FEM simulation analysis of TiO$_2$/ZnO/SiO$_2$/Si multilayer structure for CMOS compatible acousto-optic tunable filter

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Abstract. In this paper, TiO$_2$/ZnO/SiO$_2$/Si layer structures with different thickness of ZnO and TiO$_2$ is discussed and explained. The study is carried out in order to obtain optimal normalized thickness of the multilayer structure for fabricating acousto-optic tunable filter with high figure of merit (FOM). Based on simulation and study of SAW propagation characteristics like, electromechanical coupling co-efficient, figure of merit and phase velocity, it is inferred that this structure is suitable for the desired application.

1. Introduction

Photonics has gained a lot of attraction in the field of electronics after the formation of lasers, optical fibers, semiconductor optoelectronic detectors, and sources. Out all the applications of photonic integrated circuits (PICs), on-chip sensors based on photonics have gained a lot of importance for the past few decades [1] and after their advancement integrated optic structures (gratings, waveguides, etc.) gained considerable importance in different applications domain. For instance, communication, medical instrumentation etc.

For the past few decades, technology based on surface acoustic wave (SAW) is used commercially on large scale. For example, in surface acousto-optic devices, sensors and in communication field [2, 3]. Till date, usually bulk piezoelectric material is used in acousto-optic devices, for example lithium niobate (LiNbO$_3$), lithium tantalite (LiTaO$_3$), langasite (La$_3$Ga$_5$SiO$_{14}$), quartz (SiO$_2$) and tellurium dioxide (TeO$_2$) [4]. Use of these bulk materials is not cost effective and, it is difficult to integrate with microelectronics. With the advancement in fabrication technology, thin film deposition has become feasible and thin film-based devices have become more popular [3, 5]. Even though the demand of single layer-based devices has increased but due to the attractive features of different materials, there is an increase in demand of multilayer films for numerous applications. For example, for the designing of computer disks, optical filters, optical reflectors, solar cells etc [6, 7]. In comparison with doped semiconductors, broad tunability can be achieved from multilayer films which gives the optical response desired for specific application [8]. One such example is acousto-optic tunable filter (AOTF) [9-17]. The multi-layered structure device performance mainly depends on the acoustic, optic and acousto-optic properties of the material medium in which interaction of both waves occur (i.e. sound and light wave). To increase the efficiency of acousto-optic interaction in such devices, optical waveguiding with low loss and strong SAW interaction is important. Therefore, the selection of suitable layer structure is important. The layer structure used in AOTF should have the attributes like high electromechanical coupling co-efficient ($k^2$), phase velocity ($\nu$) and good figure of merit (FOM)
In order to do it, it’s better to make the combination of layer structure with using the materials possessing the said properties [7, 19]. Zinc oxide (ZnO) thin film possess excellent piezoelectric properties with high $k^2$, high sensitivity and reliability as well. In addition to that, another feature is, that it can be grown on numerous substrates, which includes silicon (Si) as well [20-23]. Titanium dioxide (TiO₂) film possess excellent optical properties, like high refractive index, high transmittance and large band gap which make it appropriate for multilayer thin film [19].

In current work, TiO₂/ZnO/SiO₂/Si layer structure with different thickness of ZnO and TiO₂ is discussed. By comparing the SAW propagation properties of said structure, figure of merit of the device is also calculated.

2. Methodology

For designing low cost and high-quality SAW devices, very precise SAW filter simulations are required to select the suitable material and geometrical shapes of electrodes [24]. To achieve the accurate quantitative description of SAW devices analytical and numerical studies are required [25-27]. Finite element method (FEM) analysis of infinite gratings of IDTs in SAW is a perfect performing tool to serve the reason. To analyse the effect of different possible geometries of the SAW device and electrode shape, it is the easiest way to analyse it. It also enables us to do the analysis of whole device geometry by the computation of half period infinite structure with the application of inverted periodical boundary conditions [28, 29]. COMSOL software is used to carry out the simulations. The simulation is carried out to study the SAW propagation characteristics (i.e. electromechanical coupling co-efficient and phase velocity) of Rayleigh wave mode as a function of normalized layer thickness. For this reason, FEM 2-dimensional models of the structure TiO₂/ ZnO/ SiO₂/ Si is built.

In the matrix form the constitutive piezoelectric equations can be written as

$$T = C_E S - e^T E$$  

$$D = e S - \varepsilon \varepsilon E$$

Here $T$ is the stress, $C_E$ is the elasticity matrix (N/m²), $S$ is strain, $e^T$ is the piezoelectric matrix (C/m²), $E$ is electric field (V/m), $D$ is the electrical displacement (C/m²), $e$ is the stress matrix and $\varepsilon$ is the dielectric matrix.

