FEM MODELING SAW HUMIDITY SENSOR BASED ON ZNO/IDTS/ALN/SI STRUCTURES

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ABSTRACT

In this study, we demonstrate a finite element method (FEM) simulation approach of surface acoustic wave (SAW) humidity sensors. The polycrystalline Zinc oxide (ZnO)/ Aluminum nitride (AlN)/Si-layered structure was simulated for SAW resonators and compared with experiment results. The humidity absorption behaviors of ZnO films coating on the propagation characteristics of the SAW were investigated by FEM modeling in the absence and presence of water vapor. The simulation frequency shift in different relative humidity (RH%) agreed with experiments values and gave a new approach to SAW sensor designing based on piezoelectric thin films.

KEYWORDS

FEM modeling, SAW sensor, humidity sensor

1. INTRODUCTION

Recently, chemical sensors based on a surface acoustic wave (SAW) have been widely investigated due to several attractive advantages such as high sensitivity, small size, reliability and wireless ability [1]. Among many factors, coated sensitive materials and piezoelectric substrates play important roles in improving SAW sensor properties and need to be investigated in detail by theory and experiment. Accurate SAW sensor response simulations have become indispensable for understanding and designing high-performance sensors. In comparison with the previous methods as δ function model, P-matrix model, or coupling-of-modes (COM) theory; the finite element method, which may be implemented via commercial software, such as ANSYS or COMSOL, has proven to have excellent capability for modeling and analyzing SAW sensors [2, 3, 4].

A finite element method (FEM) uses simple methods to analyze complicated geometries. FEM modeling hydrogen SAW sensor are described in [2] or applied to SAW organic vapor sensors in [3]. However, SAW simulations constructed in previous reports focused on bulk piezoelectric materials as lithium-niobate ($LiNbO_3$) [2], or quartz [3]. Recently, there have been increased efforts to identify materials as AlN or ZnO thin films that are better able to propagate SAWs swiftly and effectively, with an eye towards achieving higher frequencies and full compatibility with micro-electromechanical systems (MEMS). Hence, the simulated approach for SAW sensors based on a piezoelectric thin film of AlN or ZnO are necessary to research [4].

In this work, we constructed an FEM model of a SAW humidity sensor using a ZnO film as the sensing layer on interdigital transducers (IDTs)/AlN/Si and compared it to experimental results. ZnO thin films with varying thickness and humidity absorption were also investigated via FEM simulation, and a humidity absorption coefficient (k) of a ZnO thin film was conduced in this work.

2. MODEL DESCRIPTION

SAW resonator modeling

SAW propagation is governed by both differential equations that must be solved along with design problems, including the geometric complexity of the device, the material properties, and the boundary conditions. FEM provides numerical solutions defined by associated differential equations. We used the FEM method in COMSOL to analyze the piezoelectric effects [5]. The IDTs, metallic electrodes fabricated on top of the piezoelectric substrate, convert electrical energy to mechanical energy and vice versa for piezoelectric effects. The IDT has a comb-like structure, where the distance between the fingers in the IDT determines the frequency of the waves propagating over the substrate. The distance p between successive electrodes, as shown in Fig. 1, determines the elastic wavelength λ, where $\lambda = 2p$. The associated frequency, f, of waves propagating with a velocity, v, is given by $f = v / \lambda$. IDTs are periodic in nature, alternating between positive and negative potentials. Thus, one period of the electrode is sufficient to model the SAW resonator as a whole, as shown in Fig. 1. The SAW resonator may have hundreds of electrodes, each far longer than it is wide. Therefore, edge effects can be ignored, and the model geometry can be reduced to a periodic cell [3, 4], as shown in Fig. 1.

We used the multiphysics finite element package COMSOL 3.3 in the two-dimensional (2D) piezo plane strain mode (smppn) to simulate SAW propagation in piezoelectric thin films. This application mode assumes that the out-of-plane strain is zero (x_2 direction). This work modeled an AlN piezoelectric thin film 1 μm thick on a 2λ (8 μm)-thick silicon substrate with a fixed bottom boundary. A 1 V polarization was assigned to the aluminum electrode, which was 100 nm thick. The periodic boundary conditions, wherein the left Γ_L and the right Γ_R boundaries are applied, are shown in Fig. 1, and the detailed boundary conditions are listed in Table 1. Using the previously reported material constants [4] to describe the ZnO and AlN material, we also determined the Young's modulus to be 131 Gpa, the Poisson ratio to be 0.27, and the silicon density to be 2330 kg/m^3. The IDT finger was 1 μm wide with a 4 μm fixed periodicity (λ). The ZnO humidity sensing layers were 180 nm and 300 nm thick.

