Khatkevich’s theory for acoustic axes in 6mm piezoelectric CdS

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Abstract. The simplest derivation of Khatkevich’s equation based on Fedorov’s mathematics is presented here in view of recent confusions on the subject discussed in the literature. In the development of Khatkevich’s theory of acoustic axes the general equation is extended by introducing into consideration piezoelectric interaction. It is shown that the linear piezoelectric effect doubles the order of equation for the degenerated roots in hexagonal media in comparison with that obtained at taking into account pure elasticity only. Method is provided for control of phonon focusing anisotropy by investigation of acoustic axes in the piezoelectric medium. Examples of equilibrium dynamics of the acoustic axes for phonon modes in the temperature range from 4.2 to 500 K in CdS and of the phonon focusing factor in ZnO are supplied.

1. Motivation
Different methods have been elaborated to study phonon transport properties in bulk media (see, e. g., [1]). They have provided a solid basis for modeling phonon behavior in nanoscale materials [2]. An insight into energy transport carried by nonequilibrium phonons has great importance for both designing and optimizing electronic and optical devices for various working medium scale. To contribute into advancing of this field, the relationship is studied in this paper between degeneracy of the phonon phase velocities and both the material elasto-piezoelectric anisotropy and focusing factor distribution in hexagonal media. This is done by extending Khatkevich’s theory of acoustic axes that has been worked out for the case of purely elastic media only [3]. Quantitative modeling is performed for cadmium sulphide with 6mm symmetry class. A relation between the acoustics axes and phonon focusing properties is briefly exemplified for cadmium sulphide and zinc oxide materials.

2. Phonon focusing onset
The first data on phonon focusing in cadmium sulphide have been reported by McCurdy [4, 5], and the detail 2D calculation of the focusing directions in this crystal has been fulfilled in the following [6] to check the streamer breakdown theory based on the phonon streams. It has been revealed that there are unusual, in comparison with the literature data, properties in STA mode to possess directions of infinite focusing in CdS. New evidences for this finding have been obtained and possibility of the control modification of the phonon fluxes in hexagonal medium has been recently demonstrated by the 3D simulation of the focusing factor in ZnO single crystals and films including ones doped with Li impurity [7, based on 2D data [8]]. To highlight the role
of both elastic and piezoelectric anisotropy in the effect, it is supposed in the present paper that this can be effectively accompanied by the acoustic axes investigation method.

3. Acoustic axes background

Clear general theory of specific directions in elastic media has been worked out by Khatkevich since 1962 [3, etc., e.g., [9]]. This comprises both acoustic axes and longitudinal normals in crystals of arbitrary classes of symmetry. There has been both strong interest in degenerated directions study in different media [10, 11, 12, 13] and revision of the theory introduced in 1962 for the past decade. The theory background has been called into question [10] by claiming that Khatkevich has proposed his general equation without derivation and has used Fedorov’s book [14] where the rigorous proof of the equation is absent. The opponents have also stated that new arguments which have been proposed by Fedorov later in the next monograph [15] to support the validity of Khatkevich’s work are rather tangled.

Norris [11] has called attention to the confusions and proposed own proof of the Khatkevich starting equation without using, in fact, Fedorov’s formulae [14]. Evidently, there can be different methods of proof of the Khatkevich equation. To confirm this statement, without analysis of the revision that might be given elsewhere, both the simplest and based on the Fedorov data [14] derivation of Khatkevich’s equation is presented in the next section.

4. Khatkevich’s equation derivation

The cofactor matrix is well known tool used in linear algebra. By analogy, Fedorov has widely used cofactor tensor and has introduced a definition for this in general coordinateless form [14]. Let this definition be a starting point to derive Khatkevich’s equation. A rewritten Fedorov’s coordinateless expression that determines the cofactor tensor is

\[ \alpha_{ik} \alpha_{kj} = \begin{vmatrix} \alpha_{kl} \end{vmatrix} \delta_{ij}, \]

where the source tensor \( \alpha \) has the square matrix \( (\alpha)_{I1}^{m} \), its cofactor tensor \( \bar{\alpha} \) is correspondingly expressed in the form of the cofactor matrix \( (\bar{\alpha})_{I1}^{m} \), and \( |\alpha| \) is the determinant of the matrix \( (\alpha)_{I1}^{m} \). The order of the matrix \( m \), in general, can be an arbitrary number.

As the coordinateless form of the definition (1) is rarely met, one passes to the coordinate form for more clearness. In the following, delimiters are used to denote the determinant instead of Fedorov’s notation of the determinant in Eq. (1). Then expression (1) looks as

\[ \alpha_{ik} \bar{\alpha}_{lj} = \begin{vmatrix} \alpha_{kl} \end{vmatrix} \delta_{ij}, \]

where \( i \) and \( k \) are the row and column indices of the source matrix, \( l \) and \( j \) are the row and column ones of the cofactor matrix, \( \delta_{ij} \) is the Kronecker symbol, and as the matrices are the square ones, \( l \equiv k \). The proof of the accepted definition can be provided by direct substitution.

