Theoretical analysis of acoustic wave propagation in ZnO/Si bi-layered system using transfer matrix method

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1. Introduction

In the past two decades, acoustic-wave devices, such as filters, sensors and actuators have got enormous applications [1,2]. Several acoustic devices using the multi-layered structure of piezoelectric thin films on substrates, in which various acoustic modes were used, such as love modes, lamb modes, surface horizontal acoustic plate modes (SH-APM), etc. Therefore, the modeling of the acoustic wave propagation in the multi-layered piezoelectric plates is very important for designing these devices.

Some works have been done for the analysis of the acoustic wave propagation. One of the methods, called the transfer matrix method [3], is a robust method to deal with the system with many layers. In this paper, we have introduced the theory of acoustic wave propagation in layered piezoelectric media. Then, we use the transfer matrix method to give an exact analysis of the acoustic wave propagation in a system of a ZnO thin film deposited on a Silicon wafer. By numerical calculations we get the dispersion relation of the system. For a specific propagation direction, in which the SH-APM wave and the flexural plate wave (FPW) do not couple, we get the dispersion relations of these two kinds of waves respectively. Meanwhile, the displacement and stress distributions are also obtained.

Generally, in the ZnO/Si system the acoustic waves are excited by an interdigital transducer (IDT). The electromechanical coupling of these acoustic modes is a very important parameter in the design of the electro-acoustic devices. A method to estimate the electromechanical coefficient of the acoustic wave modes propagating in this system is also provided. An analysis of these wave modes is also given.

2. Theory

2.1. Partial wave method of wave propagation in piezoelectric materials

The system configuration under consideration is shown in Fig. 1.

In a piezoelectric medium, under quasi-static approximation, the coupled piezoelectric field equations are given by the equations of motion and electrostatic charge [4].

\[
\begin{align*}
&c_{ijkl}u_{jk} + e_{ij}\phi_{ik} - \rho_{ij} = 0 \\
&e_{ij}\phi_{ij} - e_{ij}u_{ij} = 0
\end{align*}
\]  \hspace{1cm} (1)

The constitutive relations are as following:

\[
\begin{align*}
T_{ij} &= c_{ijkl} S_{lj} + e_{ikj}\frac{\partial \phi}{\partial k} \\
D_{k} &= e_{kij} S_{ij} - e_{ikj}\frac{\partial \phi}{\partial i}
\end{align*}
\]  \hspace{1cm} (2)

In which,

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]

\[
E_{k} = -\frac{\partial \phi}{\partial x_k}
\]  \hspace{1cm} (3)

In the equations above, \( u_i \) and \( \phi \) are the displacements and the electric potential respectively. \( c_{ijkl}, e_{ikj} \text{ and } e_{ij} \) are the elastic stiffness constants, piezoelectric stress constants and dielectric constants respectively. \( T_{ij}, S_{ij}, D_{k} \text{ and } E_{k} \) are the stress, strain, electric displacement and electric field respectively.

For an acoustic plane waves propagating in the direction of \( x_1 \), using the partial wave method, the solution of the displacements for each layer is expressed by Eq. (4-1).

\[
(u_1, u_2, u_3, \phi) = \sum_{q=1}^{8} (X_{1q}, X_{2q}, X_{3q}, X_{4q})B_q \times \exp(i\xi(x_1 + \alpha_q x_3 - ct))
\]  \hspace{1cm} (4-1)

In this equation, \( u_1, u_2, u_3 \) are the displacements along \( x_1, x_2, x_3 \) respectively, \( \xi \) is the wave number along \( x_1 \) direction, \( c \) is the phase velocity of the wave along \( x_1 \), \( \alpha_q \) are the eight solutions of the Christoffel equation. \( (X_{1q}, X_{2q}, X_{3q}, X_{4q}) \) is the null space of the singular matrix in Christoffel equation, which denotes the ratio of the amplitude of \((u_1, u_2, u_3, \phi)\) of the \( q \)th partial wave. \( B_q \) is the weight coefficient for the \( q \)th partial wave.

Then, with the constitutive relation we can get the solution of stress tensor \( \sigma_{11}, \sigma_{22}, \sigma_{33} \) and electric displacement \( D_3 \) for each layer

\[
(\sigma_{11}, \sigma_{22}, \sigma_{33}, D_3) = \sum_{q=1}^{8} (X_{5q}, X_{6q}, X_{7q}, X_{8q})B_q \times \exp(i\xi(x_1 + \alpha_q x_3 - ct))
\]  \hspace{1cm} (4-2)
2.2. Transfer matrix method

