

Least action principle for the estimation of the slowness and the attenuation of pseudo surface acoustic waves

Vincent Laude,^{a)} Mikael Wilm, and Sylvain Ballandras

Laboratoire de Physique et Métrologie des Oscillateurs, CNRS UPR 3203, associé à l'Université de Franche-Comté, 32 avenue de l'Observatoire, F-25044 Besançon cedex, France

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The estimation of the slowness and of the attenuation of pseudo surface acoustic waves (PSAWs) has been addressed by many authors, but still represents a challenge because of the intrinsic difficulty to provide a physically consistent representation of their characteristics. In this work, we propose an alternative approach to the popular use of complex slownesses along the propagation direction. We introduce in the standard harmonic model an optimal source term exactly compensating for the energy lost by leakage, by analogy with the problem of the reflection of a bulk acoustic wave on the surface. This leads us to the minimization of a function whose minimum is the PSAW slowness and whose minimum value gives the attenuation. The method is found to be stable and reliable compared to previously published data, without requiring any change in the partial wave selection rule, and further does not require one to consider waves with increasing energy in the depth of the substrate, which generally does not correspond to the observed phenomena. © 2003 American Institute of Physics. [DOI: 10.1063/1.1574171]

I. INTRODUCTION

The problem of the exact estimation of the slowness and intrinsic attenuation of a pseudo surface acoustic wave (PSAW) has been addressed by many authors. A unique definition seems difficult to establish as a PSAW is not a true mode of the piezoelectric substrate, i.e., it does not satisfy exactly the free or shorted surface boundary conditions.

The plane wave solution in a piezoelectric material involves eight partial waves. For a semi-infinite substrate and for an excitation by sources described by real slownesses, only four of these must be physically considered, that are either inhomogeneous decreasing or propagative towards the bulk of the substrate (see, e.g., Refs. 1 and 2). With this physical partial wave selection rule, a plot of the effective permittivity (EP) in the PSAW region does not reveal a pole on the real slowness axis, which is often interpreted as a pole displaced in the complex slowness plane. When computing the EP with the physical partial wave selection rule and complex slownesses, a potential discontinuity appears (see Sec. III). Adler³ has proposed to modify this rule by selecting the propagative partial wave that is least increasing, with the result that a pole can be numerically found in the complex slowness plane. The slowness and the attenuation of the PSAW are then given, respectively, by the real and imaginary parts of the pole. Boyer, Desbois, and Zhang have obtained the slowness and the attenuation of the PSAW by relying only on the computation of the EP⁴ or of the harmonic admittance⁵ on the real slowness axis and on a first order Taylor expansion of these functions. Biryukov and Weihnacht¹ have discussed how the EP, and more generally the surface impedance matrix and the spectral Green's func-

tions, can be analytically continued in the complex plane of slowness. They also have given simple practical formulas to obtain the slowness and attenuation of a PSAW.⁶

In Sec. II, we briefly recall the theoretical procedure used to derive the partial waves and how they are connected to the description of acousto-electric fields in piezoelectric materials. A brief account of the complex slowness approach is provided in Sec. III, where we emphasize partial wave selection. In Sec. IV, we propose an alternative solution, avoiding the use of complex excitation slownesses, by analogy with the problem of the reflection of a bulk acoustic wave on the surface. Specifically, we include an optimal source term exactly compensating for the energy lost by leakage. This leads us to the minimization of a function whose minimum is the PSAW slowness and whose minimum value gives the attenuation. Numerical examples are given for several well-known shear-type PSAWs.

