

Research Paper

Design of Directional Coupler Structure in Electro-Optic Integrated Circuit Using Refractive Index Sensor Based on Silicon Nitride Substrate

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Abstract:

Ansys Lumerical software, with its powerful MODE and FDTD modules, emerges as an indispensable tool for analyzing light behavior within electro-optical integrated circuits that play a vital role in fulfilling this critical need within intricate structures and evaluating their feasibility for many applications. The MODE module, equipped with the FDE and varFDTD solvers, excels in efficiently simulating light propagation, providing rapid results that are invaluable for initial comparisons and design exploration in based on increasing the efficiency.

In this study, a simulated sensor was strategically integrated into a directional coupler structure. By meticulously analyzing light propagation through strategically placed monitors within this integrated system, were able to gain valuable insights into the sensor's performance. The findings demonstrated that the varFDTD solver within the MODE module proved highly effective in optimizing the design of the directional coupler based the TM mode behavior into the TE mode. As the light polarization changes, variations occurred at a width range between 0.66 to 0.83 micrometers.

This optimization resulted in a significant enhancement of the sensor's efficiency, ensuring its robust and reliable operation across a wide range of environmental conditions and operational scenarios.

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1. INTRODUCTION

Integrated circuits, whether optical or electronic, have brought about a major revolution in the field of information and communication technology. Initially developed with large dimensions and limited capabilities, these circuits have now become the core of many advanced electronic and optical devices. The first electronic integrated circuits, created in the 1960s, were composed of discrete transistors and had large dimensions. In contrast, the initial efforts to develop optical integrated circuits began in the 1970s. Since the 1960s, there have been remarkable advancements in electronic integrated circuit technology. With the reduction in transistor size and the increase in their numbers on a single chip, the computational power of computers has grown exponentially. Moore's Law, which states that the number of transistors in an integrated circuit doubles approximately every two years, vividly illustrates this extraordinary progress [1]. Significant progress has been achieved in the realm of optical integrated circuits, leveraging the unique properties of light and advanced optical materials. These innovations have enabled the development of circuits with vastly superior data transfer speeds and substantially reduced energy consumption compared to their electronic counterparts. Notably, these breakthroughs hold great promise in transformative fields such as optical communication and quantum computing [2].

The examination of significant advancements in silicon photonic devices and integrated circuits highlights the capabilities of this technology in transforming optical communications. Silicon photonic integrated circuits (PICs) have evolved from academic research to the development of commercial products as an efficient solution for increasing data transfer speeds and capacities. This technology, by combining silicon with other semiconductor materials in CMOS processes, enables the creation of optical devices with smaller dimensions, lower production costs, and greater integration potential [3]. This technology, utilizing advanced platforms such as silicon and silicon nitride, enables the implementation of wavelength division multiplexing (WDM) transmitters and receivers, facilitating extremely high-speed data transfer. Additionally, the design of these circuits, incorporating optical synchronization techniques and advanced modulation formats like QPSK, significantly increases the network capacity. Another key point in the article is the electronic-photonic integration, which enables close coupling between optical circuits and digital signal processors. This integration facilitates efficient communication between optical and electronic components, improving overall system performance and enabling faster, more powerful data processing.

The directional coupler, as one of the main passive components in silicon photonic integrated circuits (PICs), is introduced at the beginning of the passive device section, alongside other key components such as waveguides, multimode interference (MMI) couplers, Mach-Zehnder interferometers, Bragg gratings, and ring resonators. Hence, the theory of coupled modes and its applications for analyzing the interaction of optical waves in coupled waveguides was developed.

This theory provides a mathematical framework for describing the power exchange between waveguides during light propagation along them [4]. Among the types of directional couplers that have been studied, one can mention the photonic crystal-based coupler [5], the lithium niobate-based coupler [6], the double Y-junction coupler with a coupling range to a waveguide [7,8], and finally, the multi-channel or array couplers [8]. Although each of these structures can be adapted with modifications, they can be used in various telecommunications, industrial, or medical applications [9-11]. The difference in the design of the directional coupler in this study, compared to the aforementioned examples, lies in the structure of the directional coupler, which is designed with two waveguides placed very close to each other to couple light into the second waveguide. This structure is based on silicon nitride. This material is a perfect insulator, and unlike lithium niobate, where the refractive index can be changed by altering the electric field [12,13], the material used in this study experiences a change in the refractive index due to temperature variations or the presence of impurities, such as the analyte interacting with the light path. By comparing the physical characteristics of the light before and after the analyte attaches to the waveguide, the change in parameters will be utilized to enhance the performance of the system.

