Stable scattering-matrix method for surface acoustic waves in piezoelectric multilayers

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A scattering matrix approach is proposed to avoid numerical instabilities arising with the classical transfer matrix method when analyzing the propagation of plane surface acoustic waves in piezoelectric multilayers. The method is stable whatever the thickness of the layers, and the frequency or the slowness of the waves. The computation of the Green's function and of the effective permittivity of the multilayer is outlined. In addition, the method can be easily extended to the case of interface acoustic waves. © *2002 American Institute of Physics.*
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The increase in operating frequencies of telecommunication systems warrants the use of fast substrates with high surface acoustic wave (SAW) phase velocities, enabling the fabrication of high frequency filters. The use of piezoelectric multilayers on which guided elastic waves can propagate with high velocities and no propagation losses has often been proposed as an innovative way to avoid some classical limitations of SAW on single crystals. Consequently, efficient simulation tools are needed to characterize the electromechanical behavior of complex stratified structures. As in the case of single crystals, a basic problem is the computation of the spectral surface Green's function or of the effective permittivity.[1]

Many matrix models have been formulated for the numerical simulation of stratified structures, most of which rely on the transfer matrix (TM) approach originally proposed by Fahmy and Adler in 1973.[2–4] It will be shown that in the common situation that the frequency–slowness–thickness (FST) product becomes large for some layer, numerical instabilities occur when using the TM approach. This is because a TM links physical quantities at every interface, even though some of these quantities are decoupled for large FST products. Large FST products are, for instance, encountered when analyzing the propagation of a SAW under a grating, as all harmonics have to be included in the analysis. As an alternative, we propose the use of a scattering-matrix (SM) approach, which acts on the amplitudes of partial modes of each layer rather than on the physical quantities themselves. As a result of energy conservation, such an approach is guaranteed to be stable. Useful expressions will then be given for the computation of the Green's function or the effective permittivity of a multilayer, encompassing surface as well as interface waves.

The general configuration of Fig. 1 is considered. The multilayer is composed of a semi-infinite substrate or a plate, considered as the first layer, on top of which are layers number 2 to n. Each layer, identified by its index m, is supposed to be homogeneous, possibly piezoelectric, and has a constant thickness w_m. Propagation of plane waves with frequency f is considered along the x_1 axis, with slowness s_1. Assuming plane wave propagation in the structure, the distribution of the electromechanical fields in each layer is fully described[2] using the eight-component state vector $h=(u_1,u_2,u_3,\phi,T_{21},T_{23},T_{23},D_2)^t$ where the u_i are the mechanical displacements, ϕ is the electrical potential, T is the stress tensor, and D_2 is the normal electrical displacement. This state vector is obtained inside a layer as a superposition of eight partial modes, characterized by their eigenvalues $s_2^{(i)}$ and their associated eigenvectors.[2] The eigenvalues $s_2^{(i)}$ only depend on the material constants of the layer, and on the slowness s_1. Denoting F, the 8×8 matrix of the vertically arranged eigenvectors, this superposition reads in the mth layer

$$h(x_2)=F^{(m)}\Delta^{(m)}(x_2)a^{(m)}\exp[2j\pi f(t-s_1x_1)], \quad (1)$$

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

$$\Delta_{ii}^{(m)}(x_2)=\exp(-2j\pi f s_{2,i}^{(m)}x_2). \quad (2)$$

$a^{(m)}$ is the vector of the eight amplitudes of the partial waves, whose values are obtained when the boundary conditions are specified.

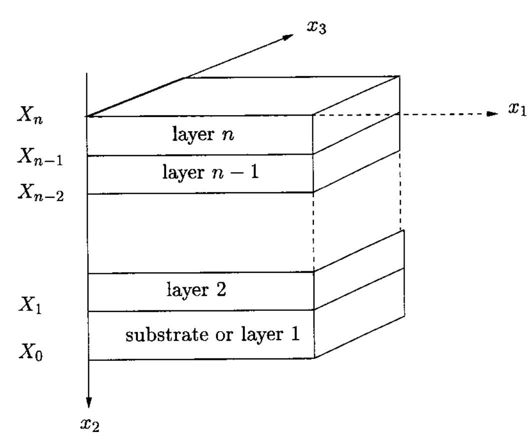

FIG. 1. Multilayer definitions.

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TABLE I. Partial modes slowness' $s_2^{(i)}$ for the $(YXl)/36°$ cut of quartz and $s_1 = 10^{-3}$ s/m.

