ZnO/AlN/diamond layered structure for SAW devices combining high velocity and high electromechanical coupling coefficient

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Prime Novelty:

In this work we propose a new Surface acoustic wave structure (ZnO/AlN/diamond) leading to perform SAW devices combining high acoustic velocity and high electromechanical coupling coefficient. Theoretical as well as experimental results demonstrate the potentiality of this new structure.

Keywords:,

Aluminium nitride (AlN), Zinc oxide (ZnO), Diamond, surface acoustic wave devices

Estimated Word Count (including figures) : 3629 words

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Abstract

A new layered structure ZnO/AlN/diamond is studied for high frequency and high electromechanical coupling (K^2) SAW devices. Theoretical study was performed to calculate the phase velocity and K^2 dispersion curves of the Rayleigh mode and its higher modes as well as the leaky waves. Both high values of K^2 (>4%) and acoustic velocities higher than 15km/s are expected with this new structure according to the theoretical results. To confirm the simulation results, SAW filters were processed on ZnO/AlN/diamond structure. First experimental results are in accordance with the theoretical ones and confirm the high potentiality of this new structure for the processing of high performances and high frequencies SAW filters.

Keywords: Diamond, Aluminium nitride, Surface acoustic wave, Zinc oxide

Introduction

The general increase of operating frequencies in telecommunication systems initiated the search for new high phase velocity substrates, which can be coupled to piezoelectric thin films. This allows the fabrication of surface acoustic wave (SAW) devices working at high frequency[1]. The center frequency *(f_0)* of the SAW filters is determined by the phase velocity (v_φ) and the spatial period *(λ)* of the inter-digital transducers (IDT): $f_0=v_\varphi/\lambda$. In this sense, and due to the very high acoustic phase velocity of diamond, layered structures based on diamond are a promising solution for the development of GHz-band SAW devices [1-3]. However these structures have the trade-off relationship between the acoustic phase velocity (Vφ) and the electromechanical coupling coefficient (K^2). According to the theoretical calculations, the best compromise obtained is K^2=1.2%, Vφ=11.612km/s for ZnO/diamond structure and K^2=1.36, Vφ=12.120km/s for the structure AlN/diamond [4]. Even if a better compromise is expected for $LiNbO_3$/diamond structures [4], the deposition of highly oriented $LiNbO_3$ film on diamond presents serious difficulties to date.

In this work, we propose the use of a three-layers structure ZnO/AlN/diamond in order to combine, with the very high velocity of diamond substrate, the advantages of both piezoelectric materials: the high K^2 of ZnO and the high velocity of AlN. In fact, ZnO exhibits a relatively high K^2 (3.2%) but low velocity (2558m/s) an opposition to the AlN that exhibits a low K^2 (0.24%) but a relatively high velocity (5600m/s). Note that the shear wave velocity of diamond is around 12400m/s. The studied structure offers also the interest to present a progressive variation of acoustic impedance of layers forming the structure (Z_{ZnO}= 34.5 MR Z_{AlN}= 41.6 MR Z_{Diam}=63.3 MR). In fact a strong variation of this impedance in film interface limit the device performances. Three configurations depending, on the Aluminium inter-digital transducers (IDT) position in the structure, are considered (Fig. 1).

Theoretical study

Theoretical study based on Campbell and Jones model [5] was performed to calculate the phase velocity and K^2 dispersion curves of the Rayleigh mode as well as its higher modes considering various thicknesses of ZnO and AlN layers. Details of theoretical analysed were published elsewhere [6]. A compilation of the elastic constants and the piezoelectric constants used for calculation are reported in table I.

According to the theoretical calculation, the best compromises between K^2 and V_φ are obtained for the propagation mode 3, thus the discussion will be focused on this propagation mode.

