What are the interface acoustic modes of twins in quartz?

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Abstract - Interface acoustic waves (IAWs) at the boundaries of Dauphiné and Brazil twins in quartz are studied using numerical and analytical techniques. It is assumed that the boundary is coincident with the *YZ* mirror plane of quartz. The numerical solution of the problem for Dauphiné twins reveals that non-leaky waves exist only for the propagation directions within 0.02-degree deviations from the *Y*-axis. For the *Y*-propagation direction, the depth of wave localization is about 25 wavelengths, and the predominant displacement component at the boundary is shear-vertical, although all displacement components are present and they are comparable. For Brazil twins, the conditions of the existence of interface modes are less restricted but the depth of wave localization in the case of propagation along the *Y*-axis is about two times more than that for Dauphiné twins. A possibility to derive the secular equation of the problem in explicit form by direct integrating the equations of motion is demonstrated in a particular case of IAW propagation along the *Y*-axis at the boundary of Dauphiné twins under ignoring piezoelectricity. The analysis of this equation allows one to separate qualitatively the contributions of different elastic constants to the occurrence of IAWs.

I. INTRODUCTION

The crystalline quartz is one of the most extensively studied materials used in frequency control and SAW devices. The characteristic natural objects of internal structure of quartz are twin boundaries. Nevertheless, the acoustic modes of a quartz twin boundary are not investigated until now. The aim of the present paper is to study a possibility of the existence of localized (non-leaky) interface acoustic modes at such a boundary.

Interface acoustic waves (IAWs), as is known, do not always exist at the boundary of solids contrary to surface acoustic waves. For example, it is mentioned in the review by Owen [1] that only 30 metal interface combinations among over 900 ones considered are favourable for the existence of Stoneley waves. Hence, the existence of IAWs in solids may be considered as the exception rather than the rule. Several studies of IAWs at twist boundaries of cubic crystals [2,3] and a 180° ferroelectric domain boundary in $BaTiO_3$ [4,5], including our preliminary results on a 90° ferroelectric domain boundary, show that interface waves without leakage exist, as a rule, only in high-symmetry geometries. For this reason, we have restricted ourselves to the case of twin boundaries coinciding with the *YZ* crystallographic plane which is a mirror plane for untwinned quartz.

II. NUMERICAL CALCULATIONS

Since the piezoelectric effect in quartz is not very strong, one might expect that the most pronounced interface wave localization will occur if not only piezoelectric constants but also elastic constants are changed at the boundary. This is the case for Dauphiné twins.

The geometry of the problem under consideration for Dauphiné twins is the same as for the bulk wave reflection problem studied by Lyamov *et al.* [6]. We assume that the boundary plane is coincident with the *YZ* crystallographic plane. Dauphiné twins are distinguished by rotation around the *Z*-axis through 180° [7]. This is equivalent to simultaneous inversion of the *X*- and *Y*-axes. In this case, as can be readily appreciated, the signs of the elastic constant c_{14} and the independent piezoelectric constant e_{11} are changed at the twin boundary. The other independent piezoelectric constant e_{14} is not changed in this case. The numerical study of this problem reveals that non-leaky waves at the *YZ* boundary of Dauphiné twins exist only for propagation directions within 0.02-degree deviations from the *Y*-axis (Fig. 1). The reason of this very narrow range of existence of

0-7803-4153-8/97/$10.00

IAWs for Dauphiné twins is discussed in Sect. III. For the Y-propagation direction, the depth of wave localization is about 25 wavelengths, and the predominant displacement component at the boundary is shear-vertical, although all displacement components are present and they are comparable (Fig. 2).

