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Abstract

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PHYSICS

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ALLOWANCE FOR THE PIEZOELECTRIC EFFECT IN THE THEORY OF ELASTIC WAVES FOR CRYSTALS OF VARIOUS SYMMETRY

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When elastic waves propagate in crystals possessing piezoelectric properties, the local mechanical stresses σ and strains γ must lead to local polarization of the medium and to the appearance of induction \mathbf{D} (the direct piezoelectric effect). On the other hand, the electric fields \mathbf{E} that arise in this process must influence the strains and stresses in the crystal (the converse piezoelectric effect). Until now, allowance for the piezoelectric effect in the theory of elastic waves has been carried out only by ordinary coordinate methods ^(1,2). This leads to cumbersome and complicated expressions, which do not lend themselves to investigation in the general case of a crystal of arbitrary symmetry for an arbitrary direction of wave propagation. Concrete results here have been obtained only for individual crystals in those special cases when the waves propagate along certain special directions determined by the symmetry elements of the crystal, so that the final formulas are greatly simplified ^(3-7,17). However, the use of coordinate-free, or covariant, methods, which are being applied ever more widely in the theory of elastic waves ⁽⁸⁾, makes it possible to approach the problem under consideration in a new way. We shall take below the equations of state of a piezoelectric medium in the form ⁽⁹⁾

$$\sigma_{ij} = c_{ijkl}^E \gamma_{kl} - e_{kij} E_k, \quad D_i = \varepsilon_{ij}^\gamma E_j + 4\pi e_{ikl} \gamma_{kl}. \quad (1)$$

Here the elastic constants c_{ijkl}^E , the piezoelectric moduli e_{kij} , and the dielectric permittivity ε_{ij}^γ are taken at constant entropy (in what follows, for brevity, we shall omit the upper indices on these constants). Using the equation of motion of an elastic medium $\rho \ddot{u}_j = (\partial/\partial x_i) \sigma_{ij}$ (here \mathbf{u} is the displacement vector; ρ is the density of the medium), the electrodynamic equations $\text{div } \mathbf{D} = \text{rot } \mathbf{E} = 0^*$ and carrying out calculations analogous to ⁽¹⁾, we obtain the equation

$$\left(\Lambda^n + \frac{1}{\varepsilon^n} \mathbf{e}^n \cdot \mathbf{e}^n - v^2 \right) \mathbf{u} = 0. \quad (2)$$

Here

$$\Lambda_{il}^n = \lambda_{ijkl} n_j n_k = \frac{1}{\rho} c_{ijkl} n_j n_k$$

is the Green-Christoffel tensor;

$$e_i^n = e_{kij} n_k n_j; \quad \varepsilon^n = \frac{\rho}{4\pi} \mathbf{n} \mathbf{n};$$

\mathbf{n} is the wave normal; v is the phase velocity of the wave. If (2) is written in the usual coordinate form, then the result obtained coincides, up to notation, with the result of (1). However, the covariant form of the fundamental equation of the theory of elasticity of piezoelectric crystals used here, (2), is considerably more convenient for further investigations. Equation (2) differs from the corresponding equation of the ordinary theory of elastic waves only by the addition to Λ^n of the simple dyad

$$\frac{1}{\varepsilon^n} \mathbf{e}^n \cdot \mathbf{e}^n$$

and by replacing the tensor Λ^n by

$$\Lambda^{n'} = \Lambda^n + \frac{1}{\varepsilon^n} \mathbf{e}^n \cdot \mathbf{e}^n$$

(in what follows we shall omit the index n almost everywhere).

* The last equation means that a quasistatic approximation is considered here. The more general case of the joint solution of the equations of motion with Maxwell's equations leads to negligibly small additional corrections, which, according to estimates (5,10), amount to 10^{-9} – $10^{-12}\%$ (the influence on the phase velocity of elastic waves). See also (11).

