Finite element modeling for improved SAW sensor response.

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Abstract:

Surface acoustic wave sensors detect chemical and biological species by monitoring the shifts in frequency of surface acoustic waves generated on piezoelectric substrates. These devices are conveniently small, relatively inexpensive and quite sensitive. Considerable attention has been focused on the development of response models to understand the characteristics of surface acoustic waves generated in SAW devices. Most of the analytical techniques require simplification of second order effects such as backscattering, charge distribution, diffraction and mechanical loading. Finite element approach has proven to be a viable option to model wave propagation in SAW devices operating in MHz-GHz range

A 3-D finite element model based on a micron sized piezoelectric substrate with a thin Pd sensing layer was simulated to gain insights into the sensor response. The effect of the Palladium film on the wave propagation characteristics was studied in the presence and absence of hydrogen. The center frequency of the device simulated was around 100 MHz. Displacement and voltage profiles at the output IDT nodes were used to identify the gas adsorption. The study demonstrates the effectiveness of finite element models in understanding the gas sensor response.

1. Introduction:

Considerable attention has been dedicated to the development of analytical and modeling techniques in order to understand the characteristics of surface acoustic waves generated in SAW devices. The recent advances in sensors and wireless communication systems indicate the need for high performance SAW devices often operating in high frequency (GHz) range. Most of the analytical techniques require simplification of second order effects such as backscattering, charge distribution, diffraction and mechanical loading. However, these effects become significant for SAW devices operating in the high frequency range.

The models commonly used to simulate the mechanical and electrical behavior of piezoelectric transducers generally introduce simplifying assumptions that are often invalid for actual designs (Morgan, 1998). The geometries of practical transducers are often two (2-D) or three dimensional (3-D) (Lerch, 1990). Simulations of piezoelectric media require the complete set of fundamental equations relating mechanical and electrical quantities to be solved. The finite difference or finite element scheme are sufficient to handle the differential equations (Xu, 2000(a), 2000 (b); Ippolito et al., 2002, 2003 (a), 2003 (b)). The finite element method has been preferred because it allows handling of complex geometries.

Finite element was applied by Lerch (1990) to calculate the natural frequencies with related eigen modes of the piezoelectric sensors and actuators as well as their responses to various dependent mechanical and electrical perturbations. A direct finite element analysis was carried out by Xu to study the electromechanical phenomena in SAW devices (Xu, 2000 (a)). The influence of the number electrodes on the frequency response was analyzed. The finite element calculations were able to evaluate the influence of the bulk waves at higher frequencies. Ippolito et al. have investigated the effect of electromagnetic feed through as wave propagation in layered SAW devices (2003 (a)). The same model was extended to study electrical interactions occurring during gas sensing (Ippolito et al., 2003 (b)). Recently, a 3-D finite element model was developed for a SAW palladium thin film hydrogen sensor (Atashbar et al., 2004). The effect of the palladium thin film on the propagation characteristics of the SAW was studied in the absence and presence of hydrogen. The variations in mass loadings, elastic constants and conductivity were the factors used in evaluating the velocity change of the wave. All the above demonstrate the feasibility of finite element models to adequately model SAW sensor response under varying conditions.

2. Finite Element Model:

The propagation of acoustic waves in piezoelectric materials is governed by the mechanical equations of motion and Maxwell's equations for electrical behavior (Auld, 1973; Ballantine et al., 1997). The constitutive equations of piezoelectric media in linear range coupling the two are given by:

$$T_{ij} = c_{ijkl}{}^{E} S - e_{kij}{}^{t} E \qquad \textbf{(2.1)}$$

$$D_i = e_{ikl} S_{kl} + \varepsilon_{ik}{}^{S} E_k \qquad \textbf{(2.2)}$$

The quasistatic assumptions help reduce Maxwell's equation to $\frac{\partial D_i}{\partial x_i} = 0$ and $E_i = -\frac{\partial \phi}{\partial x_i}$. The components of strain are defined by $S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$.

The above equations give a system of four coupled wave equations for the electric potential and the three component of displacement in piezoelectric materials.

$$-\rho \frac{\partial^2 u_i}{\partial t^2} + c_{ijkl}^{E} \frac{\partial^2 u_k}{\partial x_j \partial x_l} + e_{kij} \frac{\partial^2 \phi}{\partial x_k \partial x_j} = 0 \qquad \textbf{(2.3)}$$

$$e_{ikl} \frac{\partial^2 u_k}{\partial x_i \partial x_l} - \varepsilon_{ik}^{S} \frac{\partial^2 \phi}{\partial x_i \partial x_j} = 0 \qquad \textbf{(2.4)}$$

These coupled wave equations can be discretized and solved for generating displacement profiles and voltages at each element/nodes. We use the commercially available FEM code ANSYS. The main advantage of using ANSYS lies in the flexibility in modeling different physical phenomena and also the pre- and post-processing capabilities.

