Mathematical modelling of magnetoelectric effect in multiferroic in thickness-shear mode region

V M Petrov, A F Saplev and O I Malyshev
Yaroslav-the-Wise Novgorod State University, ul. B. St. Peterburgskaya, 41
173003, Veliky Novgorod, Russia
E-mail: Vladimir.Petrov@novsu.ru

Abstract. The article discusses the magnetoelectric effect in the thickness-shear mode region in a layered structure of a piezoelectric bimorph and a magnetostrictive material. Numerical estimates according to the proposed theoretical model of the magnetoelectric effect in the structure of the langatate bimorph and yttrium-iron garnet show that the value of ME voltage coefficient is much higher than for the bilayer of langatate and yttrium-iron garnet.

1. Introduction
The interaction of the piezoelectric and piezomagnetic properties of the composite multiferroic through elastic deformations leads to the appearance of the magnetoelectric (ME) effect [1, 2]. The mechanism of the ME effect is as follows: when an external magnetic field is applied, the piezomagnetic component is deformed. This deformation is transmitted to the piezoelectric component, in which mechanical stresses arise and the electric polarization appears due to the piezoelectric effect. One also can observe an inverse ME effect, in which the deformation of the piezoelectric component is caused by an external electric field. The deformation is transmitted to the piezomagnetic component, while the piezomagnetic component is magnetized due to the piezomagnetic effect. As a result, multiferroic acquires a new property – the magnetoelectric effect. The purpose of this work is to study the features of the ME effect in the region of the thickness-shear mode in the layered structure of a piezoelectric bimorph and a magnetostrictive layer.

2. Magnetoelectric composites
The ME effect may be present in a multiferroic characterized by a combination of piezomagnetic and piezoelectric phases or combinations of magnetostrictive and piezoelectric phases. It has been established that the ME effect in composites is more than a hundred times larger than that for a single-phase ME material, such as Cr$_2$O$_3$ [1].

Since the ME effect is due to the interaction of the magnetostrictive and piezoelectric phases through the elastic sublattice, we should expect the appearance of a giant ME effect in the electromechanical resonance (EMR) region. At this point, the ME effect in composites in the magnetic resonance longitudinal, flexural, and shear modes has been studied in detail.

The second resonance of importance that can be used to increase the ME coupling strength is magnetic resonance for the magnetic phase. At the overlapping of EMR and magnetic resonances, further enhancement of the ME effect can be observed [3]. The ME effect in the magnetoacoustic resonance region can facilitate implementation of nanosensors and high-frequency transducers.
Magnetically ordered materials, as a rule, are magnetostrictive. However, the piezomagnetic effect in these materials is not observed. Thus, the ME effect in single-crystal materials is linear in a wide range of electric and magnetic fields, in contrast to the ME effect in composite materials, in which this effect is non-linear. The use of a bias magnetic field enables linearizing the ME effect in composite materials. For ac magnetic fields with the magnitude small compared to the magnitude of the bias field, the ME effect approaches to linear one.

Substances with significant piezoelectric properties belong to the class of piezoelectric materials. Polycrystalline ferroelectric solid solutions are also piezoelectric materials after polarization in a dc electric field.

Currently, over a thousand compounds with piezoelectric effect are known. However, in practice, a limited number of materials are used as piezoelectrics, which are divided into single-crystal piezoelectrics, piezoelectric ceramics, and polymer piezoelectric elements.

Ceramics based on lead zirconate titanate (PZT) is a good piezoelectric material that is widely used in electronic devices. However, this ceramics contains more than 60% of lead. Lead is currently excluded from many applications and materials due to toxicity. It is well-known that the lead-free piezoelectric ceramics \( \{(K_{0.5}Na_{0.5})_{3-x}Li_{x}\}(Nb_{1-x}Ta_{x})O_3 \) has piezoelectric coefficients comparable to PZT. The compound \( K_{0.5}Na_{0.5}NbO_3 \) (KNN) is of particular interest. Material properties can easily be changed by doping the material in tetragonal or octahedral positions.