Let us compute the expression for the reciprocal tensor Λ' and the principal invariants of the tensor Λ' , i.e., those main characteristics by means of which the theory of elastic waves is constructed. These results will be used in further investigations. The use of coordinate-free methods makes it possible to explicitly single out the terms depending on the piezomoduli and leads to the results:

$$\begin{aligned}
\bar{\Lambda}' &= \bar{\Lambda} + \frac{1}{\mathcal{E}}\{(\mathbf{e} \cdot \mathbf{e}\Lambda + \Lambda\mathbf{e} \cdot \mathbf{e}) - \Lambda_c\mathbf{e}^{\times 2} - \mathbf{e}^2 \cdot \Lambda - \mathbf{e}\Lambda\mathbf{e}\}; & \Lambda'_c &= \Lambda_c + \frac{1}{\mathcal{E}}\mathbf{e}^2; \\
(\Lambda'^2)_c &= (\Lambda^2)_c + \frac{1}{\mathcal{E}}(2\mathbf{e}\Lambda\mathbf{e} + \mathbf{e}^4); & (\bar{\Lambda}')_c &= (\bar{\Lambda})_c + \frac{1}{\mathcal{E}}(\mathbf{e}^2\Lambda_c - \mathbf{e}\Lambda\mathbf{e}); \\
|\Lambda'| &= |\Lambda| + \frac{1}{\mathcal{E}}\mathbf{e}\bar{\Lambda}\mathbf{e}; & \mathbf{n}\Lambda'\mathbf{n} &= \mathbf{n}\Lambda\mathbf{n} + \frac{1}{\mathcal{E}}(\mathbf{e}\mathbf{n})^2; \\
\mathbf{n}\Lambda'^2\mathbf{n} &= \mathbf{n}\Lambda^2\mathbf{n} + \frac{1}{\mathcal{E}}\mathbf{e}\mathbf{n} \cdot (2\mathbf{e}\Lambda\mathbf{n} + \mathbf{e}^2 \cdot \mathbf{e}\mathbf{n}); \\
\mathbf{n}\bar{\Lambda}'\mathbf{n} &= \mathbf{n}\bar{\Lambda}\mathbf{n} + \frac{1}{\mathcal{E}}\{2\mathbf{e}\mathbf{n} \cdot \mathbf{e}\Lambda\mathbf{n} + \Lambda_c[\mathbf{e}\mathbf{n}]^2 - \mathbf{e}^2 \cdot \mathbf{n}\Lambda\mathbf{n} - \mathbf{e}\Lambda\mathbf{e}\}.
\end{aligned} \tag{3}$$

Knowledge of the specific form of the polar tensors of third rank used in crystal physics, taken in coordinate ^(9,12) or covariant ^(13,14) form, makes it possible to calculate the vectors \mathbf{e}^n for an arbitrary direction \mathbf{n} for a piezoelectric crystal of any symmetry G_k . According to their own symmetry G_e , the piezomodulus tensors are divided into 15 groups

