Available online at www.sciencedirect.com
ScienceDirect
Journal of the European Ceramic Society 27 (2007) 2949–2952
www.elsevier.com/locate/jeurceramsoc

Electromechanical coupling coefficient of isotropic sample with a marked electrostriction

Orest Vendik, Irina Vendik *

St. Petersburg Electrotechnical University, 5 Prof. Popov Str., 197376 St. Petersburg, Russia

Available online 4 January 2007

Abstract

Isotropic sample of single ferroelectric crystal (STO) with cubic symmetry or the epitaxial BSTO film does not exhibit a piezoelectric effect, but is characterized by electrostriction. The induced piezoelectric effect occurs under the dc electric field. Using electromechanical equations for this material in presence of both the dc and ac electric field makes possible to describe the transformation of energy of electromagnetic field into acoustic oscillations. The transformation intensity is estimated by the electromechanical coupling coefficient determined as the ratio of the energy of alternating electromechanical interaction to the geometric mean of alternating electrical and mechanical energy. For the induced piezoeffect, the analytical model for the electromechanical coupling coefficient is obtained using phenomenological description of the dc electric field dependence of the dielectric permittivity. There is a maximum on the dependence of the electromechanical coupling coefficient on the dc field. The value of maximum and related dc field depend on the ferroelectric film quality.

Keywords: Ferroelctric; $SrTiO_3$; $BaSrTiO_3$; Acoustic resonator

1. Introduction

High-Q microwave acoustic resonators were suggested and employed in microwave high quality filters.[1–3] In these resonators, materials with highly pronounced piezoelectric effect are used. In the case of $SrTiO_3$ (STO) and $BaSrTiO_3$ (BSTO) materials with centro-symmetric cubic lattice no piezo-effect should be observed. Very small piezoelectric effect in STO was revealed and explained by the influence of mechanical stress and slightly non-cubic structure.[4] At the same time the distinctive peaks of loss factor of the parallel-plate varactor based on a thin BSTO film[5] were observed in ref.[6] The peak height was correlated with the dc biasing voltage applied to the varactor. The nature of the peaks was explained by the induced piezoelectric hypersound generation.[7] The hypersound generation on STO and BSTO materials was also observed in refs.[8–10] and theoretically estimated in refs.[11,12] The explanation was based on the model of the induced piezo-effect due to electrostriction in the material existing by applying dc biasing field.

The most promising microwave application of the effect observed is using the induced piezoelectricity for tuning resonant frequency of the acoustic resonator.[7] The intensity of the bulk acoustic waves in the BSTO or STO acoustic resonator is determined by the electromechanical coupling, which is estimated numerically by the electromechanical coupling coefficient.[1,13]

The goal of this paper is to develop a model of the induced piezoelectrictricity in non-piezoelectric material described by the elctromechanical coupling coefficient depending on the dc biasing field.

2. Electromechanical coupling coefficient

For a description of the electromechanical phenomena in the crystals, the expansion of the free energy over powers of the dielectric polarization and the mechanical deformation can be used.[14,15] The expansion contains components of the electric field vector E_m, components of the permittivity tensor ε_{ij}, components of the strain tensor σ_{ij}, the compliance tensor components s_{ijkl}, and the components of the electrostriction tensor R_{ijmn}. We suggest that the piezoelectric modulus is zero. The tensor $||R||$ is a function of the biasing field. The most convenient form of the electrostriction tensor is the tensor $||Q||$, which enters into the free energy equation in the form of $Q_{ijkl}D_iD_j\sigma_{kl}$. For BSTO and other perovskite type crystals or ceramics the

* Corresponding author. Tel.: +7 812 346 0867; fax: +7 812 346 0867.
E-mail address: ibvendik@eltech.ru (I. Vendik).

0955-2219/$ – see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.jeurceramsoc.2006.11.068

terms of the tensors of the electrostriction Q_{ijpq} do not depend on the biasing field and slightly depend on temperature in both the ferroelectric state and in the paraelectric state[16] and can be taken constant for a practical use.