SAW humidity sensor modeling

The adsorption of water vapor was presented as a slight increase in the density of the coating film. If ρ_0 and h_0 are the density and thickness of the ZnO coating film in the absence of water vapor, the density and thickness in the presence of water vapor vary with the concentration of absorbed water species according to [3,6]:

$$\rho(c_v) = \rho_0 + \frac{kc_v}{1 + kc_v / \rho_v} \tag{1}$$

$$h(c_v) = h_0 (1 + \frac{kc_v}{\rho_v}) \tag{2}$$

where k is the air/coating film partition coefficient for water vapor, ρ_v is the water density, and c_v is the water concentration in air (absolute values).

Experimental

In order to evaluate the FEM simulation for accuracy, we fabricated two-port SAW resonators for a humidity sensor on an AlN/Si structure with λ = 40 µm. The fabrication process and SAW device geometry were similar to those previously described [7]. High-quality polycrystalline layers were deposited as 1-µm-thick (002)-oriented AlN thin films onto (100)-Si wafers using a sputtering system. Thin aluminum layer 100-nm-thick was deposited onto the AlN/Si samples using the thermal evaporator method. IDTs and reflectors were made using UV lithography and Al wet etching. The ZnO humidity sensing layer was synthesized via a sol-gel method and was coated onto the IDT/AlN/Si structure through spin coating to 180 nm and 300 nm thick [1]. The SAW humidity measurement system was setup as our previous work [1]. The frequency shift in the SAW humidity sensor was monitored with an Agilent 8802A Network Analyzer.

3. RESULTS AND DISCUSSIONS

We used an eigen-frequency analysis to determine the eigen-frequencies and the modes of deformation in the modeled structure. The model was meshed with pre-defined "normal" parameters in a free mesh. Since the SAW displacements were largest near the substrate surface, the meshing domain was meshed to higher densities near the surface than it was near the bottom, as in Fig. 2. The number of meshing elements was chosen as a trade-off between the simulation run time and accuracy level. The simulation contained over 11,000 elements. Figure 2(a) shows the total simulated deformed displacement of SAW resonators based on IDTs/AlN/Si structures. The eigen-frequency detected in this structure was 1.294983e9. The surface acoustic wavelength is equal to the width of the modeled periodic cell (λ = 4 µm) at the lowest eigen-frequency with surface acoustic wave characteristics. The surface acoustic phase velocity can be calculated using $V_{SAW} = f \times \lambda$, hence a phase velocity of 5180 m/s existed in the IDTs/AlN/Si structures. However, with a ZnO thin film 300 nm thick on top, as in Fig. 2(b), the ZnO/IDTs/AlN/Si SAW structure had a resonant frequency of 1.134777e9 (a 4 µm wavelength), giving a phase velocity of 4539 m/s.

Table 1: Boundary conditions of the simulation.

	Mechanical boundary condition	Electrical boundary condition
Γ_0	Free	Zero charge/symmetry
Γ_1, Γ_2	Free	Continuity
Γ_3	Fixed	Ground
$\Gamma_{R0}, \Gamma_{R1}, \Gamma_{R2}$ $\Gamma_{L0}, \Gamma_{L1}, \Gamma_{L2}$	Periodical boundary condition	

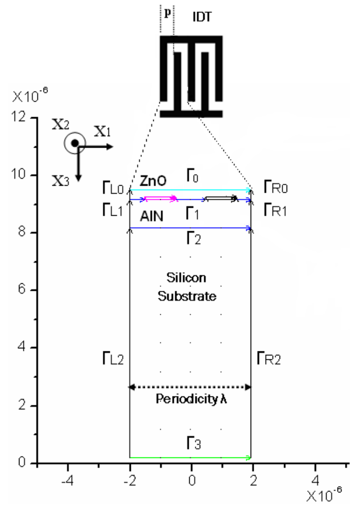

Figure 1: Geometry of a periodic cell in the simulated ZnO/IDTs/AlN/Si SAW humidity sensor.

