Development and investigation of micro- and nanostructures of metamaterials to form the necessary characteristics and coefficients of piezoelectric elements

V.S. But^{1,2}, S.V. Karpeev¹, E.S. Karlin^{1,2}

¹Samara National Research University, Moskovskoye shosse 34, Samara, Russia, 443086 ²KROHNE – Automatic LLC, Samara, Russia, 443004

Abstract. The development and research of micro and nanostructures for the manufacture of ultrasonic piezoacoustic elements has been carried out. The structures obtained in this work have practical applications for the manufacture of piezoelectric and piezoacoustic elements, in particular, for using in liquid flowmeters as receivers and emitters of an ultrasonic signal. A structure of nanocells was obtained that was different from standard piezoelectric elements (disk, cylinder), but with the same coefficients, characteristics, and radiation pattern.

1. Introduction

The piezomaterials are of great interest because of their unique properties since the discovery of the direct and inverse piezoelectric effect of single crystals by the Curie brothers in 1880 and 1881. And the discovery of the possibility of polarizing ceramic material with an electric field in 1946 led to the widespread distribution of piezoelectric and piezoelectric elements. The ability of piezoelectric materials to convert mechanical energy into electrical energy and vice versa allows them to be used in ultrasonic measurements, in pressure measurements, in medicine, in flow detectors, seismic sensors and energy collection systems. In addition, applying an AC voltage to the material causes it to vibrate and thus creates mechanical waves with the same frequency as the electric voltage, which can be used in micro-positioning devices, such as attenuators, scanning tunnelling microscopes, etc. Similarly, if mechanical vibration is used, a charge of a proportional size and the same frequency will be generated [1]. In some problems, piezoelectric materials are indispensable, since without this physical process it will be impossible to make studies or measurements.

But all the characteristics, coefficients, and piezoelectric constants of existing standard piezoelectric elements, such as a disk, cylinder, etc., are dictated by their structure and chemical composition. This leads to the fact that the properties of the piezoelectric elements, such as the radiation pattern or conversion coefficient, remain constant for the whole wide range of tasks. It is necessary to find such technical solutions in which the maximum response of the piezoelectric element and the complexity of the entire system design. In non-trivial problems, the necessary radiation pattern, which will correspond to the best signal emission result, cannot be obtained with standard piezoelectric elements. Even the addition of impurities to the crystallographic structures of piezoelectric materials cannot lead to the possibility of dynamically adjusting the piezoelectric constants in certain directions, since the set of alloying components is limited, and any changes to the geometry of standard piezoelectric elements, in an attempt to obtain the desired characteristics, will lead to a change in the

Секция: Компьютерная оптика и нанофотоника

Development and investigation of micro- and nanostructures of metamaterials to form the necessary characteristics and coefficients of piezoelectric elements

electrical and acoustic properties. One way to avoid losing the necessary parameters is to use metamaterials with a specific geometry to create piezoacoustic and piezoelectric elements. In this case, it will be possible to select material for a given geometry, and not vice versa [1].

With a certain structure of the connection of the nanocells (3 - 200 nm) of the piezoelectric materials, electromechanical bonds are formed, in which the piezoelectric properties are improved by changing parameters such as the electromechanical coupling coefficient, conversion coefficient, quality factor, piezoelectric module, etc. Due to these improvements, the efficiency of piezoelectric elements is significantly increased. These nanocells are three-dimensional (3D) structural nodes, as shown in Figure 1 [1].

3-strut, N = 5 (+ + +)	3 1		3 1,2	4 strut, N = 8 ()	3 L.1	S L2	3 -2	×
3-strut, N = 5 (+) and ()	-3-11 -1	3 1_2	3 1_2	5-strut, N = 9 (+ + +)	3 1.1	3 1_2	3 1_2	H
4-strut, N = 8 (+ + +)			3	5-strut, N = 9 (+) and ()	3 1_1	3 2	3 1_2	

Figure 1. Three-dimensional structural units [1].

Nanocomposite piezoelectric metamaterials from these structures achieve a high conversion coefficient and a piezoelectric voltage coefficient, and also have a high flexibility of characteristics, which is not achievable using standard piezoelectric and piezoelectric elements [3].

When using these structures, the field of application of piezoelectric elements significantly expands and their efficiency increases several times. There is the possibility of manufacturing piezoelectric elements with the necessary geometry for the user based on the task.

The purpose of this work is to obtain new structures to form the necessary characteristics.

2. Piezoelectric elements

One of the standard versions of piezo-acoustic elements are discs of various diameters (figure 2).



Figure 2. Standard piezoacoustic element with a diameter of 4 mm for a frequency of 1 MHz.

This element has certain characteristics and coefficients, which are key parameters. For this type of piezoelectric elements, there can be the following modes, presented in table 1[12].

