Recursive asymptotic stiffness matrix method for analysis of surface acoustic wave devices on layered piezoelectric media

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# Recursive asymptotic stiffness matrix method for analysis of surface acoustic wave devices on layered piezoelectric media

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Based on a simple second-order thin layer asymptotic expansion for the transfer matrix, an asymptotic solution for the stiffness matrix for a general anisotropic piezoelectric thin layer is obtained. The total stiffness matrix for thick layers or multilayers is calculated with arbitrary precision by subdividing them into thin sublayers and combining recursively the thin layer stiffness matrices. It is shown that this method converges to the exact solution and is computationally stable, efficient and easy to implement. A semispace substrate is substituted for by a finite thickness layer loaded by a perfectly matched attenuating layer. The effective permittivity and general Green's functions for a layered system on a substrate are formulated in terms of stiffness and compliance matrices. The advantage of the method is that one does not need to compute the exact wave propagation solution for an anisotropic piezoelectric layer or semispace. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1522831]

The demand for high frequency surface acoustic wave (SAW) devices in telecommunication systems at frequencies above 2 GHz leads to the use of piezoelectric multilayers with high surface wave phase velocity to increase the distance between lines in interdigital transducers. To analyze these devices, efficient and stable computation of the general Green's functions and effective permittivity is required.[1–6] Exact solutions based on the transfer matrix,[1–3] invariant embedding[4,7,8] and the stiffness matrix[9,10] have been developed. However, these solutions are rather complicated and some suffer from numerical instabilities. As an alternative to these exact solutions, the thin layer finite element method (FEM) has been developed.[11,12] The FEM method requires solving a global stiffness matrix and is not easily adaptable to surface Green's function and effective permittivity calculations. For the design of SAW devices one needs to measure SAW properties of the deposited layers and to determine the effect and existence of residual stresses. All these require better physical understanding of SAW propagation in multilayered piezoelectric media and the ability to solve an inverse measurement problem. Thus one needs alternative, simplified solutions that are better suited to this analysis. In this letter, we develop a recursive asymptotic stiffness matrix (RASM) method by combining a simple asymptotic stiffness matrix and an efficient recursive algorithm. The recursive stiffness matrix method is perfectly suitable for computation of the generalized Green's function and the effective permittivity for surface or imbedded transducers and converges to the exact solution. Furthermore, one does not need to compute the exact wave propagation solution for an anisotropic piezoelectric layer or a substrate.

Let us consider generally anisotropic piezoelectric media as shown in Fig. 1. We define the four-dimensional general displacement $\mathbf{U}(=[\mathbf{u},\phi]^{\mathrm{T}})$, the general stress $\mathbf{T}=[\boldsymbol{\sigma},D_3]^{\mathrm{T}}$ vectors and the state vector $\boldsymbol{\xi}=\left[\begin{smallmatrix}\mathbf{U}\\ \mathbf{T}\end{smallmatrix}\right]$, where $\mathbf{u}$ and $\boldsymbol{\sigma}$ are the particle displacement and normal stress vectors, respectively, and $\phi$ and $D_3$ are the electrical potential and normal electric displacement, respectively. We consider a harmonic wave propagating along $x$ of the form $\xi(z)e^{i(\omega t-k_x x)}$; $\omega$ is angular frequency, $k_x=\omega/V$ is wave number and $V$ is phase velocity along the $x$ axis. The governing equation for the state vector is[1,2]

$$\frac{d\xi}{dz}=i\mathbf{A}\xi, \tag{1}$$

where $\mathbf{A}$ is the fundamental acoustic tensor which is given in Ref. 2. For one homogeneous layer, the differential Eq. (1) has the well-known transfer matrix solution $\mathbf{B}$ in exponential form, which relates the state vector at the layer top $(z+h)$ to that at the layer bottom $(z)$

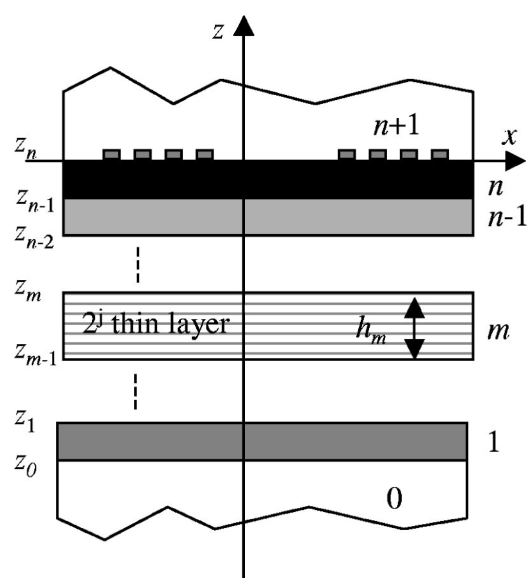


FIG. 1. Schematic of SAW on a layered structure and coordinate system. Each layer is subdivided into $2^j$ thin layers with the same thickness $h$.

