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LEAKY SAW BRANCHES COUPLED WITH OBLIQUE ACOUSTIC AXES IN TRIGONAL CRYSTALS

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ABSTRACT

The relationship between leaky surface acoustic wave (SAW) branches and acoustic axes for bulk waves is studied in the case of trigonal crystals. Three types of inclinations of acoustic axes are considered: 1) axes lying in the mirror planes of acoustic properties, oblique to the Z axis, 2) axes oblique to the mirror planes, 3) inclinated axes with respect to the boundary plane of the crystals. A new leaky SAW branch is found on the X cut of quartz. This branch is coupled with an acoustic axis lying in the boundary plane at an angle of about 66.3° from the Z axis. The other border of its existence region is determined by an acoustic axis oblique to the mirror planes. The theory by Khatkevich (1962) of acoustic axes of general position is revised and the results for trigonal crystals are corrected. It is shown that the relationship under study still holds when small deviations from the boundary plane are introduced in the acoustic axes. However, the permissible angles of deviation are smaller, as a rule, than the angles expected when the degeneracy solution is interpreted in terms of a bulk-wave-reflection problem.

1. INTRODUCTION

Leaky surface acoustic waves (SAWs) may be preferable to normal (non-attenuating) SAWs for device applications in specific cases when they have a higher electromechanical coupling coefficient or better thermal stability. The higher phase velocity of leaky SAWs is an additional advantage for high-frequency applications. However, the computational search for leaky SAWs in crystals involves the difficulties caused by restrictions on their existence region and a wide range of probable complex values of the wave number. The direct relationship between leaky SAW branches and acoustic axes (directions along which phase velocities coincide) for bulk acoustic waves in crystals has been recently indentified and explained by us [1,2]. In particular, new leaky SAW branches coupled with the acoustic axis coincident with the Z-axis of trigonal crystals have been found in berlinite and langasite. The objective of the present paper is to study the possibilty of using the oblique acoustic axes as reference points to search for new leaky SAW branches in trigonal crystals. We restrict our study to the case of trigonal crystals since they are the main substrate materials for SAW devices. The term "oblique axes" is used here in three different senses. Firstly, we consider leaky SAW branches coupled with acoustic axes oblique to the Z-axis when these axes lie in a symmetry plane of elastic properties of the crystal. Leaky SAWs on the YZ plane of quartz coupled with such an axis are found at the azimuthal angle about 66.3° from the Z-axis. Secondly, we study acoustic axes of general position which are oblique to symmetry planes. The previous statement on the absence of such axes in trigonal crystals [3], as we show, is incorrect. Correct equations for angles determining directions of acoustic axes oblique to symmetry planes are derived. Such oblique acoustic axes and associated leaky SAW branches are present in berlinite and quartz. Thirdly, the possibility of a relationship between leaky SAW branches and acoustic axes deviating from the boundary plane is examined.

2. LEAKY WAVES ON X-CUT QUARTZ

Quartz is a standard piezoelectric material for surface acoustic waves. It has been widely used both in ultrasonic devices and in physical investigations for many years. The X cut of quartz is one of the most

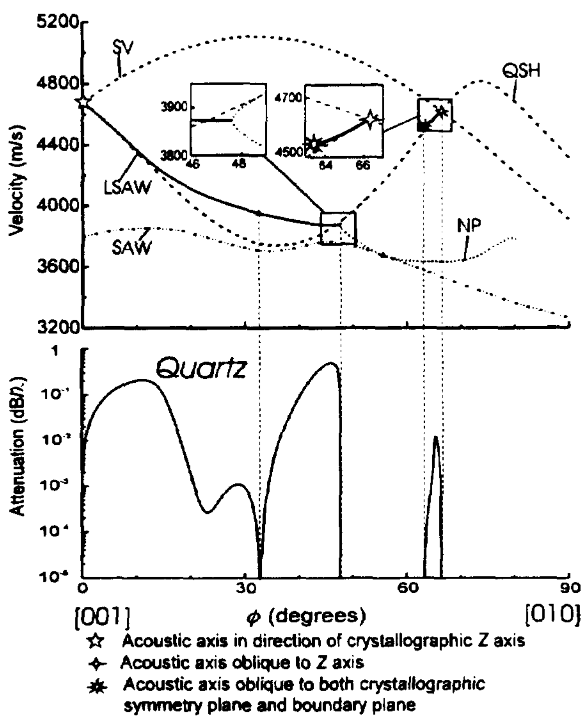

Fig. 1. Phase velocity and attenuation of leaky SAWs (LSAW) on X-cut quartz as a function of azimuthal angle ϕ. Velocity curves for bulk acoustic waves (SV and QSH), surface acoustic waves (SAW), and nonphysical solutions (NP) are also given. The inset on the right-hand side of the figure shows an additional leaky SAW branch on an enlarged scale.