2.2.1. General theory

Omitting the general term exp(iξ(x₁ - ct)), Eqs. (4-1) and (4-2) can be combined into a matrix form: \[ P^{[r]} = X^{[r]}W^{[r]}(\alpha^{[r]}), \]
in which \([r]\) denotes the \(r\)th layer, \(P^{[r]}\) is a column vector made up of field quantities. \[ P^{[r]} = \begin{bmatrix} u_1, u_2, u_3, \phi, \sigma_1, \sigma_2, \sigma_3, D_1, D_2 \end{bmatrix}^T, \]
\(X^{[r]}\) is a 8×8 matrix composed of the \(X_{mn}\) elements, \(W^{[r]}(\alpha^{[r]})\) is a diagonal matrix with the nonzero elements \(W_{mn} = \exp(i\alpha_m x_3)\), \(B^{[r]}\) is a column vector of \(B_{3n}\) for the \(r\)th layer.

\[ B^{[r]} = \begin{bmatrix} B_1, B_2, B_3, B_4, B_5, B_6, B_7, B_8 \end{bmatrix}^T, \text{here } T \text{ represents the transposition of the vector.} \]

In the lower and upper interface of the \(r\)th layer, we have \(x_3^{[r-1]} = 0\) and \(x_3^{[r+1]} = h^{[r]}\), so \(P^{[r+1]} = X^{[r]}W^{[r]}(\alpha^{[r]}), B^{[r]}\), \(P^{[r]} = X^{[r]}B^{[r]}. \%

We can get \(P^{[r+1]} = \psi^{[r]}P^{[r]}, \psi^{[r]} = X^{[r]}W^{[r]}(\alpha^{[r]}), X^{[r+1]} \)

Equation (5) is called the transfer matrix for the \(r\)th layer.

Since the elements of \(P^{[r]}\) must be continuous at the interfaces of the system, that is, \(P^{[r+1]} = P^{[r]}\) thus we get the relation \(P^{[r+1]} = \psi P^{[r]} \%

Where \(P^{[r]}\) and \(P^{[r]}\) are the values of \(P\) at the top and bottom surfaces of the system respectively. \(\psi\) is called the transfer matrix of the system.

2.2.2. Stress free and open circuit boundary condition

The stress free and open circuit boundary condition is given as the following equations.

\[ P^{[N]+} = (u_1^+, u_2^+, u_3^+, \phi^+, 0, 0, 0, 0) \]

\[ P^{[1]-} = (u_1^-, u_2^-, u_3^-, \phi^-, 0, 0, 0, 0) \]

Insert the boundary conditions into Eq. (6), we get,

\[ \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \psi_{51} & \psi_{52} & \psi_{53} & \psi_{54} \\ \psi_{61} & \psi_{62} & \psi_{63} & \psi_{64} \\ \psi_{71} & \psi_{72} & \psi_{73} & \psi_{74} \\ \psi_{81} & \psi_{82} & \psi_{83} & \psi_{84} \end{bmatrix} \begin{bmatrix} u_1^- \\ u_2^- \\ u_3^- \\ \phi^- \end{bmatrix} \]

If the nontrivial solution to Eq. (8) exists, the determinant of the matrix must be zero, which gives the relation between \(\xi\) and \(c\). For each given value of \(\xi\), there is a set of values of \(c\) that can meet the requirement. This dispersion relation includes all the acoustic wave modes that can propagate in the system.

For each acoustic wave mode we can also get the distribution of the displacements, electric potential and the stresses in the system. When determinant of the matrix is zero, we can also get the nontrivial solution of Eq. (8) from the null space of the singular matrix. Then, the field quantities of the bottom surface \(P^{[1]+} = [u_1^+, u_2^+, u_3^+, \phi^+, 0, 0, 0, 0]^T \) are obtained. We can get the vector \(B^{[1]+} = X^{[1]}B^{[1]} \) with the interface relation we get \(B^{[1]+} = X^{[1]}W^{[1]}(\alpha^{[1]}), B^{[1]} \). With the same method, we can get the weight coefficient of all the layers, so finally we get the distribution of the field quantities in the system.

2.2.3. Stress free and short circuit boundary condition

If the electric boundary condition is short circuit, say, a conductive film is deposited on the surface of the system; we can also obtain the dispersion relation and the distribution of the field quantities with the same procedure described above. The difference is in the detailed description of the electric boundary condition. In the bottom and top surface the electric potential \(\psi^+\) and \(\psi^-\) are zero, while the electric displacement \(D^+\) and \(D^-\) will be the quantities to be determined by the calculation.

\[ P^{[N]+} = (u_1^+, u_2^+, u_3^+, 0, 0, 0, 0, D^+) \]

\[ P^{[1]-} = (u_1^-, u_2^-, u_3^-, 0, 0, 0, 0, D^-) \]

From the determinant and the null space of the corresponding part of matrix \(\Theta\), the dispersion relation and the field quantities distribution can also be obtained.

2.2.4. Electromechanical coefficient

With the relation \(k^2 = 2(C_o - C_s)/C_o [5]\), we can estimate the electromechanical coupling of each wave mode. Here \(C_o\) and \(C_s\) are the phase velocities of the acoustic waves under open circuit and short circuit boundary conditions respectively. The calculation of electromechanical coupling coefficient will provide further information on the character of different wave modes.