3. Simulation Details:

A 3-D finite element model based on a micron sized piezoelectric substrate with dimensions (400µm width x 1600µm propagation length x 500µm depth) was simulated to gain insights into the sensor response. Two IDT finger pairs in each port were defined at the surface of X-cut, Y-propagating LiNbO3 substrate. The fingers were defined with periodicity of 40 µm and aperture width of 200 µm. The IDT fingers were modeled as mass-less conductors and represented by a set of nodes coupled by voltage degrees of freedom (DOF). A total of approx. 80,000 elements (more than 100000 nodes) were generated. The model was created to ensure higher node density at the surface and throughout the middle of the device to study the different modes of surface acoustic waves and the use of tetragonal elements with 4 DOF ensured the same. Three DOF's provided the displacements in the longitudinal (x), normal (y), and the shear horizontal (z) directions and a fourth for the voltage.

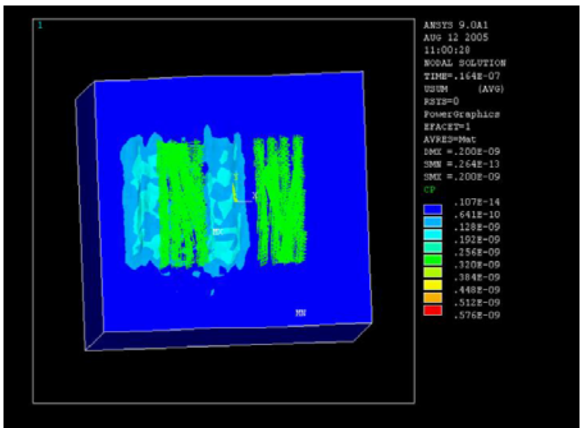


Figure 1. Finite element model of wave propagation in YZ $LiNbO_3$.

The structure (with and without sensing layer) was simulated for a total of 100 nanoseconds (ns), with a time step of 1 ns. The excitation of the structure was provided by applying an impulse function on the transmitter IDT fingers.

$$V_i = \begin{cases} \frac{1}{T_s}, 0 < t \le T_s \\ 0, t > T_s \end{cases} \qquad \textbf{(3.1)}$$

4. Sensing Layers:

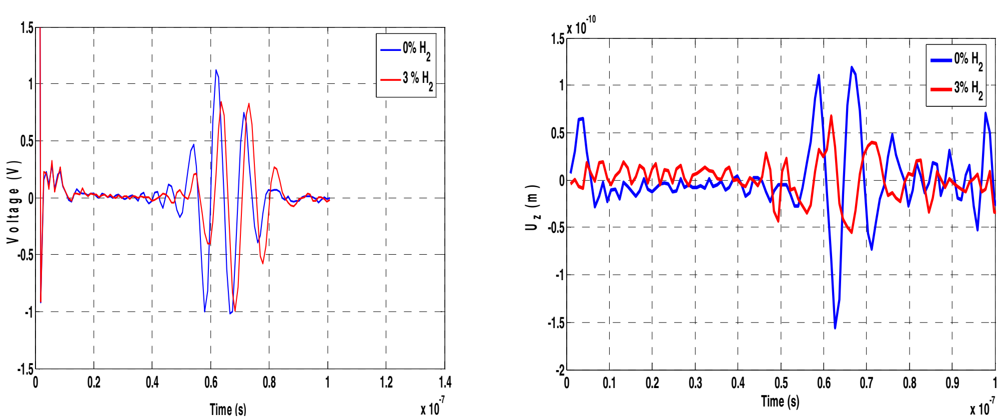
The simulations of SAW gas sensor device were carried out for two different material properties of the sensing layer. The first part of the simulation involved calculating response at the output IDT for material property of the sensing layer without any gas adsorbed. In the second part, the material property of the film was varied in accordance with the changes expected for 3% hydrogen gas adsorption. This would require the sensing film size to be increased by 10% to compensate for the expansion due to mass change. The structure density was decreased by 2% and Young's modulus of elasticity changed from 128 GPa to 110 GPa.

Thin palladium films which are known to have high affinity for hydrogen were utilized as sensing layers in the present study. A 500 nm thick palladium film was defined between the two IDT ports. The film width and length were taken as 100 and 88 microns respectively. Adsorption of H_2 gas results in changes in the palladium film properties which in turn affects the wave propagation velocity. For a known change in propagation velocity, the concentration of hydrogen gas could be calculated. The key factors contributing to the velocity change are variations in mass loadings, elastic constants and conductivity. Adsorption of H_2 leads to a decrease in density and Young's Modulus of elasticity.

Other sensing layers employed in this work would include nanowire arrays aligned in different directions. Nanowires with their high ratio of surface to bulk Pd atoms provide increased surface area for hydrogen adsorption, thereby increasing the mass loading. This in turn manifests itself as increased sensitivity of the gas sensor. It is expected that quantitative predictions of changes in wave propagation characteristics for different sensing layers would be possible using finite element models. The model would then be used to optimize the design of sensing layer by varying factors such as nanowire thickness and array spacing to arrive at best H_2 sensors possible for a given crystal orientation.