Figure 2 shows calculated dispersion curves of velocity as a function of normalized thicknesses (kh_{AlN}) of AlN film (where $k=2\pi/\lambda$ is the wave vector and h_{AlN} the AlN film thickness). Several values of ZnO film thicknesses where investigated (kh_{ZnO}=0.2, 0.4, 0.6, 0.8 and 1). Electromechanical coupling coefficient dispersion curves calculated for the two structures ZnO/IDT/AlN/diamond and IDT/ZnO/AlN/diamond are shown in figures 3-a and 3-b. The ZnO/AlN/IDT/diamond structure was also investigated theoriticaly. However, obtained results, not presented her, show less intersest compared to the two first structures. From figure 2 and 3-a, we can observe that a combination of high acoustic velocity and a relatively high K^2 value (>4%) are expected for the mode 3 on the new structure ZnO/IDT/AlN/diamond. As example V=15000m/s and K^2=4.1% are obtained with kh_{ZnO}=0.2 and kh_{AlN}=2.3. Same combinations could be also obtained with kh_{ZnO}=0.4 and kh_{AlN}=1.5.

Figure 3-b shows the dispersive curves of electromechanical coefficient of the mode 3 for the structure IDT/ZnO/AlN/Diam. One can observe that the obtained values of K^2 are lower than those obtained for the structure ZnO/IDT/AlN/Diam. Nevertheless interesting combination of K^2 and V are registered.

Experimental study

In order to confirm simulation results, SAW filters based on ZnO/IDT/AlN/diamond structure was processed and characterized. The main steps of fabrication process are summarized in following:

1- One hundred micrometers thick polycrystalline diamond layers were deposited on (100) silicon substrate by microwave plasma enhanced chemical vapour deposition method. After deposition, the silicon substrates are etched in HNA solution leading to clean freestanding diamond layers, free of non-diamond carbon impurities. This process leads to avoid the tedious step of mechanical polishing and offers a smooth surface on nucleation side [10,11].-

2- Highly oriented c-axis AlN film was deposited by RF reactive magnetron sputtering process on nucleation side of freestanding CVD diamond. The AlN film thickness was fixed to 4.7 μm. The experimental growth conditions have been described elsewhere [12]. The microstructural characterisation shows a high (002) preferred orientation of AlN thin film. The X-ray diffraction (XRD) rocking curve shows a FWHM of 1.8° that is very low compared to results obtained in other works from AlN films synthesised by magnetron sputtering [13-15] .

Morphological analysis was carried out using atomic force microscopy (AFM) measurements. The surface roughness of our AlN film exhibits a very low rms roughness of 0.7nm, which is required to limit the SAW propagation losses and consequently enhance device performances. Furthermore, transmission electron microscopy (TEM) and field emission scanning electron microscopy (FESEM) analysis have shown that AlN films present a columnar structure and each column in this structure consists of only one single grain [12]. The grain column size was estimated, from these observations, at 30 nm that is in concordance with the low surface roughness measured by AFM.

3- Aluminium IDT, with uniform finger spacing and spatial period (λ=24 μm) was patterned by conventional contact UV photolithography. The number of IDT pair fingers, the IDT aperture and the inter-IDT distance were respectively fixed at 50, 2mm and 200μm. The metallization ratio (η) of IDT was chosen to generate the 3rd and 5th harmonic of the fundamental modes excited in the structure [16]. The IDT were deposited on AlN or on ZnO surface depending on considered structure. According to theoretical calculations, the better results are expected with the ZnO/IDT/AlN/diamond structure, why the experimental results presented her will concern only this structure.

4- Zinc oxide film (1.4μm) with c-axis orientation was then also deposited by reactive magnetron sputtering process on IDT/AlN/diamond realized structure. These films were deposited by a DC planar magnetron sputtering system with a Zinc target (purity 99.99%). The distance between the cathode and the substrate holder was 80 mm. The deposition chamber was pumped down to a base pressure of 5.10^{-7} mbar by a turbomolecular pump prior to the introduction of the argon-oxygen gas mixture for ZnO thin film production. The gas discharge mixture was Ar/O_2 and the total working pressure was 2.10^{-3} mbar. The oxygen percentage in the Ar/O_2 gas mixture was fixed at 70 % and the DC power delivered by the DC generator was 120W. The substrate and the chamber wall were grounded and the substrate holder temperature was fixed at 200 °C. The crystallographic properties of the film exhibit a (002) orientation and the film composition determined by Energy Dispersive X-ray Spectroscopy (EDXS) is Zn_1O_1.