The main coefficients and characteristics for piezoelectric elements, which determine their properties and are determined by the structure, geometry and impurities [2]:

- 1. Dielectric constant
- 2. Conversion coefficient
- 3. Dielectric loss factor
- 4. Quality factor of the elastic system
- 5. Frequency constant
- 6. Electromechanical coupling coefficient
- 7. Coefficient of the piezoelectric charge

Development and investigation of micro- and nanostructures of metamaterials to form the necessary characteristics and coefficients of piezoelectric elements

- 8. Piezoelectric voltage factor
- 9. Coefficient of elastic compliance
- 10. Rate of aging
- 11. Curie point



To describe these constants, it is necessary to consider elements as 3D objects with three possible directions of action of forces and three rotation axes, as shown in Figure 6. Also in this figure, directions (1 - 6) are numbered [3].



Figure 3. Stress application directions [12].

All characteristics and constants are indicated in accordance with the position of the electrodes on the cell, the direction of the applied voltage or load, the direction of shear, etc. Examples of these designations are presented in table 2 [12].

3. Modeling

Figure 3 shows a model of a standard piezoelectric element, which is used as a receiver and transmitter of an ultrasonic signal.

Figure 4 shows a micro-cell, which is used as a structural unit for constructing a new piezoelectric element (this cell was used in [1], a microscope image of the structure from these cells is shown in Figure 5 [1]).

Секция: Компьютерная оптика и нанофотоника

Development and investigation of micro- and nanostructures of metamaterials to form the necessary characteristics and coefficients of piezoelectric elements



Figure 4. Piezoelectric element.

 Table 2. Designations [12]

Relative dielectric	$K_{3}^{S} \rightarrow All$ strains in the material are constant or mechanical deformation is blocked in any direction $K_{3}^{S} \rightarrow Electrodes$ are perpendicular to 3 axis						
constant $\varepsilon_3^S/\varepsilon_0$ and $\varepsilon_1^T/\varepsilon_0$	$K_1^T \rightarrow \text{All stresses on material are constant or no external forces.}$						
Flactromachanical	$k_p \rightarrow \text{Stress}$ or strain is equal in all directions perpendicular to 3 axis						
coupling factor	$k_{15} \rightarrow$ Stress or strain is equal in all directions perpendicular to 3 axis						
	9 Electrodes are perpendicular to 1 axis.						
Diazoalactric charge	$d_h \rightarrow {\rm Hydrostatic}$ stress or stress is applied equally in all directions.						
coefficient	$d_{33} \rightarrow Applied stress, or piezoelectrically induced strain is in 3 direction$						
	 Electrodes are perpendicular to 3 axis. 						
	$g_{15} \rightarrow$ Applied stress,or the piezoelectrically induced strain is in shear form around 2 axis.						
Piezoelectric voltage	Electrodes are perpendicular to 1 axis.						
coefficient	$g_{31} \rightarrow$ Applied stress,or the piezoelectrically induced strain is in 1 direction.						
	Electrodes are perpendicular to 3 axis.						
	SE- Compliance is measured with closed circuit. S36- Stress or strain is shear around 3 direction Strain or stress is in 3 direction						
Elastic compliance	SD- Compliance is measured with open circuit. 11- Stress or strain is in 1 direction						
	Strain or stress is in 1 direction.						



Figure 4. Microcell.

Figure 5. Microcell piezoelectric structure [1].

Секция: Компьютерная оптика и нанофотоника Development and investigation of micro- and nanostructures of metamaterials to form the necessary characteristics and coefficients of piezoelectric elements

The piezoelectric element shown in Figure 6 was constructed from these cells with the same geometric parameters as the standard one. In this sample, the upper and lower platforms of the model were chosen as electrodes for positive and negative potentials.



Figure 6. Piezoelectric element design.

The standard model (Figure 3) and designed (Figure 6) were modeled under conditions of creating a potential difference between their surfaces. Figure 7 shows the deformation diagrams of element when applying a voltage of 5V.



Figure 7. Standard element deformation diagram.

4. Conclusion

A theoretical study of the constants and coefficients for piezoelectric elements was carried out, as well as the influence of various physical properties on the characteristics and response of piezoelectric and piezoelectric materials. It was found that the dielectric constant, conversion coefficient, dielectric loss coefficient, Q factor of the elastic system, frequency constant, electromechanical coupling coefficient, piezoelectric charge coefficient, piezoelectric stress coefficient, elastic compliance coefficient, aging rate and Curie point for the piezoelectric element depend on its structure and composition.

The processes of the piezoelectric effect for a standard piezoelectric element with a diameter of 4 mm and a thickness of 2 mm were simulated, as well as a piezoelectric element constructed from microcells with preserved geometric parameters. A unit cell option was proposed for piezoelectric material structures from which a non-standard element was assembled.

This element allows you to achieve different characteristics and efficiency compared to standard piezoelectric elements, while maintaining the same overall dimensions. The use of various configurations of microcells to create structures of piezoelectric materials allows you to change the properties, parameters and characteristics of piezoelectric elements made from these structures.

5. Acknowledgments

This work was supported by the Russian Foundation for Basic Research under project No. 18-29-20045.

