Conversion of elastic waves as a result of diffraction in anisotropic layer

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Abstract. The transfer matrix method for the theory of elastic wave scattering in anisotropic layered medium is developed. The cases of the six-beam diffraction are considered. The method of the transfer matrix \( \exp(Wz) \) computation is based on the use of polynomials of principal minors in combination with scaling of matrix \( W \). This method, in contrast to the Lagrange-Sylvester and others known polynomial approaches does not require solution of eigenvalue problem. Evaluations of the scaling parameter and relative truncation error of the method are made. Some features of the conversions of shear waves and longitudinal wave are demonstrated by calculations of the diffraction on a crystalline silicon layer. It is shown that the conversion \( SH \) wave into \( SV \) waves and \( SV \) wave into \( SH \) waves are equivalent.

1. Introduction
The anisotropy of the elastic properties in a layered medium leads to the possibility of interactions between elastic waves of all possible types. As a result of these, each type of the incident elastic wave, namely, longitudinal \( (P) \), shear horizontal \( (SH) \) and shear vertical \( (SV) \) waves, can produce six elastic waves in an anisotropic layer (Fig. 1a).

The most effective way of wave field calculation in a multilayer medium is the transfer matrix method. According to this method, the stress-strain state of an elastic medium is characterized by a vector function \( \Psi(x_3) = \|\psi_i(x_3)\| \), where \( \psi_j \), \( i = 1, \ldots, 6 \) are components of displacement vector and stress tensor. So-called transfer matrix \( T_i \) relates the values of vector function \( \Psi(x_3) \) at thicknesses \( d_i \) and \( d_{i+1} \): \( \Psi(d_{i+1}) = T_i \Psi(d_i) \). Thus \( \Psi(d) = T \Psi(0) \), where \( T = \prod_{i=1}^N T_i \) is a global transfer matrix and \( d = d_1 + \cdots + d_N \) is the thickness of \( N \)-layer plate.

Figure 1. The geometry of scattering.
In the usual approaches [1, 2, 3] transfer matrices $T_i$ are represented as a functions of six exponentials of wave numbers. In the general case of six-beam diffraction in $N$-layer structure the result of transfer matrix computation depends on accuracy of $6N$ wave numbers definitions and reliability of corresponding exponentials computations. That’s why one of the substantial values that affect the accuracy of the transfer matrix calculation is propagation parameter $\kappa = \nu d$, where $\nu$ is a frequency. The computation of transfer matrix for inhomogeneous (or evanescent) waves at large values of $\kappa$ can lead to unsatisfactory results [4].

This paper uses calculations of transfer matrix $T = \exp(\text{Wd})$ by means of method of polynomials of principal minors (MPPM) of the matrix $W$. MPPM, unlike the Lagrange-Sylvester method and other polynomial approaches [5], does not require finding the eigenvalues of the matrix $W$. An elastic wave scattering by an anisotropic structure bounded by isotropic solid media (layers 0 and $N + 1$ in Fig. 1a) are considered.

2. Method of computations

2.1. Main equations

The system of equations of motion and Hooke’s law can be written in the following form

$$\frac{\partial^2 u_1}{\partial t^2} = \frac{\partial P_1}{\partial x_1} + \frac{\partial P_2}{\partial x_2} + \frac{\partial P_3}{\partial x_3}, \quad \frac{\partial u_1}{\partial x_1} = \sum_{g=1}^{6} S_{1g} P_g,$$

$$\frac{\partial^2 u_2}{\partial t^2} = \frac{\partial P_2}{\partial x_1} + \frac{\partial P_1}{\partial x_2} + \frac{\partial P_3}{\partial x_3}, \quad \frac{\partial u_2}{\partial x_2} = \sum_{g=1}^{6} S_{2g} P_g,$$

$$\frac{\partial^2 u_3}{\partial t^2} = \frac{\partial P_3}{\partial x_1} + \frac{\partial P_1}{\partial x_2} + \frac{\partial P_2}{\partial x_3}, \quad \frac{\partial u_3}{\partial x_3} = \sum_{g=1}^{6} S_{3g} P_g,$$

