

# Aspects of symmetry of Electromechanical Coupling Factors in Piezoelectric Single Crystals

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**Abstract.** This paper presents the method for the calculation of anisotropic piezoelectric properties of single crystals and the graphical display of the results in 3 D. Crystallographic preferred orientations were determined for piezoelectric modules and electromechanical coupling factor, which measures the ability of a material to interconvert electrical and mechanical energy.

## 1. Introduction

Certain materials produce electric charges on their surfaces as a consequence of applying mechanical stress. The induced charges are proportional to the mechanical stress. This is called the direct piezoelectric effect and was discovered in quartz by Piere and Jacques Curie in 1880.

The direct effect can be written as the relationship between the 2nd rank stress tensor  $x_{jk}$  and 1st rank electric polarization vector  $P_i$ , linked by the 3rd piezoelectric tensor  $d_{ijk}$  as follows:

$$P_i = \sum_{j=1}^3 \sum_{k=1}^3 d_{ij} X_{jk}, \quad i = 1, 2, 3 \quad (1)$$

In the literature the tensor  $d_{ijk}$  is reported for single crystals in the practical and compact Voigt matrix notation. The conversion from Voigt notation  $d_{il}$  to tensor  $d_{ijk}$  notation  $d_{ijk} = d_{il}$  when  $l = 1; 2; 3$  and  $d_{ijk} = \frac{1}{2} d_{il}$  when  $l = 4; 5; 6$ . The direct effects can also be written in Voigt matrix notation as:

$$P_i = \sum_{l=1}^6 d_{il} \sigma_j, \quad i = 1, 2, 3 \quad (2)$$

All crystals belong the 21 non-centrosymmetric points groups are piezoelectrically active, with the exception of the cubic 432, [1].

However, the description of the properties of piezoelectric materials is impossible without the involvement of the elastic and dielectric coefficient as the piezoelectric property by definition implies the connection between the elastic and dielectric characteristics. From this point of view, for comparison of their piezo properties useful so-called electromechanical coupling factor  $k$  (ECF):

$$k^2 = (\text{Stored mechanical energy} / \text{Input electrical energy}) \quad (3)$$

or

$$k^2 = (\text{Stored electrical energy} / \text{Input mechanical energy}) \quad (4)$$

A system of the ECFs is introduced to describe the conversion and takes into account the symmetry of a piezoelectric material, orientations of its crystallographic axes, etc. A larger absolute value of the



ECF  $|k|$  implies a more efficient performance of a piezoelectric material at a specific mode of oscillation and  $k^2$  is used to characterize the magnitude of the transducer bandwidth. Knowledge of the ECF values of piezoelectrics is important for energy-harvesting applications in the context of relationships between the amount of stored and supplied energy.

The single crystals (SCs) are anisotropic, exhibiting different material properties depending on the cut of the materials. The single crystal piezoelectric tensor can be visualized by indicatory surfaces, which radius vector is proportional to the value of the property in arbitrary direction  $n$ , [2]. For the construction of three-dimensional models of surfaces of piezoelectric coefficients was used MTEX open-source package, [3].

## 2. Research method

The work presents the aspects of anisotropy and symmetry of longitudinal piezoelectric effect. The piezoelectric effect is called longitudinal when the polarization and mechanical stress directions coincide.

Since the electromechanical coupling factor depends on the number of anisotropic properties: electrical  $\epsilon$  (2nd rank tensor), piezoelectric  $d$  (3rd rank tensor) and elastic properties  $s$  (4th rank tensor), it is also anisotropic and can be described via the indicatory surface.

The base of visualizations of surface orientation dependence of ECF is the value of the  $k$  in a direction  $n$ :

$$r = k_n = d/(\epsilon_0 \epsilon S)^{1/2} \quad (5)$$

The analysis of the received indicatory surfaces allows to define the symmetry and the anisotropy of the properties, and, if necessary, establish the directions of its extreme value.