5. Results and Discussion:

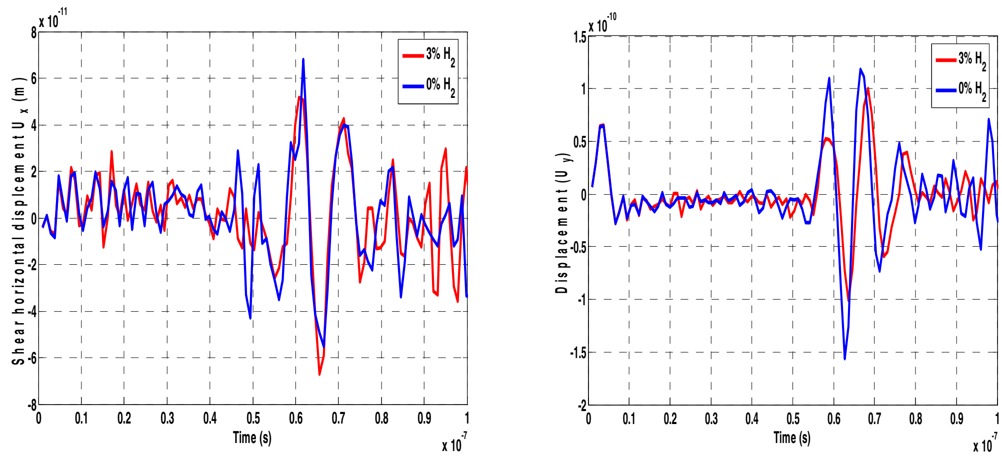
The voltage and displacement waveforms with and without hydrogen adsorbed on a thin Pd film are shown in the Figs. 1 and 2. The changes in material properties in accordance with hydrogen adsorption results in a time delay of around 3ns in these waveforms at the nodes representing the output IDT's. The substrate is anisotropic and hence the displacement profiles along the different directions independent of each other. The maximum time shift occurs in the surface normal displacement component (Uz) which is the closest to the Rayleigh mode.



(a) (b)

Figure 2. Voltage and surface normal displacement (U_z) profile with and without hydrogen adsorbed at the output IDT.

Also, the adsorption of H_2 results in wave attenuation of the voltage and displacement waveforms. The least attenuation and time delay is experienced in the x direction which represents the shear horizontal component (Fig. 3 (a)) of the generated wave. A 3D representation of the wave propagation in the YZ substrate is shown in Fig. 1. The input and the output IDT's are placed on the right and left side of the substrate. The wave travels from the input IDT to the output. The generated wave also travels outside the aperture of the IDT along the x-axis thereby dispersing part of the energy in the shear horizontal direction.



(a) (b)

Figure 3. Displacement along the x (shear horizontal) and y direction at the output IDT with and without hydrogen adsorbed.

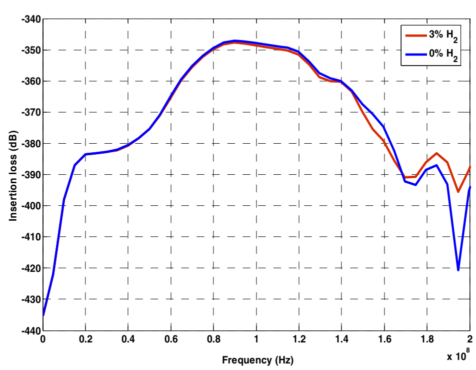


Figure 4. Frequency response with and without hydrogen adsorbed.

Figure 4 shows the frequency response at the output IDT. The adsorption of hydrogen results in approx. 1.5 dB insertion loss for a 100 MHz device. This result is comparable to those observed in experiments.

6. Limitations of Finite Element Simulations:

A fine mesh generation is required for accurate modeling of a SAW gas sensor. The incorporation of a nanomaterial sensing layer would result in significant differences in the length scales of substrate and sensing layer, thereby requiring much higher node densities. Also, the simulations are time consuming and increase with increasing mesh size. Another major setback arises from acoustic wave reflection from the edges if the simulations are carried for sufficiently longer times. One of the ways to overcome this limitation would be employment of damping elements at the ends of the substrate. While longer simulation times are necessary to attain stable state, too long a simulation time results in wave reflections causing instabilities to set in. A simulation time of 100 ns was found to be optimum for the substrate dimensions considered in the present study.

7. Conclusions:

A 3-D finite element model of SAW sensor with and without sensing layer was developed. The hydrogen gas adsorption was modeled for by changing the material properties of the sensing layer. The changes in the Young's Modulus of elasticity and density of the palladium film were utilized for the same. The displacement and voltage profiles were calculated at the output nodes of the receiving IDT's. The finite element model reveals that the Rayleigh mode (z-direction displacement) is the most suitable for gas sensing. A time shift of 3 ns was observed when the gas sensor was exposed to 3% H_2.

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