where $\rho$ is a density; $t$ is a time; $x_1, x_2, x_3$ are Cartesian coordinates; $u_1, u_2, u_3$ are components of displacement vector; $P_g$ and $S_{gl}, g, l = 1, \ldots, 6$ are accordingly components of stress tensor ($P_1 = P_{11}, P_2 = P_{22}, P_3 = P_{33}, P_4 = P_{23} = P_{32}, P_5 = P_{13} = P_{31}, P_6 = P_{12} = P_{21}$) and compliance tensor in the matrix form [6, §52].

The density $\rho = \rho(x_3)$ and elastic parameters of medium $S_{gl} = S_{gl}(x_3)$ depend only on one coordinate $x_3$ along an axis perpendicular to the surface of anisotropic layer. The deformations in an anisotropic layer $0 \leq x_3 \leq d$ are generated by a plane wave $\vec{u}_0 = \vec{\omega}_0 \exp[i(\vec{k}_0 \cdot \vec{r} - \omega t)]$ incident from the region $x_3 < 0$. Here $\vec{u}_0$, $\vec{\omega}_0$, $\vec{k}_0$ and $\omega$ are displacement vector, amplitude, wave vector and circular frequency of incident wave respectively and $i$ is imaginary unit. These assumptions make it possible to reduce the system (1) to the equation

$$\frac{\partial}{\partial x_3} \Psi = W \Psi \equiv \begin{bmatrix} w_{11} & w_{12} & w_{13} & w_{14} & w_{15} & w_{16} \\ w_{21} & w_{11} & w_{23} & 0 & w_{25} & w_{26} \\ w_{25} & w_{15} & w_{33} & w_{34} & w_{35} & w_{36} \\ w_{26} & w_{16} & w_{43} & 0 & w_{36} & w_{46} \\ w_{23} & w_{13} & w_{53} & 0 & w_{33} & w_{43} \\ 0 & w_{14} & 0 & w_{64} & w_{34} & 0 \end{bmatrix} \Psi_i,$$
where column vector \( \Psi = \| w_2, p_{23}, u_1, u_3, p_{13}, p_{33} \|^T \),

\[

t_{11} = -i(k_{01}a_7 + k_{02}a_4), \\
t_{13} = -i(k_{01}a_1 + k_{02}a_7), \\
t_{15} = S_{14}a_2 + S_{24}a_3 + S_{34}a_8 + S_{45}, \\
t_{21} = k_{01}^2\gamma_6 + k_{02}^2\gamma_4 - 2k_{01}k_{02}\gamma_5 - \rho_2^2, \\
t_{25} = -i(k_{01}a_8 + k_{02}a_5), \\
t_{33} = -i(k_{01}a_2 + k_{02}a_8), \\
t_{35} = S_{15}a_2 + S_{25}a_3 + S_{35}a_8 + S_{55}, \\
t_{43} = -i(k_{01}a_3 + k_{02}a_9), \\
t_{53} = k_{01}^2\gamma_1 + 2k_{01}k_{02}\gamma_3 + k_{02}^2\gamma_6 - \rho_2^2, \\
w_{12} = S_{14}a_1 + S_{24}a_4 + S_{34}a_7 + S_{44}, \\
w_{14} = -ik_{02}, \\
w_{16} = S_{14}a_3 + S_{24}a_6 + S_{34}a_9 + S_{44}, \\
w_{22} = k_{01}^3\gamma_7 + k_{01}k_{02}(\gamma_6 - \gamma_1) - k_{02}^3\gamma_5, \\
w_{26} = -(k_{01}a_9 + k_{02}a_6), \\
w_{34} = -ik_{01}, \\
w_{36} = S_{15}a_3 + S_{25}a_6 + S_{36}a_9 + S_{56}, \\
w_{46} = S_{13}a_3 + S_{23}a_6 + S_{36}a_9 + S_{33}, \\
w_{64} = -\rho_2^2,
\]

