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AlN/ZnO/Silicon Structure Combining Surface Acoustic Waves and Waveguiding Layer Acoustic Wave

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Abstract: In this work, the theoretical study for the realization of waveguiding layer acoustic waves devices based on AlN/IDT/ZnO/Silicon structure using the modeling software COMSOL Multiphysics (2D) is presented. The effect of thicknesses of AlN and ZnO thin films on the evolution of frequency response, phase velocity and electromechanical coupling is studied. The adequate structure is determined for an experimental investigation.

Keywords: *WLAW, SAW*

1. Introduction

Surface Acoustic Waves (SAW) devices are very innovative due to their multiple advantages: robustness in extreme environments; high sensitivity and mainly a unique capability to be interrogated remotely without embedded electronics, which present a great interest in various domains and industrial applications. However, these devices are very sensitive to environmental variations such as oxidation and humidity. Consequently, a package structure is needed to protect the surface which limits the extreme miniaturization of these devices.

An alternative way to realize a new generation of devices is a combination of a SAW and a waveguiding layer acoustic wave (WLAW) in the same structure. The surface wave is sensitive to the temperature, pressure and the surface perturbation while the isolated wave is only sensitive to the temperature and strain. However, there are a few reported studies on WLAW structures [1 - 3].

Therefore, the aim of this work was to confine a wave in a low acoustic velocity layer enclosed in between two high acoustic velocity materials. A rigorous theoretical study on WLAW devices based on AlN/IDT/ZnO/Silicon (IDT-interdigital transducer) structure has been realized, using the modelling software COMSOL Multiphysics (2D). Theoretical model, modelling results on standard ZnO/Si structure and the influence of aluminium nitride and zinc oxide thicknesses on performance of WLAW devices are discussed. The optimized final structure of WLAW devices is proposed for experimental tests.

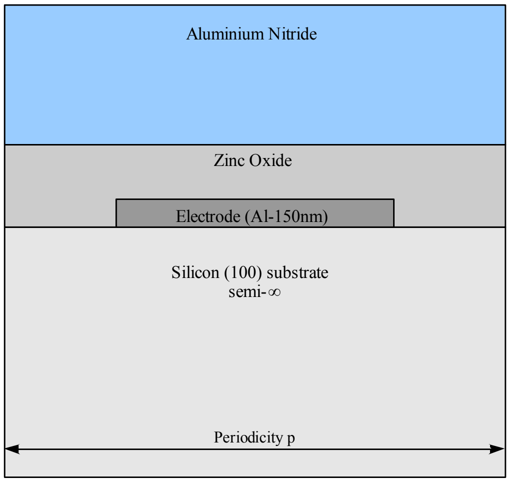


Figure 1. Schematic representation of the AlN/IDT/ZnO/Si structure.

2. Model

The COMSOL Multiphysics model used in this work was built in 2D Structural Mechanics Module. Figure 1 shows a schematic representation of the AlN/IDT/ZnO/Si structure considered in the modelling. The package structure is composed of a ZnO layer surrounded by a silicon substrate and an aluminium nitride layer. The aluminium electrode (IDT) with a wavelength of 8 µm is deposited on the ZnO surface. The orientated (100) silicon is assumed to be a semi-infinite substrate. Orientation of ZnO and AlN films corresponds to c-axis perpendicular to the substrate plane.

The physical constants of various materials, reported in literature [4 - 7], are used for our model and are given in Table 1.

Table 1. Material constants used in the model

	Silicon	ZnO	AlN	Al
Elastic constant (10^{11} N/m^2)				
C_{11}	16,6	2,1	3,45	1,12
C_{12}	6,39	1,21	1,25	0,6
C_{13}	6,39	1,25	1,2	0,6
C_{33}	1,66	2,11	3,95	1,12
C_{44}	7,95	0,425	1,18	0,26
Piezoelectric constant (C/m^2)				
e_{15}	—	-0,61	-0,58	—
e_{31}	—	1,14	1,55	—
e_{33}	—	-0,59	-0,48	—
Dielectric constant (10^{-11}F/m)				
ε_{11}	11,8	8,34	9,03	—
ε_{33}	11,8	8,84	10,7	—
Density ρ (Kg/m^3)	2329	5676	3260	2700

Phase velocity V, electromechanical coupling coefficient K^2 and wave confinement can be easily extracted from the model. Phase velocity V is determined by the eigenfrequency f and the spatial period λ following the basic expression:

$$V = f * \lambda.$$

The electromechanical coupling coefficient is calculated from admittance modulus curves obtained in modelling by using the expression:

$$k^2 = \frac{\pi}{2}\frac{f_r}{f_a} tg\left(\frac{\pi}{2}\frac{f_a - f_r}{f_a}\right)$$

where f_r is resonance frequency and f_a is anti-resonance frequency.