3. Mathematical modeling of the magnetoelectric effect in the thickness-shear mode region

The presented paper is devoted to the study of the direct ME effect in the thickness-shear mode region [4] in the laminate of a piezoelectric bimorph and a magnetostrictive layer. The use of yttrium-iron garnet (YIG) as a magnetostrictive phase is caused by the fact that YIG has low losses in a single-domain state. That is important for obtaining a strong ME effect in the microwave range. As the piezoelectric phase, the lead-free single-crystal langatate is used. We consider the laminates with Y-cut langatate bimorph. In this case, two piezoelectric layers have opposite directions of Y-axis. The choice of langatate (LGT) is related to the fact that despite the small piezoelectric module, the ratio of the piezoelectric modulus to the dielectric constant for langatate exceeds this parameter for PZT. It is known that the direct ME effect is determined by the ratio of the piezoelectric modulus to the dielectric constant, therefore the use of langatate results in a strong ME effect. In addition, Y-cut langatate is sensitive only to shear deformations. In this work, a sample is considered with X-axis of langatate parallel to the [100] axis of the ferrite. The bias magnetic field is perpendicular to the sample plane and parallel to the [110] axis of the ferrite as in figure 1. An ac magnetic field in the sample plane is used to excite the thickness-shear oscillations.

**Figure 1.** Schematic diagram showing a laminate of LGT bimorph and YIG.

It should be noted that for the out-of-plane bias magnetic field and in-plane ac magnetic field, only shear deformation can be excited. It is evident that electric field along Y-axis in langatate can be produced by thickness shear mode and face shear mode. In this paper, we consider the most high-frequency vibrations that correspond to thickness shear mode. Note that the thickness shear strains do not result in ME coupling in the low-frequency region. The point is that vibrations occur in \( XY \) plane.
and displacement $u_t$ is a function of $y$. In this case, strain component $S_i$ is zero and there is no strain transfer between the layers. However in the EMR region, the inertia force increases and enables the magnetostrictive and piezoelectric layers to be mechanically coupled. For exciting the shear vibrations in XY-plane, bias magnetic and ac magnetic fields should be applied in Y-direction and X-direction, respectively.

For the first piezoelectric layer, it is possible to write the equation for the thickness-shear oscillations in the following form:

$$\rho_p \frac{\partial^2 u_1}{\partial t^2} = \frac{\partial p^1 T_{p5}}{\partial z}$$

where $p^1 u_1$, $\rho_p$, and $p^1 T_j$ denote the displacement, density of the piezoelectric phase, and stress tensor component of first piezoelectric layer.

Thickness-shear vibrations for the second piezoelectric layer, as well as the magnetic layer, are described by similar equations. As already mentioned, the ME effect in composites is due to the interaction of the electric and magnetic phases through elastic deformations, therefore, to model the ME effect based on the solution of the equations of motion, it is necessary to use boundary conditions at the interfaces of the layers for the displacement components and stresses corresponding to the structure under consideration. We assume the piezoelectric and piezomagnetic layers to be perfectly bonded together. The open circuit condition allows one to obtain the expression for the ME voltage coefficient after substituting the found components of mechanical stresses.

Numerical estimates of the ME voltage coefficient have been obtained based on a one-dimensional model. It is assumed that multiferroic samples have the form of a long plate of length $L$, width $b \ll L$ and thickness $t \ll b$, with the X-axis directed along the length of the sample, and the Y-axis along the thickness. When finding estimates of the ME voltage coefficient, it was taken into account that the components of the deformation $S_b$ and electric induction $D_2$ are expressed in terms and stresses of according to the elasticity law.

$$p^1 S_b = p^1 S_{66} p^1 T_6 \cdot 2p^1 d_{11} p^1 E_2 ;$$
$$p^2 S_b = p^2 S_{66} p^2 T_6 \cdot 2p^2 d_{11} p^2 E_2 ;$$
$$m S_b = m s_{44} m T_6 + m q_{15} H_1 ;$$

where $p^1 S_{66}$, $p^1 d_{11}$, $p^2 S_{66}$, $p^2 d_{11}$ denote elastic compliance and piezoelectric coefficient of first and second piezoelectric layers, $m s_{44}$ and $m q_{15}$ are compliance and piezomagnetic coefficient of the magnetostrictive layer, $p^1 E_2$ and $p^2 E_2$ are electric fields in the piezoelectric layers.

