Generalized Continuum and Linear Theory of Piezoelectric Materials*

Abstract

Theory of the piezoelectric materials had been developed many years ago. It was supposed that the stress state of the piezoelectric material can be described by means of the symmetrical stress tensor. However it can be shown that as a matter of fact the particles of the piezoelectric material must be considered as dipoles. It means that the theory of the piezoelectric materials must be constructed on the base of the generalized continuum. The theory of such a kind is presented in the report. The basic equations are derived from the fundamental laws of Eulerian mechanics. It is shown that the type of the electric field vector is important, since it influences on the structure of the basic equations.

1 Introduction

The brothers Pierre and Jacques Curie, in 1880, were the first to experimentally demonstrate piezoelectric behavior in a series of crystals, including quartz and Rochelle salt. The first attempt to derive the theory of piezoelectricity was made by Voigt in 1910.

Crystals with piezoelectric properties are very useful for different scientific and industrial applications. The direct piezoelectric effect occurs when an applied stress produces an electric polarization. The inverse piezoelectric effect occurs when an applied electric field produces a strain. These coupled effects let the electronic industry to produce many useful devices such as piezoelectric crystals, filters and resonators. First crystals were created by W. Cady in 1923 on the base of the natural α-quartz. To the present time the construction and characteristics of crystals were essentially improved.

There exist a several theories of the piezoelectricity. All of them lead to the very complicated equations. The exact solutions of these equations may be found only for very particular cases. By this reason it is not easy to compare theoretical and experimental results. At the present time it seems to be possible to say that there is no qualitative discrepancies between theory and experiments. From the pure theoretical point of view in the theory of the piezoelectricity there are some serious problems. The first problem. In electrodynamics the choice of the type of the electric field vector **E** does not matter and there are no reasons to make this choice. In the

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piezoelectricity it is not so and the type of **E** is important. In conventional theories the vector **E** is supposed to be a polar vector. In what follows we consider the theories when the type of **E** may be changed. The second problem. At least some piezoelectric materials are the dipole crystals. In such a case the rotation degrees of freedom must be taken into account.

2 The classical theory of piezoelectricity

There are several theories [1, 2, 3] to describe piezoelectricity. All of them are almost the same and based on classical theory of elasticity with the symmetrical stress tensor. Below the notation of a book [4] will be used. The basic equations can be represented in the conventional form.

The equations of motion:

$$\nabla \cdot \boldsymbol{\tau} + \rho \mathbf{F} = \rho \ddot{\mathbf{u}}, \quad \boldsymbol{\tau} = \boldsymbol{\tau}^{T}, \tag{1}$$

where $\boldsymbol{\tau}$ is the stress tensor, ρ is the mass density, $\mathbf{u}$ is the displacement vector.

The Poisson equations for crystal and vacuum respectively:

$$\nabla \cdot \mathbf{D} = 0, \quad \nabla \cdot \mathbf{E}' = 0, \tag{2}$$

where $\mathbf{D}$ is the electrical induction, $\mathbf{E}'$ is the electrical field in the vacuum.

The piezoelectric effect equations

$$\boldsymbol{\tau} = \mathbf{C} \cdot \cdot \varepsilon - \mathbf{E} \cdot \mathbf{e}, \quad \mathbf{D} = \varepsilon \cdot\cdot \mathbf{e} + \boldsymbol{\epsilon} \cdot \mathbf{E}, \tag{3}$$

where $\mathbf{E}$ is the electrical field in the crystal, $\boldsymbol{\varepsilon}$ is the tensor of the linear deformation, $\mathbf{C}$ is the elasticity tensor, $\mathbf{e}$ is the tensor of piezoelectric modulus, $\boldsymbol{\epsilon}$ is the dielectric tensor.

This conventional theory is supposed to be able to give the description of all known experimental data. It is not so easy to confirm this point of view. In many practical cases we have the conspicuous discrepancy between the theoretical and experimental results — see, for example, the paper [5]. However the exact reasons of this discrepancy are not known. May be the reason is that the exact solutions of the system (1)–(3) can be found only in very particular cases. As a rule it is possible to find the approximation solution and because of this the solution does not coincide with an experiment.

However, it is quiet possible that the conventional theory (1)–(3) must be improved in some points. First of all, at least some piezoelectric crystals must be considered as dipole media. For example, it is easy calculate that the α-quartz is dipole crystal. It means that the rotational degrees of freedom must be taken into account.

The present paper is an attempt to consider piezoelectricity from this point of view.

3 The Euler Laws of Dynamics

Let us consider the elastic body. Let x_s be material (Lagrangian) coordinates. Let $\mathbf{r}(x_s)$ and $\mathbf{R}(x_s)$ be radius-vectors of the points in the reference and the actual configuration respectively. Bases in the reference and actual configurations are defined by following equations:

$$\mathbf{g}_s = \frac{\partial \mathbf{r}}{\partial x^s}, \quad \mathbf{G}_s(\mathbf{x}, t) = \frac{\partial \mathbf{R}(\mathbf{x}, t)}{\partial x^s}.$$

Let us introduce the reciprocal bases $\mathbf{g}^s$ $\mathbf{G}^s$ by means of the next expressions:

$$\mathbf{g}^s \cdot \mathbf{g}_m = \delta^s_m, \quad \mathbf{G}^s \cdot \mathbf{G}_m = \delta^s_m.$$

In the nonlinear theory it is necessary to use two the Hamilton operators [6]:

$$\overset{\circ}{\nabla} = \mathbf{g}^s \frac{\partial}{\partial x^s}, \quad \nabla = \mathbf{G}^s(\mathbf{x}, t) \frac{\partial}{\partial x^s}$$

for reference and actual configurations respectively.

