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FEM modeling of SAW organic vapor sensors

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ABSTRACT

A finite element method (FEM) simulation approach of surface acoustic wave (SAW) organic vapor sensors was investigated. The effects of the polymer coating on the propagation characteristics of the SAW were studied by FEM modeling in the absence and presence of vapor. The sensitivities for each vapor-coating combination can be obtained from the simulation frequency shift in different vapor concentration. Comparisons of the simulation sensitivities of SAW vapor sensors with the experimental values reported by Edward T. Zellers and co-workers confirm the general validity of the approach. The approach is expected to select polymer, which offers the best sensitivity for particular vapor.

1. Introduction

SAWs have most of their energy localized within 1.5 wavelengths of the surface and are sensitive to changes of surface characteristics [1]. Therefore, the gas to be sensed reacts upon sensitive film coated on surface of SAW device and this reaction has an effect on velocity of surface wave. Most gases can be detected by using different sensitive materials.

Design considerations for high sensitivity implementation require a detailed analysis of the effects of sensor geometry as well as the properties of the chemical sensitive layer [2,3]. The fabrication and systematic measurements of SAW sensors are extremely time consuming [4]. Accurate SAW sensor response simulations have become indispensable for designing high performance sensors. Changes in the propagation characteristics of the SAW in terms of the time delay in the voltage and particle displacements due to exposure of palladium thin film to hydrogen and insertion loss of the device are studied in [5]. The effects of film properties on the sensitivity of SAW chemical sensors are studied in [6]. Owing to the easy way of analyzing complicated geometries particularly, the FEM has proved to be a well performing tool to derive the influence of geometrical variations of the electrode shape and the surface perturbation of the sensors. A suited numerical method for estimating polymer coated SAW organic vapor sensor responses is important to help experimental sensor development.

This work presents a FEM modeling applied for SAW organic vapor sensors. The eigenfrequency and sensitivity of the SAW organic vapor sensors are investigated. Compared with experimental data in [7], the simulation results show that FEM modeling is an efficient tool for choosing sorbent polymer to help guide experimental sensor development.

2. Model description

To advance the use of finite element analysis for simulating the SAW sensors, the system was modeled by two steps: the SAW device with polymer coating was modeled in the absence of organic vapor; then the effects of the polymer coating were studied in the presence of organic vapor.

2.1. Design considerations of SAW organic vapor sensors

For the purpose of detecting the changes of SAW due to absorption of gas molecules, it is efficient to measure oscillation frequency of oscillator composed of SAW delay-line and feedback RF amplifier, as shown in Fig. 1. The oscillation frequency depends on the operation frequency of SAW delay-line that acts as frequency control element. The SAW delay-line is coated with sensitive polymer that acts as a chemical sensitive layer. Oscillation frequency of the oscillator is employing sensitive film changes and we can directly acquire the oscillation frequency corresponding to the amount of absorption gases [1,8].

To improve the frequency stability, low insertion loss is achieved by electrode width control single phase unidirectional transducer (EWC/SPUDT) configuration, which consists of three fingers per cell with nominal widths of $\lambda/8$, $\lambda/4$ and $\lambda/8$ (λ is the wavelength corresponding to the operation frequency) on positions of 1/8, 4/8 and 7/8, respectively [9]. Single-crystal ST-cut, X-propagating quartz

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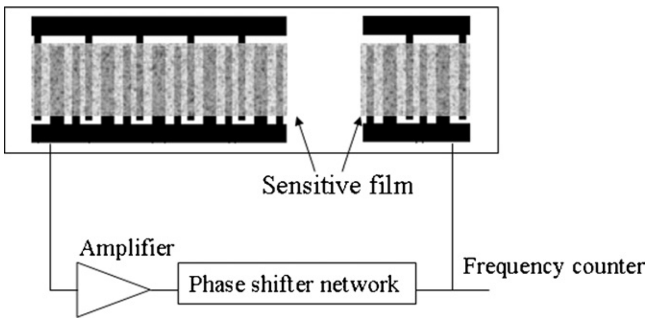

Fig. 1. The schematic of sensor system with SAW delay-line oscillator.

was used as a piezoelectric substrate for its relatively low temperature coefficient of delay. Au is often chosen for chemical detection applications because of its inertness and resistance to corrosion.

2.2. SAW delay-line modeling

SAW delay-line may have hundreds of electrodes, and each electrode's length can be far larger than it's width. The edge effects can therefore be neglected and the model geometry can be reduced to the periodic unit cell. We denote the direction of periodicity by X_1, the surface normal direction by X_2 and their perpendicular direction by X_3, as shown in Fig. 2. The dimensional extension of electrodes in X_1 direction is huge in comparison to the periodicity. Moreover, we assume homogenous material topology in X_3 direction. We are mainly interested in the propagation of Rayleigh-waves and their interaction with the periodic structure. The amplitude of waves, which live near the surface, decreases rapidly within depth and becomes negligibly small within the depth of a few wavelengths.

We set up the model in the Piezo Plane Strain application mode, which requires the out-of-plane strain component to be zero. This should be a valid assumption, considering that SAW is generated in the model plane and that the sensor is thick in the out-of-plane direction.