Expressions for electric displacements $D$ for the piezoelectric layers are as follows:

$$p^1 D_2 = -2p^1 d_{11} p^1 T_5 + p^1 E_{11} p^1 E_2 ;$$
$$p^2 D_2 = -2p^2 d_{11} p^2 T_5 + p^2 E_{11} p^2 E_2$$

with $p^1 E_{11}$ and $p^2 E_{11}$ being the dielectric constants of piezoelectric layers.

The solution of Eq. (1) taking into account Eq. (2) allows us to calculate the stress components in the piezoelectric layers. Substituting the found values of stress into the open-circuit condition leads to the expression for the electric fields in the piezoelectric layers. Average electric field induced across the sample is determined by expression:

$$E_2 = \frac{p^1 E_{11} t_{p1} + p^2 E_{11} t_{p2}}{t_{p1} + t_{p2}}$$

with $t_{p1}$ and $t_{p2}$ denoting the thickness of piezoelectric layers.

ME voltage coefficient $a_2$ is calculated as the ratio of average electric field induced across the sample to the applied magnetic field.
\[ \alpha_E = \frac{E_2}{H_1} \] (5)

Because of space limitation, this expression for \( \alpha_E \) is not given in the article. The numerical calculation was carried out for samples with a YIG layer 3.26 mm thick and a langatate layer 1.1 mm thick.

As an example, the calculation results for the ME voltage coefficient are shown in figure 2 for the fourth resonant frequency.

We used the following material parameters for estimates: \( p_{d_{11}} = -6.5 \times 10^{-12} \text{ C/N}, p_{s_{66}} = 25 \times 10^{-12} \text{ m}^2/\text{N}, \varepsilon_{33}/\varepsilon_0 = 80.3, m_{q_{15}} = -25 \times 10^{-12} \text{ m/A}, m_{s_{44}} = 13.1 \times 10^{-12} \text{ m}^2/\text{N} \).

The data in figure 2 for the fourth resonant frequency show that, a significant increase in the ME voltage coefficient (approximately 6 times) is observed for the sample of YIG and langatate bimorph compared to the bilayer of YIG and langatate with the same total thickness of piezoelectric phase.

![Figure 2](image_url)

**Figure 2.** Frequency dependence of ME voltage coefficient for YIG – langatate bilayer (1) and layered structure of YIG and langatate bimorph (2).

The increase in ME coupling strength is associated with the features of the sample geometry. Using the piezoelectric bimorph with appropriate geometry enables one to obtain the high-order harmonic modes that are suppressed in ferrite-piezoelectric bilayers. In the main case, by selecting the number of in-series piezoelectric bimorphs with appropriate layer thicknesses, ME transducer with desired resonance frequency may be produced.

4. **Conclusion**

The paper presents a theoretical model of the ME effect in the thickness-shear mode region in a layered structure based on magnetostrictive layer and piezoelectric bimorph. The model was used to estimate the ME voltage coefficient for the structure of YIG and lead-free langatate bimorph. At the fourth resonant frequency, a significant increase in the ME voltage coefficient was obtained for the sample of YIG and langatate bimorph in comparison with the YIG-langatate bilayer.

The results obtained can be used to investigate the giant ME effect at overlapping of EMR and magnetic resonances. These types of resonance phenomena are of interest for the study of the energy exchange between spin waves and phonons.
References

[1] Freeman A J et al. 1975 Magnetoelectric Interaction Phenomena in Crystals (London, N.-Y., Paris: Gordon and Breach) p 228

[2] Bichurin M I and Petrov V M 2014 Modeling of Magnetoelectric Effects in Composites Springer Series in Materials Science 201 108

[3] Bichurin M I, Petrov V M, Ryabkov O V et al. 2005 Theory of magnetoelectric effects at magnetoacoustic resonance in single-crystal ferromagnetic-ferroelectric heterostructures Phys. Rev. B 72 060408(R)

[4] Bichurin M I, Petrov R V and Petrov V M 2013 Magnetoelectric effect at thickness shear mode in ferrite-piezoelectric bilayer Applied Physics Letters 103 092902