Simulation Of Surface Acoustic Wave NO_2 Gas Sensor Based On Zno/ XY $Linbo_3$ Structure

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ABSTRACT

Surface Acoustic Wave gas sensors use a sensitive layer to detect the Nitrogen dioxide. In this paper, the simulation of the surface acoustic wave propagation using the finite element method of COMSOL Multiphysics, in piezo plane strain, convection and diffusion and incompressible Navier stroke modes is presented. The development of the 2 Dimensional Finite element mode provides a deep insight in understanding of the acoustic wave propagation in an isotropic media. This paper presents a sensitive layer of the zinc oxide with a thickness of 3 μm on a XY $LiNbO_3$ piezoelectric substrate for nitrogen dioxide (NO_2) gas sensing application at room temperature and NO_2 concentration of 100 ppm. The center frequency of the SAW device is found to be 200 MHz. This paper presents a 2 Dimensional simulation of a SAW wave propagation, furthermore it will assist understanding the behavior of the SAW gas sensor without having to perform the actual fabrication.

Keywords: SAW sensor, Nitrogen Dioxide, Zinc Oxide, Sensitivity.

1.INTRODUCTION

Pollutant gases released by factories, power plants and automobiles are hazardous to health and the environment. NO_2 is recognized as a significant air pollutant. NO_2 is a reactive gas which is formed through the oxidation of nitric oxide (NO) in an ambient air. The only protection from these hazardous gases is by direct detection. NO and NO_2 cause short and long term health issues such as serious lung damage especially for people suffering from asthma and bronchitis, thus detecting NO and NO_2 gases play a major role in health care and environmental protection [1]. The first application of a SAW device as a gas sensor was reported by Wohltjen and Dessy in 1979 [6]. Ricco and Martin [7] first reported SAW sensors based on the conductometric sensing mechanism, using a non layered device. In their paper, they investigated the operation of a $LiNbO_3$ based SAW device operating as a gas detector. Following their work, a variety of SAW sensors were developed for sensing sulphur dioxide (SO_2) [8], hydrogen (H2) [9, 10], water, carbon dioxide (CO) [11], hydrogen sulphide (H_2S) [12], nitrogen oxide (NO) [13, 14], organophosphorous compounds [15] as well as many others. The mechanism of operation for SAW Based vapour sensors has also been extensively investigated [16]. Comprehensive surveys detailing the developments of SAW sensors were then completed by D'Amico et al.[17] in 1989, Ballantine and Wohltjen [18] in 1989 and Grate et al. [8, 19] in 1993. Since then, several other reviews of acoustic wave gas sensor technology has been completed by Martin et al. [20] in 1996, Cheeke and Wang [21] in 1999, Vellekoop [22] in 1998, Drafts [23] and Anisimkin et al. [24] in 2001.

2. BRIEF OVERVIEW OF SAW GAS SENSOR

The main goal is to develop a SAW sensor by utilizing a high electromechanical coupling coefficient substrate such as $LiNbO_3$. The thin film of semiconductor metal oxides are used in NO gas sensors [1]. Metal oxide thin films such as zinc oxide (ZnO), provides sensitivity towards NO_2. The electromechanical coupling coefficient K^2 is considers as [3]

$$K^2 = 2\frac{v_f - v_m}{v_f} \qquad (1)$$

Where v_m is the metalized surface phase velocity and v_f is the free surface phase velocity. A basic SAW device can be considered as shown in fig.1. The center frequency is described by [2]

$$f_0 = \frac{v_0}{\lambda} \qquad (2)$$

Where f_0 is the center frequency, v_0 is the wave velocity and λ is the wavelength [2]. The velocity of the acoustic wave travelling along the surface of the piezoelectric materials is governed by the material properties. gas absorption on the surface of the device changes the electric properties and surface density which causes velocity perturbations [3]. The response of a SAW sensor is defined as [4]

$$R = \frac{\Delta v}{v} = \frac{\Delta f}{f_0} \qquad (3)$$

Where f_0 is the center frequency of the acoustic wave, v is the phase velocity and Δf is the frequency shift [4]. SAW sensors with polymeric films are utilized for humidity control which are competitive with hygrometers in region of the ambient humidity. It has been reported that SAW sensors with polymeric films have high sensitivity towards NO_2 [5].

