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Diamond/ZnO/LiNbO$_3$ structure for packageless acoustic wave sensors

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Abstract—This paper studies the Diamond/ZnO/LiNbO$_3$ structure, numerically and experimentally, as a candidate for a packageless sensor based on the surface acoustic wave technology. The structure is compared with an AlN/ZnO/LiNbO$_3$ structure, in order to highlight better performances of diamond with respect to AlN. Early experimental results of nanocrystalline diamond growth on ZnO/Si are presented.

Keywords—packageless sensor; waveguiding layer acoustic wave; diamond

I. INTRODUCTION

Surface acoustic wave (SAW) technology is mainly known in mobile communications [1,2]. The devices used are relatively small, simple, robust and also have the advantage of being passive (batteryless) and remotely searchable (wireless). The major disadvantage of these devices comes from the package. This hermetic enclosure, which is useful to protect the SAW device from external perturbations is also bulky and costly. A packageless structure is thus highly desirable to introduce SAW devices in new fields such as the biomedical domain. For example, it will allow the monitoring of the human body’s parameters due to the close proximity between the sensor and the target i.e. the skin. The bottleneck of the packaging can be solved with the concept of Waveguiding Layer Acoustic Wave (WLAW) [3,4]. The principle is based on wave confinement in a low acoustic velocity layer enclosed between two high velocity materials. The upper layers will play the role of the package by protecting the wave from external perturbations. Moreover, one of the layers has to be piezoelectric to allow the generation of the acoustic wave. ZnO is a material with a low propagation speed and with interesting piezoelectric properties [5]. Diamond has a very high propagation velocity [5,6] so that the ideal structure would be: Diamond/ZnO/Diamond. However, ZnO deposition is planned as a thin layer with a sputtering process, so it will be difficult to obtain a single crystal in order to minimize the acoustic propagation losses. It is therefore better to choose a piezoelectric single crystal substrate. LiNbO$_3$ is a good candidate, thanks to its extremely low acoustic propagation losses, its high electromechanical coupling coefficient (K$^2$) and its high velocity compared to ZnO [5,7]. Nevertheless, up to now, the high deposition temperature of diamond films has prevented the processing of the structure Diamond/ZnO/LiNbO$_3$ since conventional piezoelectric materials lose their piezoelectric properties at high temperature [8]. As an alternative to diamond, a sputtered AlN film as top layer has already been tested [9] due to its relatively high acoustic velocity [10]. A WLAW device operating at 868 MHz was fabricated based on a AlN(6µm)/ZnO(2µm)/LiNbO$_3$ structure and the confinement of the wave was obtained from a thickness of 6 µm of AlN. This previous work shows that in this case the wave mainly propagates in the ZnO layer. Therefore, the acoustic losses during propagation are increased, due to the relatively low crystalline quality of sputtered ZnO film. Recently, a low temperature process for nanocrystalline diamond (NCD) deposition has been developed [11]. This process opens a new path for high performance WLAW structures based on diamond.

This paper investigates the potential of the Diamond/ZnO/LiNbO$_3$ structure for packageless sensing applications. The Diamond/ZnO/LiNbO$_3$ structure will be studied theoretically and experimentally and the results compared to those of AlN/ZnO/LiNbO$_3$.

II. MATERIALS AND METHODS

A. FEM modeling

Both Diamond/ZnO/LiNbO$_3$ and AlN/ZnO/LiNbO$_3$ structures were studied using a 2D-FEM model (COMSOL Multiphysics). A geometry with a width of λ/2 was used and periodic conditions have been applied in order to represent the
entire structure. The thicknesses of the substrate and the ZnO layer were fixed to 20 µm and 2 µm, respectively. The thickness of the top layer was modified during the simulations. Particle displacements (due to the propagation of the wave in the material) were then computed in order to compare the wave confinement. And hence, a sufficient thickness for the upper layer was determined to have the wave confinement. Once the thickness of the top layer is known and fixed, the K^2 value was calculated with respect to the ZnO thickness to determine the best compromise between the electromechanical coupling and propagation losses that affect the quality factor of the device.

B. Experimental part

RF magnetron sputtering was used to deposit an Al (150 nm) layer on a LiNbO_3 128° Y-cut substrate (MTI Corporation). Interdigital transducers (IDT) defined with λ = 4.4 µm have been designed from a positive resist and an electron beam lithography process. More precisely, the structure of the IDT is done with 100 finger pairs at the center and 200 fingers on each side. The metallization ratio is fixed to 60% which impose the width of the finger (1.32 µm). The aperture is also set at the value of 269 µm (see Fig. 1). Chemical etching and a removing process for the resist were used to finalize the IDT manufacturing. ZnO was deposited using RF magnetron sputtering with the following parameters: 4-inch ZnO target, 170°C, 150 W, 6x10^{-3} mbar, 6 sccm O_2 and 6 sccm N_2.