In order to simplify the problem, we assume that the BSTO film is isotropic. In an isotropic medium the permittivity tensor is converted into a scalar $\varepsilon_{mn} = \varepsilon_0\, \varepsilon_r$, where ε_r is the relative permittivity of the medium, ε_0 is the permittivity of the free space. The electrostriction tensor $||Q||$ has two independent components: the diagonal component Q and the off-diagonal component Q_k. For the BSTO, $Q \cong 0.066\ \mathrm{m^4/C^2}$ and $Q_k = 0.01\ \mathrm{m^4/C^2}$.[16] For an isotropic medium[14]

$$R = Q \cdot \varepsilon_0^2 \varepsilon_r^2 \quad R_k = Q_k \cdot \varepsilon_0^2 \varepsilon_r^2. \tag{1}$$

Let us assume that the electric field vector $\boldsymbol{E}$ consists of ac and dc components: $\boldsymbol{E} = \boldsymbol{E}^{\mathrm{ac}} + \boldsymbol{E}^{\mathrm{dc}}$. The free energy can be taken as a sum of three terms:

$$F_\Sigma = F_0 + F^{(\mathrm{dc})} + F^{(\mathrm{ac})}, \tag{2}$$

where $F^{(\mathrm{dc})}$ and $F^{(\mathrm{ac})}$ are contributions into the free energy by dc and ac electric field components, respectively. If no dispersion of $\varepsilon(\omega)$ is observed in the range of operational frequency, the total ac free energy for an isotropic medium is

$$F^{(\mathrm{ac})} = \frac{1}{2}\varepsilon \cdot (E^{(\mathrm{ac})})^2 + \frac{1}{2}s \cdot (\sigma^{(\mathrm{ac})})^2 + R \cdot E^{(\mathrm{dc})} E^{(\mathrm{ac})} \sigma^{(\mathrm{ac})} + \ldots, \tag{3}$$

where s and R are the diagonal terms of the tensors of the compliance and the electrostriction. The first term in (3) is the energy density of alternating electric field, the second term is the energy density of alternating mechanical strain, and the third term is the energy density of alternating electromechanical interaction.

In accordance with,[13] the electromechanical coupling coefficient can be presented as

$$K = \frac{|R \cdot E^{(\mathrm{dc})} E^{(\mathrm{ac})} \sigma^{(\mathrm{ac})}|}{\sqrt{\varepsilon \cdot (E^{(\mathrm{ac})})^2 s \cdot (\sigma^{(\mathrm{ac})})^2}}. \tag{4}$$

Using Eq. (1), we replace the diagonal terms of the tensors of electrostriction R by the term Q and obtain:

$$K(E^{(\mathrm{dc})}) = \frac{Q \cdot |E^{(\mathrm{dc})}| \cdot \varepsilon_r (E^{(\mathrm{dc})})^2 \varepsilon_0^2}{\sqrt{\varepsilon_r (E^{(\mathrm{dc})}) \varepsilon_0 s}}. \tag{5}$$

In this equation, the electromechanical coupling coefficient depends on the dc electric field directly and indirectly via the dielectric permittivity of the ferroelectric material $\varepsilon_r(E^{(\mathrm{dc})})$, which depends strongly on the biasing field. The results of simulation of the electromechanical coupling coefficient as a function of the dc biasing field for typical dielectric and acoustic parameters of the BSTO film are shown in Fig. 1. In the simulation, the correct model[17] of the dielectric response $\varepsilon_r(E^{(\mathrm{dc})})$ of the ferroelectric material was used. The most important feature of the results obtained is the presence of the maximum on the characteristics. The position of the maximum and related value of the dc field depends on the BSTO film quality determined by the model parameter ξ_S: the higher ξ_S, the lower is the film quality, the higher dc field corresponds to the maximum value of the coupling coefficient, and the smaller is this maximum value of K. Evidently, a high quality ferroelectric material should be used for a highly pronounced induced piezoelectric effect.