Silicon, due to its abundance, transparency in the near and mid-infrared wavelength ranges, and compatibility with CMOS technologies, is one of the best options for photonic integrated circuits. This material enables the fabrication of small and highly functional devices, making it suitable for applications such as optical communications, advanced computing, and biosensors. Additionally, silicon is highly effective in designing high-performance waveguide channels with a small footprint due to its high refractive index and its potential for controlling and optimizing light.

The refractive index of silicon nitride is approximately 1.98 at 1550 nm, providing an index contrast of 0.5 when combined with silica cladding. This allows for the realization of devices such as waveguides or resonators, which can be integrated with other components of the silicon photonics toolbox to create the final product.

By combining this material with silicon and other materials such as graphene and using multilayer waveguides, an integrated platform has been created for the fabrication of active photonic devices such as high-speed modulators, switches, and photodiodes.

Simulations and experiments have been conducted to investigate the sensitivity of the silicon nitride-based waveguide sensor to changes in the refractive index of the cladding material (n_{clad}). Based on the results of three-dimensional simulations, it was found that the coupling coefficient (κ) increases with an increase in the refractive index of the cladding material.

Over the years of development in refractive index-based sensors, it can be observed that silicon nitride has been used as the primary material in sensors

because of its high refractive index, which reduces light leakage and increases sensor sensitivity. This type of sensor does not require complex equipment and is highly suitable for practical applications, such as biosensing and material detection [14,15].

2. MATERIALS AND METHODS

The continuous advancement of technology, computer simulations have become an essential tool for researchers and engineers. Software like Lumerical, by providing powerful virtual environments, enables in-depth investigation of physical and engineering phenomena without the limitations of laboratory experiments.

In Lumerical software, to simulate a waveguide, the MODE module is first used to obtain the modes that propagate during the electromagnetic field's transmission. This module helps determine the pattern of the expanding mode, providing insights into how the mode behaves as it propagates through the waveguide.

This method numerically solves Maxwell's equations to determine the optical modes that can exist in a specific waveguide. After defining the structure and setting the boundary conditions, Perfectly Matched Layer (PML) is applied. By preventing wave reflections and limiting the computational domain, PML increases the accuracy and speed of the simulation. PML is an artificial layer surrounding the computational domain, where material properties are modified in such a way that electromagnetic waves are gradually attenuated and eventually absorbed. This is achieved by altering the material parameters, such as magnetic permeability and electrical conductivity, in the direction perpendicular to the computational boundary.

This solver, by taking a cross-sectional slice of the structure, shows which modes are capable of propagating in the waveguide. At the beginning of the structure, where the two waveguide ports one as the source and the other as the reflection port are placed, this cross-sectional slice is positioned to reveal the results. After defining the simulation environment for the solver, the structure must be specified. The default Lumerical directional coupler sample is made of silicon, and this material is optimally used for these dimensions. Figure1 shows that is perfectly symmetrical, and the port arrangement is as follows the source input is at the top left, with the first output labeled "Through" located at the top right of the same waveguide. The coupled light in the second waveguide exits from the third port at the bottom right of the structure. The fourth port, located at the bottom left, serves as the reflection output.

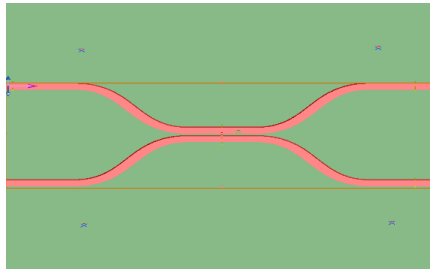


Fig. 1. Top view of the directional coupler

Figure 2 shows the application of FDE windowing, which is defined by the input of the structure. This window must include both the waveguide and its underlying layer, which is the waveguide isolating layer made of silicon. This allows the simulator to analyze the behavior of light as it passes through the waveguide and interacts with the waveguide walls, making it easier to detect the boundary of the walls and the isolating layer.