Brazil twins are distinguished by inversion of the X-axis [7]. This results in change of signs of both independent piezoelectric constants e_{11} and e_{14} at the

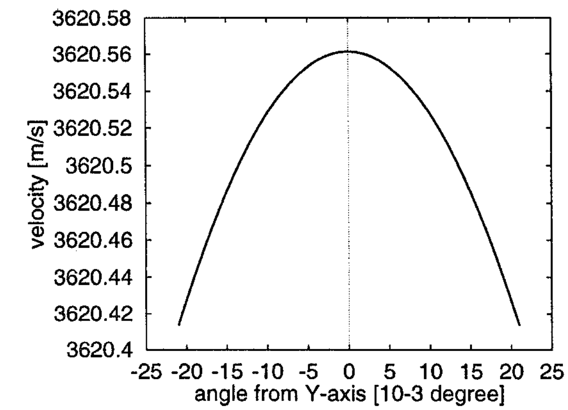

Fig. 1. Interface acoustic wave (IAW) velocity for propagation at the YZ boundary of Dauphiné twins.

boundary. In this respect the problem under consideration is equivalent to the problems of IAW propagation along a domain boundary in ferroelectrics [4,5] and along a perfectly conducting plane embedded in a piezoelectric medium [8]. The conditions of the existence of non-leaky interface acoustic waves on the YZ boundary of Brazil twins are less restricted than for Dauphiné twins (Fig. 3) but the depth of wave localization in the case of propagation along the Y-axis is about two times more than that for Dauphiné twins (Fig. 4).

III. ANALYTICAL CONSIDERATION

A possibility to derive the secular equation of the problem in explicit form is demonstrated below in a particular case of IAW propagation along the Y-axis at the boundary of Dauphiné twins under ignoring piezoelectricity. The analysis of this equation allows one to separate qualitatively the contributions of different elastic constants to the occurrence of IAWs.

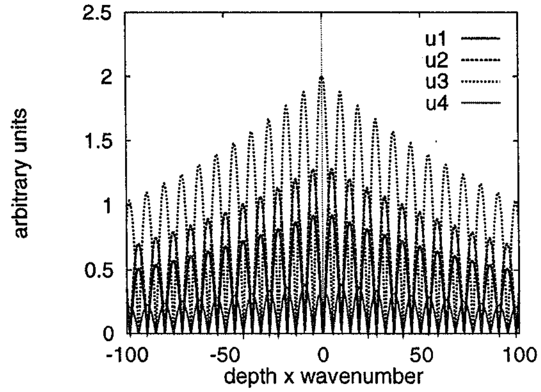

Fig. 2. Amplitude of displacement components and electric potential as a function of depth for IAWs propagating along the Y-axis at the YZ boundary of Dauphiné twins.

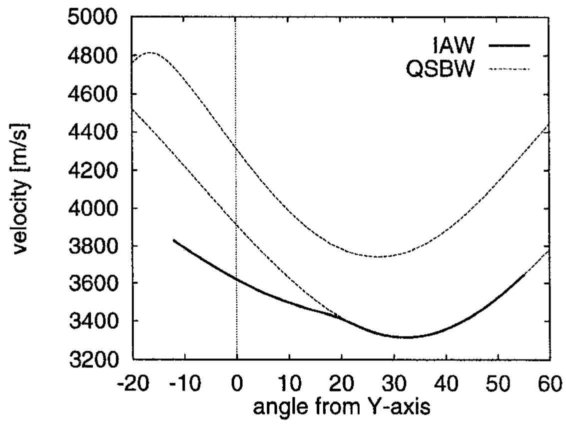

Fig. 3. Interface acoustic wave velocities for propagation at the YZ boundary of Brazil twins. Velocities of quasishear bulk waves are included.

To derive the secular equation, we use a new method of direct integrating the equations of motion [9]. The same method has been recently applied by us to study IAWs at the boundary of ferroelectric domains in barium titanate [4,5]. We assume that a plane harmonic interface wave propagates along the Y-axis in a quartz bicrystal with a normal to the boundary directed along the X-axis. The wave factor in this case is equal to $\exp(iky-i\omega t)$.

