Theoretical analysis of a surface acoustic wave gas sensor mechanism using electrical conductive bi-layer nanostructures

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**A B S T R A C T**

A theoretical investigation of the surface acoustic wave (SAW) propagation on a piezoelectric substrate was performed. The elemental theory of acoustoelectrical interactions between SAWs and bi-layer sensor nanostructures is outlined. The analysis of the SAW sensing mechanism was conducted on the basis of the velocity and attenuation changes. Three varying configurations of bi-layer nanostructures: semiconductor – metal, metal – semiconductor, and dielectric – metal, have been considered. The calculations were executed for three different thicknesses of the film layered on the substrate: 50, 250 and 750 nm. Additionally, dispersion effects, i.e. the influence of various SAW wavelengths (8, 80 and 800 μm) for sensing mechanism is discussed. The experimentally achieved data of surface electrical conductivities, construction parameters and acoustoelectric parameters for the selected single- and bi-layer sensor structures is also presented.

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1. Introduction

Surface acoustic wave sensors are well utilised because of their high sensitivity, small geometrical dimensions, relatively simple electronic setup, and, often, low production costs. The high sensitivity is principally a consequence of the energy trapping on the surface of a piezoelectric substrate. The most regularly applied power range of surface acoustic waves is 0.1–1 W/m (over the path width), and the energy density of the surface region is very high, typically 10^8–10^9 J/m^2. An interesting feature (which is not frequently mentioned) is the corrugation of a sensor thin film’s surface due to wave propagation, illustrated in Fig. 1. This surface corrugation is a unique feature of the SAW sensors, not present in other types of gas sensors (such as resistive) and can cause more effective adsorption and desorption of various analytes [1,2].

Electrically conductive bi-layer nanostructured sensors have recently been extensively used to improve the sensitivity and reliability of conventional chemical and biological sensors. Due to the layered configuration in some of these structures, one can observe an increase in the number of the adsorption active sites, as well as an increase in the surface/volume ratio, and, sometimes, the creation of molecular sieves giving selectivity improvement [3–17].

In SAW gas sensors, the configuration of the layers for the applied multi-layered sensor nanostructure is an important consideration. Apart from the mass sensitivity of SAW gas sensors, in some configurations (between piezoelectric substrate and electrical conductive sensor nanostructure), acoustoelectric sensitivity utilization is possible. The possibility of acoustoelectric interactions between the electrical potential is associated with a wave propagating on a piezoelectric substrate and mobile electric charges in the conductive structure. The perturbation of SAW attenuation and the propagation velocity can be considerably greater than the mass interactions in SAW gas sensors [18–20]. However, such a condition is only possible for a specific range of the applied acoustoelectric (AE) parameters, \( \xi = \sigma_j \gamma_0 \xi_j \) (where \( \sigma_j \) is the structures surface electrical conductivity, \( \gamma_0 \) is the unperturbed SAW velocity for the substrate, and \( \xi_j = \varepsilon_0 + \varepsilon_p \) is the sum of the dielectric permittivity of the region directly above the film and the substrate). The “work point” of the selected sensor structure is defined as the surfaces electrical conductivity (\( \sigma_r \)) of the film, the SAW velocity in the piezoelectric substrate, and the dielectric permittivity of the substrate. One can tune the acoustoelectric sensitivity of the structure by tailoring the sensor material (with various electrical properties) and by changing the thickness (\( h \)) of the sensor film, recalling that \( h \) must be considerably less than the wavelength, \( \lambda \), of the exited SAW (\( h < \lambda \)). Consequently, such an adjustment, for single film, is only possible within a restricted range. An improved fit can be achieved by designing bi-layer or even multi-layer nanos-
structured sensors. As will be presented, in such configurations there are newly achievable ranges for the AE parameter, where the interaction can be much higher than for a single sensor structure. For a SAW gas sensor, with bi-layer nanostructures, the new AE parameter, \( \xi_1 = \sigma_1/v_0 C_s \) (normalized surface electrical conductivity to the substrate parameters), is defined as \( \sigma_1 \) is the electrical surface conductivity of the first film on the substrate. Additionally, the construction parameter, \( x \), can be determined by \( x = \sigma_2/s_1 \), where \( \sigma_2 \) is the surface electrical conductivity of the second film.