II. PLANE WAVE SOLUTIONS

Propagation of plane waves with frequency f is considered along the x_1 axis, with slowness s_1 . Assuming plane wave propagation, the distribution of the electro-mechanical fields in a piezoelectric material is fully described^{7,8} using the eight-component state vector $\mathbf{h} = (u_1, u_2, u_3, \phi, T_{21}, T_{22}, T_{23}, D_2)^t$ where the u_i are the mechanical displacements, ϕ is the electrical potential, T_{ij} is the stress tensor, and D_2 is the electrical displacement normal to the propagation surface. This state vector is obtained inside a layer as a superposition of eight partial waves, characterized by their eigenvalues $s_2(n)$ and their associated eigenvectors, for $n=1, \dots, 8$. The eigenvalues $s_2(n)$ only depend on the material constants, and on the slowness s_1 . Denoting F the 8×8 matrix of the vertically arranged eigenvectors, this superposition reads

^{a)} Author to whom correspondence should be addressed; electronic mail: vincent.laude@lpmo.edu

$$\mathbf{h}(x_1, x_2) = F\Delta(x_2)\mathbf{a} \exp[j\omega(t - s_1x_1)], \quad (1)$$

where the dependence of the fields along axis x_2 is contained in the 8×8 diagonal matrix $\Delta(x_2)$ whose elements are

$$\Delta_{nn}(x_2) = \exp(-j\omega s_2(n)x_2). \quad (2)$$

The term \mathbf{a} is the vector of the eight amplitudes of the partial waves, whose values are obtained when the boundary conditions are specified. The matrix F of eigenvectors can also be written as

$$F = \begin{pmatrix} U \\ T^{(2)} \end{pmatrix}, \quad (3)$$

where U and $T^{(2)}$ are 8×4 matrices containing, respectively, the generalized displacements and the generalized constraint parts of the eigenvectors. The components of the generalized stress tensor that are not involved in the state vector are linearly dependent on the displacements and there is a 4×8 matrix $T^{(i)}$ such that

$$\mathbf{t}^{(i)}(x_1, x_2) = T^{(i)}\Delta(x_2)\mathbf{a} \exp[j\omega(t - s_1x_1)] \quad (4)$$

for $i = 1, \dots, 3$ and where $\mathbf{t}^{(i)} = (T_{i1}, T_{i2}, T_{i3}, D_i)^t$.

III. COMPLEX SLOWNESSES AND PARTIAL MODE SELECTION

As we have recalled in the previous section, the plane wave solution in a piezoelectric material involves eight partial waves. These eight partial waves can be classified in two groups of four partial waves, which we term reflected (+) or incident (-), with reference to the upper interface of the substrate. In the case of a semi-infinite substrate, reflected partial waves are just those selected by the physical partial wave selection rule. The principles for this classification have been given in detail, for instance, in Refs. 1, 2, 9, and 10, in the case of purely real excitation slownesses, and are generally well agreed on. The extension of the partial wave selection rule to complex slownesses has been a matter of some controversy and it has been shown that different approaches are possible.^{1,3} In this section, we wish to emphasize that the process of extending the physical partial wave selection rule to complex slownesses can lead to a discontinuity. In order to be descriptive and to make analytic computations possible, let us consider the simple case of the spherical slowness curve

$$s_1^2 + s_2^2 = S^2. \quad (5)$$

When s_1 is restricted to the real axis, s_2 is readily obtained as

$$s_2 = \epsilon \sqrt{S^2 - s_1^2} \quad (6)$$

if $s_1 \leq S$ and

$$s_2 = -\epsilon j \sqrt{|S^2 - s_1^2|} \quad (7)$$

if $s_1 \geq S$. In these equations, $\epsilon = 1$ for reflected partial waves and $\epsilon = -1$ for incident partial waves. The reason for this choice is that the semi-infinite substrate is assumed to extend in the half plane $x_2 \geq 0$; then homogeneous (propagative) partial waves must enter the substrate and the amplitudes of inhomogeneous (evanescent) partial waves must decrease in the depth of the substrate. In the case of an arbitrary piezo-

electric, and hence anisotropic, material, the rule for reflected homogeneous partial waves is that the component of their Poynting vector along axis x_2 be positive; the rule for inhomogeneous partial waves is unchanged.