Table 1

G_e	Basis	\mathbf{e}^n ($\mathbf{a}^2 = \mathbf{b}^2 = \mathbf{c}^2 = 1$; $\mathbf{ab} = \mathbf{bc} = \mathbf{ca} = 0$; $n_1 = \mathbf{na}$, $n_2 = \mathbf{nb}$, $n_3 = \mathbf{nc}$)
$\bar{4}3m\infty 22$	$\mathbf{a}, \mathbf{b}, \mathbf{c} \parallel \bar{4}\mathbf{c} \parallel \infty$	$2e_{14}(n_2n_3\mathbf{a} + n_3n_1\mathbf{b} + n_1n_2\mathbf{c}) - e_{14}(\mathbf{nc})[\mathbf{nc}]$
$\bar{6}m2$ ∞mm	$\mathbf{a} \parallel 2, \mathbf{c} \parallel \bar{6}$ $\mathbf{a} \perp m, \mathbf{c} \parallel \bar{6}\mathbf{c} \parallel \infty$	$e_{11}[(n_1^2 - n_2^2)\mathbf{a} - 2n_1n_2\mathbf{b}] - e_{22}[2n_1n_2\mathbf{a} + (n_1^2 - n_2^2)\mathbf{b}] + (e_{15} + e_{31})n_3\mathbf{n} + [e_{15}(1 - 2n_3^2) + (e_{33} - e_{31})n_3^2]\mathbf{c}$
$\bar{4}2m$	$\mathbf{a} \parallel 2, \mathbf{c} \parallel \bar{4}\mathbf{a} \perp m, \mathbf{c} \parallel \bar{4}$	$(e_{14} + e_{36})n_3(n_2\mathbf{a} + n_1\mathbf{b}) + 2e_{14}n_1n_2\mathbf{c}(e_{15} + e_{31})n_3(n_1\mathbf{a} - n_2\mathbf{b}) + e_{15}(n_1^2 - n_2^2)\mathbf{c}$
222	$\mathbf{a}, \mathbf{b}, \mathbf{c} \parallel 2$	$(e_{25} + e_{36})n_2n_3\mathbf{a} + (e_{14} + e_{36})n_3n_1\mathbf{b} + (e_{14} + e_{25})n_1n_2\mathbf{c}$
$mm2$	$\mathbf{a} \perp m, \mathbf{c} \parallel 2$	$(e_{15} + e_{31})n_1n_3\mathbf{a} + (e_{24} + e_{32})n_2n_3\mathbf{b} + (e_{15}n_1^2 + e_{24}n_2^2 + e_{33}n_3^2)\mathbf{c}$

G_e	Basis	\mathbf{e}^n ($\mathbf{a}^2 = \mathbf{b}^2 = \mathbf{c}^2 = 1$; $\mathbf{ab} = \mathbf{bc} = \mathbf{ca} = 0$; $n_1 = \mathbf{na}$, $n_2 = \mathbf{nb}$, $n_3 = \mathbf{nc}$)
m	$\mathbf{c} \perp m$	$[e_{11}n_2^2 + e_{26}n_2^2 + (e_{16} + e_{21})n_1n_2 + e_{35}n_3^2]\mathbf{a} + [e_{16}n_1^2 + e_{22}n_2^2 + (e_{26} + e_{12})n_1n_2 + e_{34}n_3^2]\mathbf{b} + [(e_{13} + e_{35})n_1 + (e_{23} + e_{34})n_2]n_3\mathbf{c}$

(^{12,15}). In this case it is sufficient to compute the vectors \mathbf{e} only for 8 groups G_e (Table 1). For the remaining 7 groups G_e , the vectors \mathbf{e} can be represented as the sum of the various \mathbf{e}' s included in Table 1:

$$\begin{aligned}
 \mathbf{e}_\infty &= \mathbf{e}_{\infty 22} + \mathbf{e}_{\infty mm}; & \mathbf{e}_{32(a\parallel 2)} &= \mathbf{e}_{\infty 22} + \mathbf{e}_{\bar{6}m2(a\parallel 2)}; \\
 \mathbf{e}_{3m(a\perp m)} &= \mathbf{e}_{\bar{6}m2(a\perp m)} + \mathbf{e}_{\infty mm}; & \mathbf{e}_{3m(b\perp m)} &= \mathbf{e}_{\bar{6}m2(a\parallel 2)} + \mathbf{e}_{\infty mm}; \\
 \mathbf{e}_3 &= \mathbf{e}_{\infty 22} + \mathbf{e}_{\infty mm} + \mathbf{e}_{\bar{6}m2(a\parallel 2)} + \mathbf{e}_{\bar{6}m2(a\perp m)}; \\
 \mathbf{e}_{\bar{4}} &= \mathbf{e}_{\bar{4}2m(a\parallel 2)} + \mathbf{e}_{\bar{4}2m(a\perp m)}; & \mathbf{e}_1 &= \mathbf{e}_2 + \mathbf{e}_m; & \mathbf{e}_2 &= \mathbf{e}_{222} + \mathbf{e}_{mm2}.
 \end{aligned} \tag{4}$$

Analogous relations are also valid for the piezomoduli e_{hij} themselves. From Table 1 it is seen that, for example, for $G_e = \bar{4}3m$ when $\mathbf{n} \parallel \bar{4}$, $\mathbf{e} = 0$, and consequently the piezoeffect will have no influence at all either on the phase velocity or on the polarization of waves propagating in this direction. A similar situation also occurs for $G_e = \infty 22$ when $\mathbf{n} \parallel \infty$ or $\mathbf{n} \perp \infty$, etc.