Figure 3 shows the experimental frequency response, S_{12}, of the two-port SAW resonators of IDTs/AlN/Si measured using a network analyzer with and without a ZnO film at room temperature. The resulting device had a 130.2 MHz resonant frequency, corresponding to a 40 µm wavelength and a 5208 m/s phase velocity of the Rayleigh wave. With 300-nm-thick ZnO thin film coated onto the IDT/AlN/Si structure, the SAW velocity decreased to approximately 5060 m/s. Additionally, the insertion loss of the structure increased by 2.7 dB. These changes might originate from a change in the mass loading of the ZnO thin film onto the SAW resonator. Compared to the experiment values, the FEM model had SAW velocity errors of 0.54 % and 10.3 % when simulating the IDTs/AlN/Si and ZnO/IDTs/AlN/Si structures, respectively.

The FEM models of SAW resonators based on IDTs/AlN/Si structures had a phase velocity with a low error (0.54 %), which increased significantly in the ZnO/IDTs/AlN/Si structure (10.3 %) using the material constants in [4]. The very different mass densities between the dense ZnO thin film (ρ = 5675 kg/m^3) and porous ZnO film likely created this high simulation error.

The ZnO mass density depends on the formation method [8] and the morphology of the ZnO film; a dense film has a higher density than does a porous film [9]. The initial density of a ZnO film (3405 kg/m^3 with 40 % porosity) was chosen for this simulation due to the low error rate (2.8 %) compared with those of the experimental values and its agreement with the ZnO film morphology formed via the sol-gel method in our previous work [1].

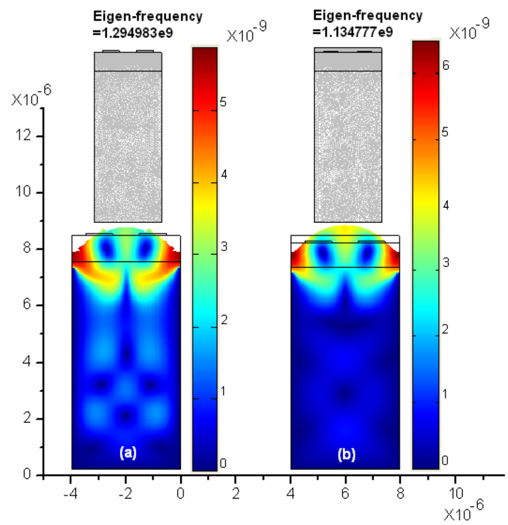

Figure 2: SAW sensors with (a) IDTs/AlN/Si and (b) ZnO/IDTs/AlN/Si structures (300-nm-thick ZnO) at the resonant frequency. Color is the deformation strength of the SAW resonator.

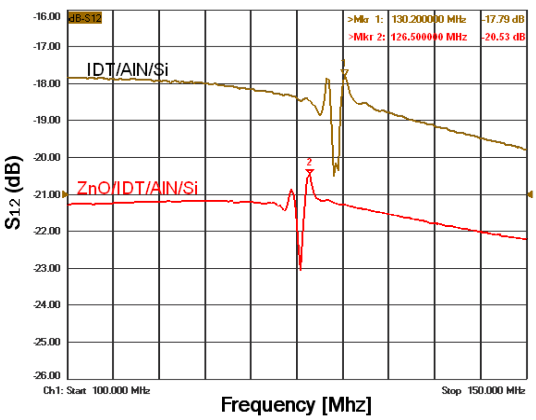

Figure 3: Frequency response, S_{12}, of two-port SAW resonators of AlN/Si structures with and without ZnO.

Exposing the sensor to absorbed water vapor shifted the eigen-frequency to lower values. The shift in the resonant frequency could be due to changed mass density, viscoelastic properties, electric conductivity, or dielectric properties of the propagation medium when water molecules were absorbed into the film surface and pores [10]. However, the simulation is limited to the SAW sensor responding solely to mass loading on the surface [2, 3]. The ZnO film absorbed water vapors (using absolute values converted from relative humidity), and the increased mass density $\rho(c_v)$ and film thickness $h(c_v)$ were calculated using Equations (1, 2). By inserting these values into the simulation for water vapor concentration, Fig. 4 shows that the SAW resonator frequency shifted at various relative humidities (RH %).

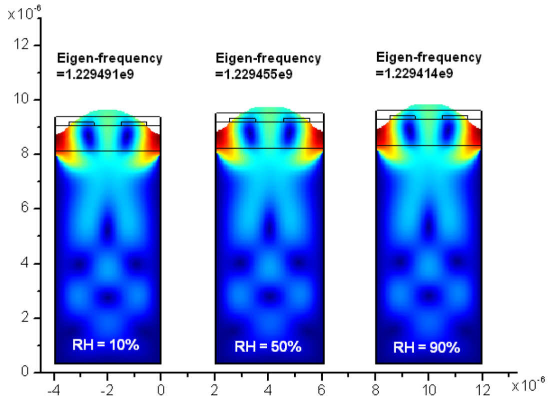

Figure 4: Frequency response of a SAW humidity sensor with a 300-nm-thick ZnO sensing layer in FEM at various relative humidities (RH%).