The first law of dynamics by Euler in the integral form of momentum balance Law takes the following form:

$$\frac{d}{dt} \int_V \rho \dot{\mathbf{u}}_1 \, dV = \int_V \rho \mathbf{F} dV + \int_S \mathbf{T}_{(n)} dS, \tag{4}$$

where $\mathbf{u}(x_s) = \mathbf{R} - \mathbf{r}$ is displacement of the particle, $\mathbf{T}_{(n)}$ is the stress vector, $\mathbf{F}$ is an external force. Making use of Eq.(4) the Cauchy formulae

$$\mathbf{T}_{(n)} = \mathbf{n} \cdot \mathbf{T} \tag{5}$$

can be proved, where the second rank tensor $\mathbf{T}$ is called the Cauchy stress tensor. Taking into account Eqs. (4), (5) and the divergence theorem one can derive the local form of the first law of dynamics

$$\nabla \cdot \mathbf{T} + \rho \mathbf{F} = \rho \ddot{\mathbf{u}}. \tag{6}$$

Here and below we suppose that the displacement vector $\mathbf{u}$ is small, i.e. we shall consider the linear theory. The stress tensor can be represented as decomposition

$$\mathbf{T} = \boldsymbol{\tau} - \frac{1}{2}\mathbf{q} \times \mathbf{I}, \quad \boldsymbol{\tau} = \boldsymbol{\tau}^T, \quad \mathbf{q} = \mathbf{T}_\times \quad ((\mathbf{a} \otimes \mathbf{b})_\times \equiv \mathbf{a} \times \mathbf{b}), \tag{7}$$

where the vector $\mathbf{q}$ determines the antisymmetric part of the stress tensor, $\mathbf{I}$ is the unit tensor. In such a case the Eq.(6) can be rewritten in the form

$$\nabla \cdot \boldsymbol{\tau} - \frac{1}{2} \nabla \times \mathbf{q} + \rho \mathbf{F} = \rho \ddot{\mathbf{u}}. \tag{8}$$

In order to describe the rotations of a particle it is necessary to introduce the turn-tensor $\mathbf{P}$ or the vector of turn $\boldsymbol{\varphi}$. For the small rotations it is possible to use the next relation

$$\mathbf{P} \approx \mathbf{I} + \boldsymbol{\phi} \times \mathbf{I} \quad \Rightarrow \quad \boldsymbol{\omega} = \dot{\boldsymbol{\phi}},$$

where $\boldsymbol{\omega}$ is the angular velocity. According to the accepted model, particles of media are body-points and, thus, we must assign inertia tensor $\mathbf{J}$ for every such body-point. Let us note that the inertia tensor $\mathbf{J}$ is determined in the reference position, thus it has the constant value. In the actual position the inertia tensor must be calculated in the form $\mathbf{P} \cdot \mathbf{J} \cdot \mathbf{P}^T$. For small angular velocities we may use the following expression for kinetic momentum $\mathbf{K}_2$:

$$\mathbf{K}_2 = \rho(\mathbf{J} \cdot \dot{\boldsymbol{\phi}}(\mathbf{x}, t) + \mathbf{r} \times \dot{\mathbf{u}}),$$

where $\boldsymbol{\phi}(\mathbf{x}, t)$ is the vector of turn of the body-point.

The second law of dynamics can be written down in an integral form

$$\frac{d}{dt}\int_V \mathbf{K}_2 dV = \int_V \rho\left(\mathbf{r}\times\mathbf{F}+\mathbf{L}\right) dV + \int_S \left(\mathbf{r}\times\mathbf{T}_{(n)}+\boldsymbol{\mu}_{(n)}\right) dS, \tag{9}$$

where $\mathbf{L}$ is an external moment, $\boldsymbol{\mu}_{(n)}$ is the coupled stress vector. For the couple stress tensor $\boldsymbol{\mu}$ the Cauchy formula

$$\boldsymbol{\mu}_{(n)} = \mathbf{n}\cdot\boldsymbol{\mu} \tag{10}$$

is valid. After some standard transformations one can obtain the kinetic moment balance equation in local form

$$\boldsymbol{\nabla}\cdot\boldsymbol{\mu}+\mathbf{q}+\rho\mathbf{L} = \rho\mathbf{J}\cdot\ddot{\boldsymbol{\phi}}. \tag{11}$$

The equations (8) and (11) are well known in the theory of micropolar media. However, we shall use a special form of the coupled stress tensor

$$\boldsymbol{\mu} = \mathbf{m}\times\mathbf{I}. \tag{12}$$

This means that the coupled stress tensor is antisymmetric. The vector $\mathbf{m}$ determines the antisymmetric part of tensor $\boldsymbol{\mu}$. Of course, the assumption (12) must be justified. Maybe it will be necessary to do this justification in the future. Substituting representation (12) into equation (11) we obtain

$$\boldsymbol{\nabla}\times\mathbf{m}+\mathbf{q}+\rho\mathbf{L} = \rho\mathbf{J}\cdot\ddot{\boldsymbol{\phi}}. \tag{13}$$

4 The equation of the Energy Balance

Now we have to discuss the energy balance equation. The integral form of this equation can be represented as

$$\frac{d}{dt}\int_V\{\frac{1}{2}\rho\dot{\mathbf{u}}^2+\frac{1}{2}\rho\dot{\boldsymbol{\phi}}\cdot\mathbf{J}\cdot\dot{\boldsymbol{\phi}}+\rho\mathbb{U}\}dV = \int_V\{\rho\mathbf{F}\cdot\dot{\mathbf{u}}+\rho\mathbf{L}\cdot\dot{\boldsymbol{\phi}}+Q\}dV + \\ + \int_S\{\mathbf{T}_{(n)}\cdot\dot{\mathbf{u}}+\boldsymbol{\mu}_{(n)}\cdot\dot{\boldsymbol{\phi}}+\mathbf{H}\cdot\mathbf{n}\}dS, \tag{14}$$

where Q is the volume external energy supply and $\mathbf{H}$ is energy flow vector.