\[k_{01} = k_0 \sin \theta_0 \cos \alpha, \quad k_{02} = k_0 \sin \theta_0 \sin \alpha \] are projections of the wave vector \( \vec{k}_0 \) on the axes \( x_1 \) and \( x_2 \) (see Figure 1b) and \( \gamma_j = \Delta_j/(S_{11}\Delta_1 - S_{12}\Delta_2 + S_{16}\Delta_3), \) \( j = 1, \ldots, 6, \) \( \Delta_1 = S_{22}S_{66} - S_{26}^2, \)
\( \Delta_2 = S_{12}S_{66} - S_{16}S_{26}, \)
\( \Delta_3 = S_{12}S_{26} - S_{16}S_{22}, \)
\( \Delta_4 = S_{11}S_{66} - S_{16}^2, \)
\( \Delta_5 = S_{11}S_{26} - S_{16}S_{12}, \)
\( \Delta_6 = S_{11}S_{22} - S_{12}^2. \)

2.2. Transfer matrix

The integration of the equation (2) for a uniform layer \( 0 \leq x_3 \leq d \) gives solution in the form

\[
\Psi(d) = T\Psi(0),
\]

where matrix

\[
T = \sum_{j=0}^{\infty} \frac{W^j d^j}{j!} \equiv \exp(Wd)
\]

is called transfer matrix. If a structure consists from a set of \( N \) layers \( 0 \leq x_3 < d_1, \)
\( d_1 \leq x_3 < d_2, \), \ldots, \( d_{N-1} \leq x_3 < d_N = d \) with transfer matrices \( T_1, \ T_2, \ T_3, \ldots, T_N \), then
\( \Psi(d) = T_N T_{N-1} \ldots T_1 \Psi(0). \) In particular, \( \Psi(d) = T^N \Psi(0) \), if \( T_i = T, \ i = 1, \ldots, N. \)

Transfer matrix \( T \) can be decomposed in the basis of the first six powers of the matrix \( Wd \):

\[
T = \exp(Wd) = \sum_{h=0}^{5} \mathcal{T}_h(Wd)^h.
\]

We use representation of coordinates \( \mathcal{T}_h \) by means of method [8]:

\[
\mathcal{T}_h = \frac{1}{h!} + \sum_{j=0}^{\infty} \frac{1}{j!} \sum_{g=0}^{h} p_{6-h+g} \mathcal{B}_{j+g}(6), \hspace{1em} h = 0, 1, \ldots, 5, \hspace{1em} j = 0, 1, \ldots;
\]

\( p_m \ (m = 1, \ldots, 6) \) are coefficients of characteristic equation of matrix \( Wd = \| w_{gh}d \| \), and polynomials \( \mathcal{B}_g(6) \) are defined by recurrence relations

\[
\mathcal{B}_0(6) = \ldots = \mathcal{B}_4(6) = 0; \hspace{1em} \mathcal{B}_5(6) = 1; \hspace{1em} \mathcal{B}_g(6) = \sum_{h=1}^{6} p_h \mathcal{B}_{g-h}(6), \hspace{1em} g \geq 6.
\]

It should be noted that the calculation according to the formulas (5) – (7) does not use the eigenvalues of the matrix \( Wd \), in contrast to the method of Lagrange-Sylvester, which was
applied in propagator matrix method[3]. We use here a well known representation of coefficients $p_m$ as a sums of principle minors of the matrix:

$$
p_1 = \sum_{g=1}^{6} w_{gg} d, \quad p_2 = -\sum_{j>i} \begin{vmatrix} w_{ii} d & w_{ij} d \\ w_{jj} d & w_{jj} d \end{vmatrix}, \quad \ldots, \quad p_6 = -\det(Wd).
$$

Therefore, the functions $\mathcal{B}_g(6)$, which are determined by formulas (7), are called in this paper polynomials of principal minors.