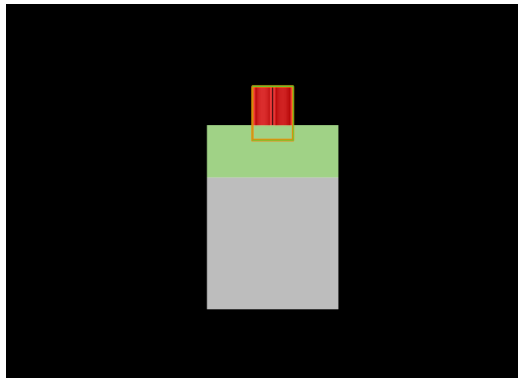


Fig. 2. Side view of a directional coupler in the varFDTD environment.

Given that in the intended structure, according to the sensing application, both the TE and TM fundamental modes need to propagate, a directional coupler is required that, based on the defined dimensions and light's behavioral pattern, generates the desired modes along the waveguide. This ensures that the modes are properly excited and maintained for optimal performance in the sensing application.

It should be noted that the solver is a Finite Difference Eigen (FDE) solver, so the cross-section is taken along the X and Y axes. Therefore, the mesh is applied to the structure in the XY plane, and the light propagates in the Z direction. This setup is essential for correctly simulating the propagation of modes and analyzing the behavior of light in the waveguide structure.

After defining these effective materials, the Lumerical software uses a complex mathematical model to precisely describe the properties of these materials. This mathematical model enables the software to simulate the behavior of light in this simplified two-dimensional structure with very high accuracy.

Thus, in this software, the MODE Solutions module simplifies the computations by transforming a complex three-dimensional problem into a simpler two-dimensional one, making the calculations much faster and easier while maintaining the accuracy of the simulation. The main assumption is that the coupling between different modes of the vertically supported waveguide structure is negligible. For many devices, such as waveguide structures based on SOI (Silicon-On-Insulator) that only support two vertical modes with different polarizations, this is a very reasonable assumption. In this case, varFDTD can provide results comparable to 3D FDTD simulations while using only the simulation time and memory of a 2D FDTD simulation.

After reviewing the VarFDTD and FDE methods to finalize the results and achieve simulation outcomes with very high accuracy and realism, the three-dimensional space is used to solve the wave equations. In the FDTD method (Finite Difference Time Domain), the chosen space is three-dimensional. Therefore, solving Maxwell's equations does not straightforwardly yield the desired results. In the FDTD method, Maxwell's differential equations are rewritten as finite difference equations to solve them numerically. This formulation is used for electromagnetic simulations in the time domain.

The FDTD method is like a movie that shows events step by step. At each moment, using electromagnetic laws (Maxwell's equations), the values of the electric and magnetic fields in each cell are calculated. Then, the simulation progresses to the next time step, and these calculations are repeated. In this way, the evolution and change of the electromagnetic fields over time can be observed. This step-by-step temporal approach provides a detailed understanding of how light interacts with the structure throughout the simulation.

Figure 3 proposed the three-dimensional space set for the simulation, ensuring that it penetrates the depth of the underlying layers. This allows for the behavior of the waveguide to be examined along with the other layers, providing a comprehensive analysis of how light interacts with the entire structure, including the lower layers.

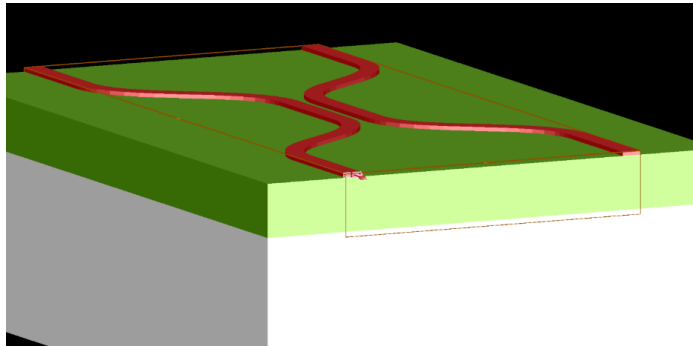


Fig. 3. A 3D view of a directional coupler in the FDTD environment

As previously mentioned, to obtain results on how light propagates, a source and a monitor are required. However, in this module, there are two different types that return the output results. These types can be used to capture the propagation behavior of light and provide insights into the mode distribution and coupling effects within the waveguide structure.