Equation (14) may be transformed to the following form

$$\int_V\{\rho\dot{\mathbb{U}}+\dot{\mathbf{u}}\cdot(\rho\ddot{\mathbf{u}}-\rho\mathbf{F}-\boldsymbol{\nabla}\cdot\mathbf{T})+\dot{\boldsymbol{\phi}}\cdot(\rho\mathbf{J}\cdot\ddot{\boldsymbol{\phi}}-\rho\mathbf{L}-\boldsymbol{\nabla}\cdot\boldsymbol{\mu})- \\ -\mathbf{T}^T\cdot\cdot\boldsymbol{\nabla}\dot{\mathbf{u}}-\boldsymbol{\mu}^T\cdot\cdot\boldsymbol{\nabla}\dot{\boldsymbol{\phi}}-Q-\boldsymbol{\nabla}\cdot\mathbf{H}\}dV = 0. \tag{15}$$

Making use the laws of dynamics the equation (15) may be rewritten in the local form

$$\rho\dot{\mathbb{U}} = \mathbf{T}^T\cdot\cdot\boldsymbol{\nabla}\dot{\mathbf{u}}-\mathbf{q}\cdot\dot{\boldsymbol{\phi}}+\boldsymbol{\mu}^T\cdot\cdot\boldsymbol{\nabla}\dot{\boldsymbol{\phi}}+\boldsymbol{\nabla}\cdot\mathbf{H}+Q. \tag{16}$$

It is easy to proof the identity

$$\mathbf{T}^T\cdot\cdot\boldsymbol{\nabla}\dot{\mathbf{u}}-\mathbf{q}\cdot\dot{\boldsymbol{\phi}} = \boldsymbol{\tau}\cdot\cdot\dot{\boldsymbol{\varepsilon}}-\mathbf{q}\cdot\dot{\boldsymbol{\theta}},$$

where

$$\boldsymbol{\varepsilon} \equiv \frac{1}{2}\left(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathsf{T}}\right), \quad \boldsymbol{\theta} \equiv \boldsymbol{\phi} - \frac{1}{2}\nabla \times \mathbf{u}. \tag{17}$$

The symmetric tensor $\boldsymbol{\varepsilon}$ is called the tensor of linear deformation and the vector $\boldsymbol{\theta}$ is the turn of the body-point with respect to its small neighborhood. Equation (16) takes the form

$$\rho\dot{\mathbb{U}} = \boldsymbol{\tau} \cdot\cdot\, \dot{\boldsymbol{\varepsilon}} + \mathbf{q} \cdot \dot{\boldsymbol{\gamma}} + \boldsymbol{\mu}^{\mathsf{T}} \cdot\cdot\, \nabla\dot{\boldsymbol{\phi}} + \nabla \cdot \mathbf{H} + \mathrm{Q}. \tag{18}$$

Making use an idea of the paper [8], let us introduce into consideration two vectors **E** and **D** such that

$$\nabla \cdot \mathbf{H} + \mathrm{Q} = \mathbf{E} \cdot \dot{\mathbf{D}}, \tag{19}$$

where the vectors **E** and **D** will be called the electric field vector and the electric displacement vector respectively. Thus, we may write down the energy balance equation in the final form

$$\rho\dot{\mathbb{U}} = \boldsymbol{\tau} \cdot\cdot\, \dot{\boldsymbol{\varepsilon}} - \mathbf{q} \cdot \dot{\boldsymbol{\theta}} + \boldsymbol{\mu}^{\mathsf{T}} \cdot\cdot\, \nabla\dot{\boldsymbol{\phi}} + \mathbf{E} \cdot \dot{\mathbf{D}}. \tag{20}$$

From this it follows that the volume density of intrinsic energy $\rho\mathbb{U}$ depends on the arguments: $\boldsymbol{\varepsilon}$, $\boldsymbol{\theta}$, **D** and $\nabla\boldsymbol{\phi}$. In many cases it is more convenient to consider the vector **E** as independent variable instead of **D**. In such a case it would be better to use the free energy

$$\rho\mathbb{F} = \rho\mathbb{U} - \mathbf{E} \cdot \mathbf{D}. \tag{21}$$

Free energy depends on $\boldsymbol{\varepsilon}$, $\boldsymbol{\theta}$, **E** and $\nabla\boldsymbol{\phi}$. In terms of the free energy equation (20) may be rewritten as

$$\rho\dot{\mathbb{F}} = \boldsymbol{\tau} \cdot\cdot\, \dot{\boldsymbol{\varepsilon}} + \boldsymbol{\mu}^{\mathsf{T}} \cdot\cdot\, \nabla\dot{\boldsymbol{\phi}} - \mathbf{q} \cdot \dot{\boldsymbol{\theta}} - \mathbf{D} \cdot \dot{\mathbf{E}}. \tag{22}$$

We have

$$\rho\dot{\mathbb{F}} = \left(\frac{\partial\rho\mathbb{F}}{\partial\boldsymbol{\varepsilon}}\right)^{\mathsf{T}} \cdot\cdot\, \dot{\boldsymbol{\varepsilon}} + \frac{\partial\rho\mathbb{F}}{\partial\boldsymbol{\theta}} \cdot \dot{\boldsymbol{\theta}} + \frac{\partial\rho\mathbb{F}}{\partial\mathbf{E}} \cdot \dot{\mathbf{E}} + \left(\frac{\partial\rho\mathbb{F}}{\partial\nabla\boldsymbol{\phi}}\right)^{\mathsf{T}} \cdot \nabla\dot{\boldsymbol{\phi}}. \tag{23}$$

From the comparison of equations (22) and (23) the Cauchy – Green relations follow

$$\boldsymbol{\tau} = \frac{\partial\rho\mathbb{F}}{\partial\boldsymbol{\varepsilon}}, \quad \boldsymbol{\mu} = \frac{\partial\rho\mathbb{F}}{\partial\nabla\boldsymbol{\phi}}, \quad \mathbf{q} = -\frac{\partial\rho\mathbb{F}}{\partial\boldsymbol{\theta}}, \quad \mathbf{D} = -\frac{\partial\rho\mathbb{F}}{\partial\mathbf{E}}. \tag{24}$$