Calculation of coefficients $p_m$ conveniently carried out by the recurrence formulas (see method of Le Verrier[7]):

$$
mp_m = s_m - p_1 s_{m-1} - \ldots - p_{m-1} s_1, \quad m = 1, 2, \ldots, 6,
$$

where $s_m$ are traces of the matrices $(Wd)^m, \quad m = 1, \ldots, 6$.

For numerical calculations of transfer matrix $T$ by the formula (5) one must approximate the series $\sum_{j=6}^{\infty}$ in the formulas (6) by sum of finite number of terms, let’s say $J$:

$$
\mathcal{T}_h \approx \frac{1}{h!} + \sum_{j=6}^{J-1} \frac{1}{j!} \sum_{g=0}^{h} p_{6-h+g} \mathcal{B}_{j-1-g}(6), \quad J = 6 + N, \quad N = 0, 1, \ldots.
$$

2.2.1. The relative truncation error. Obviously, the values (9) depend on $J$: $\mathcal{T}_h = \mathcal{T}_h(J)$. Equality in the formula (9) becomes exact, when $J \to \infty$, i.e. $\mathcal{T}_h(\infty), \quad h = 0, \ldots, 5$ conform the exact values of coordinates of the matrix $T = \exp(Wd)$ in the basis $I, Wd, \ldots, (Wd)^5$.

The value

$$
\epsilon = \max \left| \frac{\mathcal{T}_h(\infty) - \mathcal{T}_h(J)}{\mathcal{T}_h(\infty)} \right|
$$

is called the relative truncation error in calculating the coordinates $\mathcal{T}_h$ by the formulas (9).

It can be shown that if

$$
\eta = 8.5 \frac{\omega d}{\min v} < 1,
$$

then

$$
\epsilon < \frac{\eta^{N_1+1}}{(6 + N_1) \prod_{h=1}^{N_1}(6 + h)}.
$$

The following notation is used in formulas (11) and (12): $\min v$ is minimum propagation velocity of elastic waves in the layer, $N_1 = J - 7$ is a difference between the limits of summation in $\sum_{j=6}^{J-1} C_{j!}/j!$. The values of parameters $\eta$ and $N_1$ can be regulated by scaling.

2.2.2. Scaling. If the condition (11) for the matrix $Wd$ is not satisfied, we can always choose an integer $m$, for which

$$
\eta = 8.5 \frac{\omega d}{\min v m} < 1.
$$

In other words, we first calculate the matrix $\exp(Wd/m)$ with a given accuracy. And then we use the remarkable property of the exponential function:

$$
T = \exp(Wd) = \left[ \exp \left( \frac{Wd}{m} \right) \right]^m,
$$

where the integer $m$ is called scaling parameter.
Example. Let us consider the scaling procedure on the example of crystalline silicon. The density of Si $\rho = 2.329 \cdot 10^3$ kg/m$^3$. Non-zero elements of compliance tensor have values: $S_{11} = S_{22} = S_{33} = 7.69$, $S_{12} = S_{13} = S_{23} = -2.14$, $S_{44} = S_{55} = S_{66} = 12.58$ (in units $10^{-12}$m$^2$/N). $d = 10^{-3}$m, $\nu = 10^7$Hz. The value $\min v$ can be estimated by the formula: 
\[ \min v \approx 1/\sqrt{\rho \max S_{ij}}. \]
So, from (2.2.2) we find $m > 17\pi d\sqrt{\rho \max S_{ij}} > 91$. The smallest number of matrix multiplications (namely seven) and, consequently, the smallest round-off errors will be when $m = 2^7 = 128$ and the last operation in (13) is performed by repeated squaring.