When s_1 is allowed to be complex, we write $s_1 = a - jb$. The minus sign is consistent with an attenuating wave; s_2 then satisfies

$$s_2^2 = (S^2 - a^2 + b^2) + 2jab. \quad (8)$$

We wish to examine whether the selection of partial waves is continuous as b continuously increases from $b=0$, while remaining very small. Let us first eliminate the case $S=a$. Then $s_2 = \pm \sqrt{b^2 + 2jab}$ and the choice of the sign can always be made continuous since $s_2=0$ for $b=0$.

If $a > S$, then we choose $0 < b \ll \sqrt{a^2 - S^2}$, and we define $c = \sqrt{a^2 - S^2 - b^2}$. Then we have

$$s_2 \approx -\epsilon \left(jc + \frac{ab}{c} \right). \quad (9)$$

This choice is continuous as a comparison with Eq. (7) reveals.

If $a < S$, then we choose $0 < b \ll \sqrt{S^2 - a^2}$, and we define $c = \sqrt{S^2 - a^2 + b^2}$. Then we have

$$s_2 \approx -\epsilon \left(c + j \frac{ab}{c} \right). \quad (10)$$

A comparison with Eq. (6) shows that this time the partial wave selection is discontinuous, since a reflected homogeneous partial wave is selected for $b=0$, while the reflected inhomogeneous partial wave selected for b infinitesimally greater than zero originates from an incident homogeneous partial wave when $b=0$.

This property has been demonstrated for an isotropic slowness curve only, but it generalizes straightforwardly to any slowness curve in a piezoelectric medium by considering a local approximation of the slowness curve. As an example, Fig. 1 displays the slowness curves for bulk acoustic waves in Y+42 lithium tantalate, in the sagittal plane. The PSAW slowness lies in between the slow and fast shear slowness curves. When s_1 is real in this region, two homogeneous partial waves are slow shear bulk acoustic waves, one reflected and one incident. When s_1 is allowed to become complex, they change from reflected to incident, and vice versa.

The above discussion shows that the EP cannot be an analytic function of s_1 if the physical partial wave selection rule is strictly employed, but that the modified partial wave selection rule of Adler³ is continuous in the complex plane. Also, assuming that the EP is analytic implies the Adler partial wave selection rule is implicitly selected in the PSAW region. This implies that the estimation methods in Refs. 3 and 4 must give equivalent results. We have indeed estimated the slowness and attenuation of PSAWs on various substrates, as reported in Table I, and have obtained identical results, but for numerical differences. The material constants used for the computations were the same in both cases.

We remark that the use of complex excitation slownesses to represent the attenuation of a PSAW might well not be firmly grounded. Indeed, complex wave vectors naturally oc-

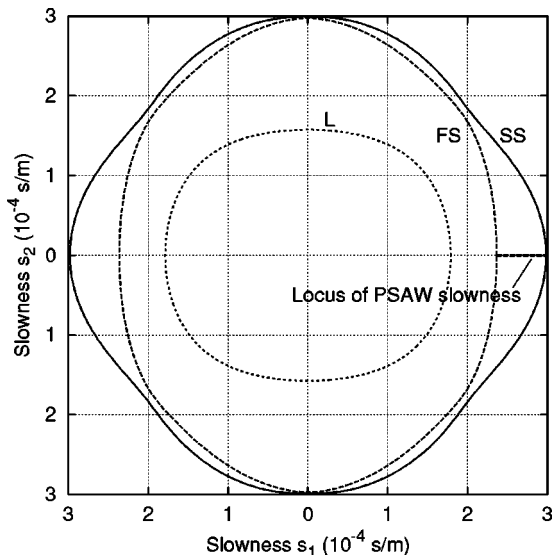


FIG. 1. Slowness curves for slow shear (SS), fast shear (FS), and longitudinal (L) bulk acoustic waves in Y+42 lithium tantalate, in the sagittal plane. The slowness of the PSAW is between the slowness of the FS and the SS bulk acoustic waves propagating along the surface.

cur when friction-type terms are added to the wave equation (see, e.g., Refs. 11 and 12). However, the leakage phenomenon of PSAWs cannot directly be accounted for by friction terms, as the materials considered are not themselves lossy. To avoid this possible issue, we propose in the next section an alternative solution to the problem of the determination of the slowness and the attenuation of a PSAW.

