1 - \frac{1}{{}^{m}v^2}\, {}^{m,p}C\right)^2} \cdot \frac{{}^{m}Y\, {}^{p}\rho\, {}^{p}t\, {}^{m,p}C}{{}^{m}\rho\, {}^{m}t + {}^{p}\rho\, {}^{p}t}.$$

Variation (3) allows to consider partial variations of α_E with respect to parameters ${}^{m}q_{xx,z}$, ${}^{m}Y$ and ${}^{m}\rho$.

2.1 Optimization over set of values

In this subsection, the variation (3) is evaluated at certain sets of values of ${}^{m}q_{xx,z}$, ${}^{m}Y$ and ${}^{m}\rho$. The aim is to maximize α_E by choosing ${}^{m}q_{xx,z}$, ${}^{m}Y$ and ${}^{m}\rho$ among materials which are usually used in such structures. Such materials are gathered in Table 1.

Table 1. Parameters of materials used in structures under consideration

Material	${}^{m}q_{xx,z}$ [m/A]	${}^{m}Y$ [N/m^2]	${}^{m}\rho$ [kg/m^3]
Permendur	$1062 \cdot 10^{-12}$	$1.81 \cdot 10^{11}$	8100
Nickel	$1156 \cdot 10^{-12}$	$2.04 \cdot 10^{11}$	8900
NFO	$125 \cdot 10^{-12}$	$1.53 \cdot 10^{11}$	5200
Metglas	$7514 \cdot 10^{-12}$	$1.86 \cdot 10^{11}$	8200
CFO	$556 \cdot 10^{-12}$	$1.54 \cdot 10^{11}$	4600
Manganite	$-120 \cdot 10^{-12}$	$0.6 \cdot 10^{11}$	4400
Terfenol-D	$6108 \cdot 10^{-12}$	$0.55 \cdot 10^{11}$	9300

The absolute values of α_E in the case of chosen materials are presented in Table 2. As piezoelectric material the standard PZT is chosen with ${}^{p}\varepsilon_{zz} = 1.55 \cdot 10^{-12}$, ${}^{p}d_{xx,z} = -175 \cdot 10^{-12}$ m/V, ${}^{p}Y = 0.65 \cdot 10^{11}$ N/m^2, ${}^{p}\rho = 7600$ kg/m^3. Geometric characteristics are chosen to be ${}^{p}t$=0.4mm, ${}^{m}t$=0.29mm.

2.2 Optimization over interval

A better result can be obtained by maximizing α_E over the interval between the lowest and highest values of ${}^{m}q_{xx,z}$, ${}^{m}Y$ and ${}^{m}\rho$, respectively. Choosing the restrictions

120 · 10-12 $120 \cdot 10^{-12} \le {}^{m}q_{xx,z} \le 7514 \cdot 10^{-12}$, $0.6 \cdot 10^{11} \le {}^{m}Y \le 2.04 \cdot 10^{11}$, $4400 \le {}^{m}\rho \le 8900$,

it is derived $|\alpha_E| = 2.44$ for ${}^{m}q_{xx,z} = 7514 \cdot 10^{-12}$ m/A (Permendur), ${}^{m}Y = 2.04 \cdot 10^{11}$ N/m^2 (Nickel), ${}^{m}\rho = 9208.9$ kg/m^3.

Table 2. Magnetoelectric voltage coefficients for materials used in structures under consideration

Material	$\lvert\alpha_E\rvert$
Permendur	0.331
Nickel	0.375
NFO	0.036
Metglas	2.2
CFO	0.162
Manganite	0.021
Terfenol-D	1

On the other hand, removing the restriction from above on ${}^{m}Y$ and ${}^{m}\rho$, a better result is obtained: $|\alpha_E| = 3.67$

for ${}^{m}q_{xx,z} = 7514\cdot10^{-12}$ m/A (Permendur), ${}^{m}Y = 3.05\cdot10^{11}$ N/m^2, ${}^{m}\rho = 4403.5$ kg/m^3.

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