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Investigation of guided surface acoustic wave sensors by analytical modeling and perturbation analysis

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ABSTRACT

In this paper, shear horizontal polarized guided surface acoustic wave propagation was investigated with analytical modeling and perturbation analysis for biosensing applications. The model was also verified experimentally. The analytical model was developed for multilayer systems taking viscoelasticity into consideration. Detailed parametric investigation of dispersion curves was conducted using various substrate materials and guiding layers. The effects of frequency and degree of viscoelasticity were also studied. Perturbation equations were developed with first order approximations by relating the dispersion curve slopes to sensitivity. Among the guiding layers investigated, Parylene C showed the highest sensitivity followed by gold, chrome and silicon dioxide. The perturbation investigations were also extended to protein layers for immunosensing applications. It was observed that viscous behavior resulted in slightly higher sensitivity, and protein layers showed almost identical sensitivity similar to polymers investigated (SU-8, Parylene, etc.). The optimum configuration is found to be Parylene-C guiding layer on a ST-cut quartz substrate for protein layer sensing and this configuration has 40 times the sensitivity of gold guiding layer on quartz substrate. Our results indicate that chrome and silicon dioxide have low sensitivity when used as guiding layers. Also, lithium tantalate substrate with gold and Parylene-C guiding layers results in ∼10% lower sensitivity as compared to quartz substrate.

1. Introduction

Biosensing applications aim to detect biological target analytes such as biomarkers, fungi, bacteria, viruses and DNA [1]. Acoustic biosensors are viable alternative to alternative methods and offer the capability of low-cost, portable, rapid, sensitive, selective and point-of care detection [2]. Biosensors are used in broad range of applications such as clinical diagnosis, biomedicine, food production and analysis, microbiology, pharmaceutical and drug analysis, pollution control and monitoring, and military applications [3]. Biosensors that utilize antibody–antigen interactions are commonly referred as immunosensors. They are based on the same principles as conventional immunoassays such as enzyme linked immunosorbent assay (ELISA).

Surface acoustic waves (SAWs) show good sensitivity to surface perturbations due to their energy being concentrated at or very close to the surface [4]. SAW biosensors typically utilize shear horizontal polarized surface acoustic waves (SH-SAWs) allowing sensing under liquid loading. SH-SAWs propagate on the surface of materials with particle displacement and propagation in the plane of the surface [1]. They are minimally attenuated or damped by liquid loading. The typical cuts and materials for SH-SAWs are ST-Cut quartz, 41° YX lithium niobate ($LiNbO_3$), 64° YX $LiNbO_3$, 36° YX lithium tantalate ($LiTaO_3$), potassium niobate ($KNbO_3$) and langasite (pure SH waves) [1]. Material and SAW properties of these cuts of materials has been investigated in detail [5,6], enabling various designs. Among guiding layer and sensing materials, gold was used as the non-specific adsorptive layer in almost all early biosensing applications [7]. The guiding layers that are frequently employed for SAW biosensors include polymers such as photoresists [8], Parylene C [9], zinc oxide [10,11] and chemical vapor deposited silicon dioxide (SiO_2) [12].

To date, there are numerous reported immunosensor applications utilizing several designs with different methods, SAW types, configurations, materials and surface treatments as presented in review papers [1,7,13]. There are also several reported studies that employs different mathematical approaches for guided layer waves [14,15], however there hasn't been a particular study focusing on universal guidelines for sensitivity optimization. The wave propagation and sensitivity to mass loading was investigated in several papers in literature [16–25], however, no similar detailed parametric analysis has been presented elsewhere. The method discussed in this paper can be employed to investigate gravimetric sensors in detail for optimization and prediction of sensor performance. The mass loading sensitivity presented is applicable to thin film perturbations including viscoelastic layers and biosensors. Prediction

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of sensor performance is essential in order to investigate the effect of material properties (substrate, guiding layer, and sensing layer). As presented in this paper, for some specific design parameters, the optimum sensitivity can only be obtained in a narrow band, which may be a concern for the application. In order to investigate the design space of sensors, various typical substrate types, guiding and mass layer materials were used and sensitivity of several configurations were compared. In this study, the guiding effects of multi-layer thin films were treated by analytical modeling of wave equation with boundary conditions by dispersion curves. The sensitivity problem and optimization of sensing mechanism was investigated by perturbation methods which was first presented by Auld for acoustic wave propagation [26]. A detailed parametric study on dispersion, sensitivity and perturbation analysis was done for each case and results were compared.

2. Analytical modeling

In the wave propagation investigations, the substrate and the guiding layer were modeled as ideal elastic and isotropic. The shear velocities in substrates were taken as the SH-SAW velocities in the specified SH direction. The wave propagation was assumed as mechanical only. The leaky nature of SH waves was also neglected, since layer-guided waves are effective in energy confinement to the surface. Viscoelasticity was also taken into account for all layers other than substrate using Maxwell's model for fluids, polymers and layers of proteins [19,27].