2. Results

In previous research, [2] the elemental theory of an acoustoelectrical effect in SAW gas sensor with electrical conductive bi-layer nanostructures has been derived. Here, additional results are presented and discussed from a sensing mechanism perspective. To fully understand the discussion in this chapter, we present the equations for the attenuation [1] and the end velocity [2] relative changes of the surface acoustic wave in bi-layer sensing structure:

\[
\frac{\Delta \varpi}{\varpi_0} = \frac{K^2}{2(1 + e^{-2\varpi_0 h_1})} \frac{v_0}{v_1} \left\{ \begin{array}{c}
\square_1^2 \left( \sigma_1 + \sigma_2 e^{-2\varpi_0 h_1} \right) + \sigma_1 \sigma_2 \left( \sigma_1 + \sigma_2 e^{-2\varpi_0 h_1} \right) \\
\square_1^2 \left( \sigma_1 \sigma_2 + \sigma_1^2 e^{-2\varpi_0 h_1} \right) + \sigma_2 \left( \sigma_1^2 + \sigma_1 e^{-2\varpi_0 h_1} \right)
\end{array} \right\}
\]

\[
\frac{\Delta v}{v_0} = \frac{K^2}{2(1 + e^{-2\varpi_0 h_1})} \left\{ \begin{array}{c}
\square_1^2 \left( \sigma_1^2 + \sigma_2^2 \right) + \sigma_1 \sigma_2 \left( \sigma_1^2 + \sigma_2 \right) \\
\square_1^2 \left( \sigma_1^2 + \sigma_2^2 + \sigma_1 \sigma_2 \right) + \sigma_1 \left( \sigma_2 \right)
\end{array} \right\}
\]

where:

\( K^2 \) is the electromechanical coefficient of the piezoelectric substrate,

\( v_0 = 2\pi / \lambda \) is the wave number, \( k_0 = 7.85 \times 10^4 \text{m}^{-1} \) (for \( \lambda = 80 \mu\text{m} \)),

\( v_0 \) is the unperturbed SAW velocity,

\( C_s = \varepsilon_0 + \varepsilon_p \), is the dielectrical permittivity sum of the region above the films and the substrate,

\( \sigma_1 = \sigma_1 h_1 \) is the surface electrical conductivity of the first film with a bulk conductivity \( \sigma_1 \) and thickness \( h_1 \),

\( \sigma_2 = \sigma_2 h_2 \) is the surface electrical conductivity of the second film with a bulk conductivity \( \sigma_2 \) and thickness \( h_2 \).

2.1. The influence of the first film thickness

To obtain accurate acoustoelectrical curves we applied three different values of the initial layer thickness, \( h_1 \) (50, 250 and 750 nm). The chosen values are within a range of typical sensor layer thicknesses, used in experimental gas sensor investigations. Fig. 2 presents the changes of the SAW velocity and the attenuation with respect to the AE parameter, \( \xi_1 \), for a given construction parameter of \( x = 10 \) (i.e. the semiconductor – metal configuration), and three thicknesses of the primary film (50, 250 and 750 nm). A construction parameter of \( x = 10 \), means that the electrical surface conductivity of the second metal film is 10 times greater than the primary semiconductor film.

We observe that the influence of the primary layer thickness, \( h_1 \), on the SAW velocity changes throughout most of the analyzed range by very small amount. Differences are observable for only the AE parameter, \( \xi_1 \), between 0.1 and 1, especially in case of the attenuation. The least changes occur for the structure with the highest \( h_1 \) (green curve shows \( h_1 = 750 \text{ nm} \)). This is explained by the fact that the second layer, in this case, is further from the surface of the piezoelectric crystal than for thinner primary layers.

![Fig. 2. The influence of three different thicknesses of the first film \( h_1 = 50, 250 \) and 750 nm on a SAW velocity and attenuation changes of a semiconductor – metal structure with a parameter \( x = 10 \)– the curves in black are for the single film structure with \( x = 0 \).](image-url)
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