Figure 5 shows the simulated and experimental frequency responses of a two-port SAW resonator (ZnO coated) examined at approximately 10 %, 30 %, 50 %, 70 %, and 90 % relative humidities. Figure 5 also shows the frequency shifts with 300-nm- and 180-nm-thick ZnO thin films. The downward shift in frequency was due to a thicker sensitive layer, which increased the mass of the layer and also explained the SAW resonator response to humidity. The partition coefficient, k, described for water vapor absorption of a ZnO porosity film, was assumed to be 40 for the simulation results in Fig. 5 but does not agree with the experimental values across the relative humidity range (10-90 %). Additionally, in the large RH range (50-90 %), the sensors shifted farther than that in the low RH range (below 50 %) [1]. Hence, we chose a partition coefficient, k_1 = 17, in the low RH range (below 50 %) and one, k_2 = 40, in the high RH range (50-90 %). The simulation results were close to the experimental values, as shown in Fig. 6, in the low RH range. In the high RH range, the conductivity and dielectric properties of a ZnO film changed the experimental humidity sensor response, hence producing differences between the simulated and experimental results. The two different linear responses of the SAW resonator at different RH agree with the results of other reports [10, 11]. The water vapor absorption, k, should be separated into two values, k_1 = 17 at low RH (below 50 %) and k_2 = 40 at high RH (50-90 %), to obtain better results from the simulation. The SAW humidity sensor showed a downward shift in frequency of 0.32~0.58 kHz per 1% RH in the low RH range and 0.56~0.82 kHz per 1% RH in the high RH range, depending on the ZnO layer thickness.

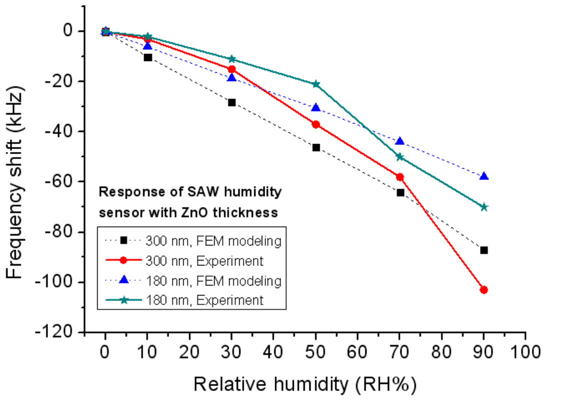

Figure 5: Frequency shift curves according to FEM modeling for a SAW humidity sensor coated with ZnO layers of varying thickness compared with the experiment results (water vapor absorption, k = 40).

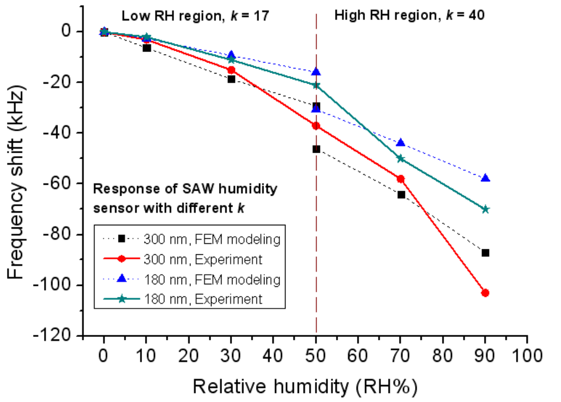

Figure 6: SAW humidity sensor response to RH: two linear stages with k *= 17 at the low RH range (RH<50%) and* k *= 40 at the high RH range (RH>50 %).*

4. CONCLUSION

We illustrated FEM modeling of a SAW resonator based on IDTs/AlN/Si structures using a ZnO film as the humidity-sensing layer. The simulation results were confirmed by the experimental values, with good agreement given a suitable water vapor absorption constant (k) of a ZnO porous film in humid environments. Because of the limitations of the simulation, these values are estimates, not precise predictions; they are aimed to help guide the development of an experimental SAW sensor based on piezoelectric thin films. Future research efforts should investigate the varied conductivity of a ZnO film in humid environments to enhance the simulation accuracy.

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