The flexibility to handle a wide range of applications is a key feature of this method. Using the varFDTD solver, the broadband light transmission into various modes in an expanded cone can be accurately calculated. The high accuracy is because in this method, the vertical structure is effectively converted into a single layer, and this conversion works well in broad regions such as the cone. In other words, no approximations are made regarding how light propagates within the waveguide layer, and the results obtained from this method are very similar to the more accurate results from 3D FDTD simulations.

Nonlinear optical phenomena, such as second and third-order harmonic generation, frequency mixing, and self-phase modulation, are the result of the nonlinear dependence of polarization on the electric field [15]. These phenomena have numerous applications in various fields, including optical communications, lasers, and sensors. They enable the creation of new wavelengths, enhanced signal processing, and the development of highly sensitive detection methods, making them critical in advancing technologies related to photonics and optoelectronics.

As light travels through the waveguide, after covering a distance equal to its wavelength (λ), it returns to its initial state [9]. In other words, light undergoes a full oscillation at each wavelength, which is derived from equation (1). This periodic behavior of light in the waveguide is essential for understanding wave propagation, resonance effects, and the interaction of light with the material properties of the waveguide. Equation (1) describes the relationship between the wavelength, propagation constant, and the structure's dimensions [12].

$$\theta_c = \sin^{-1} \frac{n_l}{n_h} \quad (1)$$

In space, light waves propagate at a speed of $c=299,792,458$ m in a bulk material, this speed is divided by the refractive index. Therefore, the number of cycles per unit length is multiplied by the refractive index, and the propagation constant in the bulk material [12] is given by equation (2):

$$\beta = \frac{2\pi}{\lambda} n \quad (2)$$

Since there are no nonlinear losses such as two-photon absorption or free carrier absorption at the desired wavelength (1.55 micrometers), the nonlinear parameter [12] is defined as follows in equation (3):

$$\gamma = \frac{\omega n_2}{c A_{eff}} \quad (3)$$

The effective length L_{eff} in nonlinear regions is given by the following equation (4), which plays a role in reducing longitudinal losses for the nonlinear parameter [12]:

$$L_{eff} = \frac{1 - e^{-\alpha L}}{\alpha} \quad (4)$$

Table 1. Physical parameters of silicon nitride and related materials in a waveguide

Material	n	n_2 [10^{-17} m^2/W]	β_{TPA} [cm/GW]	γ [W^{-1} m^{-1}]	FOM	α [dB/cm]
c-Si	3/47	0/385	0/9	300	0/3	0/4
a-Si	N/A	N/A	0/25	1200	5	4/5
SiO ₂	1/44	0/0022	Negligible	N/A	N/A	0/0005
Si ₃ N ₄	1/97	0/03	Negligible	1/4	>>1	0/004
AlGaAs	3/3	2/6	N/A	660	21	1/3
GaInP	3/1	0/06	0/22	450	1/7	N/A

3. Results And Discussion

In this paper, when using this structure as a sensor, both the TE and TM modes should maintain similar behavior throughout the waveguide's path. The emphasis on the fundamental modes is due to their ability to preserve their stability during light propagation. This stability helps reduce distortion and losses in the optical signal, thereby improving the sensor's performance.

Besides, the sensors typically require high sensitivity. The TE and TM modes, due to their differing behaviors in interaction with environmental materials (such as changes in refractive index), can be effective tools for enhancing the accuracy and sensitivity of the system.

Hence, the use of both TE and TM modes in a single sensor offers greater design flexibility for the optical structure. By properly adjusting the waveguide's geometry and selecting the appropriate materials, conditions can be created that

allow both modes to propagate optimally. This provides the user with selective control over the sensor's functionality. It also facilitates simultaneous multi-functional applications within a single sensor.

Finally, combining the information from both modes allows for a more comprehensive analysis of optical phenomena. This way, the information can be analyzed once with the TE mode and again with the TM mode, allowing for a more thorough and detailed understanding of the sensor's behavior and its interaction with the surrounding medium.

According to the experimental simulation of these two modes in the waveguide, simultaneous use of both modes with a height of less than 0.8 microns is not feasible for a laser source with a wavelength of 1550 microns. Therefore, in this mode, a transverse sweep was applied to the waveguide to show the optimal coupling of light in the form of the TM mode.

These results, according to the Figure 4 are for the waveguide with widths ranging from 0.1 to 0.5 microns.