Frequency characterization of SAW filter was performed before and after ZnO deposition using a network analyzer (HP8752A) and micro-probe system (Suss Microtech). Figure 4 and 5 show the wide range frequency responses obtained respectively for IDT/AlN/Diamond and ZnO/IDT/AlN/Diamond structures. We can observe several peaks related to the different

Rayleigh wave modes and the corresponding different harmonics. The frequency value, the propagation mode order and the harmonic order are indicated for each peak (M2h3 means mode 2 and harmonic 3). The phase velocity (v_φ) were determined from the peak's frequency f_i using the following equation:

$$f_i = \frac{v_\varphi}{\lambda} \qquad (1)$$

with $\lambda = P/n$. n being the order of considered harmonic and P, the spatial periodicity of IDT. The delay time to determine the group velocity was also measured for each peak to avoid any confusion between the mode's order and the harmonic's order.

In order to compare experimental results with theoretical ones, dispersive curves of velocity calculated by varying simultaneously AlN and ZnO film thicknesses with a constant h_{AlN}/h_{ZnO} ration. Hence, experimental velocity determined from fundamental and harmonics peaks could be presented together in the same graph. Figure 6 shows a compilation of dispersive curves calculated for modes 0, 1, 2 and 3 (line) and experimental points related to identified peaks in figure 5, determined from SAW device realized with the following parameters: AlN film thickness h_{AlN}=4.7µm; ZnO film thickness h_{ZnO}=1.4µm; and spatial periodicity of IDT P=24µm. The related kh are: kh_{AlN}=1.23 and kh_{ZnO}=0.366 for fundamental peaks and kh_{AlN}=1.23n, kh_{ZnO}=0.366n for the peaks related to the n^{th} harmonic of considered mode.

One can observe that the identified peaks agree well with theoretical prediction. However, some peaks remind unidentified and the expected high velocity and high electromechanical coupling coefficient was not obtained with the tested SAW device. This is due to the fact that the SAW device was processed before to completely finish the simulation and with the used thicknesses, the leaky waves of modes 3 are not excited. In fact, from figure 2 and 3-a, and by considering the used AlN normilized thickness kh_{AlN}=1.23, the optimum ZnO thickness leading to a combination of high K^2 and high velocity is located between kh_{ZnO}=0.4 and 0.6 instead the used value kh_{ZnO}=0.36. Realization of SAW devices with the optimum piezoelectric films thicknesses is in progress to confirms theoretical results.

Conclusion

In summary, we have demonstrated by calculation that the three-layered structure ZnO/AlN/Diamond, offers a good combination of high surface acoustic velocity and high electromechanical coupling. First experimental results obtained from this structure are in accordance with the theoretical results. Realization of additional devices with optimum normalized thicknesses determined by calculation are in progress in order to confirm the high potentiality of the new ZnO/AlN/diamond structure for the processing of high performances and high frequencies SAW filters.

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Table I: Material elastic, piezoelectric and dielectric constants used in the calculations.

		AlN [7]	ZnO [8]	Diamond [9]
Elastic constants (10^{11}N/m^2)	C_{11}	3.45	1.57	11.45
	C_{12}	1.25	0.89	0.893
	C_{13}	1.20	0.83	0.893
	C_{33}	3.95	2.08	11.45
	C_{44}	1.18	0.38	5.255
Piezoelectric constants (C/m^2)	e_{15}	-0.48	-0.45	-------
	e_{31}	-0.58	-0.51	-------
	e_{33}	1.5	1.22	-------
Relative dielectric Constants (10^{-11}F/m)	ε_{11}	8	6.69	5.04
	ε_{33}	9.5	7.9	5.04
Masse density (10^3Kg/m^3)	ρ	3.26	5.72	3.515

Figure captions:

Figure 1: The three structures configurations considered in calculation (a) IDT/ZnO/AlN/diam, (b) ZnO/IDT/AlN/diam and (c) ZnO/AlN/IDT/diam.

Figure 2: kh_{AlN} dependence of phase velocity of ZnO/AlN/Diamond structure calculated for various ZnO film thicknesses. Horizontal lines correspond to shear wave (SW) and Rayleight wave (RW) of diamond substrate.

Figure 3: kh_{AlN} dependence of electromechanical coupling coefficient (K2) calculated for the mode 3 for various ZnO film thicknesses; (a) ZnO/IDTS/AlN/Diamond structure (b) IDT/ZnO/AlN/Diam structure.