Let the source matrix represent the set of homogeneous linear equations and its order be equal to the number of unknown values. Then rank \( r_{s} \) of the source matrix is equal to rank \( r_{e} \) of the augmented matrix and there is the only solution: it is zero if \( |\alpha| \neq 0 \). This directly results from Kronecker-Capelli’s theorem which allows more than one solution if and only if the following conditions are fulfilled: \( r_{s} = r_{e} < m \) and \( |\alpha| = 0 \). As the existence of more than one solution is of interest to the present study, the expression (2) accepts the form

\[ \alpha_{ik} \bar{\alpha}_{kj} = \begin{vmatrix} 0 & 0 & \ldots & 0 \\ 0 & 0 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & 0 \end{vmatrix} = 0. \]
The source matrix \((α)_{i}^m\) is a non-zero matrix. Consequently, in any case Eq. (3) will be satisfied if the cofactor matrix is zero. In general case its degenerated roots are provided by the Perron-Frobenius (or Frobenius) theorem. Besides, for the case of interest, this is also true if its elements are dyads [14], and vice versa in line with Fedorov’s theorem [14, 15]. Therefore the corresponding cofactor tensor should satisfy the same equality \(α = 0\). In other words, by applying these conclusions to the wave equation for elastic displacements in the case of degenerated roots, Khatkevich’s equation (Eq. (5) in Ref. [3]) has been proved.

5. Piezoelectrically modified equation

In development of the Khatkevich theory piezoelectricity is taken into account by augmenting the general Eq. (4) yields the following set of four linear homogeneous equations

\[
\begin{aligned}
(\Gamma_{il} + G_{il} - ρu^2 δ_{il}) &= 0, \\
(L_{22} - ρu^2) (L_{33} - ρu^2) &= 0, \\
(L_{11} - ρu^2) (L_{33} - ρu^2) - L_{13}^2 &= 0, \\
(L_{11} - ρu^2) (L_{22} - ρu^2) &= 0, \\
(L_{22} - ρu^2) L_{13} &= 0.
\end{aligned}
\]  

(5)

As the axes of symmetry are not considered, \(L_{13} \neq 0\) and therefore the first root for the transverse mode is determined from the forth equation of the Eqs. (5): \(L_{22} = ρu^2\). Substituting it into the second equation of (5) results in the equation to be solved:

\[
(L_{11} - L_{22}) (L_{33} - L_{22}) - L_{13}^2 = 0.
\]  

(6)

Again, regardless of the properties of dyads, validity of the solution is controlled by the Frobenius theorem, namely, if the solution of Eq. (6) exists, the sought roots are degenerated, and vice versa. Therefore, in line with the transverse isotropy in hand, the derived solution which determines directions of the acoustic axes in hexagonal media via the polar angle \(θ\) is:

\[
b_1 \tan^4 θ + b_2 \tan^2 θ + b_0 = 0,
\]  

(7)

where the acoustic axes directed along the symmetry axes have been excluded. Comparison of Eq. (7) with Eq. (23) [3] shows that linear piezoelectric effect doubles the order of the equation obtained by Khatkevich (\(c_0 \tan^2 θ + c = 0\)) for media with pure elastic properties. This difference is also involved in both the number and structure of the polynomial coefficients which are:

\[
\begin{aligned}
b_1 &= c_0 e_{11}^S + e_{15}^2 (c_{11} - c_{66}), \\
b_2 &= c_6 e_{11}^S + c_0 e_{33}^S + e_{44}^2 (c_{44} - c_{66}) + 2e_{15}e_{33} (c_{11} - c_{66}) - 2e_{15}e_5 (c_{13} + c_{44}), \\
b_0 &= c_6 e_{33}^S + e_4^2 (c_{33} - c_{44}) + e_{33}^2 (c_{11} - c_{66}) - 2e_{33}e_5 (c_{13} + c_{44}).
\end{aligned}
\]  

(8)
where $c_{\alpha\beta}$ are the elastic moduli, $e_s = e_{15} + e_{31}$, $e_{i\alpha}$ are the piezoelectric coefficients, $c_0$ and $c$ are the coefficients which correspond to these $b_0$ and $b_2$ from Eq. (22a) in Ref. [3] if $c_{14}$ is dropped, namely, $c_0 = (c_{11} - c_{66})(c_{44} - c_{66})$ and $c = (c_{11} - c_{66})(c_{33} - c_{44}) - (c_{13} + c_{44})^2$.

6. Examples: acoustic axes and energy flux dynamics
As it can be seen from Eq. (7) there are eight conditions which determine existence of the acoustic axes in piezomedia. In turn, perturbation of the direction of acoustic axes affects the anisotropy of focusing factor. The piezoelectric deflection of the axis direction can reach up to $5^\circ$ in the CdS crystal at 300 K (see also Fig. 1). However, this effect can result in drastic modification of the focusing factor anisotropy. Fig. 1 shows such an example for transverse modes in ZnO [7, to be published].

Figure 1. The acoustic axis in CdS (left) and phonon focusing factor dynamics in ZnO (rest).

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