NCD films were deposited using a Distributed Antenna Array (DAA) microwave system operating in H_2/CH_4/CO_2 (96.4:2.6:1) gas mixture under 0.25 mbar and 3 kW at 250°C substrate temperature (see Fig. 2). The morphology and the thickness of the diamond films were investigated by scanning electron microscopy (SEM) and reflectometry, respectively. X-ray diffraction (XRD) and Raman spectroscopy were carried out to estimate the microstructure of the diamond layer grown on ZnO. Finally, SAW devices were characterized using a probe station and a vector network analyzer (VNA Agilent N5230A).

III. RESULTS AND DISCUSSIONS

A. FEM modeling

Based on a previous study [9], the confinement of the acoustic wave is obtained with a thickness of 6 µm of AlN when the ZnO thickness is fixed to 2 µm. While using diamond instead of AlN, a thinner layer is required to achieve the confinement. Indeed, 2.5 µm of diamond are sufficient to confine the wave (see Fig. 3). The confinement appears much rapidly with diamond due to its exceptional hardness. More precisely, the confinement is proved with the very limited displacement at the surface of the WLAW structure (see Fig. 4). Therefore, the structure Diamond/ZnO/LiNbO_3 can be used for packageless applications.

![Fig. 3. 2D COMSOL modeling of particle displacements in a LiNbO_3/ZnO structure with, (a) 6 µm of AlN, (b) 2.5 µm of AlN and (c) 2.5 µm of diamond on top of it, respectively.](image)

![Fig. 4. 1D COMSOL modeling of particle displacements in a LiNbO_3/ZnO structure with AlN or diamond on top of it.](image)

Compared to the AlN case, with the diamond layer, the maximum deformation is shifted to the substrate. The wave tends to propagate more in the low loss single crystal LiNbO_3, rather than in the ZnO (see Fig. 3c vs 3a), thus reducing the acoustic propagation losses and improving performance.

With the fixed value of 2.5 µm of diamond, the ZnO layer has been optimized to maximize the wave deformation in the substrate with a reasonable K^2 value. A thickness of 1.2 µm of ZnO is suitable because the main portion of the energy of the wave propagates in LiNbO_3 (see Fig. 5) and the
electromechanical coupling factor value remains relatively high (K^2= 3.9%).

![ZnO 2 μm ZnO 1.2 μm](image)

**Fig. 5.** 2D COMSOL modeling of particle displacements in 2 μm and 1.2 μm of ZnO, respectively.

**B. Experimental part**

Preliminary NCD deposition experiments on ZnO/Si substrates are promising. Indeed, the SEM pictures (see Fig. 6) showed that NCD layer can be grown on relatively rough ZnO surface. The Raman spectrum (see Fig. 7) exhibiting an intense peak at 1332 cm^{-1} also confirms that diamond is deposited on the considered samples. The diamond deposition on ZnO/LiNbO₃ structures and on entire SAW devices, including IDT, are in progress.

![SEM top view of the Diamond/ZnO/Si structure](image)

**Fig. 6.** SEM top view of the Diamond/ZnO/Si structure

![Raman spectrum of a Diamond/ZnO/Si structure](image)

**Fig. 7.** Raman spectrum of a Diamond/ZnO/Si structure

**IV. CONCLUSION AND PERSPECTIVES**

The comparison between the Diamond/ZnO/LiNbO₃ and the AlN/ZnO/LiNbO₃ structures has shown that the wave confinement is done more rapidly with the diamond layer than with the AlN layer. In other words, the minimum diamond thickness required for confinement is significantly lower than that of AlN. Moreover, with the diamond layer, the wave propagation tends to take place in the substrate which is a single crystal and therefore the propagation losses are reduced.

The first experimental diamond growth tests on ZnO layers, backed by Raman measurements, are promising.

As a short-term perspective, the aim is to prove that the Diamond/ZnO/LiNbO₃ structure can be used for packageless applications. This could be proved with the wave confinement by measuring S-parameters of the SAW sensor with and without an absorber. The Solaris elastomer, with almost the same properties as the skin, will be used as absorber as in [9]. The structure could then be validated for biomedical applications.

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