popular cuts. The boundary plane for this cut is coincident with the mirror plane for elastic and acoustic properties of the crystal. Leaky SAWs on this cut exist in the sector of azimuthal angles adjacent to the Z crystallographic axis [4]. As shown in our previous papers [1,2], the leaky SAW solution for the propagation direction along the Z axis on this cut degenerates into a peculiar solution of a bulk-wave-reflection problem. Such a reflection problem was considered for the first time in Ref. [5]. The incident wave in this case impinges on the boudary plane at glancing angle and is called incident only due to the anisotropic deviation of its power flow from the wave vector to the boundary. This well-known leaky SAW branch exists when the propagation direction deviates from the Z axis no more than approximately 47.65°. Besides, there is an additional acoustic axis in the YZ plane of quartz. This axis is inclined with respect to the Z axis by 66.3°. The relationship under study between leaky SAW branches and acoustic axes and also corresponding results for lithium tantalate [6] allow us to assume that this additional acoustic axis can give rise to an additional leaky SAW branch on the X cut of quartz. This assumption is confirmed by our calculations (Fig. 1). Material constants for calculations are taken from Ref. [7]. The sector of existence of this new leaky branch is rather small (about 2°). The other end point of this branch also corresponds to an acoustic axis, this time slightly tilted to the bulk. In the next section, we consider in detail the theory of such acoustic axes of general position with arbitrary oblique orientations with respect to the symmetry planes of crystals.

3. ACOUSTIC AXES OUT OF THE SYMMETRY PLANES

The general theory of acoustic axes was developed by Khatkevich [3]. Khatkevich noticed that the orientations of acoustic axes lying out of the symmetry planes of crystals may be found from the condition that all cofactors, A_{ik}, of matrix $a_{ik} \equiv (\Gamma_{ik} - \rho v^2 \delta_{ik})$ be equal to zero

$$A_{ik} = 0, \quad i,k = 1, 2, 3. \tag{1}$$

Here Γ_{ik} is the Green-Christoffel tensor, ρ is the mass density of the crystal, δ_{ik} is Kronecker delta, v is the phase velocity of bulk waves. This condition is much simpler than the one obtained from the analysis of the secular equation. It is given in the paper by Khatkevich [3] without derivation, with reference to the book by Fedorov [8]. However, the formulae of Ref. [8] can give the condition (1) only if one assumes that the solution for the displacement vector is not unique in this case. Although such an assumption is not erroneous, it is not explicitly proved in the mentioned references and so rigorous proof of Eqs. (1) is absent there. Arguments in support of the validity of this condition presented in the other book by Fedorov [9] are rather tangled. Besides, only symmetrical three-dimensional matrices are discussed by Fedorov [8,9]. We present below a simple and general proof of Eqs. (1). This proof is valid for matrices of arbitrary dimension and their symmetry is not essential in this case. The problem of calculating the phase velocities of bulk acoustic waves in crystals is equivalent to the following eigenvalue problem

$$E_i \equiv (\Gamma_{ik} - \lambda \delta_{ik})\, u_k = 0, \tag{2}$$

where $\lambda = \rho v^2$ is an eigenvalue of Γ_{ik}, u_i is the particle displacement (eigenvector of Γ_{ik}). A nontrivial solution of Eqs. (2) is obtained if

$$D(\lambda) \equiv \det(\Gamma_{ik} - \lambda \delta_{ik}) = 0. \tag{3}$$

When Eq. (3) does not have coincident roots, these roots correspond to the points of sign change in the curves $D(\lambda)$, $E_i(\lambda)$. It is evident from geometrical analysis that there is no change of sign in these curves at the points of coincidence of two roots. Such contact points correspond, obviously, to local extrema of the functions which implies

$$\partial D/\partial \lambda = \partial E_i/\partial \lambda = 0. \tag{4}$$

This synchronous behaviour of several functions at the degeneracy points is in fact a true reason of great simplification of degeneracy conditions. Substituting E_i into Eqs. (4) produces