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$$\xi(z+h)=\mathbf{B}\xi(z), \mathbf{B}=e^{i\mathbf{A}h}, \tag{2}$$

where $h$ is the layer thickness. Exact computation of $\mathbf{B}$ requires finding the eigenvalues and eigenvectors of $\mathbf{A}$. For small thickness $h$, a second-order asymptotic transfer matrix can be written as[13]

$$\mathbf{B}_{\mathrm{II}}(h)=\left(\mathbf{I}-i\frac{h}{2}\mathbf{A}\right)^{-1}\left(\mathbf{I}+i\frac{h}{2}\mathbf{A}\right). \tag{3}$$

The asymptotic solution can accurately represent the exact transfer matrix for small frequency $f$ on thickness $h$ products ($fh<0.1$).[13] For a thick layer with thickness $H$, one can subdivide it into $N$ thin layers with thickness $h=H/N$. The total transfer matrix $\mathbf{B}(H)$ for the thick layer is the product of the $N$ thin layers

$$\mathbf{B}(H)=\prod_{j=1}^{N}\mathbf{B}_{\mathrm{II}}(H/N)=\left[\left(\mathbf{I}-\frac{iH\mathbf{A}}{2N}\right)^{-1}\left(\mathbf{I}+\frac{iH\mathbf{A}}{2N}\right)\right]^{N}. \tag{4}$$

Because $(\mathbf{I}-iH\mathbf{A}/2N)^{-1}$ and $(\mathbf{I}+iH\mathbf{A}/2N)$ commute,[13] Eq. (4) can be written as $\mathbf{B}(H)=[(\mathbf{I}-iH\mathbf{A}/2N)^{-1}]^{N}[(\mathbf{I}+iH\mathbf{A}/2N)]^{N}$. Since $(e^{-iH\mathbf{A}/2})^{-1}=e^{iH\mathbf{A}/2}$, and $e^{iH\mathbf{A}/2}e^{iH\mathbf{A}/2}=e^{iH\mathbf{A}}$, the approximate transfer matrix $\mathbf{B}(H)$ converges to the exact transfer matrix $\mathbf{B}=e^{i\mathbf{A}H}$ as the number of subdivisions $N$ approaches infinity.

One should distinguish analytical convergence from computational convergence due to the limited number of computational digits. It is well known that the transfer matrix method is numerically unstable at high frequencies and therefore the recursive algorithm (4) for the transfer matrix is also computationally unstable and will not converge computationally. Recently Wang and Rokhlin[9,10] have developed a recursive algorithm based on the stiffness matrix which has been demonstrated to be unconditionally stable. Therefore we will transform the asymptotic transfer matrix $\mathbf{B}_{\mathrm{II}}$ into the stiffness matrix $\mathbf{K}_{\mathrm{II}}$ using the relation between the transfer matrix $\mathbf{B}$ and the stiffness matrix $\mathbf{K}$

$$\mathbf{K}=\begin{bmatrix} -(\mathbf{B}_{12})^{-1}\mathbf{B}_{11} & (\mathbf{B}_{12})^{-1} \\ \mathbf{B}_{21}-\mathbf{B}_{22}(\mathbf{B}_{12})^{-1}\mathbf{B}_{11} & \mathbf{B}_{22}(\mathbf{B}_{12})^{-1} \end{bmatrix}. \tag{5}$$

Substituting Eq. (3) into Eq. (5) and replacing the acoustic tensor $\mathbf{A}$ by submatrices $\mathbf{\Gamma}_{ik}$ (see Refs. 1 and 2), the second-order stiffness matrix can be written as $\mathbf{K}_{\mathrm{II}}$

$$\mathbf{K}_{\mathrm{II}}=\begin{bmatrix} -\frac{\mathbf{\Gamma}_{33}}{h}+(\mathbf{\Gamma}_{31}-\mathbf{\Gamma}_{13})\frac{ik_x}{2}-\frac{\mathbf{\Gamma}_{11}hk_x^2}{4}+\frac{\rho h\omega^2}{4}\mathbf{I}' & \frac{\mathbf{\Gamma}_{33}}{h}+(\mathbf{\Gamma}_{31}+\mathbf{\Gamma}_{13})\frac{ik_x}{2}-\frac{\mathbf{\Gamma}_{11}hk_x^2}{4}+\frac{\rho h\omega^2}{4}\mathbf{I}' \\ -\frac{\mathbf{\Gamma}_{33}}{h}+(\mathbf{\Gamma}_{31}+\mathbf{\Gamma}_{13})\frac{ik_x}{2}+\frac{\mathbf{\Gamma}_{11}hk_x^2}{4}-\frac{\rho h\omega^2}{4}\mathbf{I}' & \frac{\mathbf{\Gamma}_{33}}{h}+(\mathbf{\Gamma}_{31}-\mathbf{\Gamma}_{13})\frac{ik_x}{2}+\frac{\mathbf{\Gamma}_{11}hk_x^2}{4}-\frac{\rho h\omega^2}{4}\mathbf{I}' \end{bmatrix}, \tag{6}$$