Partial differential equations of motion are reduced for such a wave to ordinary differential equations with respect to x. Under ignoring piezoelectricity these equations have the form

$$c_{11}u_1'' - \gamma_1 u_1 + i\beta u_2' + i2c_{14}u_3' = 0, \quad (1)$$

$$c_{66}u_2'' - \gamma_2 u_2 + i\beta u_1' + c_{14}(u_3'' + u_3) = 0, \quad (2)$$

$$c_{44}u_3'' - \gamma_3 u_3 + i2c_{14}u_1' + c_{14}(u_2'' + u_2) = 0, \quad (3)$$

where $\gamma_1 = c_{66}-X$, $\gamma_2 = c_{11}-X$, $\gamma_3 = c_{44}-X$, $\beta = c_{12}+c_{66}$, $u_i' = du_i / d(kx)$, $X = \rho v^2$, ρ is the mass density, and v and k are the phase velocity and wavenumber of interface waves, u_i are the particle displacement components (i = 1-3), c_{IJ} are the elastic constants (I, J = 1-6). From the symmetry of the problem, it is easy to determine the following effective conditions to be satisfied by quasiflexural interface waves at the boundary of twins

$$u_1' = u_2 = u_3' = 0. \quad (4)$$

As integrating factors for Eqs. (1)-(3), it is convenient to use such functions of which derivatives are included as separate terms in these equations, that is,

u_1', iu_2, iu_3 for Eq. (1),

u_2', iu_1, u_3' for Eq. (2),

u_3', iu_1, u_2' for Eq. (3),

Multiplying Eqs. (1)-(3) by integrating factors and integrating over x, we obtain a system of 9 linear algebraic equations which include the following 6 nonintegrable terms

$$F_4=i\int u_1u_2dx,\ F_5=i\int u_1'u_2'dx,\ F_6=i\int u_1u_3dx,$$

$$F_7=\int u_2u_3'dx,\ F_8=i\int u_1'u_3'dx,\ F_9=\int u_2'u_3''dx.$$

The boundary conditions, Eqs. (4), allow us to transform this system of equations to the form

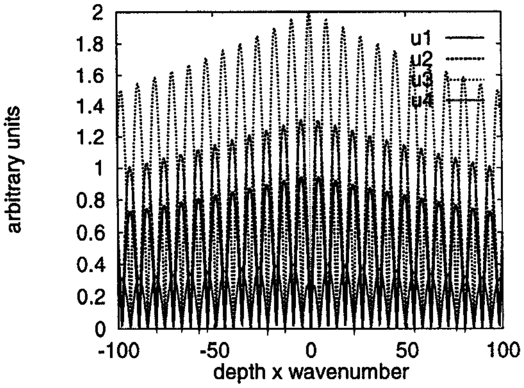

Fig. 4. Amplitude of displacement components and electrical potential as a function of depth for IAWs propagating along the Y-axis at the YZ boundary of Brazil twins.

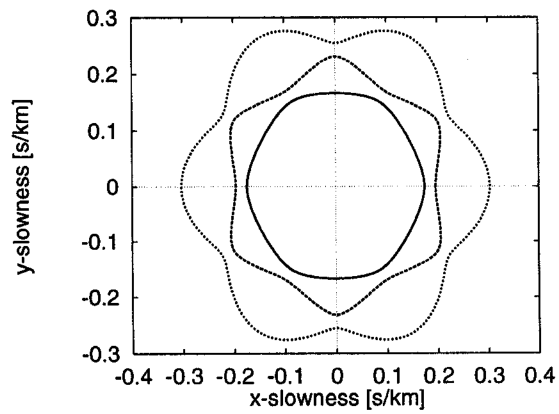

Fig. 5. Slowness curves of bulk waves for propagation in the XY plane of quartz.

$$A_{mn}F_n = B_m iu_1{}'u_2, \qquad m,n = 1\text{-}9 \qquad (5)$$

where

$$F_1 = u_1^2/2,\ F_2 = (u_2{}')^2/2,\ F_3 = u_3^2/2,$$

and the matrix A_{mn} is

$$\begin{matrix}
-\gamma_1 & 0 & 0 & 0 & \beta & 0 & 0 & 2c_{14} & 0 \\
0 & 0 & 0 & -\gamma_1 & -c_{11} & 0 & -2c_{14} & 0 & 0 \\
0 & 0 & -2c_{14} & 0 & 0 & -\gamma_1 & \beta & -c_{11} & 0 \\
0 & c_{66} & 0 & 0 & \beta & 0 & -c_{14} & 0 & c_{14} \\
-\beta & 0 & 0 & -\gamma_2 & -c_{66} & c_{14} & 0 & -c_{14} & 0 \\
0 & 0 & c_{14} & 0 & 0 & 0 & -\gamma_2 & \beta & -c_{66} \\
0 & 0 & -\gamma_3 & 0 & 0 & 0 & c_{14} & 2c_{14} & -c_{14} \\
-2c_{14} & 0 & 0 & c_{14} & -c_{14} & -\gamma_3 & 0 & -c_{44} & 0 \\
0 & c_{14} & 0 & 0 & 2c_{14} & 0 & \gamma_3 & 0 & c_{44}
\end{matrix}$$