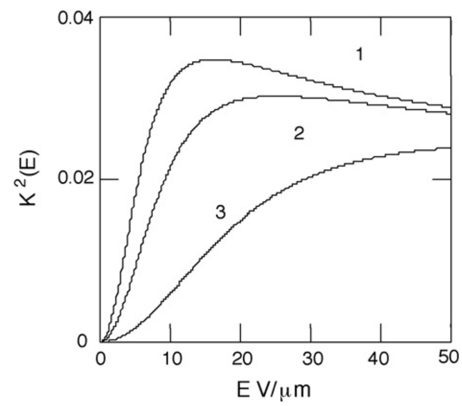

Fig. 1. Electromechanical coupling coefficient vs. dc biasing field for the BSTO film with the acoustic parameters $Q \cong 0.066\ \mathrm{m^4/C^2}$ and $s = 6.12.10^{-12}\ \mathrm{m^2/N}$ and the dielectric model[17] parameters: $E_N = 440$ kV/cm, $T_C = 240$ K, $\varepsilon_{00} = 430$, $\theta_F = 175$ K: $\xi_S = 1$ (1), $\xi_S = 2$ (2), $\xi_S = 5$ (3).

3. Tuneability of the BSTO based bulk acoustic resonator

A thin film bulk acoustic resonator (TFBAR) is formed by a thin piezoelectric film, in which the bulk acoustic oscillations are exited. In the case of the BSTO film, the acoustic oscillations are caused by the electric voltage applied to the electrodes on the surfaces of the film in presence of the dc field providing the induced piezoeffect. In general case, the active acoustic region is terminated in input acoustic impedance of the electrodes Z_L and Z_R on the left and right sides of the structure (Fig. 2). The acoustic resonator modeling[1] gives the following equation for the input electrical impedance of the acoustic resonator:

$$Z_{\mathrm{eq}} = \frac{1}{Y_{\mathrm{eq}}} = \frac{1}{i\omega C}\left[1 - K^2 \frac{tg\phi}{\phi} \cdot \frac{(Z_R + Z_L)\cos^2\phi + i\,\sin 2\phi}{(Z_R + Z_L)\cos 2\phi + i(Z_R Z_L + 1)\sin 2\phi}\right], \tag{6}$$

where C is the capacitance of the parallel plate capacitor formed by the resonator structure and ϕ is the acoustic length dependent

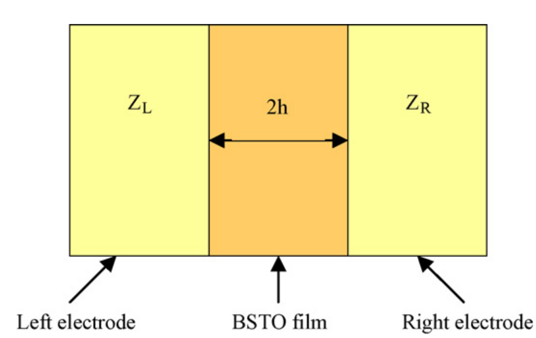

Fig. 2. Structure of a tuneable bulk acoustic resonator.

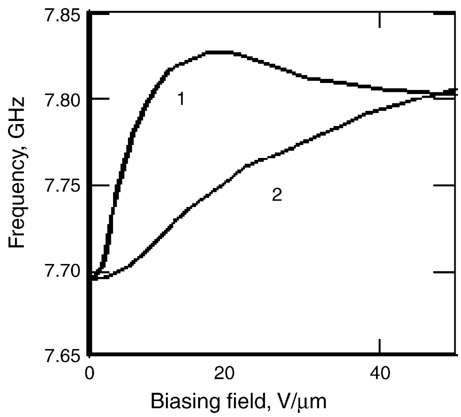

Fig. 3. Resonant frequency of the antiresonance as a function of the dc biasing field for different crystallographic quality of the BSTO film: $\xi_S = 1$ (1), $\xi_S = 5$ (2). Other parameters are the same as in legend to Fig. 1.

on the biasing voltage:

$$\phi(E^{(dc)}) = k(E^{(dc)}) \cdot h = \frac{\omega}{V_{ac}(E^{(dc)})} \cdot h \tag{7}$$

$$V_{ac}(E^{(dc)}) = V_{ac}^{(0)} \cdot \sqrt{1 + K(E^{(dc)})^2}, \quad V_{ac}^{(0)} = \sqrt{\frac{c}{\rho}} \tag{8}$$

Here c is the elastic constant and ρ is the material density.