To determine the conditions of wave confinement, data on displacement along Y-direction is needed which is obtained from a Y-axis cross-section of the structure.

Eigenfrequency, admittance modulus and Y-displacement are largely exploited in modelling of WLAW structure.

3. Results and discussion

3.1 ZnO/Si structure

Due to the complexity of the studied AlN/IDT/ZnO/Si structure, investigation was started by a basic ZnO/Si structure, where silicon substrate is considered as semi infinite and the thickness of ZnO thin film was modulated from 1 µm to 10 µm.

Figure 2 shows the dispersion curves of the acoustic wave velocity calculated for the 0th, 1st and 2nd acoustic modes. The X-axis corresponds to the normalized thickness of the ZnO film ($kh_{ZnO} = 2\pi h/\lambda$); where h is the film thickness, λ is the acoustic wave wavelength fixed by the spatial periodicity of the IDTs and k is a wave vector. The 2nd mode exists only at $kh_{ZnO} > 3.14$, its phase velocity is higher than those of other two modes. The dispersion curves of the electromechanical coupling coefficient for 0th, 1st and 2nd mode, presented in Figure 3, depend on the type of mode considered and on the normalized thickness. The coupling coefficient of the first mode increases with the increase of ZnO film thickness up to a maximum value at $kh_{ZnO} = 3.14$ and decrease soon after. Contrary, the curves of 0th mode and 2nd modes increase slightly with kh_{ZnO} and stabilize at high ZnO thickness.

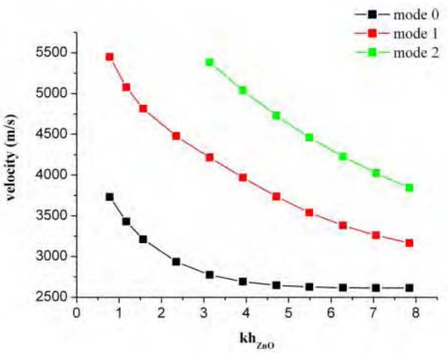


Figure 2. Dispersion curves of phase velocity V of 0th, 1st, and 2nd modes for ZnO/Si structure.

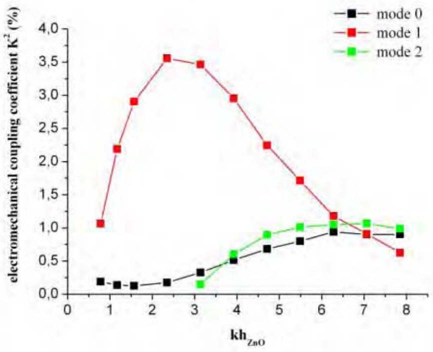


Figure 3. Dispersion curve of electromechanical coupling coefficient of 0th, 1st, and 2nd modes for ZnO/Si structure.

High electromechanical coupling coefficient (more than 3.5 %) is obtained for $2.35 < kh_{ZnO} < 4.71$. In the case of $\lambda = 8$ µm, the related thickness of ZnO film should be comprised of between 3 and 6 µm. Good accordance of this results with previous works, realized on ZnO/Si structure [7 - 9], validated our used model.

3.2 Thickness of AlN film

Thickness of AlN film is the key parameter for achieving the waveguiding layer. The influence of this parameter on the evolution of different acoustics modes must be evaluated.