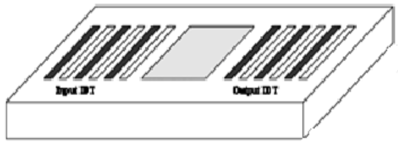

Fig.1 SAW delay line with input and output IDTs

3. SIMULATION RESULTS

SAW sensors were tested towards different gases such as Hydrogen and Nitrogen Dioxide. This paper investigated the ZnO / YX LiNbO3 structure employing the 3 µm Zno sensitive layer and its response towards Nitrogen Dioxide in 100 ppm concentration. The result presents the high sensitivity towards NO_2. Frequency measurement is presented when the sensor is exposed to Nitrogen Dioxide. As H_2 is a reducing gas, it increases the conductivity of the Zno sensitive layer by injecting electrons into the device surface. Therefore, the acoustic wave velocity decreases, resulting in a decrease in the center frequency f_0 when the device is exposed to H_2 gas. Unlike hydrogen, NO_2 gas decreases the conductivity of the Zno selective layer by stripping an electron from the conduction band; resulting in an increase in acoustic wave velocity and thus, in center frequency. With regards to NO_2, the interaction mechanism is assumed to be the similar to the interaction between ozone and other n-type metal oxides. According to Moseley et al. [19] and Galatsis [20], it is unlikely the NO_2 molecules interact with the oxygen atoms in the metal oxide sensitive layer. Instead, a direct chemisorptions reaction occurs, such that

$$NO_2 + e^- \rightleftarrows NO_2^- \qquad (4)$$

Therefore it is assumed that the Nitrogen Dioxide molecule strips an electron from the conduction band, which results in a decrease in film conductivity. During the interaction of Hydrogen and Nitrogen Dioxide gas species, the layer is assumed to be either reduced or oxidized, leading to a change in sheet conductivity and as a result, perturbation of the propagating SAW occurs. By exposing to Nitrogen Dioxide, conductivity of the thin film was changed, therefore it resulted in a slight change in velocity. The definition of the mass sensitivity of a SAW mode is [3]

$$S_m^v = lim_{\Delta m \to 0}\left(\frac{\Delta v/_v}{\Delta m/_a}\right) \qquad (5)$$

where *v* is the propagation velocity and *Δv* is velocity change due to mass change *Δm* per area *a*[3].

mass and acoustoelectric effect can be described as change in the mass density of the film and a change in its electrical conductivity. both of these effects can be considered separately, assuming that the total effect of a relative change of the propagation wavenumber, $\frac{\Delta K}{K_0}$, is the sum of both these component disturbances [21]

$$\frac{\Delta K}{K_0} \sim \left(\frac{\Delta K}{K_0}\right)_m + \left(\frac{\Delta K}{K_0}\right)_\sigma \qquad (6)$$

If the mass effect occurs, the relative change of the propagation velocity is considered as [21]

$$\left(\frac{\Delta v}{v_0}\right)_m \sim -c_{m1} f_0 \rho_s + c_{m2} f_0 h\mu \frac{\lambda + \mu}{\lambda + 2\mu} \qquad (7)$$

Where cm_1 is mechanical coupling factor, which is depending on the substrate, $\rho_s = \rho_h$ surface density of the layer, c_{m2} is the coupling factor of the surface, μ and λ are the Lame constants of the layer for non-disturbing frequency of the propagating wave. The first component in expression (7) is always larger than the second one.

If the mass effect occurs, two components are to be differentiated: the negative one, which causes a decrease in velocity and the positive effect which increases the velocity.
Assuming that the mass of the layer is approximately zero, there will be relative changes in propagation wavenumber [21]

$$\left(\frac{\Delta K}{K_0}\right)_{\sigma,D} \sim \frac{K^2}{2}\frac{(\sigma_s^2 + c_s K_0 D \sigma_s) + i c_s v_0 \sigma_s}{v_0^2 c_s^2 + (\sigma_s + c_s K_0 D)^2} \qquad (8)$$

And [21]

$$\left(\frac{\Delta v}{v_0}\right)_\sigma \sim -\frac{k^2}{2}\frac{\sigma_s^2}{\sigma_s^2 + v_0^2 c_s^2} \qquad (9)$$

For simulating the SAW sensor in this paper, two steps are chosen. During the first step, two simulations are performed. The first simulation presents the SAW sensor with Zno thin film and the second simulation presents the SAW on the surface of the device. As a result, the SAW velocity of the center frequency is obtained. In the second step, the effect of NO_2 on the SAW sensor is studied. In this study the 2D piezo plain strain, convection and diffusion and incompressible Navier Stroke modes of the COMSOL Multiphysics are used. Convection and diffusion mode is used for chemical reaction and incompressible Navier Stroke mode is used for gas flow. In this simulation, chemical reaction and SAW propagation simultaneously occurred. In this simulation, a SAW delay line consisting of a finger pair for each IDT is used. The Dimension of the piezoelectric substrate are 400 µm in the X axis and 160 µm in the Y axis. To avoid the electrical conduction path that might be created between the two IDTs, the bottom layer of the piezoelectric substrate is grounded, thus in the boundary condition section, for the bottom layer of the piezoelectric substrate, the term "Fixed" and for the other layers of the piezoelectric substrate the term "Free" is selected. The term "electrical potential" is chosen for the bottom layer of the electrodes. Quad method is used for the mesh generation and the predefined mesh size is extremely fine. For more accuracy a maximum size of 0.05×10^{-6} is set for the surface of the device.