Assuming linear material and steady state sinusoidal time dependence, the quasi-static equations for the modeling of piezoelectric devices are Newton's law, Gauss's law and the constitutive relations. More details on the theoretical aspect are found in [10]. In this two-dimensional problem, we neglect the diffraction effect

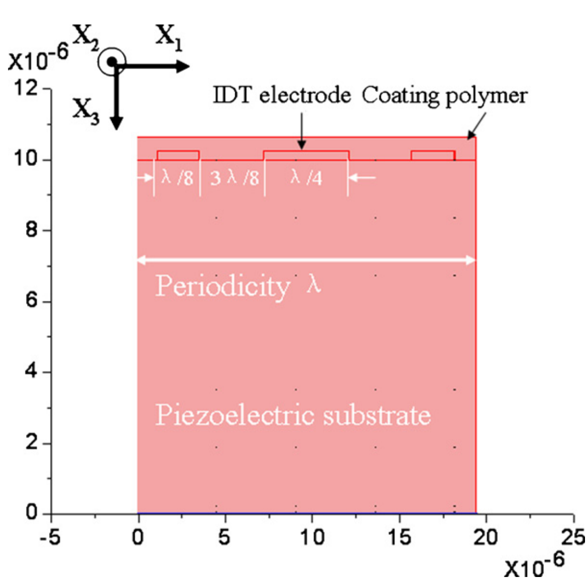

Fig. 2. The modeled geometry of the studied EWC/SPUDT unit cell in the model.

in the X_2 direction. Consequently no variation is permitted in the X_2 direction and all the derivatives are equal to zero. As we are interested in harmonic response of the device, the governing differential equations that define the mechanical and electrical properties in the volume have to be established for the amplitudes of the mechanical displacement ξ_l (only in the X_1 and X_3 directions) and the electrical scalar potential φ in Eq. (1).

$$\sum_{i=1}^{3}\sum_{l=1}^{3}\sum_{m=1}^{3} c_{iklm}^{E} \frac{\partial^2 \xi_l}{\partial X_i \partial X_m} + \sum_{i=1}^{3}\sum_{m=1}^{3} e_{mik} \frac{\partial^2 \varphi}{\partial X_i \partial X_m} = \rho \frac{\partial^2 \xi}{\partial t^2}; k = 1, 2, 3$$
$$\sum_{i=1}^{3}\sum_{l=1}^{3}\sum_{m=1}^{3} e_{ikl} \frac{\partial^2 \xi_k}{\partial X_i \partial X_l} - \sum_{i=1}^{3}\sum_{m=1}^{3} \varepsilon_{im} \frac{\partial^2 \varphi}{\partial X_i \partial X_m} = 0 \quad (1)$$

where C_{iklm} is elastic constant, e_{ikl} piezoelectric constant, ρ density, ε_{im} dielectric permittivity.

Here, mathematical modeling, analysis and solution strategies get more technical due to the governing piezoelectric equations. First, the model deals only with free SAW propagation in the piezoelectric substrate by using FEMLAB solver, without any applied electric field. In order to find the velocity of the wave, we use periodic boundary conditions to dictate that the voltage and the displacements are the same along both vertical boundaries of the geometry. This implies that the wavelength will be an integer fraction of the width of the geometry. The lowest SAW eigenmode has its wavelength equal to the width of the geometry. The eigenfrequency of this mode multiplied by wavelength hence gives the velocity of the wave. Second, based on the Auld's perturbation theory [11], the model deals with perturbations of the SAW velocity by changes in the mechanical and electrical surface boundary conditions, due to the deposition of IDT electrodes as well as coating sensitive film overlay. Within the overlay, the perturbed fields satisfy the acoustic field equations and a lowest eigenfrequency that acts as a reference frequency for sensor responses is obtained.

2.3. SAW organic vapor sensors modeling

The amount of vapor sorbed by the polymer layer and hence the sensor responses depend on the interactions between the vapor and the polymer. Giving an understanding of these interactions and the transduction mechanisms of the device, it should be possible to estimate the responses of such a sensor. It has long been recognized that acoustic wave vapor sensors coated with an absorbent material produce responses proportional to the partition coefficient [2]. The linear solvation energy relationships (LSERs) could be used to model sorption of vapors by polymer layers on SAW sensors [12]. This LSER models the sorption process as a linear combination of terms representing the contributions of particular interactions to the overall sorption process.

The adsorption of organic vapor is represented as a slight increase of the density of the coating film. Based on the Martin et al.'s perturbational approach [13], if ρ_0 and h_0 are the density and thickness of coating film in the absence of vapor, the film density and thickness in the presence of vapor vary with the concentration of absorbed species as

$$\rho(c_v) = \frac{\rho_0 + kc_v}{1 + kc_v/\rho_v} \quad (2)$$

$$h(c_v) = h_0 \left(1 + \frac{kc_v}{\rho_v}\right) \quad (3)$$

where k is the air/coating film partition coefficient for detected vapor, ρ_v is the vapor density and c_v is the vapor concentration in air.

In the final modeling, the sensor is exposed to organic vapor in air at atmospheric pressure and room temperature, and the