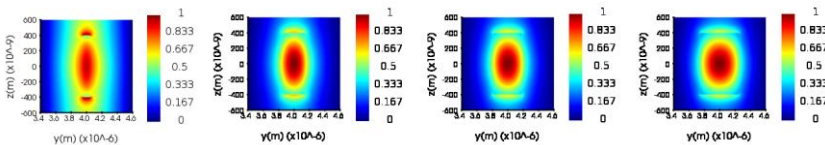


Fig. 4. Sweep across the waveguide width in TE mode

Based on these images, it can be inferred that at a width of 0.5 microns and height of 0.8 microns, the fundamental TM mode is well coupled in the waveguide. However, as the width is increased from 0.5 microns to 1 micron, the results diverge from expectations, and the TM mode transitions into the TE mode. According to figure 5, from the second image onward, this difference is noticeable as the light polarization changes. This variation occurred at a width range between 0.66 to 0.83 micrometers.

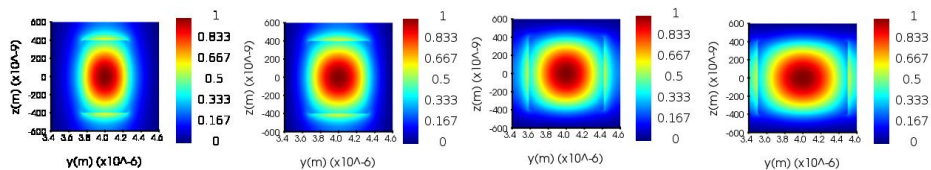


Fig. 5. Sweep across the width of the waveguide in TM mode

When selecting the waveguide width during the determination of optical modes, careful consideration must be given to the specific application of the structure. The required precision for physical phenomena and the ability to predict the behavior of light along the structure are crucial. In this case, the mode change in the waveguide is undesirable for sensing applications, as it introduces

complexity in predicting light behavior, which can lead to inaccuracies or challenges in optimizing the sensor's performance. Ensuring stability in the chosen mode is key to maintaining reliable and consistent sensing results.

To maintain both TE and TM modes in the structure, the waveguide height must be kept constant, with only the width of the waveguide being adjusted. This means that by keeping the waveguide height at 0.8 microns and varying the width from 0.1 to 0.5 microns, efforts are made to preserve both modes throughout the waveguide. In simulations conducted for the TE mode, adjustments to the width of the waveguide help fine-tune the coupling of light and the behavior of the TE mode. This approach helps prevent unwanted mode changes and maintains stability in the system.

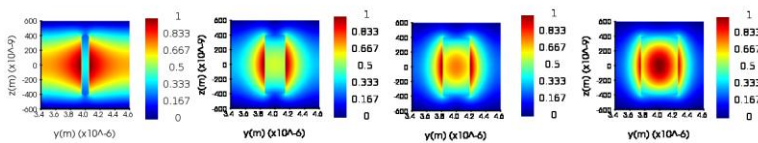


Fig. 6. Sweep across the waveguide width in TE mode

Table 2 shows the TE and TM modes, where the first and second options represent the modes for the magnetic and electric fields, respectively.

Table 2. Method for determining the fundamental mode of the electric and magnetic fields in Lumerical software

Mode	Effective index	Wavelength (um)	Loss (dB/cm)	Group index	TE polarization (Ey)	Waveguide TE/TM fraction (%)	Effective area (um ²)
1	1.456466+7.307292e-06i	1.55	2.5729	1.864147+8.935042e-06i	1	97.9/80.59	0.744846
2	1.337439+8.085108e-07i	1.55	0.28467	1.670011+6.279056e-07i	100	99.1/81.09	0.881698
3	1.248834+4.624917e-06i	1.55	1.6284	1.872937-1.203893e-06i	10	77.49/93.32	0.796716
4	1.145041+8.034508e-07i	1.55	0.28289	1.849466-9.995896e-07i	81	96.26/66.56	0.953277

In the next step, the coupling section of the structure is analyzed. This is the region where the waveguides are placed parallel to each other with a very small gap between them. The analysis focuses on the cross-sectional view to examine the coupling behavior and determine the optimal gap distance.

With a waveguide width of 0.5 micrometers and a height of 0.8 micrometers, a sweep over the gap was performed. The results indicate that beyond a gap of 0.5 micrometers, the evanescent field is no longer able to overcome the distance effectively, and the light fails to couple properly into the second waveguide.

The sweep is performed over a gap range of 0.1 to 0.5 micrometers, as shown in Figure 7.