ZnO thickness is fixed at 5µm which corresponds to a good electromechanical coupling (as shown above). The phase velocity and electromechanical coupling coefficient of 0th, 1st and 2nd modes are summarized in Figure 4 and 5. The calculations were carried out on typical AlN/ZnO/Si structure with increasing the thickness of AlN film until the wave confinement is achieved. One can see that the AlN thickness has a large impact on the structure performance. One should notice that the modes evolve differently with the increase of AlN layer thickness. Electromechanical coupling coefficient of the 1st and 2nd mode decreases up to 0.06 % and stabilizes. Contrary, K^2 of 0th mode increases up to a plateau around 2.33 %. The wave velocity of each mode in this structure increases by increasing the AlN thickness due to the fact that velocity in AlN is almost two times larger than that in ZnO. At $kh_{AlN} > 6$ the AlN thickness doesn't influence on the wave, resulting in stabilization of the velocity and of the electromechanical coupling coefficient.

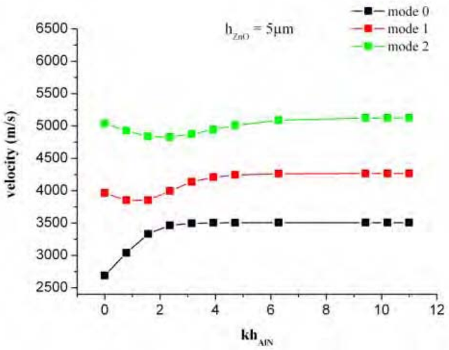


Figure 4. Phase velocity of 0th, 1st, and 2nd mode of Rayleigh wave as a function of the AlN thickness.

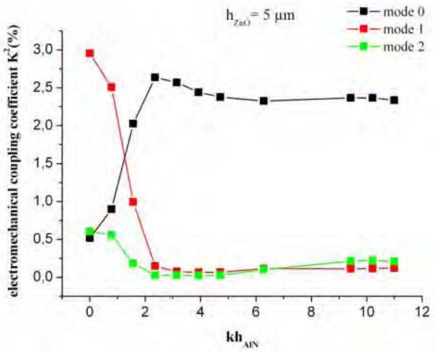
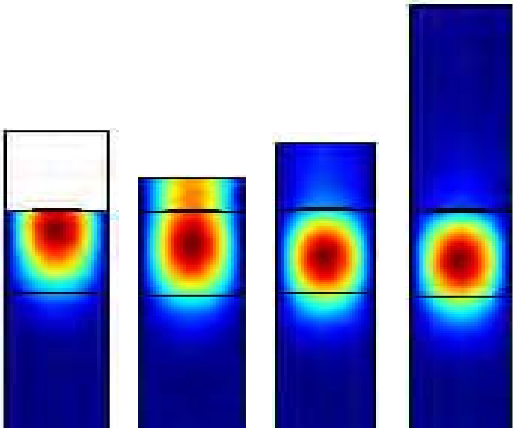


Figure 5. Electromechanical coupling coefficient K^2 of 0th, 1st, and 2nd mode of Rayleigh wave as a function of the AlN thickness.

The Figure 6 illustrates the shape deformation along Y-axis of 0th mode in AlN/IDT/ZnO/Si structure with AlN thickness of 0, 2, 4 and 12 µm. Figure 7 shows, the displacement normalized along Y-direction, for AlN/ZnO/Si structure. It is considered that the confinement is achieved by using 10 µm thick AlN layer; afterward the wave confinement can be assured with 12 µm thick AlN film.



0 µm 2 µm 4 µm 12 µm

Figure 6. Shape deformation along Y-axis of 0th mode in AlN/IDT/ZnO/Si structure.

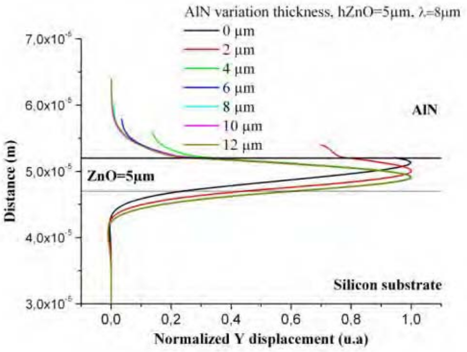
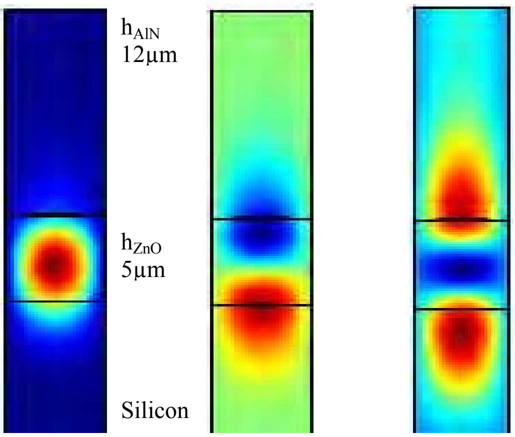


Figure 7. Y-direction normalized displacement in AlN/ZnO=5µm/Si structure of 0th mode for different AlN thickness.