Figure 4: Wide band attenuation characteristic of IDT/AlN/diamond filter performed with kh_{AlN}= 1.25

Figure 5: Wide band attenuation characteristic of ZnO/IDT/AlN/diamond filter performed with kh_{AlN}= 1.25 and kh_{ZnO}= 0.37

Figure 6: Compilation of dispersive curves calculated for modes 0, 1, 2 and 3 (line) and experimental points determined from SAW device realized with the following parameters: AlN film thickness h_{AlN}=4.7µm; ZnO film thickness h_{ZnO}=1.4µm; and spatial periodicity of IDT P=24µm.

Figure 1 :

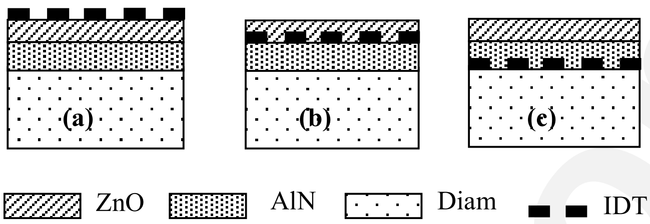


Figure 2 :

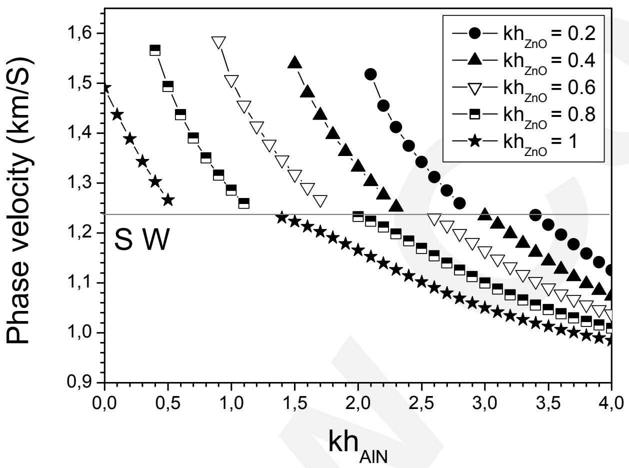
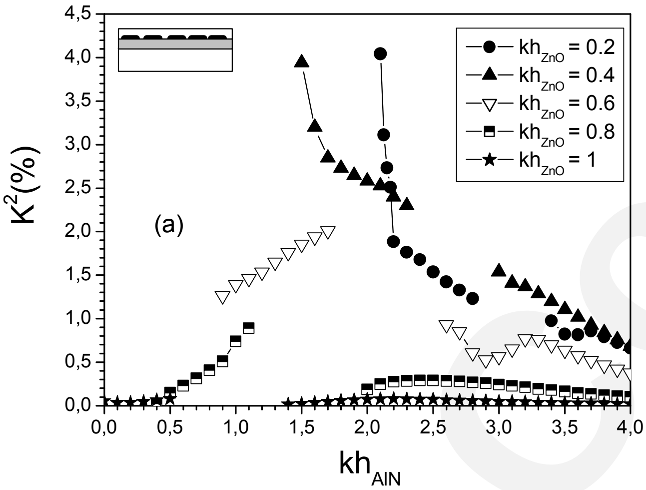

Phase velocity (km/S)
kh$_{AlN}$
S W
kh$_{ZnO}$ = 0.2
kh$_{ZnO}$ = 0.4
kh$_{ZnO}$ = 0.6
kh$_{ZnO}$ = 0.8
kh$_{ZnO}$ = 1
1,6
1,5
1,4
1,3
1,2
1,1
1,0
0,9
0,0
0,5
1,0
1,5
2,0
2,5
3,0
3,5
4,0

Figure 3

(a)


K²(%)
kh_AlN
(a)
kh_ZnO = 0.2
kh_ZnO = 0.4
kh_ZnO = 0.6
kh_ZnO = 0.8
kh_ZnO = 1

(b)