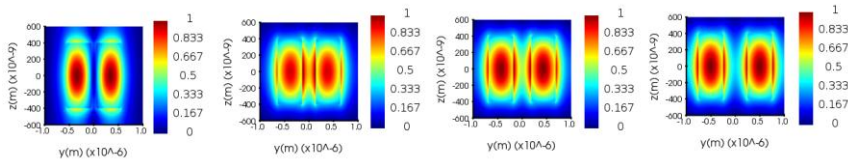


Fig. 7. Sweep of the gap between two waveguides

Figure 8 demonstrates that the coupling boundary becomes unsuitable beyond 0.5 micrometers, where the coupling phenomenon no longer occurs. This sweep covers a gap range of 0.61 to 0.66 micrometers, and similar results are repeated beyond this range.

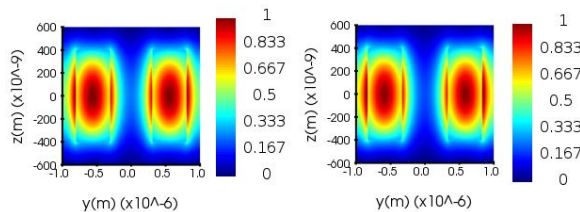


Fig. 8. Large distance between two waveguides and no coupling

In the final stage of this analysis, it is expected that the output of the directional coupler will replicate the fundamental TE and TM modes introduced at the input. An ideal directional coupler would transfer exactly what was coupled at its input to the output without any differences. However, depending on the application such as the sensor-focused analysis in this study it is anticipated that the presence of the target material along the light path will alter these characteristics. This aspect will be explored further in the subsequent analysis.

According to the obtained results, the waveguide's width is 0.5 micrometers, its height is 0.8 micrometers, and the distance between the two waveguides is 400 nanometers. These dimensions differ from those in the reference paper [13], where the silicon nitride height is specified as 0.22 micrometers. This discrepancy arises due to fabrication constraints that prevent the use of such thicknesses on the chip. Additionally, the reference paper does not explicitly mention the waveguide width. The waveguide length is only approximately indicated and was shown to produce results up to 100 micrometers.

From this section onward, we use the VarFDTD solver. According to the primary reference article [13], the directional coupler length is optimized by fine-tuning the coupling region, as this section has the most significant impact on the waveguide's output. A length of 71.3 micrometers is used; however, due to the symmetry of the structure, the optimal value derived from the script based on the coupling and bending sections is 87.3 micrometers. The structure in this research

uses a smaller dimension compared to the 100-micrometer reference value, demonstrating successful size reduction for optimizing the device's dimensions.

Thus, Figure 9 and Figure 10 show the top view of the electric and magnetic field intensities within the coupled waveguide. Initially, the electric and magnetic fields are shown to analyze their distributions effectively.

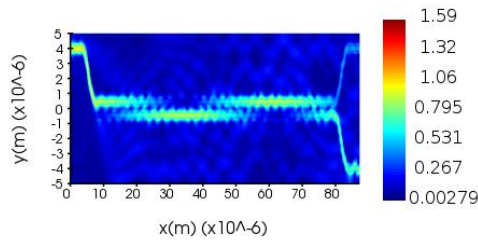


Fig. 9. Fundamental TE Mode in a Silicon Nitride Directional Coupler

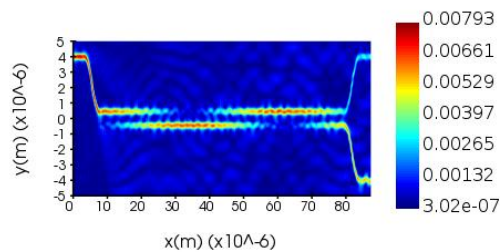


Fig. 10. Fundamental TM Mode in a Silicon Nitride Directional Coupler

In Figure 11 and Figure 12, the intensity of the electric and magnetic fields is also shown. Due to the sensor application, the coupling length is appropriately set at this size so that the desired materials interact properly with the waveguide, maintaining high accuracy and sensitivity.