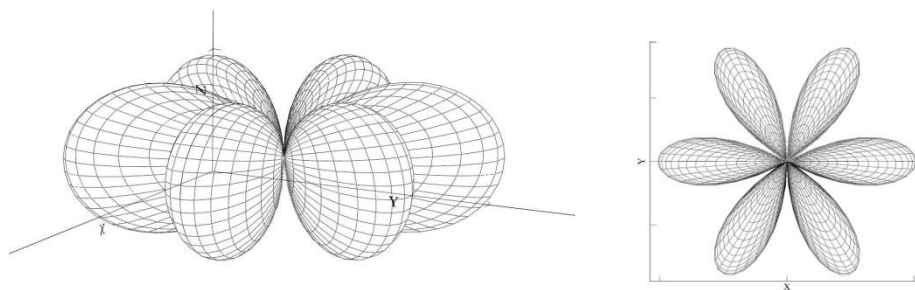
## 3. Analysis and discussion

Although piezoelectric ceramics are widely used for a large number of applications, single crystal materials retain their utility, being essential for applications such as frequency stabilized oscillators and surface acoustic devices.

The most popular single-crystal piezoelectric materials are quartz ( $\text{SiO}_2$ ), lithium niobate ( $\text{LiNbO}_3$ ), lithium tantalate ( $\text{LiTaO}_3$ ), barium titanate ( $\text{BaTiO}_3$ ) and etc.

Quartz has been the first and widespread piezoelectric material. Below  $T = 847$  K quartz is related to the 32 symmetry class. According to room-temperature experimental data, these piezoelectric coefficients are  $d_{11} = 2.30$  pC/N and  $d_{14} = -0.693$  pC/N, table 1.

Taking into account elastic compliances of the quartz and its dielectric permittivity, we obtain the ECFs as follows, figure 1.



**Figure 1.** The indicatory surface of longitudinal electromechanical coupling factor  $k$  of quartz ( $\text{SiO}_2$ ) and its projection onto the plane (XOY).

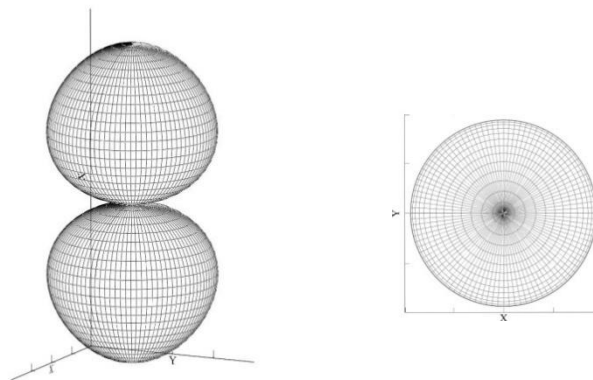
This indicatory surface consisting of alternating positive and negative parts is related to the  $\bar{6}m2$  symmetry class. Maximum longitudinal piezoelectric effect (as well as the maximum value of  $k$ ) is

observed along the polar axis of symmetry of the second order. Along the Z-axis of the longitudinal piezoelectric effect is not observed.

**Table 1.** Experimental values of elastic compliances  $s$  (in  $10^{-12}$  Pa $^{-1}$ ), piezoelectric coefficients  $d$  (in pC/N), dielectric permittivities  $\varepsilon/\varepsilon_0$  of some piezoelectric SCs at room temperature, [4].

	BaTiO <sub>3</sub>	CdS	SiO <sub>2</sub>
$S_{11}^E$	7,92	20,69	12,79
$S_{12}^E$	-3,80	-9,93	-1,54
$S_{13}^E$	-1,28	-5,81	-1,10
$S_{14}^E$			4,46
$S_{22}^E$	8,05		
$S_{23}^E$	-3,80		
$S_{33}^E$	7,92	16,97	9,56
$S_{44}^E$	11,9	66,49	19,78
$S_{55}^E$	30,2		
$S_{66}^E$	13,6	61,36	
$d_{11}$			2,3
$d_{14}$			-0,693
$d_{15}$	126	-13,98	
$d_{24}$	269		
$d_{31}$	-189	-5,18	
$d_{32}$	-24,5		
$d_{33}$	225	10,32	
$\varepsilon_{11}^T/\varepsilon_0$	265	9,35	4,520
$\varepsilon_{33}^T/\varepsilon_0$	2130	10,38	4,6

To the best of our knowledge, the important group of piezoelectric SCs consist of compounds such as  $\alpha$ -ZnS, CdS, CdSe, ZnO, etc. from the 6mm symmetry class. The ECFs for the CdS have the form on figure 2.