$$(\Gamma_{ik} - \lambda \delta_{ik})\, u'_k = u_i. \tag{5}$$

Eqs. (5) can be transformed into the form

$$D\, u'_k = A_{jk} u_j. \tag{6}$$

The well-known Cramer solution is obtained from Eqs. (6) dividing them by D under the condition that $D \neq 0$. However, in our case $D = 0$ and therefore

$$A_{jk} u_j = 0. \tag{7}$$

Eqs. (2) and (7) should be fulfilled simultaneously. Decomposing the determinant of Eqs. (2) in arbitrary i-th line gives

$$D = \sum_j a_{ij} A_{jk} = 0. \tag{8}$$

There is no summation over i in Eqs. (8) and (9). On the other hand, if we replace one of Eqs. (2) with fixed subscript i by one of Eqs. (7) with the same subscript ($k = i$), then the condition of existence of nontrivial solution of this combined system of equations takes the form

$$D = \sum_j A_{jk}{}^2 = 0. \tag{9}$$

From this it follows that Eqs. (1) should be fulfilled if the matrices under consideration are real. Only three among Eqs. (1) may be considered as independent due to additional relations imposed by Eq. (3). As such independent equations, it is convenient to consider the cofactors of elements a_{23}, a_{13}, a_{12}

$$\begin{bmatrix}\Gamma_1-\lambda & \Gamma_6\\ \Gamma_5 & \Gamma_4\end{bmatrix}=\begin{bmatrix}\Gamma_6 & \Gamma_2-\lambda\\ \Gamma_5 & \Gamma_4\end{bmatrix}=\begin{bmatrix}\Gamma_6 & \Gamma_4\\ \Gamma_5 & \Gamma_3-\lambda\end{bmatrix}=0$$

Excluding λ from these equations, we obtain two conditions derived by Khatkevich [3]

$$(\Gamma_1-\Gamma_2)\Gamma_4\Gamma_5+\Gamma_6(\Gamma_4^2-\Gamma_5^2)=0. \qquad (10)$$

$$(\Gamma_1-\Gamma_3)\Gamma_4\Gamma_6+\Gamma_5(\Gamma_4^2-\Gamma_6^2)=0. \qquad (11)$$

Analysing these equations, Khatkevich concluded that all the acoustic axes in trigonal crystals lie only in a symmetry plane, that their number is 4 or 10, and that previous numerical data for quartz available in the literature [10] are incorrectly calculated. This discrepancy and also the more recent numerical finding of out-of-plane acoustic axes in $LiTaO_3$ [11] and quartz [12] has stimulated us to recalculate Khatkevich's results on the basis of the general equations given in his paper. It has been found that the analytical results obtained by Khatkevich for trigonal crystals and therefore his conclusion mentioned above are incorrect. The correct expressions have the form

$$\tan^2\theta=\frac{(c_{33}+c_{44}+2c_{13})(c_{11}+c_{12})-2(c_{13}+c_{44})^2}{(c_{11}-c_{44})(c_{11}+c_{12})-2c_{14}^2}. \qquad (12)$$

$$\sin 3\varphi=\frac{2(c_{33}+c_{44}+2c_{13})-(2c_{11}+c_{13}-c_{44})\tan^2\theta}{c_{14}\tan^3\theta}. \qquad (13)$$

where θ and φ are the polar and azimuthal angles, respectively, and c_{ij} are elastic constants.

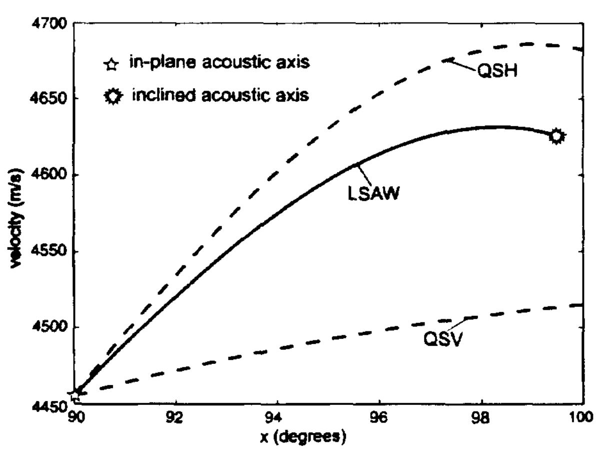

Fig. 2. Leaky SAW branch derived from nonsymmetric acoustic axis in quartz.