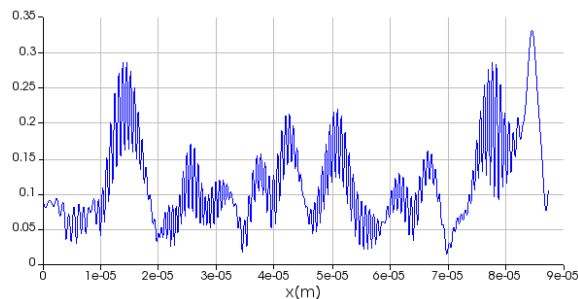


Fig. 11. Electric field intensity of the fundamental TE mode of a silicon nitride directional coupler

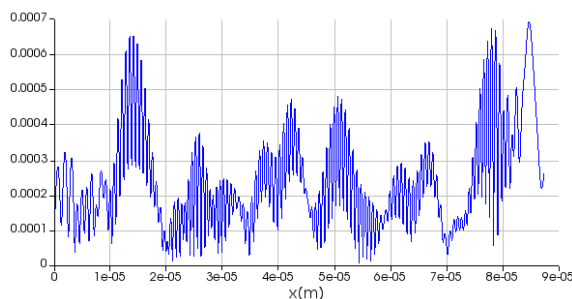


Fig. 12. Electric field intensity of the fundamental TM mode of a silicon nitride directional coupler

You can observe that the behavior of the fields is similar, but their intensities differ. This is due to the waveguide structure, where we determined in the solver that the waveguide can propagate both TE and TM modes in their fundamental states. Figure 13 shows the evanescent field for the electric field generated around the waveguide, which is also compared and obtained according to the second reference [13]. It is worth mentioning that another name for this graph is "single mode."

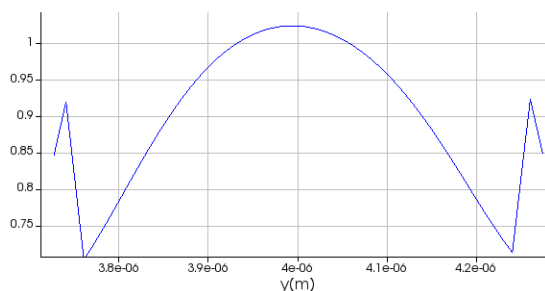


Fig. 13. Evanescent field of the fundamental TE mode around a single-mode waveguide

However, for the magnetic field, Figure 14 does not show the evanescent field on the graph. Nevertheless, based on the results mentioned, this section also exhibits coupling.

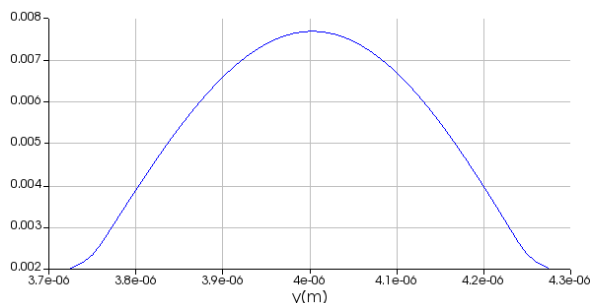


Fig. 14. Evanescent field of the fundamental TM mode around a single-mode waveguide

To ensure correct mode propagation in the structure, a Mode Expansion monitor is used. According to previous analyses, it is clear that with the current dimensions, the fundamental TM and TE modes couple in the structure.

4. CONCLUSION

Based on the results obtained in this research and a comparison with previous research, it can be concluded that the present study has made significant innovations in the field of design and simulation of direct optical couplers with respect to change material and variation behavior in sensing and nonlinear effects. By carefully comparing the optical and electrical properties of silicon nitride materials in directional coupler structures and utilizing the Variational FDTD solver, valuable insights were gained regarding the selection of suitable materials. To achieve results in the shortest time possible while ensuring a theoretical understanding of the materials, the use of the Variational FDTD solver is optimal, and if the study progresses towards fabrication, using the FDTD module would be more advantageous. Using the varFDTD simulator, highly accurate simulation results have been obtained, significantly contributing to the validation of experimental results. The simultaneous use of TE and TM modes and the detailed comparison of various materials are among the innovations of this research. Additionally, the findings of this study can be applied in the design and fabrication of directional couplers with higher efficiency and lower costs by considering nonlinear effects in sensing.

In conclusion, this research has made a significant step towards improving the design and simulation of optical directional couplers. Based on the obtained results, it can be concluded that silicon nitride can be used for the construction of such couplers. Moreover, the simultaneous use of TE and TM modes and the development of precise simulation models provide the opportunity to design couplers with higher performance and greater flexibility.

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