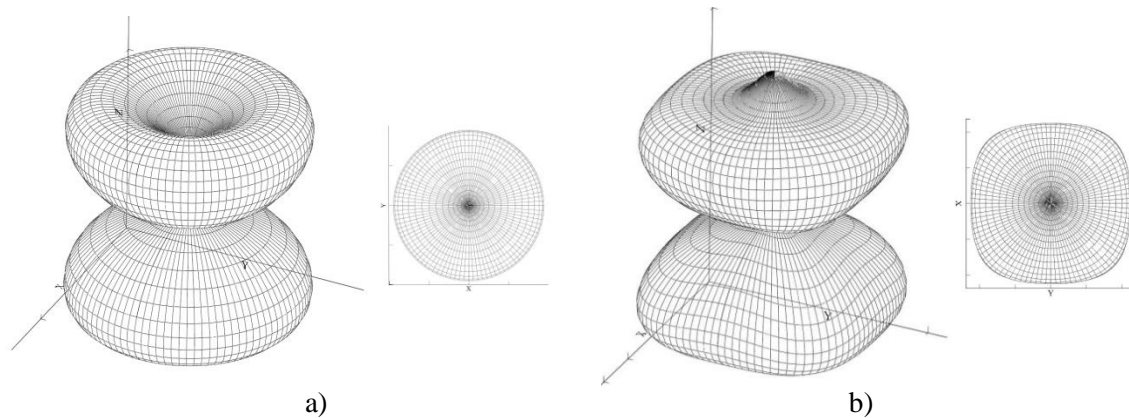


**Figure 2.** The indicatory surface of longitudinal electromechanical coupling factor  $k$  of CdS and its projection onto the plane (XOY).

The symmetry of this surface identical with the symmetry of the indicatory surface of the piezoelectric modules in CdS and describes the class  $\infty$ mm. Perpendicular to the Z-axis there is anti-symmetry plane, since its upper and lower parts have different signs.

Barium titanate BaTiO<sub>3</sub> (the perovskite-type ferroelectric crystals) is one of the most thoroughly studied and most widely used piezoelectric materials, [1, 4]. Just below the Curie temperature (120°C), the vector of the spontaneous polarization points in the [001] direction (tetragonal phase), below 5 °C it

reorients in the [011] (orthorhombic phase) and below - 90 °C in the [111] direction (rhombohedral phase). Example of electromechanical and piezoelectric constants surfaces of the BaTiO<sub>3</sub> single crystals (4mm symmetry class) are given in figure 3.



**Figure 3.** The indicatory surface of longitudinal piezoelectric effect in BaTiO<sub>3</sub> and its projection onto the plane (XOY) (a); the indicatory surface of longitudinal electromechanical coupling factor k in BaTiO<sub>3</sub> and its projection onto the plane (XOY) (b).

In contrast to the previous cases, symmetry of surfaces are different, and respectively, the directions with extreme values of properties are also different.

The indicatory surface of piezoelectric modules is the rotational surface, i.e. it possesses the symmetry axis of infinite order, directed along the coordinat Z axis, chosen along the fourth order axis in SCs. The symmetry class of this surface is  $\infty$ mm. The piezoelectric effect is zero perpendicular to the fourth order symmetry axis (Z axis). The maximum piezoelectric effect in the SCs of barium titanate can be obtained by cutting out the rod along the directions cone with the half of its internal angle of 51°5' to the Z axis.

The symmetry of electromechanical coupling factor orientation dependence is defined by the indicatory surfaces superposition of values describing it. Herewith the determining role is played by those surfaces which symmetry is lower. Thus, in the barium titanate electromechanical coupling factor indicatory surface the fourth order symmetry axis appears which caused by the aspects of its elastic properties. The symmetry of this surface 4mm is equal to the symmetry of the crystal itself. The maximum electromechanical coupling factor in this crystal can be obtained by deforming barium titanate along directions being at the angle 49°23' to the Z axis.

#### 4. Conclusion

We calculated efficiency of mechanical-to-electrical energy conversion, depending on the direction of applied load with respect to the crystallographic axes for a wide range of single piezoelectric crystals.

#### References

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