One can write the following cause–effect consecution:

$$K(E^{(dc)}) \to V_{ac}(E^{(dc)}) \to k(E^{(dc)}) \to \phi(E^{(dc)}), \tag{9}$$

The acoustic length ϕ ($E^{(dc)}$) is further used for a description of resonant conditions.

In line with (6), there are two specific cases when $Z_{in} = 0$ related to the resonance and $Z_{in} = \infty$ related to the antiresonance. Solving (6) for these two cases one can find ϕ_{res} ($E^{(dc)}$) and ϕ_{ares} ($E^{(dc)}$) for resonance and antiresonance. The corresponding frequencies are

$$f_{res} = \frac{V_{ac}(E^{(dc)})}{\lambda_{ac}^{res}(E^{(dc)})} \quad \text{with} \quad \lambda_{ac}^{res}(E^{(dc)}) = \frac{2\pi h}{\phi_{res}(E^{(dc)})} \tag{10}$$

$$f_{ares} = \frac{V_{ac}(E^{(dc)})}{\lambda_{ac}^{ares}(E^{(dc)})} \quad \text{with} \quad \lambda_{ac}^{ares}(E^{(dc)}) = \frac{2\pi h}{\phi_{ares}(E^{(dc)})} \tag{11}$$

In the case of perfect boundary conditions $Z_L = Z_R = 0$, the Eq. (6) is simplified and the resonant acoustic length for the resonance ϕ_{res} ($E^{(dc)}$) can be found form the equation:

$$K(E^{(dc)})^2 = \frac{\tan\,\phi_{res}(E^{(dc)})}{\phi_{res}(E^{(dc)})}, \tag{12}$$

and ϕ_{ares} ($E^{(dc)}$) for the antiresonance is found from

$$\tan\,\phi_{ares}(E^{(dc)}) = \infty \to \phi_{ares}(E^{(dc)}) = \frac{\pi}{2}. \tag{13}$$

The results of modeling the resonant frequency dependence on the dc biasing field (antiresonance) are presented in Fig. 3 for the BSTO film with $V_{ac}(0) = 8000$ m/s, attenuation constant $\alpha = 0.001$, and the thickness of the film $2h = 500$ nm. The results are shown for the first antiresonant mode. For the resonance, the frequency shift is slightly less as compared with the antiresonance. In the case of a real system of electrodes,[7] the input impedance exhibits multiresonance tuneable response for the both resonance and antiresonance containing additional spurious responses related to the acoustic resonances in the whole multi-electrode structure. The tuneability of the BSTO response is less pronounced in this case. Evidently, a special trouble should be taken to provide highly reflective boundary conditions. For this, the Bragg reflection structure or membrane structure made by micromachinary technique can be used.

4. Conclusion

Modeling of excitation of the acoustic wave oscillations by the induced piezoeffect in ferroelectric materials (BSTO film) revealed that there is a maximum in the dependence of the electromechanical coupling coefficient on the dc electric field. The value of maximum and the related dc field depend on the ferroelectric film quality. The tuneability of the resonant frequencies of resonance and antiresonance was demonstrated. The model developed can be used as a basis of a design of a tuneable bulk acoustic resonator for microwave application.

Acknowledgment

The investigation was supported by the Project "NANOSTAR" Project No. 016340 (IST-NMP-3), the 6th Framework Programme of the European Commission.