3. Numerical results

For a bi-layered system of RF sputtered ZnO thin film on the (100) silicon substrate. The ZnO thin film with the thickness 10 μm is grown with the c axis normal to the substrate plan. The thickness of the Si substrate is 100 μm, and the wave propagates along [0,0,1] direction of silicon.

For this system, our numerical calculation shows that there are two kinds of modes. In one kind \(u_2\) exists but \(u_1\) and \(u_3\) and \(\phi\) are zero, and in the other kind \(u_1\), \(u_3\) and \(\phi\) exist while \(u_2\) is zero. It means that in this system the piezoelectric stiffened FPW do not couple with SH-APM. We show the dispersion relation for these two kinds of modes in Figs. 2 and 3.

Since the SH-APM wave does not couple with the electric field, although this set of APM wave modes can propagate in this system, they can not be excited by IDT.

The following research is focused on the FPW. When the wavelength is 100 μm, there are six electrically coupled FPW modes that can propagate in the system, their frequencies are
40.61 MHz, 49.15 MHz, 59.60 MHz, 67.89 MHz, 81.16 MHz and 86.96 MHz. The distribution of the displacement and stress along the $x_3$ direction of these modes are shown in Figs. 4 and 5.

From Figs. 4 and 5, we can see that, in this system, because of the asymmetry of the system induced by the ZnO layer, the FPW cannot be S modes or A modes of the Lamb wave as in one layer plate. Also, because the silicon substrate discussed here is of the medium thickness, the wave modes are much more complicated than the thin substrate case, in which only the quasi-$S_0$ and quasi-$A_0$ modes can propagate.

As shown in from Figs. 4 and 5, the first two modes are the combination of the quasi-$A_0$ and quasi-$S_0$, which primary propagate in the two surfaces of the system. The first mode is the surface acoustic wave (SAW) in the top surface of ZnO thin film, which also penetrates into the Si wafer because the film thickness 10 $\mu$m is much less than the wave length 100 $\mu$m. Since the phase velocity of acoustic wave in ZnO is less than that in Si, the phase velocity of this mode is less than the second one, which propagate primary in the rear surface of the silicon wafer. Also, The frequency of the second mode is 49.15 MHz, which is the same as the Rayleigh wave of silicon wafer.

The following modes 3, 4, 5 and 6 are the higher acoustic guided wave modes. Their displacement distribution is even more complicated with the mode number goes up. Just similar to the properties of standing wave, their displacement and stress form some nodes and crests along the $x_3$ direction.

Compare the phase velocities of each mode between open circuit and short circuit boundary conditions, we get the electromechanical coefficient of these modes. Shown in Fig. 6 is the relation between electromechanical coupling $k^2$ and the wave vector along $x_1$ direction $\xi_1$ in the system of 10 $\mu$m ZnO on 100 $\mu$m Si substrate. It shows the
same result as in the dispersion relation, when $\xi$ is small, i.e., $\lambda$ is large, only two modes exist. At this case the thickness of the system is small compared to wavelength, mode 2 also has a moderate value of electromechanical coupling. But when $\xi$ increases, i.e. $\lambda$ is about three times of the thickness, the electromechanical coupling of mode 2 decreases to a very low value soon.

When the wavelength is 100 $\mu$m, the coupling coefficients of each mode are shown in the following table.

<table>
<thead>
<tr>
<th>Mode</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frequency (open circuit)(MHz)</td>
<td>40.61</td>
<td>49.15</td>
<td>59.60</td>
<td>67.89</td>
<td>81.15</td>
<td>86.95</td>
</tr>
<tr>
<td>$K^2$ ($\times 10^{-3}$)</td>
<td>4.54</td>
<td>0.16</td>
<td>7.59</td>
<td>5.99</td>
<td>0.6</td>
<td>0.22</td>
</tr>
</tbody>
</table>

4. Conclusions

From the calculation, we find that the transfer matrix method is a robust method for the acoustic wave propagation problem. It is particularly suitable for the numerical modeling of multi layer system.

The result for the ZnO/Si system shows that the SH-APM wave and FPW do not couple with each other. The SH polarized acoustic field does not couple with electric field, so SH-APM wave cannot be excited with the electro-acoustic transducer such as the method of IDT.

The dispersion relation gives the acoustic wave modes that can propagate in the particular ZnO/Si system. The distribution of field quantities together with the electromechanical coefficient give the detailed information of each modes and the coupling efficiency when the acoustic waves are excited by electric signals.

For the particular case of the 10 $\mu$m thick ZnO on 100 $\mu$m Si substrate, when the wavelength is 100 $\mu$m, there are six modes can be propagated in the system. But only the mode 1, mode 3 and mode 4 have a comparably large exciting efficiency.

The numerical results given in this paper is based on the assumption that all the material constants of the sputtered ZnO thin film are the same as those of the bulk crystal ZnO. The acoustic wave modes shown here agree with the experimental result qualitatively. In order to perform the
quantitative design of the excited wave modes by IDT, the
difference of the material constants between films and bulk
materials must be considered in future researches.

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