where $\mathbf{\Gamma}_{ik}$ depends on the elastic constants $c_{ijkl}$, piezoelectric constants $e_{ijk}$ and dielectric permittivity constants $\epsilon_{ik}$. $\mathbf{I}'$ is the $4\times4$ identity matrix but with zero (4,4) element; $\rho$ is the density of the solid. The asymptotic stiffness matrix elements are simple explicit functions of the elastic and piezoelectric properties. This provides better insight into the wave phenomena and has advantages for inverse solution. To find the stiffness matrix of a thick layer, as discussed above, the thick layer is subdivided into a set of thin layers and the total stiffness matrix of the thick layer is obtained from the thin layer stiffness matrix using a stable recursive algorithm[9,10]

$$\mathbf{K}^{M}=\begin{bmatrix} \mathbf{K}_{11}^{m}+\mathbf{K}_{12}^{m}(\mathbf{K}_{11}^{M-1}-\mathbf{K}_{22}^{m})^{-1}\mathbf{K}_{21}^{m} & -\mathbf{K}_{12}^{m}(\mathbf{K}_{11}^{M-1}-\mathbf{K}_{22}^{m})^{-1}\mathbf{K}_{12}^{M-1} \\ \mathbf{K}_{21}^{M-1}(\mathbf{K}_{11}^{M-1}-\mathbf{K}_{22}^{m})^{-1}\mathbf{K}_{21}^{m} & \mathbf{K}_{22}^{M-1}-\mathbf{K}_{21}^{M-1}(\mathbf{K}_{11}^{M-1}-\mathbf{K}_{22}^{m})^{-1}\mathbf{K}_{12}^{M-1} \end{bmatrix}, \tag{7}$$

where $\mathbf{K}^{M}$ is the total stiffness matrix for the bottom $m$ layers, $\mathbf{K}_{ij}^{M-1}$ are the submatrices of the total stiffness matrix for the bottom $m-1$ layers, $\mathbf{K}_{ij}^{m}$ are the submatrices of the $m$th layer stiffness matrix. Since Eq. (7) is obtained from Eq. (4) using Eq. (5), from the convergence of the operation (4) to the exact solution follows the convergence of the recursive algorithm (7) with increase of the number of subdivisions. However, in contrast to Eq. (4), algorithm (7) is computationally stable.

Above we described the computation of the stiffness matrix for a layered structure with finite thickness. It is impractical to represent a semi-infinite substrate directly by a series of thin layers. For this reason, we first replace the semi-infinite substrate by a substrate of finite, but larger than wavelength, thickness with absorbing boundary conditions (BC) at the bottom surface. To implement the absorbing BC we apply the perfectly matched layer concept (PML)[14] used in finite element modeling. We obtain the governing equation for the PML state vector by replacing $d/dz$ by $d/\beta dz$ in Eq. (1)

$$\frac{d\xi}{dz}=i\mathbf{A}_{\mathrm{PML}}\xi, \tag{8}$$

where $\mathbf{A}_{\mathrm{PML}}=\beta\mathbf{A}$ and $\beta$ is a complex variable. Therefore the PML layer is a lossy medium with acoustic tensor $\mathbf{A}_{\mathrm{PML}}$. Because $\mathbf{A}_{\mathrm{PML}}$ and $\mathbf{A}$ have the same eigenvectors, the surface stiffness (impedance) matrix[10] of these two media will also be the same. Due to impedance matching there is no reflection from the interfaces between PML and the substrate layer with acoustic tensor $\mathbf{A}$. Because $\beta$ is complex, all plane waves in the PML are attenuated. One can easily verify that the second-order stiffness matrix $\mathbf{K}_{\mathrm{II}}^{\mathrm{PML}}$ for a PML layer is obtained by replacing the real thickness $h$ in $\mathbf{K}_{\mathrm{II}}$ [Eq. (7)] by the complex thickness $h\beta$.