Let us use the results obtained to investigate the influence of the piezoeffect on the phase velocity of elastic waves. Without taking the piezoeffect into account, $v^{02} = \mathbf{u}^0 \Lambda \mathbf{u}^0$, where $\mathbf{u}^{02} = 1$. The presence of the piezoeffect leads to a change of v^0 and \mathbf{u}^0 . In this case one may put $v^2 = v^{02} + \Delta v^2$, $\mathbf{u} = \mathbf{u}^0 + \Delta \mathbf{u}$, and assume that $\Delta \mathbf{u} \mathbf{u}^0 = 0$. If we restrict ourselves to consideration of a weak piezoeffect, such that the terms quadratic in the small parameters $\frac{1}{\mathcal{E}} \mathbf{e} \cdot \mathbf{e}$ and $\Delta \mathbf{u} \dots$

Table 2

G_e	\mathbf{n}	\mathbf{u}^0	v_0^2	Δv^2 ($n_1 = \sin \theta \cos \varphi$; $n_2 = \sin \theta \sin \varphi$; $n_3 = \cos \theta$)	Remarks
$\bar{4}3m$	$\perp \mathbf{c}$	\mathbf{c}	λ_{44}	$\frac{4\pi e_{14}^2}{\rho \mathcal{E}} \sin^2 2\varphi$	

