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Love-mode surface acoustic wave devices based on multilayers of TeO_2/ZnO$(11\bar{2}0)$/Si(100) with high sensitivity and temperature stability

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ABSTRACT

A multilayer structure of TeO_2/interdigital transducers (IDTs)/ZnO$(11\bar{2}0)$/Si(100) was proposed and investigated to achieve both high sensitivity and temperature-stability for bio-sensing applications. Dispersions of phase velocities, electromechanical coupling coefficients K^2, temperature coefficient of delay (TCD) and sensitivity in the multilayer structures were simulated as functions of normalized thicknesses of ZnO (h_{ZnO}/λ) and TeO_2 (h_{TeO2}/λ) films. The fundamental mode of Love mode (LM) - surface acoustic wave (SAW) shows a larger value of K^2 and higher sensitivity compared with those of the first mode. TeO_2 film with a positive TCD not only compensates the temperature effect induced due to the negative TCD of ZnO$(11\bar{2}0)$/Si(100), but also enhances the sensitivity of the love mode device. The optimal normalized thickness ratios were identified to be $h_{TeO2}/\lambda = 0.021$ and $h_{ZnO}/\lambda = 0.304$, and the devices with such structures can which generate a normalized sensitivity of -1.04×10^{-3} m^3/kg, a TCD of 0.009 ppm/°C, and a K^2 value of 2.76%.

1. Introduction

Surface acoustic wave (SAW) devices have been extensively applied for communications, automotive and environmental sensing for more than 60 years [1]. Recently, SAW sensors for bio-analysis and bio-sensing have been extensively studied due to their advantages of high sensitivity, reliability and capability to respond to various measurands [2]. For chemical and biological sensing in liquid environments, shear horizontal (SH) SAW devices are widely used, because their dominant in-plane displacement parallel to the substrate provides a minimal damping of the wave in liquid [3,4]. The SH-SAW can be converted into a Love mode (LM) SAW when a wave-guiding layer is deposited on top of the piezoelectric materials [5,6]. Because of the wave-guiding effect, most of the wave energy is confined to this wave-guiding layer, thus any small perturbation on the surface will significantly influence the wave propagation. Therefore, the LM-SAW devices generally possess a high sensitivity in both air and liquid which are suitable for bio-sensing applications [5,7–10].

There are two requirements to generate the LM-SAW. Firstly, the piezoelectric substrate should excite the SH-SAW. Secondly, the shear wave velocity of the wave-guiding layer must be less than that of the piezoelectric substrate. So far, majority of the LM-SAW devices are based on thick bulk piezoelectric substrates such as lithium niobate ($LiNbO_3$), lithium tantalate ($LiTaO_3$) and quartz [11–16]. LM-SAW biosensors based on quartz commonly suffer from low electromechanical coupling coefficients (K^2), large penetration depth, and low dielectric permittivity when working in a liquid media [17], while those on $LiNbO_3$ and $LiTaO_3$ suffer from the poor temperature stability [18]. In addition, the commonly used bulk piezoelectric crystals (quartz, $LiNbO_3$ and $LiTaO_3$) are brittle, expensive and inconvenient for integration with microelectronics and multiple sensing or microfluidic functions into a lab-on-chip, thus not suitable for low-cost, disposable point of care applications.

Piezoelectric thin films deposited on Si are promising for integration with electronic circuitry, aiming for disposability, low-price and mass production [19–22]. Among the commonly used piezoelectric thin films, ZnO exhibits a high value of K^2, and is competitive for SAW sensing applications [23–26]. Furthermore, ZnO is bio-safe and shows a high affinity for binding biomolecules, making it suitable for biomedical applications to immobilize and mod-

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ify biomolecular material without toxic effects [27–29]. In order to excite an LM-SAW on the ZnO/Si structure, ZnO films should have a preferred orientation of $(11\bar{2}0)$ or $(10\bar{1}0)$ with the *c*-axis parallel to the substrate plane [30,31]. For the wave-guiding layer on top of the ZnO/Si structure, SiO_2, polymethyl-methacrylate (PMMA), TeO_2 and ZnO have frequently been used [5,23,32,33]. The shear wave velocity of PMMA is smaller than that of ZnO; however, it exhibits large acoustic losses as well as poor chemical and temperature resistance. Compared with SiO_2 (2747 m/s) film, TeO_2 has a lower shear wave velocity (1192 m/s), therefore, TeO_2 is more suitable as the wave-guiding layer on ZnO/Si. Furthermore, similar to SiO_2 films, TeO_2 films possess a positive value of temperature coefficient of delay (TCD), compared to the negative TCD value of the ZnO/Si structure [34]. Therefore, it is possible to obtain zero TCD in the TeO_2/IDT/ZnO$(11\bar{2}0)$/Si structure, which is critical for biosensing applications with a strict requirement on temperature stability.

Although there were previous reports on characterization of the TeO_2/ZnO/diamond, $TeO_2/LiNbO_3$ and $TeO_2/LiTaO_3$ SAW structures [33,35,36], as far as we know, there is none on the LM-SAW propagation in the TeO_2/ZnO$(11\bar{2}0)$/Si multilayered structure. In particular, there is no previous study on the wave-guiding effect of TeO_2 films and its effects on the sensitivity in the TeO_2/ZnO$(11\bar{2}0)$/Si LM-SAW devices. This paper aims to investigate a novel low cost Si based structure in order to compete with those conventional Love wave biosensors, and performs a theoretical investigation of the LM-SAWs based on a TeO_2/ZnO$(11\bar{2}0)$/Si multilayered structure, The dispersion effects of phase velocity V_p, K^2, TCD and sensitivity as a function of normalized thicknesses of ZnO (h_{ZnO}/λ) and TeO_2 (h_{TeO2}/λ) films are systematically studied.