IV. OPTIMAL GENERATION OF PSEUDO SURFACE ACOUSTIC WAVES

A PSAW is not a true surface mode but needs to be sustained by an external energy source, e.g., an interdigital transducer (IDT).¹ An optimal source is one that will use as

less power as possible to sustain the PSAW. For this external energy source to be efficient, it needs to be in phase with the wave. Since the wave is periodic, the source should be periodic, and its Fourier series should match that of the wave. When the PSAW is excited by a source located on the surface of the piezoelectric substrate, then the net power flux through the surface vanishes, and if the source is adapted to the PSAW, then the equilibrium equation is

$$\varphi_{\text{source}} + \varphi_{\text{PSAW}} = 0, \tag{11}$$

where φ is the flux of the Poynting vector through the surface.

Let us consider the analogy with the problem of total internal reflection of an incident bulk acoustic wave when the slowness s_1 lies between the two shear slowness curves. In this region, only two partial waves are homogeneous (one incident and one reflected) and the remaining six partial waves are inhomogeneous. Then, the incident bulk acoustic wave is the incident homogeneous partial wave, which is in principle reflected into a combination of the four reflected partial waves. For the following computations, the three reflected inhomogeneous partial waves are numbered 1–3; the reflected homogeneous partial wave is numbered 4; and the incident homogeneous partial wave is numbered 5. The three incident inhomogeneous partial waves, numbered 6–8, are not considered in this problem since they do not radiate acoustic power through the surface. φ_{source} is linked to incident partial waves, while φ_{PSAW} is linked to reflected partial waves. We postulate that an optimal source is one that creates generalized surface constraints that mimic that of the incident partial wave, while minimizing the dissipated power. We next discuss how this postulate can be used to obtain the slowness and attenuation of the PSAW.

In the case of a mechanically free surface, the normal constraints at $x_2=0$ must vanish, which results in three linear boundary conditions. We then distinguish between the

TABLE I. Comparison of PSAW slowness and attenuation estimations obtained using complex poles of the effective permittivity, either by fit from the real axis of slowness (see Ref. 4) or by a direct search in the complex plane (see Ref. 3), and using the least action principle (LAP) in this work, for several cuts of lithium tantalate (LT), lithium niobate (LN), and quartz (QTZ).

Cut	Method of Ref. 4		Method of Ref. 3		LAP	
	Slowness (10 ⁴ s/m)	att. (mdB/λ)	Slowness (10 ⁴ s/m)	att. (mdB/λ)	Slowness (10 ⁴ s/m)	att. (mdB/λ)
Y+36 LT						
free	2.365 739 59	0.204 953 01	2.365 739 42	0.204 935 05	2.365 739 42	0.051 012 40
shorted	2.433 584 23	0.263 392 44	2.433 584 23	0.263 390 77	2.433 584 25	0.009 268 54
Y+42 LT						
free	2.365 822 33	0.754 350 78	2.365 820 95	0.754 273 02	2.365 820 94	0.188 278 77
shorted	2.429 986 52	12.371 696 42	2.429 985 25	12.367 737 26	2.429 986 24	1.385 391 98
Y+41 LN						
free	2.103 931 30	0.243 616 71	2.103 931 24	0.243 550 98	2.103 931 23	0.061 051 85
shorted	2.283 694 05	14.163 903 53	2.283 693 30	14.145 821 32	2.283 697 09	1.905 401 67
Y+64 LN						
free	2.130 830 86	52.292 367 33	2.130 796 33	52.043 856 54	2.130 948 13	3.890 276 50
shorted	2.246 521 66	3.710 201 85	2.246 521 61	3.709 219 83	2.246 521 36	0.301 390 06
Y+42.75 QTZ						
free	1.967 794 57	78.392 572 60	1.967 570 14	78.297 195 10	1.967 677 76	16.162 780 22
shorted	1.968 118 59	78.875 692 28	1.967 896 53	78.766 046 19	1.968 003 04	16.307 023 91