Below the natural state hypothesis is accepted. This means absence of stress when strain is equal to zero. In such a case we have the representation for the free energy in the form

$$\begin{aligned}\rho\mathbb{F} = \rho\mathbb{F}_0 &+ \frac{1}{2}\boldsymbol{\varepsilon} \cdot\cdot\, \mathbf{C} \cdot\cdot\, \boldsymbol{\varepsilon} + \boldsymbol{\varepsilon} \cdot\cdot\, \mathbf{M} \cdot \boldsymbol{\theta} + \frac{1}{2}\boldsymbol{\theta} \cdot \mathbf{P} \cdot \boldsymbol{\theta} + \boldsymbol{\varepsilon} \cdot\cdot\, \mathbf{N} \cdot \mathbf{E} + \frac{1}{2}\mathbf{E} \cdot \boldsymbol{\epsilon} \cdot \mathbf{E} + \boldsymbol{\theta} \cdot \mathbf{X} \cdot \mathbf{E} + \\ &+ \frac{1}{2}\nabla\boldsymbol{\phi} \cdot\cdot\, \boldsymbol{\Phi}^{\mu} \cdot\cdot\, \nabla\boldsymbol{\phi} + \boldsymbol{\theta} \cdot \boldsymbol{\Phi}^{\times} \cdot\cdot\, \nabla\boldsymbol{\phi} + \boldsymbol{\epsilon} \cdot\cdot\, \boldsymbol{\Phi}^{\tau} \cdot\cdot\, \nabla\boldsymbol{\phi} + \mathbf{E} \cdot \boldsymbol{\Phi}^{\mathsf{E}} \cdot\cdot\, \nabla\boldsymbol{\phi}.\end{aligned} \tag{25}$$

The intrinsic energy must be a positively defined function. This means that the known restrictions must be superposed on the tensors of elasticity: **C**, **M**, **N**, **X**, **P**, $\boldsymbol{\Phi}^{\mu}$, $\boldsymbol{\Phi}^{\times}$, $\boldsymbol{\Phi}^{\mathsf{E}}$, $\boldsymbol{\Phi}^{\tau}$.

Substituting expression (25) into the Cauchy – Green relations (24) we shall get the stress – strain relations

$$\boldsymbol{\tau} = \frac{\partial \rho \mathbb{F}}{\partial \boldsymbol{\varepsilon}} = \mathbf{C} \cdot\cdot \boldsymbol{\varepsilon} + \mathbf{M} \cdot \boldsymbol{\theta} + \mathbf{N} \cdot \mathbf{E} + \boldsymbol{\Phi}^{\tau} \cdot\cdot \nabla \boldsymbol{\phi}, \tag{26}$$

$$\mathbf{q} = -\frac{\partial \rho \mathbb{F}}{\partial \boldsymbol{\theta}} = -\boldsymbol{\varepsilon} \cdot\cdot \mathbf{M} - \mathbf{P} \cdot \boldsymbol{\theta} - \mathbf{X} \cdot \mathbf{E} - \boldsymbol{\Phi}^{\times} \cdot\cdot \nabla \boldsymbol{\phi}, \tag{27}$$

$$\mathbf{D} = -\frac{\partial \rho \mathbb{F}}{\partial \mathbf{E}} = -\boldsymbol{\varepsilon} \cdot\cdot \mathbf{N} - \boldsymbol{\theta} \cdot \mathbf{X} - \boldsymbol{\epsilon} \cdot \mathbf{E} - \boldsymbol{\Phi}^{E} \cdot \nabla \boldsymbol{\phi}, \tag{28}$$

$$\boldsymbol{\mu} = \frac{\partial \rho \mathbb{F}}{\partial \nabla \boldsymbol{\phi}} = \boldsymbol{\Phi}^{\mu} \cdot\cdot \nabla \boldsymbol{\phi} + \boldsymbol{\theta} \cdot \boldsymbol{\Phi}^{\times} + \mathbf{E} \cdot \boldsymbol{\Phi}^{E} + \boldsymbol{\varepsilon} \cdot\cdot \boldsymbol{\Phi}^{\tau}. \tag{29}$$

Tensors $\mathbf{C}$, $\mathbf{M}$, $\mathbf{N}$, $\mathbf{X}$, $\mathbf{P}$, $\boldsymbol{\Phi}^{\mu}$, $\boldsymbol{\Phi}^{\times}$, $\boldsymbol{\Phi}^{E}$ and $\boldsymbol{\Phi}^{\tau}$ describe the physical properties of the material under consideration.

5 The special form of the energy balance equation

In order to simplify the theory let us accept the assumption (12). In such a case, instead of equation (22) we obtain

$$\rho \dot{\mathbb{F}} = \boldsymbol{\tau} \cdot\cdot \dot{\boldsymbol{\varepsilon}} - \mathbf{m} \cdot \dot{\boldsymbol{\gamma}} - \mathbf{q} \cdot \dot{\boldsymbol{\theta}} - \mathbf{D} \cdot \dot{\mathbf{E}}, \tag{30}$$

where

$$\boldsymbol{\gamma} \equiv \nabla \times \boldsymbol{\phi}. \tag{31}$$

The Cauchy – Green relations (24) take a form

$$\boldsymbol{\tau} = \frac{\partial \rho \mathbb{F}}{\partial \boldsymbol{\varepsilon}}, \quad \mathbf{m} = -\frac{\partial \rho \mathbb{F}}{\partial \boldsymbol{\gamma}}, \quad \mathbf{q} = -\frac{\partial \rho \mathbb{F}}{\partial \boldsymbol{\theta}}, \quad \mathbf{D} = -\frac{\partial \rho \mathbb{F}}{\partial \mathbf{E}}. \tag{32}$$

