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Investigation of surface acoustic waves propagating in ZnO–SiO_2–Si multilayer structure

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ABSTRACT

The investigations of the propagation of the SAW in the multilayered structures have been of great interest since the combination of the surface acoustic wave (SAW) technology with the microelectromechanical system (MEMS) technology comes true. In this paper, the recursive asymptotic method (RAM) is applied to analysis the propagation of the SAW in the ZnO–SiO_2–Si multilayered structure. The influences of the ZnO layer thickness and the SiO_2 layer thickness to the phase velocity and the electro-mechanical coupling coefficient for the Rayleigh wave and Love wave are discussed. The Love mode wave is found to be predominantly generated since the *c*-axis of the ZnO film is generally perpendicular to the substrate. In order to prove the theoretical results, a series of Love mode SAW devices based on the ZnO–SiO_2–Si multilayered structure is fabricated by micromachining, and their frequency responses are detected. The experimental results are found to be mainly consistent with the theoretical ones except the little larger velocities induced by the residual stresses produced in the fabrication process of the films. The deviation of the experimental results from the theoretical ones is reduced by thermal annealing.

1. Introduction

Surface acoustic wave (SAW) technology and devices have been in commercial use for more than 60 years. They are widely used in the fields of communication, automotive, and environmental sensing. Up to now, most of the SAW devices have been made from bulk piezoelectric materials, such as quartz (SiO_2), lithium tantalate ($LiTaO_3$), and lithium niobate ($LiNbO_3$). These bulk materials are expensive and difficult to integrate with microelectronics. With the development of fabrication technology of piezoelectric thin films, the SAW devices made from piezoelectric thin films become more and more attracting. Zinc oxide (ZnO) is an important piezoelectric thin film material, which has excellent piezoelectric property, high electro-mechanical coupling coefficient, high sensitivity and reliability. It can be grown on varies substrates, including silicon. Some SAW sensors [1–4] which are made from the ZnO–SiO_2–Si multilayered structure have the advantages of high frequency, high sensitivity, mass production and low price.

The investigations of the propagation of the SAW in the multilayered structures have been of great interest since the SAW devices made from piezoelectric films become the research focuses. The transfer matrix method (TMM) [5] and stiffness matrix method (SMM) [6,7] are two powerful techniques to analyze the SAW propagation in multilayered structure with arbitrary layers. Compared to the TMM and the SMM, the recursive asymptotic method (RAM) developed by Wang Lugen and Rokhlin [8] is much simpler and computationally efficient, because the RAM does not need to compute the exact wave propagation solution for each anisotropic layer of the system, and only the elastic piezoelectric, and dielectric constants of the layer are required.

In this work the SAW propagation in the ZnO–SiO_2–Si multilayered structure is analyzed by using the RAM. By calculating the velocity dispersion and electro-mechanical coupling coefficient for Rayleigh mode and Love mode in the ZnO–SiO_2–Si structures, the influences of the ZnO thickness and SiO_2 thickness to the SAW propagation are investigated, and the Love mode waves are found to be predominantly generated in the structure. To prove the theoretical results, a series of Love mode SAW devices with different wavelengths and layer thicknesses are fabricated by micromachining. The frequency responses of the SAW devices are detected and found to behave consistently with the calculated results.

2. Theory

2.1. Recursive asymptotic method

The ZnO–SiO_2–Si multilayered structure is simplified as Fig. 1. Let us consider a generally anisotropic piezoelectric media. We