G_e	\mathbf{n}	\mathbf{u}^0	v_0^2	Δv^2 ($n_1 = \sin \theta \cos \varphi$; $n_2 = \sin \theta \sin \varphi$; $n_3 = \cos \theta$)	Remarks
$\infty 22, \infty$	any	$\frac{[\mathbf{nc}]}{ [\mathbf{nc}] }$	$\lambda_{44} \cos^2 \theta + \lambda_{66} \sin^2 \theta$ (except $G_k = 422$ and 4)	$\frac{\pi e_{14}^2 \sin^2 2\theta}{\rho(\varepsilon_1 \sin^2 \theta + \varepsilon_2 \cos^2 \theta)}$	the polarization is completely determined
$\bar{6}m2$ ($\mathbf{a} \parallel \mathbf{m}$)	any	$\frac{[\mathbf{nc}]}{ [\mathbf{nc}] }$	$\lambda_{44} \cos^2 \theta + \lambda_{66} \sin^2 \theta$ (except $G_k = 422$ and 4)	$\frac{4\pi e_{11}^2 \sin^4 \theta \sin^2 3\varphi}{\rho(\varepsilon_1 \sin^2 \theta + \varepsilon_2 \cos^2 \theta)}$	the polarization is completely determined
$\bar{6}m2$ ($\mathbf{a} \perp 2$)	any	$\frac{[\mathbf{nc}]}{ [\mathbf{nc}] }$	$\lambda_{44} \cos^2 \theta + \lambda_{66} \sin^2 \theta$ (except $G_k = 422$ and 4)	$\frac{4\pi e_{22}^2 \sin^4 \theta \cos^2 3\varphi}{\rho(\varepsilon_1 \sin^2 \theta + \varepsilon_2 \cos^2 \theta)}$	the polarization is completely determined
$\infty mm, \infty$	$\perp \mathbf{c}$	\mathbf{c}	λ_{44}	$\frac{4\pi e_{15}^2}{\rho \varepsilon_1}$	
32 ($\mathbf{a} \parallel 2$); 3	$\perp \mathbf{a}$	\mathbf{a}	$\lambda_{44} \cos^2 \theta + \lambda_{66} \sin^2 \theta \pm 2\lambda_{14} \cos \theta \sin \theta$	$\frac{\pi (e_{11} \cos 2\theta \mp e_{14} \sin 2\theta - e_{11})^2}{\rho(\varepsilon_1 \sin^2 \theta + \varepsilon_3 \cos^2 \theta)}$	($\varphi = \pm \frac{\pi}{2}$)
$\bar{4}2m$ ($\mathbf{a} \parallel 2$)	$\perp \mathbf{c}$	\mathbf{c}	λ_{44}	$\frac{4\pi e_{14}^2 \sin^2 2\varphi}{\rho \varepsilon_1}$	same for $G_e = 4$
$\bar{4}2m$ ($\mathbf{a} \parallel 2$)	$\perp \mathbf{a}$	\mathbf{a}	$\lambda_{44} \cos^2 \theta + \lambda_{66} \sin^2 \theta^*$	$\frac{\pi (e_{14} + e_{36})^2 \sin^2 2\theta}{\rho(\varepsilon_1 \sin^2 \theta + \varepsilon_3 \cos^2 \theta)}$	same for $G_e = 4$ ($\varphi = \pm \frac{\pi}{2}$)
$\bar{4}2m$ ($\mathbf{a} \perp \mathbf{m}$)	$\perp (\mathbf{a} + \mathbf{b})$	$\frac{\mathbf{a} + \mathbf{b}}{\sqrt{2}}$	$\lambda_{44} \cos^2 \theta + \frac{1}{2}(\lambda_{11} - \lambda_{12}) \sin^2 \theta^*$	$\frac{\pi (e_{15} + e_{31})^2 \sin^2 2\theta}{\rho(\varepsilon_1 \sin^2 \theta + \varepsilon_3 \cos^2 \theta)}$	same for $G_e = 4$ ($\varphi = \frac{\pi}{4}, \frac{5\pi}{4}$)
$\bar{4}$	$\perp \mathbf{c}$	\mathbf{c}	λ_{44}	$\frac{4\pi e_{15}^2}{\rho \varepsilon_1} \cos^2 2\varphi$	
$\bar{4}$	$\perp \mathbf{c}$	\mathbf{c}	λ_{44}	$\frac{4\pi}{\rho \varepsilon_1} (e_{14} \sin 2\varphi + e_{15} \cos 2\varphi)^2$	
$\bar{4}$	$\perp \mathbf{c}$	\mathbf{c}	$\lambda_{55} \cos^2 \varphi + \lambda_{44} \sin^2 \varphi$	$\frac{\pi (e_{14} + e_{25})^2 \sin^2 2\varphi}{\rho(\varepsilon_1 \cos^2 \varphi + \varepsilon_2 \sin^2 \varphi)}$	

Fig. 1

Figure 1: Fig. 1

G_e	\mathbf{n}	\mathbf{u}^0	v_0^2	Δv^2 ($n_1 = \sin \theta \cos \varphi$; $n_2 = \sin \theta \sin \varphi$; $n_3 = \cos \theta$)	Remarks
222	$\perp \mathbf{b}$	\mathbf{b}	$\lambda_{44} \cos^2 \theta + \lambda_{66} \sin^2 \theta$	$\frac{\pi(e_{14} + e_{36})^2 \sin^2 2\theta}{\rho(\varepsilon_1 \sin^2 \theta + \varepsilon_3 \cos^2 \theta)}$	($\varphi = 0, \pi$)
222	$\perp \mathbf{a}$	\mathbf{a}	$\lambda_{55} \cos^2 \theta + \lambda_{66} \sin^2 \theta$	$\frac{\pi(e_{25} + e_{36})^2 \sin^2 2\theta}{\rho(\varepsilon_1 \sin^2 \theta + \varepsilon_3 \cos^2 \theta)}$	($\varphi = \pm \frac{\pi}{2}$)
<i>mm2</i>	$\perp \mathbf{c}$	\mathbf{c}	$\lambda_{55} \cos^2 \varphi + \lambda_{44} \sin^2 \varphi$	$\frac{4\pi(e_{15} \cos^2 \varphi + e_{24} \sin^2 \varphi)^2}{\rho(\varepsilon_1 \cos^2 \varphi + \varepsilon_2 \sin^2 \varphi)}$	
2	$\perp \mathbf{c}$	\mathbf{c}	$\lambda_{55} \cos^2 \varphi + \lambda_{44} \sin^2 \varphi$	$\frac{2\pi[(e_{15} - e_{24}) \cos 2\varphi + (e_{11} + e_{25}) \sin 2\varphi + e_{15} + e_{24}]^2}{\rho[(\varepsilon_{11} - \varepsilon_{22}) \cos 2\varphi + 2\varepsilon_{12} \sin 2\varphi + \varepsilon_{11} + \varepsilon_{22}]}$	

