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Theoretical analysis on response mechanism of polymer-coated chemical sensor based Love wave in viscoelastic media

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ABSTRACT

This paper presents a theoretical analysis on response mechanism of polymer-coated Love wave chemical sensor. A theoretical model is presented to describe wave propagation in Love wave devices with viscoelastic polymer guiding layer and to provide the optimal design parameters. A complex dispersion equation expanded into Taylor series was presented to describe the lossy mechanism of the viscoelastic polymer guiding layer. Using the polymer films (fluoropolyol (FPOL)) as the chemical interfaces to organophosphorous compounds (dimethymethylphosponate (DMMP)) detection, the response mechanism of the Love wave chemical sensor structured by ST-90°X quartz substrate and polymethylmethacrylate (PMMA) guiding layer was performed, including the perturbation of different polymer types (glassy, glassy–rubbery and rubbery) to Love wave propagation, and optimal guiding layer thickness extraction. Calculated results indicate that the glassy–rubbery polymer shows better linearity of the velocity change, and exhibits higher sensitivity over other films. A ~2 μm optimal PMMA guiding layer thickness was evaluated to yield superior sensor performance in case of 40 ppm DMMP adsorption by 0.1 μm FPOL film. And, superior sensor sensitivity was observed from chemical sensor based on Love wave mode in comparison with surface acoustic wave (SAW) mode. Experimental data mentioned that the theoretical model is valid for response mechanism analysis of Love wave chemical sensor.

1. Introduction

Love wave-based devices have been the growing interests for (bio)chemical sensing in liquid because of no elastic coupling loss in liquids and protection of the interdigital transducer (IDTs) for liquid environment [1–5]. Typical Love wave sensors are composed of a piezoelectric substrate with the IDTs pattern supporting a shear horizontal (SH) SAW propagation, a thin overlayer (waveguide layer) on the top of the substrate, and a sensitive film which responds to the chemical compound to be measured. The necessary conditions for the Love wave formation is the acoustic shear velocity in the overlayer is lower than that in the piezoelectric substrate, most of the acoustic wave generated from the IDTs is coupled to the waveguide layer and converted into a SH wave flowing in the waveguide layer. Due to the waveguide effect, the Love wave mode can be very sensitive to surface perturbation and high sensitivity to surface loading can be achieved. Recently, Love wave mode devices are introduced to operate in gaseous media using different designs and operating principles, it has been reported that these devices have superior sensitivity compared to the surface acoustic wave (SAW) sensors. For chemical sensing, a chemical sensitive film, chosen for its selectivity and affinity towards the target compound is added on the top of the Love wave device. The adsorption of the target compound in the sensitive layer results in both mass loading effect and viscoelastic effect towards to Love wave, which change the Love wave velocity. Zimmermann et al. successfully demonstrated a Love wave device on ST quartz/SiO_2 for the detection of organophosphorous vapors, and achieved approximately 10 times the sensitivity of a Rayleigh wave sensor operating at a similar frequency [6]. Jakoby et al. also reported a Love wave gas sensor on ST quartz/SiO_2 coated a molecularly imprinted thin film; high sensitivity was obtained [7].

However, despite some reported success stories, current Love wave gas sensors still suffer from many issues: (1) low piezoelectric coefficient of AT quartz substrate results in large insertion loss, which would deteriorate the frequency stability of the oscillator. Recently, a new SH wave propagating along the ST-90°X quartz substrate (with Euler angles of (0°, 132.75°, 90°)) by composing heavy metal IDTs was reported to provide superior temperature stability, large acoustic velocity (~4500 m/s) and higher electromechanical coupling factors (over three times than the AT-cut quartz with electromechanical coupling factors of ~0.1%, on which, a SH wave mode is supported) [8,9]. (2) The choice of the waveguide layer materials is also controversial. One of the conditions for the existence of Love wave mode is that the shear velocity in the guiding layer is smaller than the shear velocity in the substrate. Thus, the choices

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of the overlay material with low shear velocity, low density and low acoustic adsorption are very important. Various dielectric materials such as silicon dioxide (SiO_2), and polymers can be used as the waveguide materials [10]. SiO_2 has been widely used for Love wave sensors because it presents some advantages of good rigidity, low acoustic loss, and high mechanical and chemical resistance. Nevertheless, the polymers have some advantages over SiO_2 for Love wave sensor implementation because they are more efficient than SiO_2 in converting the bulk SH mode to the Love wave mode due to their lower shear bulk velocity and lower density as compared to that of SiO_2, resulting in an order of magnitude improvement in mass sensitivity. Also, they are easier to deposit onto the substrate than SiO_2 [10]. Until now, different structures have been tested and it has been demonstrated that generally polymers as guiding layer give a better sensitivity than oxide layers. However, the polymer guiding layer induces large signal attenuation when thicker polymer layers are applied onto the device surface because of the viscoelastic nature. To our knowledge, there is no systematic theoretical study concerning the structure parameters and their influence on the sensor sensitivity currently.

Also, due to the wide range of chemical properties available and the ease of film formation, a number of polymer films have been examined as chemically interfaces. For the sensor response mechanism of the SAW based chemical sensor, Martin et al. described the dynamics and response of polymer-coated SAW devices and effect of viscoelastic properties and film resonance [11]. Due to the viscoelastic nature, the polymer coating induces additional attenuation to wave propagation. Zimmermann et al. reported the mass loading sensitivity of the polymer-coated Love wave-based sensor. Unfortunately, there are still no any reports about the response mechanism of the polymer-coated Love wave chemical sensor considering the mass loading and viscoelastic effect, which provide more precise theoretical prediction of the sensor performance and instruction of the sensor design.