2.1. Geometry description

COMSOL Multiphysics is used to carry out the FEM simulation of the SAW devices. There is a periodicity in IDTs, hence, to model the whole SAW resonator one period of electrode is enough. For this reason, for designing a SAW resonator, a unit cell measuring one $\lambda$ is taken. $40\lambda$ is taken as the depth of a unit cell. As SAW generates on the upper surface and dies out as it goes deeper in the substrate. For the simulations a very fine triangular mesh was taken to get more accuracy in the results. Figure 1 depicts the geometry of unit cell. Table 1 gives the information of the device’s dimensions. Table 2 gives the boundary conditions used and table 3 summarizes the material constants which are used in the simulation.

| Table 1. Dimensions of the device. |
|------------------------------------|
| **Dimensions** | **Value (µm)** |
| wavelength | $4 (\lambda)$ |
| pitch of electrode | $2 (\lambda/2)$ |
| width of IDT | $1 (\lambda/4)$ |
| substrate thickness | $40 (10\lambda)$ |

| Table 2. Boundary conditions (BC). |
Table 3. Material constants of TiO₂, ZnO, SiO₂ and Si.

| Parameter                      | Symbol | TiO₂ | ZnO | SiO₂ | Si  |
|--------------------------------|--------|------|-----|------|-----|
| Density (kg/m³)                | ρ      | 4260 | 5665| 2200 | 2330|
| Elastic constants (GPa)        |        |      |     |      |     |
| C₁₁                            | 271.43 | 209.7| 78.5| 166  |
| C₁₂                            | 177.96 | 12.1 | 16.1| 64   |
| C₁₃                            | 149.57 | 105.4| 16.1| 64   |
| C₃₃                            | 483.95 | 211.2| 78.5| 166  |
| C₄₄                            | 124.43 | 42.4 | 31.2| 80   |
| C₆₆                            | 194.77 | -    | 31.2| 80   |
| Piezoelectric constants (C/m²) |        |      |     |      |     |
| e₁₅                            | -      | -0.45| -   | -    |
| e₃₁                            | -      | -0.51|     |      |
| e₃₃                            |        | 1.22 |     |      |
| Dielectric constants (10⁻¹¹ F/m) |        |      |     |      |     |
| ε₁₁                            | 63.7   | 8.55 | 3.32| 10.62|
| ε₃₃                            | 63.7   | 10.2 | 3.32| 10.62|
| Refractive Index               | n      | 2.782| 1.998| 1.5 | 3.88|

Figure 1. A 2-Dimensional unit cell geometry used in FEM simulation for the layer structure: IDT/TiO₂/AlN/SiO₂/Si.
To find the acoustic wave velocity in Eigen mode the equation is as follows:

\[ v = f \lambda \]  \hspace{1cm} (3)

Here \( f \) is the Eigen frequency which we get through simulation and \( \lambda \) is the acoustic wave’s wavelength. To find the electromechanical coupling coefficient \( (k^2) \), the equation used is as follows:

\[ k^2 = 2 \left( \frac{v - v_m}{v} \right) \]  \hspace{1cm} (4)

Where \( v \) is the free surface velocity without the metal short and \( v_m \) is the phase velocity with the metal short.

3. Results and Discussions

In the proposed layer structure (i.e. TiO\(_2\)/ZnO/SiO\(_2\)/Si) with TiO\(_2\) as top layer and interdigitated electrodes (IDTs) on top of TiO\(_2\) layer is shown in figure 1. The variation of electric field in the IDTs which travels from TiO\(_2\) to ZnO produces SAW and penetrates in SiO\(_2\) as well [30]. The light waves fall on TiO\(_2\) layer and after interacting with SAW produces an acousto-optic effect which is the main principle of acousto-optic tunable filter (AOTF) [31]. In this structure TiO\(_2\) material is chosen because of its good optical properties and ZnO because of its good piezoelectric properties [19, 32, 33]. SiO\(_2\) layer is deposited on silicon (Si) substrate because waveguide action cannot be achieved without it, as the refractive index of Si is greater than the refractive index of rest of the materials whereas the refractive index of SiO\(_2\) is less than the other materials which are deposited on top of it [3]. The electromechanical coupling coefficient of a material depends on certain properties like dielectric, piezoelectric and elastic properties. Therefore, the material is chosen based on these properties. In addition to that while choosing the material for AOTF device, the material also needs to have a good figure of merit (FOM), which is eventually dependant of photoelastic constant \( (p) \), refractive index \( (n) \), density \( (\rho) \) and acoustic phase velocity \( (v) \). In mathematical form, figure of merit \( (M) \) can be written as:

\[ M = \frac{n^6 p^2}{\rho v^3} \]  \hspace{1cm} (5)