3. Six-wave scattering

If the regions $x_3 < 0$ and $x_3 > d$ bounding the layered structure are solid isotropic, then six scattered plane waves can propagate in them: $SH$ wave with amplitude $\mathbf{a}_1$ and wave number $k_1 = 2\pi \nu \sqrt{\rho_0/\mu_0}$; $SV$ wave with amplitude $\mathbf{a}_2$ and wave vector $\mathbf{k}_2 = \mathbf{k}_1$; $P$ wave with amplitude $\mathbf{a}_3$ and wave number $k_3 = 2\pi \nu \sqrt{\rho_0/(2\mu_0 + \lambda_0)}$; $SH$ wave with amplitude $\mathbf{a}_4$ and wave number $k_4 = 2\pi \nu \sqrt{\rho_d/\mu_d}$; $SV$ wave with amplitude $\mathbf{a}_5$ and wave vector $\mathbf{k}_5 = \mathbf{k}_4$; $P$ wave with amplitude $\mathbf{a}_6$ and wave number $k_6 = 2\pi \nu \sqrt{\rho_d/(2\mu_d + \lambda_d)}$. Here $\rho_0$, $\lambda_0$, $\mu_0$ and $\rho_d$, $\lambda_d$, $\mu_d$ are density and Lamé parameters for regions $x_3 < 0$ and $x_3 > d$.

Possible directions of wave propagation in layered medium are defined by the relations $k_j \sin \theta_j = k_0 \sin \theta_0$, where $\theta_j$ is angle between wave vector $\mathbf{k}_j$ and axis $x_3$. All wave vectors $\mathbf{k}_j$ lie in the plane of incidence and
\[
\begin{align*}
k_{j1} &= k_0 \sin \theta_0 \cos \alpha, \\
k_{j2} &= k_0 \sin \theta_0 \sin \alpha, \\
k_{j3} &= -k_0 \cos \theta_1, \\
k_{j4} &= -k_0 \cos \theta_3, \\
k_{j5} &= k_0 \cos \theta_4, \\
k_{j6} &= k_0 \cos \theta_6. 
\end{align*}
\]

3.1. Components of vector functions $\Psi(0)$ and $\Psi(d)$

From the solutions of the equations (1) for an isotropic layer it follows that vector functions $\Psi(0)$ and $\Psi(d)$ are expressed in terms of the amplitudes $\mathbf{a}_h$ by formulas:
\[
\psi_g(0) = \sum_{h=0}^{3} \beta_{gh} \mathbf{a}_h, \quad \psi_g(d) = \sum_{h=4}^{6} \beta_{gh} \mathbf{a}_h, \quad g = 1, \ldots, 6, \quad (14)
\]
where \[ \beta_{1h} = c_{h1}, \beta_{2h} = i\mu(c_{h2}k_{h2} + c_{h3}k_{h3}), \beta_{3h} = c_{h1}, \beta_{4h} = c_{h3}, \beta_{5h} = i\mu(c_{h1}k_{h3} + c_{h3}k_{h1}), \beta_{6h} = i \left[ 2\mu c_{h3}k_{h3} + \lambda \sum_{j=1}^{3} c_{hj} k_{hj} \right], \]
\[
\lambda, \mu = \begin{cases} 
\lambda_0, \mu_0, & \text{if } h = 0, 1, 2, 3 \text{ (for region } x_3 < 0), \\
\lambda_d, \mu_d, & \text{if } h = 4, 5, 6 \text{ (for region } x_3 > d) 
\end{cases}
\]
and direction cosines $c_{h1}, c_{h2}, c_{h3}$ of vectors $\mathbf{a}_1, \ldots, \mathbf{a}_6$ are defined by Figures 2a, Figures 2b and Figures 3a, respectively.

3.2. Conversion coefficients

The equality (3) expresses the vector function $\Psi(d)$ through the $\Psi(0)$ with the help of transfer matrix $T = ||t_{ij}||$. Substitution of expressions (14) in the formula (3) gives a system of algebraic equations for the amplitudes $\mathbf{a}_h$, $h = 1, \ldots, 6$: 
\[
d_{j1} \mathbf{a}_1 + d_{j2} \mathbf{a}_2 + \ldots + d_{j6} \mathbf{a}_6 = f_i \mathbf{a}_0, \quad i = 1, \ldots, 6, \quad (15)
\]
where $f_i = -\sum_{j=1}^{6} t_{ij} \beta_j \theta_0$; $d_{il} = \sum_{j=1}^{6} t_{ij} \beta_{jl}$, if $l = 1, 2, 3$ and $d_{il} = -\beta_{il}$, if $l = 4, 5, 6$. 