The free energy (25) will be accepted in the more simple form

$$\rho \mathbb{F} = \rho \mathbb{F}_0 + \frac{1}{2} \boldsymbol{\varepsilon} \cdot\cdot \mathbf{C} \cdot\cdot \boldsymbol{\varepsilon} + \frac{1}{2} \boldsymbol{\theta} \cdot \mathbf{P} \cdot \boldsymbol{\theta} + \frac{1}{2} \chi \boldsymbol{\gamma} \cdot \boldsymbol{\gamma} + \frac{1}{2} \mathbf{E} \cdot \boldsymbol{\epsilon} \cdot \mathbf{E} + \\ + \boldsymbol{\varepsilon} \cdot\cdot \mathbf{M} \cdot \boldsymbol{\theta} + \boldsymbol{\varepsilon} \cdot\cdot \mathbf{N} \cdot \mathbf{E} + \boldsymbol{\theta} \cdot \mathbf{X} \cdot \mathbf{E}, \tag{33}$$

where χ is the physical constant. The stress – strain relations (26)–(29) takes a form

$$\boldsymbol{\tau} = \frac{\partial \rho \mathbb{F}}{\partial \boldsymbol{\varepsilon}} = \mathbf{C} \cdot\cdot \boldsymbol{\varepsilon} + \mathbf{M} \cdot \boldsymbol{\theta} + \mathbf{N} \cdot \mathbf{E}, \tag{34}$$

$$\mathbf{q} = -\frac{\partial \rho \mathbb{F}}{\partial \boldsymbol{\theta}} = -\boldsymbol{\varepsilon} \cdot\cdot \mathbf{M} - \mathbf{P} \cdot \boldsymbol{\theta} - \mathbf{X} \cdot \mathbf{E}, \tag{35}$$

$$\mathbf{D} = -\frac{\partial \rho \mathbb{F}}{\partial \mathbf{E}} = -\boldsymbol{\varepsilon} \cdot\cdot \mathbf{N} - \boldsymbol{\theta} \cdot \mathbf{X} - \boldsymbol{\epsilon} \cdot \mathbf{E}, \tag{36}$$

$$\mathbf{m} = -\frac{\partial \rho \mathbb{F}}{\partial \boldsymbol{\gamma}} = -\chi \boldsymbol{\gamma}. \tag{37}$$

Now we have to find the general form of the tensors $\mathbf{C}$, $\mathbf{P}$, $\boldsymbol{\epsilon}$, $\mathbf{M}$, $\mathbf{N}$, $\mathbf{X}$. For this it is necessary to use the symmetry requirements.

6 Symmetry and the tensor transformations

When using the symmetry groups we have to take into account the type of a tensor. There exist tensors of two different types: polar and axial tensors. Axial tensor depends on the choice of the orientation in 3D space, but the polar tensor does not depend on the choice of the orientation in 3D space. Usually the axial vector associates with rotations and the polar vector associates with translations in the space. As a matter of fact we do not know the type of the electrical field vector. In electrodynamics the type of the vector **E** does not matter [10]. In electro-elasticity the type of the vector **E** is very important, since the type of the tensors **N**, **X** depends on the type of the vector **E**. Let there be given tensors **A** and **B**, the symmetry groups of which are the same, but the types of these tensors are different. In such a case the structures of tensors **A** and **B** will be different. If the vector **E** is polar one, then in the case under consideration the tensors **C**, **P**, $\boldsymbol{\epsilon}$, **N**, **J** are the polar (euclidian) tensors and **M**, **X** are the axial tensors. If the vector **E** is axial one, then the tensors **C**, **P**, $\boldsymbol{\epsilon}$, **X**, **J** are the polar (euclidian) tensors and **M**, **N** are the axial tensors. This fact can be established by means of experiment.

Let us accept the definition [9]

Definition 1. *Orthogonal transformation of a tensor* **S** *of a rank* k *is a tensor*

$$\mathbf{S}' \equiv (\det \mathbf{Q})^{\alpha} \otimes_1^k \mathbf{Q} \cdot \mathbf{S} \equiv (\det \mathbf{Q})^{\alpha} S^{i_1 \ldots i_k} \mathbf{Q} \cdot \mathbf{g}_{i_1} \otimes \ldots \otimes \mathbf{Q} \cdot \mathbf{g}_{i_k}, \tag{38}$$

where $\alpha = 0$, if the tensor **S** is a polar tensor and $\alpha = 1$, if the tensor **S** is an axial tensor. Let us accept the notation for a turn-tensor

$$\mathbf{Q}(\alpha \mathbf{n}) = (1 - \cos\alpha)\, \mathbf{n} \otimes \mathbf{n} + \cos\alpha\, \mathbf{I} + \sin\alpha\, \mathbf{n} \times \mathbf{I},$$

where α is the angle of turn and the unit vector **n** determines the axis of turn. The tensors

$$\mathbf{Q} = -\mathbf{I}, \quad \mathbf{Q} = \mathbf{I} - \mathbf{n} \otimes \mathbf{n}$$

are called the central inversion tensor and the mirror inversion tensor respectively.

Let us define [8] the symmetry group of a tensor **S**.

Definition 2. *Symmetry group of a tensor* **S** *is the set of the orthogonal tensors,* $\mathbf{Q}_s$*, which are the orthogonal solutions of equation*

$$(\det \mathbf{Q})^{\alpha} \otimes_1^k \mathbf{Q} \cdot \mathbf{S} = \mathbf{S}, \tag{39}$$

where **S** *is the given tensor.*

If a tensor **S** is known, then it is easy to find its group of symmetry. If we know the symmetry group of some tensor, then it is possible to construct a general form of the tensor with this symmetry group. To this end we must use the Curie – Neumann principle.

Curie – Neumann principle: *The symmetry group of the cause is a sub-set of the symmetry group of the consequence.*

In our case we are working with a certain piezoelectric crystal, for example, α-quartz. According to the Curie – Neumann Principle, the symmetry group of tensors **C**, **M** **P** may be equivalent or wider than the symmetry group of the crystal. Additional symmetry elements may appear as effects of shape, etc. Since we consider infinite 3D crystal, it is possible to find out the form of tensors using the invariance about all symmetry elements inherited by crystal structure. Numerical values of components must be found out experimentally.