Eqs. (12) and (13) give real directions oblique to the symmetry planes for some trigonal crystals like quartz and berlinite: φ = 19.13°, θ = 63.04° for quartz and φ =25.94°, θ = 65.46° for berlinite. These values are confirmed by numerical solutions with account of piezoelectricity which give: φ = 19.64°, θ = 63.41° for quartz and φ = 25.37°, θ = 65.48° for berlinite. It is of interest to note that according to Eqs. (10) and (11) oblique acoustic axes should also exist in lithium niobate when φ = -21.40°, θ = 55.60°. However, numerical calculations of phase velocities of bulk waves in this crystal taking into account piezoelectricity reveal a small but finite spacing between two sheets of the slowness surface rather than their contact in the corresponding cone of directions. Thus piezoelectricity has a pronounced effect on the existence of acoustic axes in this special case.

The oblique acoustic axis in quartz has been used to find an associated leaky SAW branch (Fig. 2). The orientation of cut and the propagation direction are defined by the Euler angles (109.6361°, -26.5870°, x). The acoustic axis is in the boundary plane at x = 90°. At the termination of the leaky SAW branch, x = 99.49°, there is a degeneracy of leaky mode associated with an acoustic axis slightly tilted to the bulk.

4. ACOUSTIC AXES OUT OF THE BOUNDARY PLANE

Two configurations suitable to search for leaky SAWs with the aid of acoustic axes have been found in Ref. [1]. For one of them an acoustic axis should be in the plane of the surface. For the other an acoustic axis lying in the sagittal plane is directed into the bulk and one of the bulk waves propagating along it should simultaneously be a limiting wave (erroneously called exceptional wave in Ref. [1]). The interpretation of the degeneracy solution as a solution of a bulk-wave-reflection problem allows us to propose that all the orientations of acoustic axes confined between the two previously specified directions are permissible. To test this hypothesis, we have investigated some cuts of different crystals like berlinite, langasite, and potassium niobate. In all the cases studied, it is possible to tilt acoustic axes into the bulk and still maintain their coupling with the leaky SAW branch. The maximum angle of deviation corresponds to the case when one of

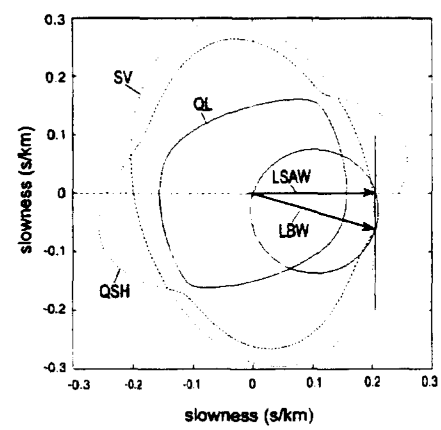

Fig. 3. Observed case of maximum deviation angle of acoustic axis from the boundary for constructing a leaky wave. Quartz, Euler angles (61.56°, 72.83°,-89.99999°). (LSAW = leaky surface acoustic wave, LBW = limiting bulk wave, SV = shear vertical wave, QSH = quasi shear horizontal wave, QL = quasi longitudinal wave)

the bulk acoustic waves propagating along the acoustic axis is simultaneously limiting bulk wave. This situation has been realized, in fact, only in special cases like rotated X-cut langasite for acoustic axis oblique to the Z-axis [13] and rotated Y-cut quartz. The best coincidence between results and predictions is observed in the case of quartz with the Euler angles (61.56°, 72.83°, -89.99999°), see Fig. 3. For comparison, the expected angle derived from the slowness curves is 72.82°. The circle in the figure represents the surface projections of slowness along the direction of acoustic axis for various angles of tilt of acoustic axis into the bulk (the sagittal plane is held constant in this case). The slowness-surface cross-section under consideration coincides practically with the *YZ* plane. Nevertheless, a small deviation from this plane is required to transform the degeneracy solution into leaky SAWs. Due to this small deviation, the direction mentioned as acoustic axis in Fig. 3 is not an acoustic axis in the strict sense, but it is very close to such an axis. The exact positioning of acoustic axis in the sagittal plane in this case results in the degeneracy of leaky SAWs into the so-called "no-motion" solution identified for the first time by Taylor [14].

Thus, our expectations concerning the limiting angle of tilt of acoustic axes coupled with leaky SAW branches are confirmed in the case shown in Fig. 3. However, the permissible angle of deviation is substantially smaller than expected one in many other studied cases. This is because of other types of leaky wave degeneracy being essential during changing the Euler angles after starting from a LSAW solution at a certain crystal orientation.

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