In the solver parameter section, the eignfrequency analysis is used. The simulation result in the Fig.2 shows the SAW wave propagation on the surface of the XY $LiNbO_3$ substrate. The input and output IDTs are placed on the right and left side of the substrate. as seen in Fig.2 the wave travels on the surface and the displacements in the bulk is negligible. The center frequency of the device is approximately 200 MHz. The surface acoustic wave sensor with a chemical chamber in the absence of NO_2 is shown in fig.3. The SAW velocity is found to be 3800 m/s. The surface acoustic wave sensor with a chemical chamber in the presence of 100 ppm NO_2 is shown in fig.4. with exposure of NO_2 in 100 ppm concentration, a 3 KHz frequency shift is obtained. The frequency shift presents the existence of NO_2 in the ambient atmosphere.

The LiNbO3 substrate is solved by the following governing equation as piezoelectric materials

$$T = C_E S - e^T E \quad (10)$$

$$D = eS + \varepsilon_s E \quad (11)$$

Where **T** is the stress tensor, **S** is the strain tensor, **D** is the electric displacement vector, **E** is the electric field vector, c_E, e and ε_s are elastic, piezoelectric and dielectric matrix respectively. In COMSOL Multiphysics both of the elastic equation and electrostatic equation are solved under this materials mode as following

$$T = c_E S \quad (12)$$

$$-\nabla.(\varepsilon_0 \varepsilon_r \nabla V) = \rho_v \quad (13)$$

where w is the egenfrequency, ε_0 is the electrical permittivity of the free surface, ε_r is the relative electrical permittivity of the materials, V is th e potential, ρ_v is the volume charge density.

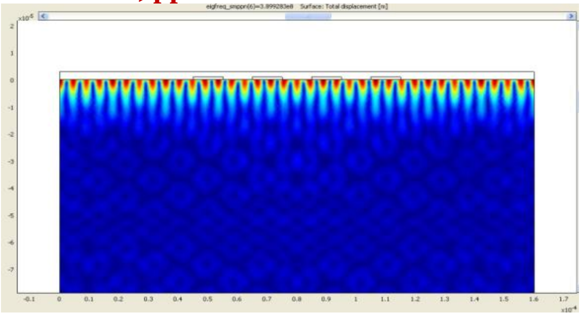

Fig.2 SAW wave propagation on XY $LiNbO_3$ substrate

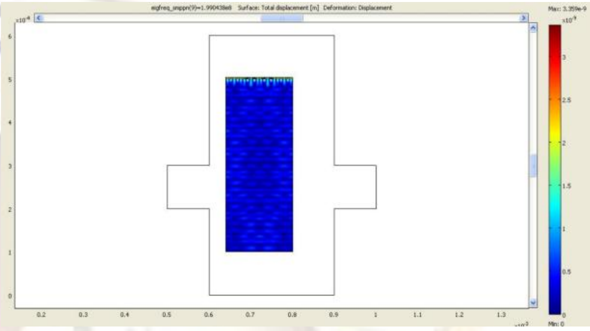

Fig.3 The surface acoustic wave sensor with a chemical chamber in the absence of NO_2.

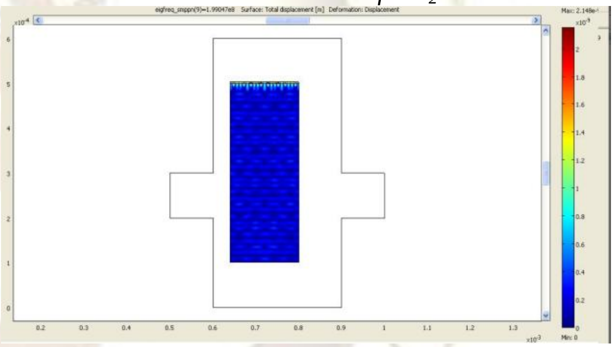

Fig.4 The surface acoustic wave sensor with a chemical chamber in the presence of 100 ppm NO_2 gas.

4.Conclusion

A 2 dimensional SAW sensor with Zinc oxide thin film for detecting NO_2 gas is modeled and simulated. XY $LiNbO_3$ piezoelectric substrate is used and simulations are performed to study the behavior of the sensor in the absence and presence of NO_2. As a result of the simulations, total displacement of the wave is obtained. A 3 KHz frequency shift is observed by exposing the sensor to 100 ppm NO_2.

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