2. Methodology of theoretical analysis

In this work, the transfer matrix [37] and compliance stiffness matrix formulation [38] of the general Green's function were used to calculate the LM-SAW propagation and sensitivity characteristics of the multilayer structures. The structure consists of a ZnO$(11\bar{2}0)$ film deposited on Si (100), a TeO_2 film deposited on ZnO films and the IDTs at the interface between the ZnO and TeO_2 films. In contrast to the SAW wavelength, the electrodes are approximately assumed as infinitely thin and massless to simplify the computation. The interface where the IDT appears is set perfectly conductive and electrically grounded. The thicknesses of the TeO_2 and ZnO$(11\bar{2}0)$ films are denoted by h_{TeO2} and h_{ZnO}, respectively. The dispersive patterns were calculated as a function of the normalized thickness h/λ, where λ is the wavelength of the LM-SAW device. The multilayered structure and the coordinate system are illustrated in Fig. 1. A Cartesian coordinate system is built in such a way that the Love wave is assumed to propagate along the X_1 axis direction, the X_2 axis is parallel to the direction of particle polarization, and the X_3 axis is normal to the surface of the substrate. The Si substrate is considered to occupy the $X_3 < 0$ half space domain. The other layers are located in the upper $X_3 > 0$ half space. All layers are considered to be rigidly coupled and, as assumed below, the continuity of displacement components across all interfaces are taken into account. All layers are assumed to be completely elastic, and material viscosity effects are neglected.

The particle motion and electric field in a piezoelectric medium are based on the following elastic wave equations:

$$\begin{cases} c_{ijkl}\dfrac{\partial^2 u_k}{\partial x_j\partial x_l} + e_{ijk}\dfrac{\partial^2 \phi}{\partial x_j\partial x_k} - \rho\dfrac{\partial^2 u_i}{\partial t^2} = 0 \\ e_{jkl}\dfrac{\partial^2 u_k}{\partial x_j\partial x_l} - \varepsilon_{jk}\dfrac{\partial^2 \phi}{\partial x_j\partial x_k} = 0 \end{cases} \qquad (1)$$

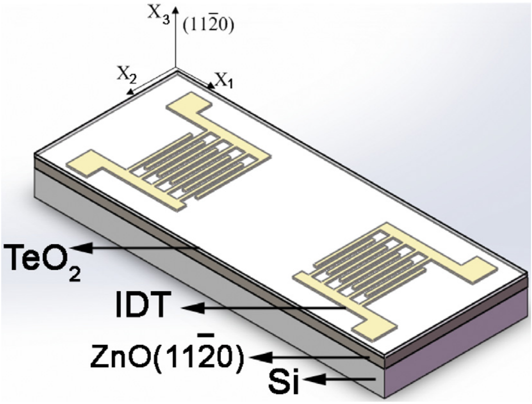

Fig. 1. Illustration of TeO_2/ZnO$(11\bar{2}0)$/Si multilayer Love mode SAW structure and the coordinate system.

where *u* is the mechanical displacement, c_{ijkl} is the elastic constants, ρ is the density, *e* is the piezoelectric constant, ε is the dielectric constant, and ϕ is the electric potential. The indices, *i*, *j*, *k*, *l*, have values 1, 2, or 3. The piezoelectric constants of non-piezoelectric medium are set at zero.

Taking account of the free boundary conditions on the surface of the top layer, the generation of mechanical displacements and electrical potential by mechanical stresses and the electrical charge on the IDT embedded at the interface can be described using a symmetric generalized Green function as shown below:

$$\begin{Bmatrix} U_1 \\ U_2 \\ U_3 \\ \varphi \end{Bmatrix} = \begin{bmatrix} G_{11} & G_{12} & G_{13} & G_{14} \\ G_{21} & G_{22} & G_{23} & G_{24} \\ G_{31} & G_{32} & G_{33} & G_{34} \\ G_{41} & G_{42} & G_{43} & G_{44} \end{bmatrix} \begin{bmatrix} T_{31} \\ T_{32} \\ T_{33} \\ \sigma \end{bmatrix} \qquad (2)$$

where σ and φ denote charge density and potential, respectively, and T_{3i} is the stress along X_i direction at the interface. The term G_{44} denotes the effective permittivity, whose poles and zeros represent the velocities of propagation modes for short and free interface conditions, respectively.

2.1. Electromechanical coupling coefficient (K^2)

The value of K^2 is determined using the following formula:

$$K^2 = 2\frac{V_{free} - V_{short}}{V_{free}} \qquad (3)$$

where V_{free} and V_{short} derived from the effective permittivity denote the Love wave phase velocities for electric free and short circuit conditions, respectively.

2.2. Mass sensitivity

The sensitivity of the LM-SAW device subjected to surface mass loading is defined as the fractional velocity change due to a small mass loading per unit area:

$$S_m = \frac{1}{v}\left(\frac{\Delta v}{\Delta m}\right)_{\Delta m \to 0} = \frac{1}{\rho_w}\frac{d\ln(v^2 - v_w^2)}{dh} \qquad (4)$$

where v is the phase velocity without mass loading perturbation, Δm is the absorbed mass per area, and Δv corresponds to the velocity shift due to the mass loading, ρ_w, v_w and *h* are the mass density, shear bulk acoustic wave velocity and thickness of the top waveguide layer, respectively.