* Same for $G_k = 422$ and 4.

can be neglected, then approximately $\mathbf{u}^2 = 1$, and from (2) we have

$$v^2 = v^{02} + \Delta v^2 = \mathbf{u}^0 \Lambda \mathbf{u}^0 + \frac{1}{\varepsilon} (\mathbf{e} \mathbf{u}^0)^2. \quad (5)$$

It is seen from (5) that always $\Delta v^2 \geq 0$ (if one takes into account that ε is a positive-definite tensor). It is important that \mathbf{u}^0 in (5) is calculated within the framework of the theory that does not take the piezoelectric effect into account. According to this theory (8), if \mathbf{n} lies

Fig. 1. Influence of the piezoelectric effect on the refraction surface M (polarities of quasi-transverse waves). The dashed lines correspond to the absence of the piezoelectric effect; the solid lines to its presence.

I— $G_e = \bar{4}3m, \bar{4}2m$ ($a \parallel 2$), $\mathbf{n} \perp c$;

II— $G_e = \bar{6}m$ ($2a \parallel 2$), $\theta = \theta_0$;

III— $G_e = \infty 22, \infty$, $\varphi = \varphi_0, \varphi_0 + \pi$ (for $G_k = \bar{4}22$ and $\mathbf{n} \perp a$ and $\mathbf{n} \perp (a+b)$);

$G_e = \bar{4}2m$ ($a \parallel 2$), $\mathbf{n} \perp a$; $G_e = 222$, $\mathbf{n} \perp a, b, c$.

in the symmetry plane m belonging to the symmetry group G_e of the elastic-moduli tensor,* then one of the waves is purely transverse, and for it $\mathbf{u}^0 \perp m$. On the basis of (5) it is convenient to investigate sections of the phase-velocity surface (the surface V) or of the refraction surface (the surface M) by such planes for the polarity of quasi-transverse waves. In doing so, all 15 symmetry

groups G_e were considered successively, and in each case an analysis was carried out for each of those symmetry planes that belong to the group G_e . The results of the investigation are summarized in Table 2, where only those cases for which $\Delta v^2 \neq 0$ are collected. Table 2 includes only crystallographically nonequivalent planes (with respect to the group G_e). For $G_e = 2$ the basis a, b, c is chosen so that $\lambda_{45} = 0$ ^(8,16). In this case a and b , generally speaking, are not eigenvectors of the tensor ε . In this basis the matrix ε contains the nondiagonal component ε_{12} , which also appears in the final expression for Δv^2 .

If, without taking the piezoelectric effect into account, the curve obtained in the sections of the surface M under consideration can only be an ellipse or a circle ⁽⁸⁾, then the piezoelectric effect leads to its distortion. In this case specific bulges and concavities appear, connected with one another by the symmetry elements belonging to the group G_e (see Fig. 1).

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* The symmetry plane m under consideration need not at all belong to G_e or to G_k ($G_k \subseteq G_e$, $G_k \subseteq G_c$).

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