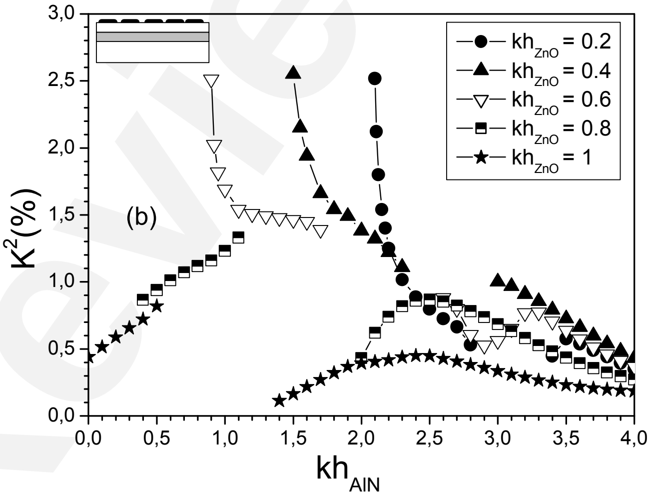

K²(%)
kh_AlN
(b)
kh_ZnO = 0.2
kh_ZnO = 0.4
kh_ZnO = 0.6
kh_ZnO = 0.8
kh_ZnO = 1

Figure 4

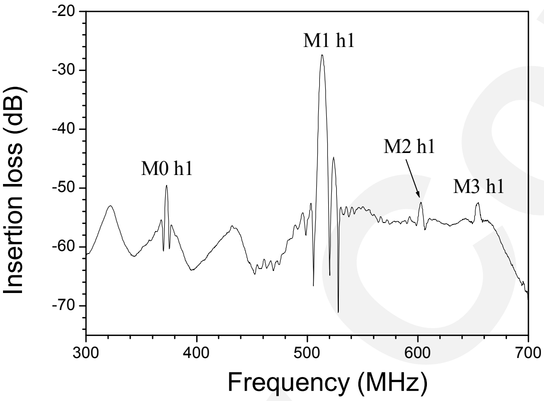

M1 h1
M0 h1
M2 h1
M3 h1
Insertion loss (dB)
Frequency (MHz)
-20
-30
-40
-50
-60
-70
300
400
500
600
700

Figure 5

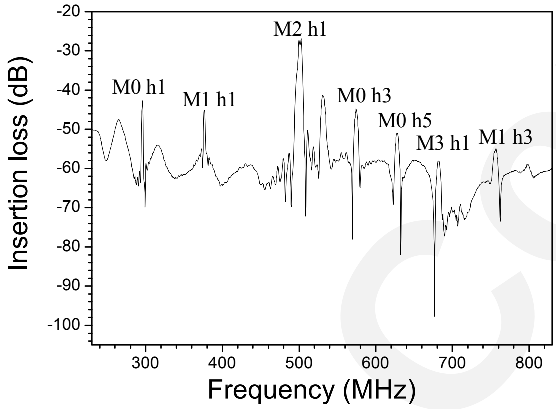
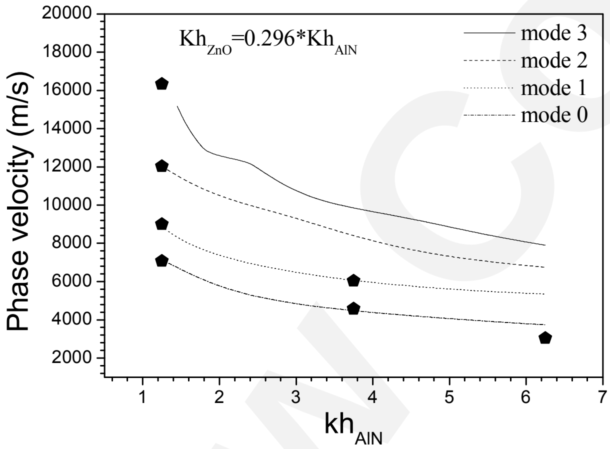

M2 h1
M0 h1
M1 h1
M0 h3
M0 h5
M3 h1
M1 h3
Insertion loss (dB)
Frequency (MHz)
-20
-30
-40
-50
-60
-70
-80
-90
-100
300
400
500
600
700
800

Figure 6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18000
16000
14000
12000
10000
8000
6000
4000
2000
Phase velocity (m/s)
1
2
3
4
5
6
7
kh_AlN
Kh_ZnO=0.296*Kh_AlN
mode 3
mode 2
mode 1
mode 0