For example let us consider 3-rank tensor **M** and present it in the following form

$$\mathbf{M} = M^{ijk}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k.$$

Transformed tensor:

$$\mathbf{M}' = (\det\mathbf{Q})^{\alpha} M^{ijk}\mathbf{Q}\cdot\mathbf{e}_i \otimes \mathbf{Q}\cdot\mathbf{e}_j \otimes \mathbf{Q}\cdot\mathbf{e}_k.$$

If **Q** is the symmetry element of the crystal it is necessary to require $\mathbf{M}' = \mathbf{M}$. In the other form:

$$M^{ijk}\left[(\det\mathbf{Q})^{\alpha}\mathbf{Q}\cdot\mathbf{e}_i \otimes \mathbf{Q}\cdot\mathbf{e}_j \otimes \mathbf{Q}\cdot\mathbf{e}_k \otimes -\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k\right] = 0 \tag{40}$$

We have 3^3 equations for every symmetry element, but the most of them are identities. If the crystal under consideration has n symmetry elements, the number of equations in (40) should be $n3^3$.

Now let us apply the conditions (40) to the tensor **N**. Let some crystal has the inversion tensor $(-\mathbf{I})$ as its element of symmetry. Let the vector **E** is the polar vector. In such a case the tensor **N** must be polar as well. The conditions (40) gives $\mathbf{N} = \mathbf{0}$. It means that the piezoeffect for this kind of crystal is impossible. If the vector **E** is the axial vector, then the tensor **N** must be axial as well. The conditions (40) are identities. It means that the piezoeffect for this kind of crystal is possible. This is an experimental way to establish the type of the vector **E**. If we find out the piezoelectric material with the central symmetry, then the vector **E** must be axial. We do not if there exist the piezoelectric material of such a kind, but theoretically such piezoelectric material may exist. From the other hand, it is well known that there exist the piezoelectric materials with two planes of the mirror symmetry. Let the tensors

$$\mathbf{Q}_1 = \mathbf{I} - \mathbf{e}_1 \otimes \mathbf{e}_1, \quad \mathbf{Q}_2 = \mathbf{I} - \mathbf{e}_2 \otimes \mathbf{e}_2 \tag{41}$$

be the symmetry elements of some crystal. According to the Curie – Neumann Principle these tensors must belong to the symmetry group of the tensor **N**. If tensor **N** is a polar tensor, then we have

$$\begin{aligned}\mathbf{N} = \left(N^{113}\mathbf{e}_1 \otimes \mathbf{e}_1 + N^{223}\mathbf{e}_2 \otimes \mathbf{e}_2 + N^{333}\mathbf{e}_3 \otimes \mathbf{e}_3\right) \otimes \mathbf{e}_3 +\\ + N^{131}\left(\mathbf{e}_1 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1\right) \otimes \mathbf{e}_1 + N^{232}\left(\mathbf{e}_2 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_2\right) \otimes \mathbf{e}_2.\end{aligned} \tag{42}$$

If tensor **N** is an axial tensor, then we have another representation

$$\begin{aligned}\mathbf{N} = N^{231}\left(\mathbf{e}_2 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_2\right) \otimes \mathbf{e}_1 +\\ + N^{132}\left(\mathbf{e}_1 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1\right) \otimes \mathbf{e}_2 + N^{123}\left(\mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1\right) \otimes \mathbf{e}_3.\end{aligned} \tag{43}$$

In conventional theory of the piezoelectricity expression (42) is used and the vector **E** is supposed to be a polar vector. However, there is some reasons in order to consider the vector **E** to be an axial one. Thus it is possible that expression (43) will be better to describe the real crystals. In any case the situation must be studied more carefully.

If the symmetry group of a crystal contains only turns, then the type of the vector **E** does not matter. Below we derive the results of treating the system (40) for α-quartz which belongs to class 32. There are two symmetry elements of class 32 structure: turn around axis x_3 about angle $2\pi/3$ and turn around axis x_1 about angle π.

Any two-rank tensor of quartz must have the following form:

$$\mathbf{T}^{(2)} = t_1(\mathbf{e}_1 \otimes \mathbf{e}_1 + \mathbf{e}_2 \otimes \mathbf{e}_2) + t_2\mathbf{e}_3 \otimes \mathbf{e}_3 = t_1\mathbf{I} + (t_2 - t_1)\mathbf{e}_3 \otimes \mathbf{e}_3. \tag{44}$$

Also, any three-rank tensor of quartz must have the form:

$$\mathbf{T}^{(3)} = t_0(\mathbf{e}_1 \otimes \mathbf{a} - \mathbf{e}_2 \otimes \mathbf{b}) + t_1\mathbf{e}_3 \otimes \mathbf{c} + t_2\mathbf{c} \otimes \mathbf{e}_3 + t_3(\mathbf{e}_1 \otimes \mathbf{e}_3 \otimes \mathbf{e}_2 - \mathbf{e}_2 \otimes \mathbf{e}_3 \otimes \mathbf{e}_1), \tag{45}$$

where

$$\mathbf{a} = \mathbf{e}_1 \otimes \mathbf{e}_1 - \mathbf{e}_2 \otimes \mathbf{e}_2, \quad \mathbf{b} = \mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1, \quad \mathbf{c} = \mathbf{e}_1 \otimes \mathbf{e}_2 - \mathbf{e}_2 \otimes \mathbf{e}_1.$$

The four-rank tensor of quartz have rather complicated form and, thus we just mention that it has 14 independent components. However when we consider the tensor of elasticity the last one has simple form due to symmetry of the stress tensor and the strain tensor. In this case we have only 6 independent components. It is common in symmetric elasticity theory to perform the 4-rank elasticity tensor as 6×6 matrix.