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define the state vector $\xi = [U, T]^T$, the general displacement $U = (u, \phi)^T$ and the general stress $T = (\sigma, D_3)^T$, where $u = (u_1, u_2, u_3)$ is the particle displacement, $\sigma = (\sigma_{13}, \sigma_{23}, \sigma_{33})$ is normal stress vector on the (x, y) plane, ϕ is the electric potential, and D_3 is the normal electric displacement. For pure elastic media, ϕ and D_3 is set to be zero. The general solution for the state vector can be represented in the form $\xi(z) = e^{i(\omega t - k_x x)}$, where ω is the angular frequency, and k_x is the wave number along the x axis. The governing equation for the state vector is [9]:

$$\frac{d\xi}{dz} = iA\xi, \tag{1}$$

where A is the fundamental acoustic tensor, which is a function of material properties, wave number and frequency. The explicit formulation is given by:

$$A = \begin{bmatrix} k_x X \Gamma_{31} & -iX \\ -i(\Gamma_{11} - \Gamma_{13} X \Gamma_{31}) k_x^2 + i\rho\omega^2 \mathrm{I}' & k_x \Gamma_{13} X \end{bmatrix}, \tag{2}$$

where ρ is the density of the material, $X = (\Gamma_{33})^{-1}$ the inverse of Γ_{33}, I' is a 4×4 identical matrix but with zero (4, 4) element, and Γ_{ik} are the 4×4 matrices which are related to the elastic, piezoelectric, and dielectric permittivity constants:

$$\Gamma_{ik} = \begin{bmatrix} c_{1i1k} & c_{1i2k} & c_{1i3k} & e_{k1i} \\ c_{2i1k} & c_{2i2k} & c_{2i3k} & e_{k2i} \\ c_{3i1k} & c_{3i2k} & c_{3i3k} & e_{k3i} \\ e_{i1k} & e_{i2k} & e_{i3k} & -\varepsilon_{ik} \end{bmatrix}. \tag{3}$$

For a single homogeneous layer, the differential (1) has the well-known exponential transfer matrix solution B, which relate the state vector at the layer top $(z + h)$ to that at the layer bottle (z) surface:

$$\xi(z + h) = B\xi(z), \quad B = e^{iAh}, \tag{4}$$

where h is the layer thickness. To compute B requires finding the eigenvalues and eigenvectors of the matrix A, and it is fairly complicated. So for a thin layer $h/\lambda \ll 1$, a second-order asymptotic approximation for the transfer matrix B has been proposed as [8]:

$$B_{\mathrm{II}} = \left(I - i\frac{h}{2}A\right)^{-1}\left(I + i\frac{h}{2}A\right), \tag{5}$$

where I is a 8×8 identical matrix. The asymptotic solution is valid only for a thin layer.

To obtain the asymptotic stiffness matrix of a thick layer with thickness H, one can subdivide it into $N = 2^n$ thin layers, every thin

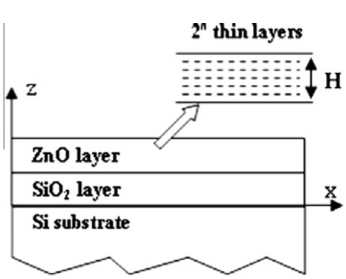

Fig. 1. Schematic of the ZnO–SiO_2–Si multilayered structure.

layer has the thickness of $h = H/N$, and then use the relation between the transfer matrix B and the stiffness matrix H [7]:

$$K = \begin{bmatrix} B_{22}(B_{12})^{-1} & B_{21} - B_{22}(B_{12})^{-1}B_{11} \\ (B_{12})^{-1} & -B_{22}(B_{12})^{-1}B_{11} \end{bmatrix}, \tag{6}$$

where B_{ij} are 4×4 submatrices of B. Substituting the second-order transfer matrix B_{II} (5) into (12), the second-order stiffness matrix K_{II} of a thin layer is obtained as [8]:

$$K_{\mathrm{II}} = \begin{bmatrix} \frac{\Gamma_{33}}{h} - (\Gamma_{31} - \Gamma_{33})\frac{ik_x}{2} + \frac{\Gamma_{11}hk_x^2}{4} - \frac{\rho h\omega^2}{4}\mathrm{I}' & -\frac{\Gamma_{33}}{h} - (\Gamma_{31} + \Gamma_{33})\frac{ik_x}{2} + \frac{\Gamma_{11}hk_x^2}{4} - \frac{\rho h\omega^2}{4}\mathrm{I}' \\ \frac{\Gamma_{33}}{h} - (\Gamma_{31} + \Gamma_{33})\frac{ik_x}{2} - \frac{\Gamma_{11}hk_x^2}{4} + \frac{\rho h\omega^2}{4}\mathrm{I}' & -\frac{\Gamma_{33}}{h} - (\Gamma_{31} - \Gamma_{33})\frac{ik_x}{2} - \frac{\Gamma_{11}hk_x^2}{4} + \frac{\rho h\omega^2}{4}\mathrm{I}' \end{bmatrix}. \tag{7}$$