Modes	number i	s_2 (10^{-4} s/m)
Reflected (+)	1	$-j$ 16.3
	2	$-j$ 13.3
	3	$-j$ 10.1
	4	$-j$ 4.55
incident (−)	5	j 16.3
	6	j 13.3
	7	j 10.1
	8	j 4.55

The components of the state vector have been explicitly chosen such that they are continuous across any interface inside the multilayer. It is then practical to construct a TM linking state vectors at two interfaces. For instance, this relation between the $(m-1)$-th to the mth interface writes

$$h(X_m) = M_{m-1}^m h(X_{m-1}), \tag{3}$$

where the transfer matrix M_{m-1}^m can be written[2]

$$M_{m-1}^m = F^{(m)} \Delta^{(m)}(w_m) (F^{(m)})^{-1}. \tag{4}$$

Equations (3) and (4) are easily generalized in a chain-matrix fashion to obtain the relation between any two interfaces, and e.g., between the first to the nth interface as

$$h(X_n) = M_1^n h(X_1), \tag{5}$$

$$M_1^n = M_{n-1}^n \times \cdots \times M_{m-1}^m \times \cdots \times M_1^2. \tag{6}$$

The TM approach is naturally well suited to the analysis of thin piezoelectric layers deposited on a substrate. However, it is numerically unstable whenever the FST product is large. To prove this, it is sufficient to consider the $\Delta^{(m)}(w_m)$ matrix in Eq. (4), which according to Eq. (2) has elements

$$\Delta_{ii}^{(m)}(w_m) = \exp(-2j\pi f w_m s_{2,i}^{(m)}). \tag{7}$$

The magnitude of these matrix elements is mostly dictated by the values $s_{2,i}^{(m)}$. In the example of Table I, the $(YXl)/36°$ cut of a layer of quartz is considered, for a propagation slowness $s_1 = 10^{-3}$ s/m, corresponding to a velocity of 1000 m/s. The eight partial modes have been classified into two groups of four partial modes, and are termed either reflected (+) or incident (−), with reference to the upper interface of the layer. The rules for this classification have been for instance given in Ref. 4. With the product $f w_m$ real and positive, the matrix elements $\Delta_{ii}^{(m)}(w_m)$ are either of unit modulus if the mode is propagative, of modulus smaller than 1 if the partial mode is reflected evanescent $[\Im(s_2) < 0]$, or of modulus larger than 1, if it is incident evanescent $[\Im(s_2) > 0]$. When s_1 is larger than the slow-shear wave slowness, all partial modes are always evanescent, whatever the material constants, and asymptotically $|s_2|$ increases linearly with s_1.[5] When the FST product $f w_m s_1$ is large, reflected, and incident evanescent partial modes will then, respectively, cause the TM or its inverse to become singular. Physically, the values of displacements and stresses at one interface can not be deduced properly from their values at a distant interface if evanescent partial modes are involved, since their influence is vanishingly small.

For the stable computation of the electromechanical response of multilayers, we propose using a SM method, based on the decomposition of reflected and incident partial modes inside each layer. Remarking that there are no sources at the bottom of a semi-infinite substrate, or outside and below a plate, the reflected partial modes in the first layer must be uniquely determined by the incident partial modes in that layer. Proceeding in a recursive manner, from the bottom to the top layer, the same argument holds for any layer from the first to the last. We now exploit mathematically this property. In order to simplify the derivation, an auxiliary variable is introduced as

$$g^{(m)}(x_2) = \Delta^{(m)}(x_2) a^{(m)}, \tag{8}$$

or using the decomposition in reflected and incident partial modes

$$g^{(m)}(x_2) = \begin{pmatrix} \Delta^{(m+)}(x_2) & 0 \\ 0 & \Delta^{(m-)}(x_2) \end{pmatrix} \begin{pmatrix} a^{(m+)} \\ a^{(m-)} \end{pmatrix}. \tag{9}$$

We then define a reflection matrix at the bottom of the mth layer as

$$g^{(m-)}(X_{m-1}) = R^{(m)} g^{(m+)}(X_{m-1}). \tag{10}$$

In the case of a semi-infinite substrate, the amplitudes of the incident partial modes must vanish so that

$$R^{(1)} = 0. \tag{11}$$

In the case of a plate, we assume no mechanical stresses or charge density at the free bottom interface, so that

$$g^{(1)}(X_0) = F^{(1)-1} \begin{pmatrix} I_4 \\ 0_4 \end{pmatrix} h(X_0) = \begin{pmatrix} A \\ B \end{pmatrix} b, \tag{12}$$

where I_4 and 0_4 are, respectively, the 4×4 identity and null matrices, A and B are 4×4 matrices, and b is some four-component vector. The reflection matrix is then easily obtained as

$$R^{(1)} = BA^{-1}. \tag{13}$$

In Eq. (12), the eigenvector matrix $F^{(1)}$ can be modified to account for the permittivity of vacuum[2] according to the rule

$$F_{8,i}^{(1)} \leftarrow F_{8,i}^{(1)} - j\epsilon_0 |s_1| F_{4,i}^{(1)}, \quad i = 1 \ldots 8. \tag{14}$$