7 The simplest piezoelectric media

There are a lot of crystals which have the piezoelectric effect. Piezoelectricity is the result of interaction of crystal with electromagnetic field. In this work a piezoelectric crystal is supposed to be dipole crystal. This means that low-level cell has dipole properties. Electric field influences over dipole and creates a torque. There are two ways to impart energy to the crystal: either through an external force, or through an external torque. In order to complete the formulation of the theory we have to calculate the volume density of force $\rho\mathbf{F}$ in equation (8) and the volume density of torque $\rho\mathbf{L}$ in equations (11) or (13). To this end we can calculate the power of the external forces by two ways

$$\rho\left(\mathbf{F} \cdot \dot{\mathbf{u}} + \mathbf{L} \cdot \dot{\boldsymbol{\phi}}\right) = q_+\mathbf{D}_+ \cdot \mathbf{v}_+ + q_-\mathbf{D}_- \cdot \mathbf{v}_-, \tag{46}$$

where the Lorentz forces are taken into account. Each point of the media is neutral dipole. Dipole is placed along the vector $\mathbf{d}_0$. Then we have

$$q_+ = -q_- = q, \quad \mathbf{D}_+ = \mathbf{D}_- = \mathbf{D}, \quad \mathbf{v}_+ = \dot{\mathbf{u}} + \frac{1}{2}\dot{\boldsymbol{\phi}} \times \mathbf{d}_0, \quad \mathbf{v}_- = \dot{\mathbf{u}} - \frac{1}{2}\dot{\boldsymbol{\phi}} \times \mathbf{d}_0.$$

Substituting these expressions into equation (46) we obtain

$$\rho\left(\mathbf{F} \cdot \dot{\mathbf{u}} + \mathbf{L} \cdot \dot{\boldsymbol{\phi}}\right) = q\left(\mathbf{d_0} \times \mathbf{D}\right) \cdot \dot{\boldsymbol{\phi}} \quad \Rightarrow \quad \rho\mathbf{F} = \mathbf{0}, \quad \rho\mathbf{L} = \mathbf{d} \times \mathbf{D}, \tag{47}$$

where $\mathbf{d} = q\mathbf{d}_0$ is the physical characteristic of the material under consideration.

Let us write down the complete system of the piezoelectric equations.

Equations of motion

$$\nabla \cdot \boldsymbol{\tau} - \frac{1}{2}\nabla \times \mathbf{q} + \rho\mathbf{F} = \rho\ddot{\mathbf{u}}, \quad \nabla \times \mathbf{m} + \mathbf{q} + \mathbf{d} \times \mathbf{D} = \rho\,\mathbf{J} \cdot \ddot{\boldsymbol{\phi}}, \quad \nabla \cdot \mathbf{D} = \mathbf{0}. \tag{48}$$

The Cauchy – Green relations

$$\boldsymbol{\tau} = \frac{\partial\rho\mathbb{F}}{\partial\varepsilon}, \quad \mathbf{m} = -\frac{\partial\rho\mathbb{F}}{\partial\gamma}, \quad \mathbf{q} = -\frac{\partial\rho\mathbb{F}}{\partial\theta}, \quad \mathbf{D} = -\frac{\partial\rho\mathbb{F}}{\partial\mathbf{E}}. \tag{49}$$

In the given paper we are not going to discuss the theory of piezoelectricity for the real crystals of a general form. Our aim is only to discuss the main features of a new theory. By this reason let us consider the simplest expression for the free energy

$$\rho\mathbb{F} = \mu\varepsilon\cdot\cdot\varepsilon + \frac{1}{2}\lambda\,(\mathrm{tr}\varepsilon)^2 + \frac{1}{2}p\,\theta\cdot\theta + \frac{1}{2}\chi\gamma\cdot\gamma + \frac{1}{2}\epsilon\mathbf{E}\cdot\mathbf{E} + \varepsilon\cdot\cdot\mathbf{N}\cdot\mathbf{E} + \theta\cdot\mathbf{X}\cdot\mathbf{E}. \quad (50)$$

In this representation only the terms relating with the piezoeffect were taken into account in general form.

The stress – strain relations

$$\boldsymbol{\tau} = 2\mu\,\varepsilon + \lambda\,\mathrm{tr}\varepsilon\mathbf{I} + \mathbf{N}\cdot\mathbf{E}, \quad \mathbf{q} = -p\,\theta - \mathbf{X}\cdot\mathbf{E}, \quad \mathbf{m} = -\chi\,\gamma, \quad \mathbf{D} = -\epsilon\mathbf{E} - \varepsilon\cdot\cdot\mathbf{N}. \quad (51)$$

The geometrical equations

$$\varepsilon = \frac{1}{2}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^T\right), \quad \theta = \boldsymbol{\phi} - \frac{1}{2}\nabla\times\mathbf{u}, \quad \gamma = \nabla\times\boldsymbol{\phi}, \quad \mathbf{E} = \nabla\varphi, \quad (52)$$

where φ is an electrostatics potential.

The classical theory of the piezoelectricity follows from equations (48)–(52) under the next conditions

$$\boldsymbol{\phi} = \frac{1}{2}\nabla\times\mathbf{u}, \quad \mathbf{X} = \mathbf{0}, \quad \chi = 0, \quad \mathbf{d}\times\mathbf{D} = \mathbf{0}, \quad \mathbf{J} = \mathbf{0}. \quad (53)$$

While equations (48)–(52) can not be applied to the crystals of general form, nevertheless they contain a several different versions of the piezoelectricity theory. At the moment it is impossible to accept the final decision what theory is better. First of all, we do not know the type of the electrical field vector **E**. However this is very important for the piezoelectricity theory. As a matter of fact it is necessary to construct electrodynamics on the base of rational mechanics. P. Zhilin is quit sure that there exist only one possibility: the vector **E** is an axial vector (this means that a charge is a pseudoscalar). This fact follows from an unpublished yet work by Zhilin on electrodynamics. In any way we have to consider the two possibilities: both when the vector **E** is a polar vector and when the vector **E** is an axial vector. Besides, from equations (48)–(52) it follows that the piezoeffect penetrate into the theory by means of two way: either when

$$\mathbf{N} \neq \mathbf{0}, \quad \mathbf{X} = \mathbf{0} \quad (54)$$

or when

$$\mathbf{N} = \mathbf{0}, \quad \mathbf{X} \neq \mathbf{0}. \quad (55)$$

Of course both tensor **N** and tensor **X** may be in general different from zero.

Let us consider the particular case. Let the dipole direction be parallel to the optic axis x_3: $\mathbf{d} = d\mathbf{e}_3$. Let the symmetry group of the piezoelectric properties of a crystal contains the tensors (41) and any turn around the axis $\mathbf{e}_3$.