For a layered structure, the computational algorithm to obtain the total stiffness matrix using the RASM method can

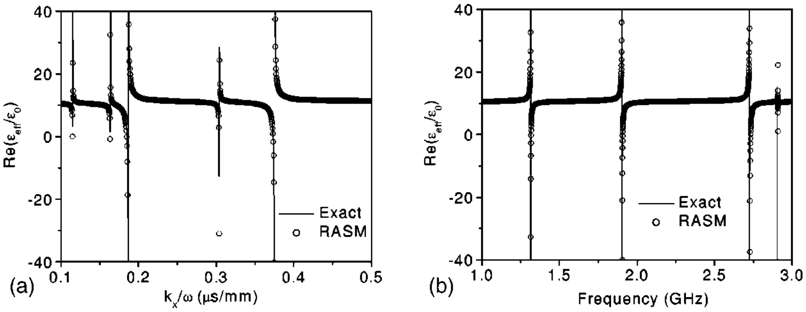


FIG. 2. Comparison of effective surface permittivity for a ZnO/diamond/silicon layered semispace calculated using exact and RASM methods. Thickness of ZnO and diamond layers is 2 and 30 $\mu$m, respectively. (a) as function of $k_x/\omega$, frequency is 2.5 GHz; (b) as function of frequency, phase velocity is 8 mm/$\mu$s.

be separated into two steps:

(1) Obtain the layer stiffness matrix for each homogeneous layer of the layered structure by dividing it into $N = 2^j$ thin layers and using the recursive algorithm (7) and the asymptotic thin layer stiffness matrix (6) to obtain the layer stiffness matrix. Because all thin layer stiffness matrices are identical, only $j$ recursive operations are needed for $2^j$ thin layers.[10]

(2) Obtain the total stiffness matrix for the layered structure by combining all layer stiffness matrices (including the PML layer) using the recursive algorithm (7). Alternatively, the top surface stiffness $\mathbf{K}_S$ ($\mathbf{T}_n = \mathbf{K}_S \mathbf{U}_n$) can be obtained directly[10] calculating recursively only the $\mathbf{K}_{11}^M$ ($= \mathbf{K}_S^M$) element in Eq. (7). Because the semi-infinite substrate is replaced by a PML layer, the value of the state vector is negligible at its bottom surface and thus in starting the recursive procedure from the system bottom the surface stiffness $\mathbf{K}_S^B$ is taken to be zero.

After the total surface stiffness matrix for the layered substrate or the total stiffness matrix for a layered plate is obtained, the generalized Green's function $\mathbf{G}$ and effective permittivity $\epsilon_{\mathrm{eff}}$ can easily be determined. Here we use the layered semispace with surface transducers as an example. For simplicity, we use the total surface compliance matrix $\mathbf{S}_S = \mathbf{K}_S^{-1}$ and decompose it into mechanical $\mathbf{S}_S^f$ $(3\times3)$, electric $S_S^e$ $(1\times1)$ and coupling $\mathbf{S}_S^{fe}$ $(3\times1)$, $\mathbf{S}_S^{ef}$ $(1\times3)$ submatrices:

$$\mathbf{S}_S = \begin{bmatrix} \mathbf{S}_S^f & \mathbf{S}_S^{fe} \\ \mathbf{S}_S^{ef} & S_S^e \end{bmatrix}.$$

Taking into account the electric field in the vacuum above the top semispace, where the electric potential satisfies the Laplace equation,[2] the generalized surface Green's function can be written as

$$\mathbf{G} = \begin{bmatrix} \mathbf{S}_S^f + \alpha|k_x|\epsilon_0 \mathbf{S}_S^{fe}\mathbf{S}_S^{ef} & -(1+\alpha|k_x|\epsilon_0)\mathbf{S}_S^{fe} \\ \alpha \mathbf{S}_S^{ef} & -\alpha S_S^e \end{bmatrix}, \tag{9}$$

where $\epsilon_0$ is the vacuum permittivity and $\alpha = 1/(1 - |k_x|\epsilon_0 S_S^e)$. The effective surface permittivity $\epsilon_{\mathrm{eff}}$ can be obtained using the $G_{44}$ element of the Green's function as

$$\epsilon_{\mathrm{eff}}(k_x) = \frac{1}{|k_x| G_{44}} = \epsilon_0 - \frac{1}{|k_x| S_S^e}. \tag{10}$$

As an example, we compare the effective surface permittivity for a ZnO/diamond/silicon layered semispace calculated using the exact recursive stiffness matrix method[10] and the RASM methods. The properties of the materials are taken from Ref. 15. Figures 2(a) and 2(b) show the comparison of the real part of the effective surface permittivity for a ZnO/diamond/silicon layered semispace versus (a) wave number $k_x/\omega$ and (b) frequency. In the RASM computation, the semispace Si substrate is replaced by a 30 $\mu$m Si layer with an additional 30 $\mu$m PML layer with $\beta = 1.0 + 0.3i$. The ZnO layer has been divided into $2^6$ thin layers and the others into $2^9$. The results calculated using RASM agree very well with the exact solution. Both solutions are free of numerical instabilities.

The RASM-based effective permittivity method provides a versatile, simple and efficient tool for SAW device analysis in layered structures and has better suitability for inverse solution in the determination of the properties of deposited layers and residual stresses.

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