The recursion to compute the reflection matrix from one layer to the next can be obtained as follows. We have first

$$g^{(m-)}(X_m) = D^{(m-)} R^{(m)} D^{(m+)} g^{(m+)}(X_m), \tag{15}$$

with the notations $D^{(m-)} = \Delta^{(m-)}(-w_m)$ and $D^{(m+)} = \Delta^{(m+)}(w_m)$. Second, from the continuity of the state vector,

$$g^{(m+1)}(X_m) = (F^{(m+1)})^{-1} F^{(m)} g^{(m)}(X_m), \tag{16}$$

from which we obtain the reflection matrix for the $(m+1)$-th layer as

$$R^{(m+1)} = DC^{-1}, \tag{17}$$

where the 4×4 matrices C and D are defined as

$$(F^{(m+1)})^{-1} F^{(m)} \begin{pmatrix} I_4 \\ D^{(m-)} R^{(m)} D^{(m+)} \end{pmatrix} = \begin{pmatrix} C \\ D \end{pmatrix}. \tag{18}$$

The key point is that the moduli of the elements of the diagonal matrices $D^{(m-)}$ and $D^{(m+)}$ involved in Eq. (18) are all

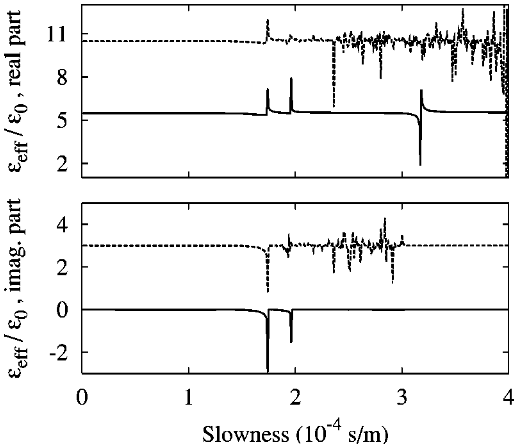

FIG. 2. Surface permittivity of a layer of $(YXl)/36°$ quartz ($fw = 33$ GHz μm) over a semi-infinite $(YXl)/36°$ quartz substrate, computed using either the TM (dotted line) or the SM (solid line) method. TM curves are translated vertically by an arbitrary amount to ease the comparison.

smaller than 1. This ensures the stability of the recursion algorithm, and justifies *a posteriori* the decomposition into incident and reflected modes.

The surface Green's function of the multilayer is easily obtained using the reflection matrix for the last layer and reads

$$G = FE^{-1}, \tag{19}$$

with the 4×4 matrices E and F defined by

$$F^{(n)}\begin{pmatrix} I_4 \\ D^{(n-)}R^{(n)}D^{(n+)} \end{pmatrix} = \begin{pmatrix} E \\ F \end{pmatrix}. \tag{20}$$

As in Eq. (12), the eigenvector matrix F_n can be modified to account for the permittivity of a vacuum. Additionally, the effective surface permittivity can be obtained from the Green's function as[1]

$$\varepsilon_{\text{eff}} = \frac{1}{j\varepsilon_0|s_1|G_{44}}. \tag{21}$$

Figure 2 shows the effective surface permittivity computed using the TM and SM methods for a $(YXl)/36°$ quartz plate, with a frequency-thickness product $fw = 33$ GHz μm, over a semi-infinite $(YXl)/36°$ quartz substrate. This combination is obviously equivalent to a single semi-infinite quartz substrate, and is considered only for illustration purposes. It can be seen that the results are strictly the same for small slownesses, but that after some point numerical instabilities arise in the TM computation. As a result, neither the second transverse mode nor the Rayleigh wave can be observed in this case. The SM result is free of numerical instabilities, as expected.

It is simple to apply the SM algorithm to simulate an excitation on the bottom side of the multilayer. In this case, the recursion must be initiated at the upper interface, the incident and reflected modes have to be interchanged, and all layer thicknesses has to be taken negative. Once these changes have been made, Eqs. (8)–(21) apply unchanged.

The SM method can also be easily extended to interface acoustic waves in multilayers. In this case, the interface permittivity can be computed by separating the multilayer into two subsets, divided by the excitation interface. The SM algorithm is then applied to both multilayers, considering an electrical excitation on the top surface of the lower multilayer, and on the bottom surface of the upper multilayer. With the reflection matrices of each multilayer, the electromechanical solutions can be connected using the boundary conditions (continuity of all fields excepted for the normal electrical displacement), which gives a relation between the electrical potential and the charge density at the excitation interface in the form

$$\phi = \varepsilon_{\text{int}}\Delta D_2. \tag{22}$$

In conclusion, a SM approach has been proposed to remedy to numerical instabilities arising with the classical TM method when analyzing surface acoustic waves in multilayers. The SM method enables the stable computation of the spectral Green's function of a multilayer, whatever the thickness of the layers, and the frequency or the slowness of the wave. In addition, the method can be extended easily to the case of interface waves.

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