cases of an electrically free or shorted surface. For a shorted surface, the surface potential vanishes; for an electrically free surface, surface charges are not allowed to exist. Summarizing both cases, we can write the boundary conditions giving the reflected partial wave amplitudes, a_1 through a_4 , as a function of the incident partial wave amplitude a_5 in the form

$$M \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{pmatrix} = 0, \quad (12)$$

where M is the 4×5 matrix constructed, for $j=1, \dots, 5$, as

$$M(i, j) = F(i + 4, j), \quad i = 1, 2, 3, \quad (13)$$

$$M(4, j) = F(4, j) \quad (14)$$

for a shorted surface, and

$$M(4, j) = F(8, j) - j \omega s_1 \epsilon_0 F(4, j) \quad (15)$$

for an electrically free surface. From the linear Eq. (12), the reflected partial wave amplitudes can be computed as a function of a_5 , according to

$$M_r \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = -a_5 \mathbf{m}_5, \quad (16)$$

where M_r is the matrix composed of the first four columns of M , and \mathbf{m}_5 is the vector equal to the fifth column of M .

The Poynting vector of the n th partial wave can be computed as

$$P_i(n) = \text{Re} \left\{ \sum_{j=1}^4 u_j^*(n) T_{ij}(n) \right\} \quad (17)$$

or using Eqs. (1)–(4),

$$P_i(n) = \text{Re} \left\{ \sum_{j=1}^4 U_{jn}^* T_{jn}^{(i)} \Delta_{nn}^*(x_2) \Delta_{nn}(x_2) \right\}. \quad (18)$$

Writing

$$s_2(n) = \beta_2(n) + j \alpha_2(n) \quad (19)$$

we have

$$\Delta_{nn}^*(x_2) \Delta_{nn}(x_2) = \exp(2 \omega \alpha_2(n) x_2). \quad (20)$$

Inhomogeneous reflected partial waves ($\alpha_2(n) < 0$) transport power along the surface; the total power flux crossing an arbitrary section normal to the surface is

$$\varphi_1(n) = \int_0^\infty dx_2 P_1(n) = \frac{-1}{2 \omega \alpha_2(n)} \text{Re} \left\{ \sum_{j=1}^4 U_{jn}^* T_{jn}^{(1)} \right\}. \quad (21)$$

Propagative partial waves have a nonvanishing power flux through the surface; the total power flux crossing a section of the surface one wavelength long is

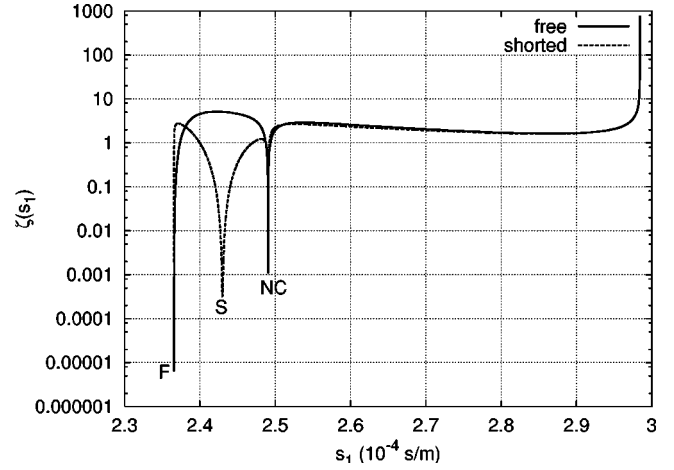


FIG. 2. Plot of attenuation function $\zeta(s_1)$ defined by Eq. (27) for Y+42 lithium tantalate, as a function of slowness s_1 . The PSAW is located by the two minima for free surface (label F) and shorted surface (label S) boundary conditions. Another minimum (label NC) appears simultaneously for both free and shorted boundary conditions, indicating the presence of a nonpiezoelectrically coupled PSAW.