References

1. Lakin, K. M., Kline, G. R. and McCarron, K. T., High-Q microwave acoustic resonators and filters. *IEEE Trans. MTT*, 1993, **41**(12), 2139–2146.
2. Park, J. Y., Lee, H. C., Lee, K. H., Ko, Y. J. and Bu, J. U., Silicon bulk micromachined FBAR filters for W-CDMA applications. In *Proceedings of the 33rd European microwave conference*, 2003, pp. 907–910.
3. Ellae, J., Pohjonen, H., Kylaekoski, J., Kulojaervi, M. and Kuisma, E., FBAR filters – key components for future cellular RF miniaturization. In *Proceedings of the 6th European Conference on Wireless Technology*, 2004, pp. 273–276.
4. Ruprecht, G. and Winter, W. H., Electromechanical behavior of single-crystal strontium titanate. *Phys. Rev. B*, 1967, **155**, 1019–1028.
5. Vorobiev, A., Rundquist, P., Kamchane, K. and Gevorgian, S., Silicon substrate integrated high Q-factor parallel-plate ferroelectric varactors for microwave/millmeterwave applications. *Appl. Phys. Lett.*, 2003, **83**, 1344–1346.
6. Gevorgian, S., Vorobiev, A. and Berge, J., Electromechanical modelling and reduction of the electroacoustic losses in parallel-plate ferroelectric varactors. In *Proceedings of the 36th European Microwave Conference*, 2006, pp. 851–853.
7. Gevorgian, S., Vorobiev, A. and Lewin, T., DC field and temperature dependent acoustic resonances in parallel-plate capacitors based on $SrTiO_3$ and $Ba_{0.25}$ $Sr_{0.75}$ TiO_3 films. Experiment and modeling. *J. Appl. Phys.*, 2006, **99**, 124112-1.
8. Pond, J. M., Kirchoffer, S. W., Chang, W., Horwitz, J. S. and Chrisey, D. B., Microwave properties of ferroelectric thin films. *Integr. Ferroelectr.*, 1998, **22**, 317–328.
9. Krowne, C. M., Daniel, M., Kirchoefer, S. W. and Pond, J. M., Anisotropic permittivity and attenuation extraction from propagation constant measurements using an anisotropic full-wave Green's function solver for coplanar ferroelectric thin film devices. *IEEE Trans. Microwave Theory Tech.*, 2002, **50**(2), 537–548.

10. Tappe, S., Boettger, U. and Waser, R., Electrostrictive resonance I $(Ba_{0.7}Sr_{0.3})TiO_3$ thin films at microwave frequency. *Appl. Phys. Lett.*, 2004, **85**(4), 624–626.
11. Vendik, O. G. and Ter-Martirosyan, L. T., Electrostrictive mechanism of microwave losses in a planar strontium titanate film capacitor. *Tech. Phys.*, 1999, **44**(8), 954–960.
12. Vendik, O. G. and Rogachev, A. N., Electrostriction mechanism of microwave losses in a ferroelectric film and experimental confirmation. *Tech. Phys. Lett.*, 1999, **25**(9), 702–704.
13. Berlincourt, D. A., Curran, D. R. and Jaffe, H., Physical acoustics. In *Methods and devices*, *vol. 1*, ed. W. Mason. Academic Press, New York, 1964 [Part A].
14. Nye, J. F., *Physical Properties of Crystals: Their Representation by Tensors and Matrices*. Clarendon Press, Oxford, 1957.
15. Zheludev, I. S., *Physics of crystalline dielectrics*, *vols. 1 and 2*. Plenum Press, New York, 1971.
16. Smolensky, G. A., *Ferroelectrics and Related Materials*. Gordon and Breach, New York, 1985.
17. Vendik, O. G. and Zubko, S. P., Ferroelectic phase transition and maximum dielectric permittivity of displacement type ferroelectrics $(Ba_xSr_{1-x}TiO_3)$. *J. Appl. Phys.*, 2000, **88**(9), 5343–5350.