Секция: Компьютерная оптика и нанофотоника Development and investigation of micro- and nanostructures of metamaterials to form the necessary characteristics and coefficients of piezoelectric elements

6. References

- [1] Cui, H. Chemical Three-dimensional printing of piezoelectric materials with designed anisotropy and directional response / H. Cui, R. Hensleigh, D. Yao, D. Maurya, P. Kumar, M.G. Kang, Sh. Priya, X. Zheng // Nature Materials. – 2019. – Vol. 18. – P. 234-241.
- [2] Jaffe, B. Piezoelectric ceramics / B. Jaffe, W. Kuk, G. Jaffe M.: Mir, 1974. P. 288.
- [3] Moulson, A.J. Electroceramics / A.J. Moulson, J.M. Herbert // Chapman and Hall, 1990. P. 121.
- [4] Setter, N. Piezoelectric Materials in Devices // EPFL-LC, 2002. P. 518.
- [5] Burfoot, J.C. Polar Dielectrics and their Applications // University of California Press, 1979.
- [6] Corker, D.L. Liquid-Phase Sintering of PZT Ceramics / D.L. Corker, R.W. Whatmore, E. Ringgaard, W.W. Wolny // Eur. Ceram. Soc. 2004. Vol. 20. P. 2039-2045.
- [7] Gómez, T.E. Ceramic Powder Polymer Piezocomposites for Electroacoustic Transduction: Modeling and Design / T.E. Gómez, F. Montero de Espinosa, F. Levassort, M. Lethiecq, A. James, E. Ringgaard, C.E. Millar, P. Hawkins // Ultrasonics. – 2010. – Vol. – 36. – P. 907-923.
- [8] Tripathi, N. Analysis and optimization of photonics devices manufacturing technologies based on Carbon Nanotubes / N. Tripathi, V.S. Pavelyev, V.S. But, S.A. Lebedev, S. Kumar, P. Sharma, P. Mishra, M.A. Sovetkina, S.A. Fomchenkov, V.V. Podlipnov, V. Platonov // Journal of Physics: Conference Series. – 2019. – Vol. 1368. DOI: 10.1088/1742-6596/1368/2/022034.
- [9] González, A.M. Determination of the Frequency Dependence of Characteristic Constants in Lossy Piezoelectric Materials / A.M. González, C. Alemany // J. Phys. D: Appl.Phys. – 2012. – Vol. 29. – P. 2476-2482.
- [10] Lethiecq, M. High Permittivity Ceramics for Medical Ultrasonic Transducers: a Study on the Optimisation of Processing Parameters / M. Lethiecq, F. Levassort, A.S. James, W.W. Wolny, J.P. Mercurio, B.M. Kulwicki, A. Amin, A. Safari // Proc. 10th IEEE International Symp. on Applications of Ferroelectrics, 1996. – P. 287-290.
- [11] Millar, C.E. Fabrication of High Density, Fine-Grained PZT Ceramics Using a Post Sinter HIP Treatment / C.E. Millar, B. Andersen, E. Ringgaard, W.W. Wolny, J. Ricote, L. Pardo // ISAF. – 1990. – Vol. 10.
- [12] Ferroperm Catalogue, 2003.
- [13] Makariev, D. I. Possibility of creating digital piezomaterials based on mixed composites "piezoceramic-polymer" / D. I. Makariev, A. N. Rybyanets, G. M. Mayak // Letter to ZhTF. – 2019. – Vol. 41. – P. 22-27.
- [14] Yasuyoshi, S. Lead-free piezoceramics / S. Yasuyoshi, T. Hisaaki, T. Toshihiko, N. Tatsuhiko, T. Kazumasa, H. Takahiko, N. Toshiatsu, N. Masaya // Nature. – 2004. – Vol. 432. – P. 84-87.
- [15] Yasuda. Origami-based impact mitigation via rarefaction solitary wave creation / Yasuda, Y. Miyazawa, E.G. Charalampidis, Ch. Chong, P.G. Kevrekidis, J. Yang // Science Advances. 2019. Vol. 5. P. 1-8.
- [16] Kornienko, V.S. Brownian dynamics of the self-assembly of complex nanostructures in the field of quasi-resonant laser radiation / V.S. Kornienko, A.S. Tsipotan, A. S. Aleksandrovsky, V.V. Slabko // Photonics and Nanostructures - Fundamentals and Applications. – 2019. – Vol. 35.
- [17] Wiegleb, G. Sensors M.: Mir, 1989.
- [18] Storozhenko, D.V. Excitonic optical nonlinearity of dielectric nanocomposites in weak optical fields / D.V. Storozhenko, V.P. Dzyuba, Y.N. Kulchin, A.V. Amosov // Computer Optics. – 2016. – Vol. 40(6). – P. 855-862. DOI: 10.18287/2412-6179-2016-40-6-855-862.
- [19] Li, F. Ultrahigh piezoelectricity in ferroelectric ceramics by design // Nat. Mater. 2018. Vol. 17. – P. 349-354.
- [20] Zhang, S. Focusing ultrasound with an acoustic metamaterial network / S. Zhang, L. Yin, N. Fang // Phys. Rev. Lett. 2009. Vol. 102.