$$\varphi_2(n) = \int_0^{2\pi/(\omega s_1)} dx_1 P_2(n) = \frac{2\pi}{\omega s_1} \text{Re} \left\{ \sum_{j=1}^4 U_{jn}^* T_{jn}^{(2)} \right\}. \quad (22)$$

We choose to normalize, respectively, propagative partial waves (numbered 4 and 5 here) by $\sqrt{\varphi_2(n)}$, and inhomogeneous reflected partial waves (numbered 1–3 here) by $\sqrt{\varphi_1(n)}$. With this normalization, Eq. (11) implies that

$$|a_4|^2 = |a_5|^2 \quad (23)$$

which states the equilibrium of power loss by radiation into the substrate to the power brought by the source. Furthermore, the total power transported by the surface wave along the surface is $|a_1|^2 + |a_2|^2 + |a_3|^2$, and the attenuation per wavelength is given by

$$\zeta(s_1) = \frac{|a_4|^2}{|a_1|^2 + |a_2|^2 + |a_3|^2}. \quad (24)$$

Using Eq. (16) we have

$$|a_1|^2 + |a_2|^2 + |a_3|^2 + |a_4|^2 = |a_5|^2 \|M_r^{-1} \mathbf{m}_5\|^2 \quad (25)$$

with

$$\|M_r^{-1} \mathbf{m}_5\|^2 = (M_r^{-1} \mathbf{m}_5)^\dagger (M_r^{-1} \mathbf{m}_5) \quad (26)$$

and \dagger stands for transpose and conjugate of a complex vector or matrix. The final expression for the attenuation per wavelength then becomes

$$\zeta(s_1) = \frac{1}{\|M_r^{-1} \mathbf{m}_5\|^2 - 1} \quad (27)$$

and the criterion for locating the PSAW slowness is to find s_1 that minimizes $\zeta(s_1)$, or equivalently that maximizes $\|M_r^{-1} \mathbf{m}_5\|$. This constitutes the least action principle (LAP) referred to by the title of this article.

As an illustration of this procedure, Fig. 2 shows functions $\zeta(s_1)$ for Y+42 lithium tantalate and electrically free and shorted boundary conditions. Minima can clearly be ob-

served, indicating the location of the classical PSAW of Y +42 lithium tantalate, plus an additional nonelectrically coupled PSAW which cannot be revealed by an EP search.

Table I shows a comparison of PSAW slowness and attenuation estimations obtained by searching for the complex poles of the EP^{3,4} and the LAP. It can be observed that the slownesses are very close, but that the attenuations predicted by the LAP are about 5–10 times smaller than that predicted using the EP. However, the figures are correlated.

V. CONCLUSION

We have shown that the consideration of complex excitation slownesses in the search for PSAWs leads to a discontinuity in the usual partial wave selection rule used in the description of the propagation of plane waves in piezoelectric media. We argue that the implicit hypothesis that the attenuation can be represented by the imaginary part of the slowness is questionable, as the leaking mechanism of PSAWs is not equivalent to the friction loss mechanism that underlies this hypothesis. Observing that a PSAW is not a true mode of the substrate and must be sustained by an external energy source to exist, e.g., by an interdigital transducer, we have proposed an optimal excitation condition for a PSAW, by analogy with the total reflection of a bulk acoustic wave. From the derived least action principle, we have computed the attenuation as a function of slowness for several widely used PSAW cuts. The numerical values we find

for the slowness are very close to those given by other methods based on a search in the complex plane. However, the attenuations we obtain are substantially smaller.

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