To summarise, the best mode for a future experimental application would be the 0th mode because the coupling coefficient of the other modes is too low to be detected.

3.3 Thickness of ZnO film

The principal function of ZnO is to form a guiding layer. In this part, the effect of ZnO film thickness on isolated wave behaviour, in the structure AlN/ZnO/Si, is studied. For total confinement of the wave, the AlN thickness is fixed at 12 µm and the ZnO thickness is varied from 1 µm to 7 µm. As noted before, the 0th mode is mainly studied which exhibits the best performance regarding electromechanical coupling coefficient. As shown in Figure 8, 0th mode is also the best to obtain a good wave confinement with a minimum AlN thickness required. Indeed, the 1st and the 2nd modes need thicker AlN layer to confine completely the wave so this reinforces our motivation to choose the 0th mode in the future experimental study.



mode 0 mode 1 mode 2

Figure 8. Shape Deformation along Y-axis of 0th, 1st and 2nd modes in AlN12/ZnO5/Si structure.

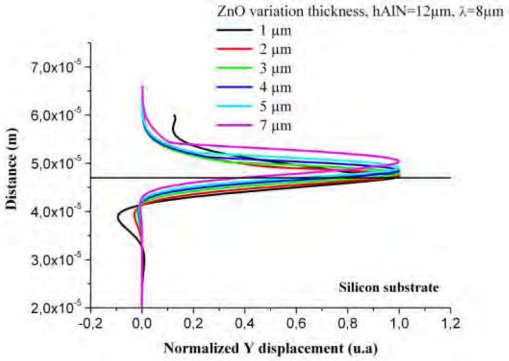


Figure 9. Y-direction normalized displacement of AlN=12µm/ZnO/Si structure of 0th mode for different ZnO thickness.

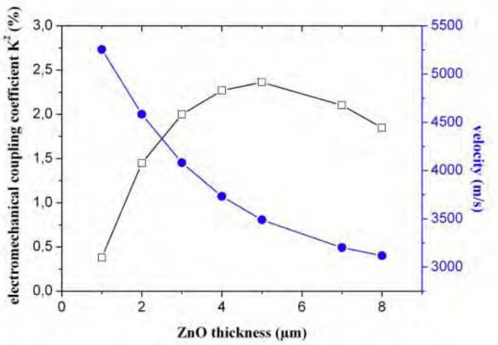


Figure 10. Phase velocity and electromechanical coupling as a function of the ZnO thickness for the 0th mode.

Figure 9 demonstrates the evolution of the Y displacement with increasing ZnO thickness. Phase velocity and electromechanical coupling of 0th mode for different ZnO thickness are given in Figure 10. The electromechanical coupling coefficient increases up to a maximum value at h_{ZnO} = 5 µm and then decreases with further increase of the ZnO thickness. The best K^2 value is obtained for ZnO thickness from 3 µm to 7 µm. Moreover, according to Figure 9, a good wave confinement is obtained at $h_{ZnO} > 4$µm.

A first experimental test has been realized with the studied structure and it confirms the results obtained in the modelling. It will be reported elsewhere.

4. Conclusion

Using powerful COMSOL Multiphysics software, the new AlN/ZnO/Silicon structure was studied. This software is an effective tool to optimize the structure before an experimental implementation which represents a good way to save the time and the money.

It was shown that an efficient AlN/ZnO/Silicon structure could be achieved with an electromechanical coupling coefficient around 2.33 %. The importance of AlN and ZnO thickness in the final device performance has been demonstrated. A minimum AlN thickness of 12 µm is required to confine completely the wave. ZnO thickness is the second important parameter for the realization of structure and it must be choosen thoroughly.

6. References

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