5
The solution of the system of equations (15) allows us to find in an obvious way the conversion coefficients

$$C_{ij} = \frac{\alpha_{ji}}{\alpha_{ij}}, \quad j = 1, \ldots, 6,$$

where $i = 1, 2, 3$ correspond to incident wave $SH$-type, $SV$-type and $P$-type, respectively.

Dependencies of the coefficients $C_{ij}$ on the angles of incidence $\theta_0$, $\alpha$ and on the propagation parameter $\kappa$ were investigated for some crystals, the elastic constants of which are available in the monograph [9]. Examples of spectra for a silicon crystal are shown in Figures 2 and 3. Numbers $h = 1, \ldots, 6$ indicates curves $C_{gh}(\theta_0)$. They were calculated for the following conditions: $\rho_0 = \rho_d = 2.65 \times 10^3 \text{kg/m}^3$, $\lambda_0 = \lambda_d = 1.67 \times 10^{10} \text{N/m}^2$, $\mu_0 = \mu_d = 3.27 \times 10^{10} \text{N/m}^2$.

![Diagram](image)

**Figure 2.** Conversion coefficients of the shear waves, $\alpha = 23^\circ$, $\kappa = 2 \times 10^3 \text{m/s}$.

### 3.3. Conversions of shear waves

The results of modeling allow us to state that

$$C_{12}(\theta_0, \alpha) = C_{21}(\theta_0, \alpha), \quad C_{15}(\theta_0, \alpha) = C_{24}(\theta_0, \alpha). \quad (16)$$

Figure 2 illustrates this relations. Here functions $C_{12}(\theta_0), C_{21}(\theta_0), C_{15}(\theta_0), C_{24}(\theta_0)$ are shown by solid lines. It should be noted that the corresponding coefficients of $SH$ and $SV$ waves...
coverions into longitudinal waves differ substantially (see Figure 2c and Figure 2d; Figure 2e and Figure 2f).

Another important feature of the spectra \( C_{1j}(\theta_0) \) and \( C_{2j}(\theta_0) \) is the resonance character of the shear waves transformation into longitudinal waves. For the spectra shown in Figure 2, this can be observed in the regions near the angles \( \theta_0 = 39^\circ \) and \( \theta_0 = 50^\circ \). It is possible complete transformation of incident SH wave into SV-type in reflected wave. For example \( C_{11} = 0, C_{12} = 0 \).

\[
\begin{align*}
\rho_0, \lambda_0, \mu_0 & \quad \rho, S_{ph} \\
\rho_d, \lambda_d, \mu_d & \quad d
\end{align*}
\]

\[
\begin{align*}
\theta_0 & \quad \theta_1 \\
k_0 & \quad k_1 = k_2 \\
k_3 & \quad \theta_3 \\
\rho_0, \lambda_0, \mu_0 & \quad \rho, S_{ph} \\
\rho_d, \lambda_d, \mu_d & \quad d
\end{align*}
\]

\[
\begin{align*}
\theta_4 & \quad \theta_0 \\
k_0 & \quad k_5 = k_6
\end{align*}
\]

3.4. \( P \) wave scattering

Conversion of a longitudinal wave into the \( SH \) wave can be as significant as transformation \( P \to SV \) and even stronger. Figure 3b shows, that for \( \theta_0 = 52^\circ \) \( SH \) wave prevails among the reflected waves. An analogous situation among the transmitted waves is observed in Figure 2c for the angle of incidence \( \theta_0 = 35^\circ \).

4. Conclusion

When performing calculations, the implementation of the law of conservation of energy flow was monitored. High accuracy of realizations of this law and relations (16) indicate the reliability of the transfer matrix calculations by means of MPPM.

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