There are only two nonzero elements in the column B_m:

$$B_5 = -c_{66}iu_1u_2{}',\quad B_8 = -c_{14}iu_1u_2{}'.$$

From Eqs. (5) one can find

$$u_1^2/2 = (\Delta_1/\Delta)iu_1u_2{}', \qquad (6)$$

$$(u_2{}')^2/2 = (\Delta_2/\Delta)iu_1u_2{}', \qquad (7)$$

where $\Delta = \det A_{mn}$, Δ_1 and Δ_2 are determinants of matrices obtained by replacing corresponding columns of A_{mn} by B_m. The secular equation sought is a condition of compatibility of Eqs. (6) and (7)

$$\Delta^2 + 4\Delta_1\Delta_2 = 0. \qquad (8)$$

Eq. (8) is the secular equation of the problem in explicit form. Only material constants of the crystal and the phase velocity of the wave are included in this equation. To solve Eq. (8) exactly, it is necessary to perform computer calculations. But for a qualitative analysis, there is a sense to consider the limiting form of this equation under c_{14} tends to zero. In this case Eq. (8) is factorized. Two main factors involved there have the form

$$D_1 = (\gamma_1c_{66}\text{-}\gamma_2c_{11}\text{-}\beta^2)^2 - 4\beta^2c_{11}\gamma_2,$$

$$D_2 = \gamma_1\gamma_2c_{44}^2\text{-}\ (\gamma_1c_{66}\text{+}\gamma_2c_{11}\text{-}\beta^2)c_{44}\gamma_3 + c_{11}c_{66}\gamma_3^2.$$

The condition $D_1 = 0$ coincides with the secular equation for a virtual boundary wave [4,5] which is the interference of two equal-amplitude limiting bulk waves. This wave exists only in the case when the slowness curve of the slowest bulk wave in the sagittal plane has a concavity along the direction of the boundary. The cross section in the *XY* plane for quartz possesses this property (Fig. 5).

Thus, it is possible to separate qualitatively the contribution of different elastic constants into the occurrence of IAWs. Namely, c_{14} changing its value at the boundary is directly responsible for the occurrence of IAWs by transforming the virtual wave into IAWs. But this is possible only in the case when the other elastic constants create a concavity of the slowness surface that is a necessary condition for the existence of the virtual waves.

The general structure of the equations in this problem is the same as in the case of IAWs at a twist boundary of crystals [3]. Therefore, the reason of a very small region of existence of IAWs is also the same. This reason is a violation of the symmetry of the problem in the case of a deviation of the propagation direction from the symmetry direction.

In conclusion, note that further investigations on the subject of the present paper may include the search for leaky IAWs at twin boundaries of quartz. As reference points for such a search at the boundary of Dauphiné twins, one can use a value of the phase velocity of bulk waves propagating along the *Z*-axis which is an acoustic axis for both twins in this case. Leaky interface waves should degenerate in this case into the solution of the bulk wave reflection problem considered by Lyamov *et al.* [6]. The explanation of the relationship with acoustic axes for leaky wave branches is given in Ref. [10]. The other possibility is related to the consideration of artificial crystals. Material constants changing their signs at the boundary of twins in a real crystal should be equal to zero in these artificial crystals. The bulk wave velocities of such crystals may be then used as starting values to search for leaky waves for both Dauphiné and Brazil twins.

ACKNOWLEDGEMENTS

This research is supported in part by INTAS (project 96-441), by Sächsiches Ministerium für Wissenschaft und Kunst and by Deutsche Forschungsgemeinschaft. The authors are grateful to Dr. R. Wobst for his programming work.

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