The first purpose of this paper is to describe the Love wave propagation along a piezoelectric substrate (ST-90°X quartz) with a polymer guiding layer (PMMA: stiffness modulus of 1.7 GPa and a density of 1.17 g/cm^3, giving a lower waveguide acoustic velocity of 1105 m/s [12]) on top of it, as shown in Fig. 1(a). A theory model of Love wave propagating in a viscoelastic polymer layer deposited on a piezoelectric substrate was considered, an analytical formula relating the attenuation coefficient of the Love wave and the viscoelastic parameters of the waveguide structure were established. The complex dispersion relationship of the Love wave was studied, in which, the attenuation induced by the viscoelastic guiding layer was calculated, and it would provide as guidelines for the optimization structure of the Love wave devices.

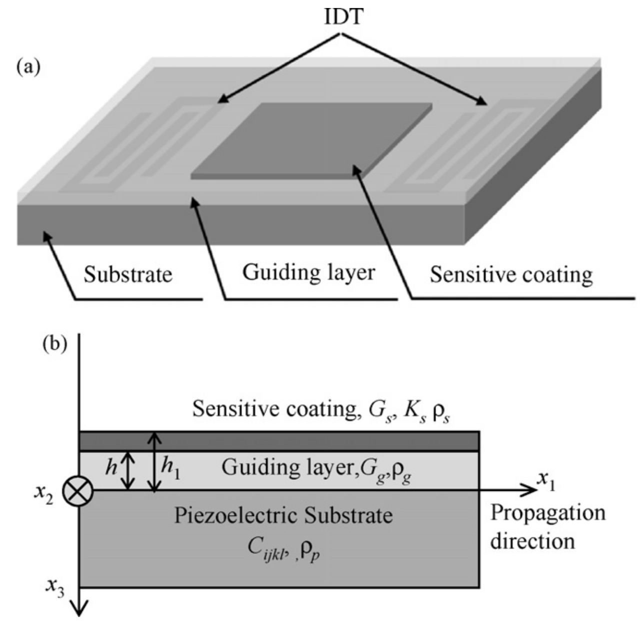

Fig. 1. (a) The schematic of the Love wave chemical sensor consists of piezoelectric substrate, guiding layer and sensitive film, (b) the coordinate system used in this work (x_1: propagation direction, x_2: SH waves polarization direction).

Another aim of this paper is investigation of the response mechanism of the Love wave chemical sensor coated with a polymer film. Due to the complex shear modulus, the polymer film was classified into three statuses as glassy, glassy–rubbery and rubbery status. The different polymer types lead to different Love wave propagation properties, such as attenuation change and velocity shift. Numerical results indicate that glassy–rubbery shows better linearity of the velocity shift and higher sensitivity than other films, an ~2 μm optimal guiding layer thickness was provided for gas sensing application of Love wave sensors in case of 40 ppm DMMP adsorption by 0.1 μm FPOL sensitive film, in which the DMMP adsorption by different type polymer sensitive film contributes the mass loading effect (change in the film thickness and density), however, the viscoelastic nature of the polymer layer decides the gas response properties. Also, a sensitivity comparison between the Love wave model and SAW model was investigated.

2. Theoretical analysis

2.1. Dispersion relationship of Love wave in viscoelastic media

For theoretical approach of the Love wave device, a structure composed of a semi-infinite piezoelectric substrate with IDT pattern, a viscoelastic guiding layer is constructed as shown in Fig. 1(a). The original feature of our theoretical work is the description of Love wave propagation by the way of an analytical resolution of motion equations, which allows obtaining analytical expressions of the dispersion relation, so the influences of different parameters to device performances appear clearly. A solution for an isotropic Love wave structure was given by Dieulesaint et al. [13]. Also, solution for the Love wave piezoelectric structure in the case of quartz with various cuts was presented by Zimmermann and Jakoby et al. [14,15], in which SiO_2 was used as the guiding layer. Kielczynski established the theory of Love wave propagating in a lossy viscoelastic layer deposited on an elastic substrate, the attenuation induced by the viscoelastic polymer guiding layer was described theoretically [16].

In this paper, we propose to resume this method of resolution for the Love wave mode structure in the case of an anisotropic piezoelectric substrate of ST-90°X with gold IDTs, a polymer guiding layer (PMMA). Due to the weak electromechanical coupling factors, we neglect the piezoelectric property of quartz. The guiding layer and the sensitive layer are considered to be isotropic. The coordinate system for the Love wave propagation analysis is shown in Fig. 1(b). Acoustic wave propagates along the x_1 axis on the x_1–x_2 plane at $x_3 = 0$. In our analysis, all material parameters of the mediums are transformed into this coordinate system. Each material in Fig. 1 is defined by its physical parameters: stiffness constants C_{ijkl}, and density ρ_p for quartz ($i, j, k, l = 1, 2, 3$), complex shear modulus G_g: $(G_g' + jG_g'')$, density ρ_g for PMMA, here, the G_g' are the storage shear modulus, G_g'' represents the so-called loss moduli, for ideal elastic film would have $G'' = 0$. The phase velocity dispersion relationship of the Love wave can be calculated by solving the elastic wave equations from particle displacement u_j within Eq. (1),

$$\frac{\rho \partial^2 u_i}{\partial t^2} = \frac{C_{ijkl} \partial^2 u_k}{\partial x_j \partial x_l} \tag{1}$$