In order to choose the optical material for AOTF all the parameters of equation (5) should be kept into consideration. The most important is refractive index and acoustic velocity. Some materials offer good optical properties like high transmittance and less losses but due to having high acoustic velocity the FOM becomes low. In order to achieve a high FOM using the same material it’s better to use the material in a combination with other materials with less velocity. The velocity of the layer structure is the combined velocity of all the materials. In this research, we have selected TiO\(_2\) as the optical material due to its good optical properties and ZnO because of its high electromechanical coupling coefficient [19, 23].

For the validation of our FEM simulation method, first we simulated ZnO/ SiO\(_2\)/ Si layer structure which was published in Reference [32]. Figure 2 and 3 depicts the ZnO/ SiO\(_2\)/ Si layer structure simulation results and it is evident from it that our simulated results are similar to the Reference [32]. This proves that our method of simulation is reliable.
Figure 2. Calculated phase velocity v/s normalized thickness of ZnO with thicknesses (ZnO = 3µm and SiO2 = 2µm) for structure ZnO/ SiO2/ Si.

Figure 3. Calculated electromechanical coupling coefficient v/s normalized thickness of ZnO, with thicknesses (ZnO = 3µm and SiO2 = 2µm) for structure ZnO/ SiO2/ Si.

The results of simulation for SAW propagation characteristics of the structure TiO2/ZnO/SiO2/Si are displayed in figure 4 and 5. It is evident from figure 4, that phase velocity increases with the increase in normalized thickness of TiO2 but decreases with the increasing normalized thickness of ZnO. In this study we calculated phase velocity on different thicknesses of TiO2 (0.4µm, 1 µm, 2 µm, and 3µm) with varying thickness of ZnO (0.4 µm, 0.8 µm, 1.6 µm, 2.4 µm, 3.2 µm and 4 µm), while keeping SiO2 as 1 µm. Moreover, from figure 5, it can be observed that the electromechanical coupling coefficient decreases with the increase in normalized thicknesses of both TiO2 and ZnO.

Figure 4. Phase velocity versus normalized thickness of TiO2 on different normalized thickness of ZnO.

Figure 5. Electromechanical coupling coefficient versus normalized thickness of TiO2 on different normalized thickness of ZnO.

In order to fabricate the AOTF we need the FOM and electromechanical coupling coefficient high at the same time. It means an optimum value among all the combinations of thickness should be chosen which gives low phase velocity, high FOM and high $k^2$ at the same time. In order to analyse that, we have plotted 3-D graphs to show the variation of phase velocity and $k^2$ with respect to normalized thickness of TiO2 and ZnO.
After the analysis of the data, using equation (5) we calculated the figure of merit of the TiO$_2$/ZnO/SiO$_2$/Si structure to be $3.04 \times 10^{-14}$ s$^3$/kg which is higher than the FOM of merit of both ZnO ($2.572 \times 10^{-15}$ s$^3$/kg) and TiO$_2$ ($0.694 \times 10^{-14}$ s$^3$/kg) individually [34, 35].

4. Conclusion

In this research, surface acoustic wave propagation characteristics of TiO$_2$/ZnO/SiO$_2$/Si layer structure (which includes phase velocity and electromechanical coupling coefficient) are investigated and using these, figure of merit of the layer structure is calculated. The chosen multilayered structure showed increase in phase velocity with the increase in normalized thickness of TiO$_2$ and showed a declined behavior with the increase in ZnO layer normalized thickness keeping lambda ($\lambda$) as 4$\mu$m. Moreover, a decreasing trend is observed in electromechanical coupling coefficient with the increase in normalized thicknesses of both ZnO and TiO$_2$. In addition to this, figure of merit is also calculated and the value of FOM is $3.04 \times 10^{-14}$ s$^3$/kg with the thickness of SiO$_2$ = 1 $\mu$m, TiO$_2$ = 0.4 $\mu$m and ZnO = 1.6 $\mu$m, which is higher than the individual FOM of TiO$_2$ and ZnO. It is clear from the data, that using this layered structure with the mentioned optimized thickness a high figure of merit can be achieved and also, depositing this thickness is practically possible. Hence, this becomes a basis for fabricating a CMOS compatible acousto-optic tunable filter.

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