The total stiffness matrix of the thick layer is obtained from the thin layer stiffness matrix using a recursive algorithm [8]:

$$K_a^J = \begin{bmatrix} K_{11}^{J-1} + K_{12}^{J-1}(K_{11}^{J-1} - K_{22}^{J-1})^{-1}K_{21}^{J-1} & -K_{12}^{J-1}(K_{11}^{J-1} - K_{22}^{J-1})^{-1}K_{12}^{J-1} \\ K_{21}^{J-1}(K_{11}^{J-1} - K_{22}^{J-1})^{-1}K_{21}^{J-1} & K_{22}^{J-1} + K_{21}^{J-1}(K_{11}^{J-1} - K_{22}^{J-1})^{-1}K_{12}^{J-1} \end{bmatrix}, \tag{8}$$

where $J = 1, \cdots n$, K_a^J is the total asymptotic stiffness matrix after J recursive operations, and K_{ij}^0 are the submatrices of the thin layer asymptotic stiffness matrix K_{II} (7).

By using the asymptotic solution for a finite thickness layer discussed above, the stiffness matrices of the ZnO layer and SiO_2 layer can be obtained respectively. However the asymptotic solution is not valid for the Si substrate, because the Si substrate should be considered as a semispace for SAW application. In the framework of the RAM, the semispace is replaced by a thick layer with appropriate wave attenuations, which is considered as a perfect matched layer (PML). The transfer matrix solution for the Si PML can be written in the form of (5) with the replacement of h by $h^* = h\beta$, and β is a complex variable which can be selected as $\beta = 1 + \beta_i$ with $0 < \beta_i < 0.5$. The introduction of the complex parameter β will accelerate the decay of wave but not change the eigenvalue of A. The asymptotic transfer and stiffness matrices for the Si PML can be obtained by replacing h by h^* in (5), (7), and (8). The PML thickness H and complex parameter β can be selected from the condition

$$\frac{2\pi f H \sin(\theta_x)}{V_{ql}}\beta_i > n_e, \tag{9}$$

where θ_x is the angle between propagation direction and x-axis and V_{ql} is the fastest velocity in this direction, f is the frequency of the wave, n_e is a parameter related to the error. For example, if n_e is selected as about 37, the semispace solution satisfies the radiation condition [8].

After the respective obtaining of the stiffness matrices for the ZnO layer, SiO_2 layer and Si substrate, the total stiffness matrix for the ZnO–SiO_2–Si multilayered structure can be obtained by using a stiffness matrix recursive algorithm, which is expressed as [7]:

$$K^M = \begin{bmatrix} K_{11}^m + K_{12}^m(K_{11}^{M-1} - K_{22}^m)^{-1}K_{21}^m & -K_{12}^m(K_{11}^{M-1} - K_{22}^m)^{-1}K_{12}^{N-1} \\ K_{21}^{M-1}(K_{11}^{M-1} - K_{22}^m)^{-1}K_{21}^m & K_{22}^{M-1} + K_{21}^{M-1}(K_{11}^{M-1} - K_{22}^m)^{-1}K_{12}^{M-1} \end{bmatrix}, \tag{10}$$

where M refers to the bottom m layers, and m refers to the mth layers. For example, $K^{M=3}$ are the total stiffness matrices for the ZnO–SiO_2–Si structure with 3 layers, $K_{ij}^{M=2}$ are the submatrix of the total of the stiffness matrices for the SiO_2 layers and Si substrate, $K_{ij}^{m=2}$