The propagation was investigated for a system illustrated in Fig. 1. The coordinate axes are placed in such a way that x_1–x_2 plane coincides with the upper surface of the substrate and x_3 as normal to this plane with $x_3 = 0$ defining the substrate's top surface. The analytical modeling method utilized in this work was based on the method presented in the Refs. [15,18,19]. Considering wave propagation in an isotropic medium, the equation of motion can be written as

$$\frac{\rho \partial^2 u_j}{\partial t^2} = \mu \nabla^2 u_j \tag{1}$$

where u_j is the particle displacement; ρ is the density; λ and μ are the Lame constants and S_{ij} is the strain tensor. The multilayer wave propagation equation is solved by trial solutions for displacements with propagation along the x_1 axis and displacement in x_2 axis. The trial solutions for substrate (s), guiding layer (g) and mass layer (m) can be constructed, satisfying these conditions as

$$u_s = (0, 1, 0)[A_s e^{-T_s x_3} + B_s e^{T_s x_3}] e^{j(\omega t - k_1 x_1)} \tag{2}$$

$$u_i = (0, 1, 0)[A_i e^{-jT_i x_3} + B_i e^{jT_i x_3}] e^{j(\omega t - k_1 x_1)} \tag{3}$$

where $k_1 = \omega/v$ is the phase speed v of the solution, $A_{s,i}$ and $B_{s,i}$ are constants that determine wave propagation characteristics and $T_{s,i}$ are wave vectors. Because of the initial assumption of propagation only along x_1 direction, strain tensor S_{ij} can be allowed to vanish. Substituting trial solutions Eq. (2) into Eq. (1) for each layer, the wave vectors can then be obtained [18]. The resulting wave vector, T_s, for the substrate is different from the others as the trial solution was chosen to ensure non-imaginary T_s. This condition arises from Love wave theory, in which shear acoustic velocities of any guiding layers should be less than that of the substrate [19]. Shear velocities of isotropic, elastic materials can be calculated using shear modulus and density values with the formula $v_i = (\mu_i/\rho_i)^{1/2}$. Love wave solution is obtained when $t_s \to \infty$. In such a case, wave vector T_s is real, leading to real v_s and particle displacement decaying with depth (i.e. surface waves) [19].

The dispersion solution is obtained by applying displacement and stress boundary conditions. The displacement boundary conditions are particle displacement continuity at interfaces and the stress boundary conditions are stress continuity at the interfaces and stress-free top and bottom surfaces. Each additional layer adds two extra rows and columns to the coefficient matrix. The elements in the new rows and column are all zero except for six elements. The constant ξ_{km} defined as the ratio of material constants and wave vectors $\xi_{km} = \mu_k T_k / \mu_m T_m$.

The dispersion solution for a system composed of the substrate and i number of additional layers is given in Eq. (4). The odd numbered rows represent the displacements and the even numbered rows represent the stress continuities. Note that the two non-zero elements added to the last row of previous layer ($a_{2i,2i+1}$ and $a_{2i,2i+2}$) represent continuity of stress between the layers, the row before the last row with non-zero elements ($a_{2i+1,2i-1}$, $a_{2i+1,2i}$, $a_{2i,2i+1}$ and $a_{2i,2i+2}$) indicates the displacement continuity, and last row with non-zero elements ($a_{2i+2,2i+1}$ and $a_{2i+2,2i+2}$) represents the top free surface. Another advantage of this representation is that it already includes the dispersion equation of the simpler systems. As an example, the first 4×4 matrix represents a two layer system, and 6×6 matrix represents a three layer system.

$$\begin{pmatrix}
1 & 1 & -1 & -1 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 \\
e^{T_s d_s} & -e^{-T_s d_s} & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 \\
1 & -1 & -j\xi_{s1} & j\xi_{s1} & 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 \\
0 & 0 & e^{-jT_1 d_1} & -e^{jT_1 d_1} & -\xi_{21} e^{-jT_2 d_1} & \xi_{21} e^{jT_2 d_1} & 0 & 0 & \cdots & \cdots & 0 & 0 \\
0 & 0 & e^{-jT_1 d_1} & e^{jT_1 d_1} & -e^{-jT_2 d_1} & -e^{jT_2 d_1} & 0 & 0 & \cdots & \cdots & 0 & 0 \\
0 & 0 & 0 & 0 & e^{-jT_2(d_2+d_1)} & -e^{jT_2(d_2+d_1)} & -\xi_{32} e^{-jT_3(d_2+d_1)} & \xi_{32} e^{jT_3(d_2+d_1)} & \cdots & \cdots & 0 & 0 \\
0 & 0 & 0 & 0 & e^{-jT_2(d_2+d_1)} & e^{jT_2(d_2+d_1)} & -e^{-jT_3(d_2+d_1)} & -e^{jT_3(d_2+d_1)} & \cdots & \cdots & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & e^{-jT_3(d_3+d_2+d_1)} & -e^{jT_3(d_3+d_2+d_1)} & \cdots & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \xi_{i,i-1} e^{-jT_i \sum_0^{i-1} d_i} & \xi_{i,i-1} e^{jT_i \sum_0^{i-1} d_i} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & e^{-jT_{i-1} \sum_0^{i-1} d_i} & e^{jT_{i-1} \sum_0^{i-1} d_i} & -e^{-jT_i \sum_0^{i-1} d_i} & -e^{jT_i \sum_0^{i-1} d_i} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & e^{-jT_i \sum_0^{1} d_i} & -e^{jT_i \sum_0^{1} d_i}
\end{pmatrix}$$