If the vector **E** is a polar vector, then the tensor **N** is a polar tensor, but the tensor **X** is an axial one. In such a case we have

$$\mathbf{N} = [N_1\mathbf{I} + (N_2 - N_1)\mathbf{e}_3\otimes\mathbf{e}_3]\otimes\mathbf{e}_3 + N_3\,[\mathbf{e}_1\otimes\mathbf{e}_3\otimes\mathbf{e}_1 + \mathbf{e}_2\otimes\mathbf{e}_3\otimes\mathbf{e}_2 + \\ + \mathbf{e}_3\otimes(\mathbf{I} - \mathbf{e}_3\otimes\mathbf{e}_3)], \qquad \mathbf{X} = X_1\,\mathbf{e}_3\times\mathbf{I}, \quad (56)$$

where N_1, N_2, N_3, X_1 are true scalars.

If the vector **E** is an axial vector, then the tensor **N** is an axial tensor, but the tensor **X** is a polar one. In such a case we have

$$\mathbf{N} = N_1 \left[\mathbf{e}_2 \otimes \mathbf{e}_3 \otimes \mathbf{e}_1 - \mathbf{e}_1 \otimes \mathbf{e}_3 \otimes \mathbf{e}_2 + \mathbf{e}_3 \otimes \mathbf{e}_3 \times \mathbf{I}\right], \quad \mathbf{X} = X_1 \mathbf{I} + (X_2 - X_1)\mathbf{e}_3 \otimes \mathbf{e}_3, \tag{57}$$

where N_1, X_1, X_2 are true scalars.

From the comparison of the expressions (56) and (57) we see the significant difference between them. It is important that this difference can be established by means of experiment. This means that it is possible to find out the type of the electric field vector **E**. In order to use the experimental data we have to solve some concrete problems and to determine what kind of theory is better to describe the experimental data. This way leads to rather complicated dispersion equations which may be represented as the roots of the equation of an order 6. It has 6 different roots, which gives 6 dispersion curves. There are 3 acoustic and 3 optic curves. Classical theory gives us only acoustic curves.

8 Conclusion

In the paper two different versions of the piezoelectricity theory were derived. Both of them are new. Now we have to investigate the consequences from these theories and compare them with the experimental data. From theoretical point of view the most interesting result is to clear if the electric field **E** is a polar vector or it is an axial vector. At the moment authors are not ready to formulate the final results, since they must be verified very carefully.

As an illustration let us consider the simplest cases, when the tensor **N** is equal to zero. We have to consider two cases.

The first case: the electric field vector **E** is a polar vector. In such a case the strain – strain relations (51) take a form

$$\boldsymbol{\tau} = 2\mu\, \varepsilon + \lambda\, \mathrm{tr}\varepsilon \mathbf{I}, \quad \mathbf{q} = -p\, \theta - X_1 \mathbf{e}_3 \times \mathbf{E}, \quad \mathbf{m} = -\chi\, \gamma, \quad \mathbf{D} = -\epsilon \mathbf{E}. \tag{58}$$

The second case: the electric field vector **E** is an axial vector. In this case the strain – strain relations (51) take the next form

$$\boldsymbol{\tau} = 2\mu\, \varepsilon + \lambda\, \mathrm{tr}\varepsilon \mathbf{I},\ \mathbf{q} = -p\, \theta - X_1 \mathbf{E} - (X_2 - X_1)(\mathbf{E}\cdot\mathbf{e}_3)\mathbf{e}_3,\ \mathbf{m} = -\chi\, \gamma,\ \mathbf{D} = -\epsilon \mathbf{E}. \tag{59}$$

If the direction of vector **E** coincides with the direction of the vector $\mathbf{e}_3$, then the piezoeffect is absent in the case (58). However in the case (59) the effect will be present. If we shall be able to find out a crystal with the property (59), then it will be established that the electric field vector **E** is the axial vector, what is very important from the theoretical point of view. It is obvious that the dispersion curves will be quiet different for the cases (58) and (59). We do not actually know if there exist the piezoelectric crystals with such properties. But the existence of such crystals is theoretically possible. Let us point out that the cases under consideration differ from the classical case (1)–(3) very significantly. Up to present time only classical theory was verified by means of the experimental data. We may hope that a new theory — not necessary like the cases (58) and (59) — will be able to describe the experimental data better and simpler then the classical theory. In any case this possibility must be investigated in all details.

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References

[1] Gerber E., Balato A. Precision frequency control. Vol. 1,2. Academic Press Inc. 1985.

[2] Cady W. An introduction to the theory and applications of electromechanical phenomena in crystals. New York – London, 1946.

[3] Smagin A., Yaroslavsky M. Piezoelectricity of quartz and quartz cryatals. M.: “Energiya”, 1970. (in Russian).

[4] Victorov I.A. Acoustic surfase waves in solids. M.: Nauka, 1981. (in Russian).

[5] Yamaguchi M., Hashimoto K., Nanjo T., Hanazawa N., Ttsutsumi S., Yoneszawa T. Ultrasonic Properties of PZT Thin Films in UHF-SHF Ranges. Proceedings of the IEEE International Frequency Control Symposium, 1997. P. 544 – 551.

[6] Lurie A.I. Nonlinear theory of elasticity. M.: Nauka, 1980.

[7] Zhilin P.A. A New Approach to the Analysis of Free Rotations of Rigid Bodies.//ZAMM Z. angew. Math. Mech. **76** (1996), **4**. P. 187 – 204.

[8] Zhilin P.A. The basic equations of theory of inelastic media. Proc.of the XXVIII Summer School “Actual Problems in Mechanics”, St. Petersburg, 2001. P. 15 – 58. (in Russian).

[9] Zhilin P. Basic equations for nonclassical theory of elastic shells. Proc. of the SPbSTU, 386, St. Petersburg: 1982. P. 29 – 46.

[10] Nye J.F. Physical properties of crystals. M.: Mir, 1967. (in Russian).