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Compact angled multimode interference duplexers for multi-gas sensing applications

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Abstract: A compact, low-loss 2×1 angled-multi-mode-interference-based duplexer is proposed as an optical component for integrating several wavelengths with high coupling efficiency. The self-imaging principle in multimode waveguides is exploited to combine two target wavelengths, corresponding to distinctive absorption lines of important trace gases. The device performance has been numerically enhanced by engineering the geometrical parameters, offering trade-offs in coupling efficiency ratios. The proposed designs are used as versatile duplexers for detecting gas combinations such as ammonia-methane, ammonia-ethane, and ammonia-carbon dioxide, enabling customization for specific sensing applications. The duplexers designed are then fabricated and characterized, with a special focus on assessing the impact of the different target wavelengths on coupling efficiency.

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1. Introduction

The ever-increasing demand for passive optical components is critical in the interconnection of photonic integrated circuits (PICs) utilized in telecommunication and sensing applications [1–3]. The couplers stand as key enablers, and ongoing advances in waveguide-based integrated optical structures will facilitate future integration between optical sources and receivers. Distinctive functions of integrated optical couplers include modulation, power splitting and combining, signal routing and filtering, wavelength division multiplexing (WDM), etc [4–7]. Some of the passive optical components useful for realizing the above functions are directional and Y-junction couplers or multimode interference (MMI) couplers, also realized in angled configuration [8,9]. The angled MMI was first proposed by Y. Hu *et al.* and shows excellent characteristics in terms of low loss, compactness, superior fabrication tolerances and the capability to filter out higher order modes [10]. Furthermore, the angled design of angled MMI couplers can boost the coupling efficiency (CE), since it shortens the coupling region, resulting in lower optical loss. Due to its excellent compatibility with mature complementary metal-oxide-semiconductor (CMOS) technology, with low cost and high-volume production capability, silicon nitride (Si_3N_4) in silicon dioxide (SiO_2) is an appealing platform for the realization of integrated devices [11,12].

The development of real-time, low-loss, portable multi-gas sensors is creating a need for high-performance duplexers. Trace gas sensing using technologies like laser absorption spectroscopy

(LAS), photoacoustic spectroscopy (PAS), and quartz enhanced photoacoustic spectroscopy (QEPAS), compared to other techniques, are considerably faster, with response times >1 s, offer high gas specificity, are capable of part-per-quadrillion (ppq) detection sensitivity and unlock real time in-situ measurements. In LAS gas detection systems, increased radiation intensity is essential as it facilitates efficient coupling of the light source with the gas sample, resulting in heightened accuracy in measurements. In PAS and QEPAS, the measured signal is directly proportional to the radiation intensity. These techniques are typically limited to detecting a single gas [13,14]. High-coupling-efficiency-based duplexers not only are essential for sensing applications requiring high sensitivity and accuracy but can also enable multi-gas detection devices with a high temporal resolution by fast switching of two or more distinct optical sources, while alleviating the issues caused by the broad spectral separation of gases absorption lines. This is true, for example, in the case of industrial processes and combustion monitoring, toxic and flammable gas detection, agricultural fumes, hydrocarbon and explosives monitoring, as well as in breath analysis. Within the near infrared range (NIR), typical wavelengths of interest are $\lambda_1 = 1530$ nm, $\lambda_2 = 1653.7$ nm, $\lambda_3 = 1684$ nm, and $\lambda_4 = 2003$ nm which correspond to the specific absorption characteristics of the following gases: ammonia (NH_3), methane (CH_4), ethane (C_2H_6) and carbon dioxide (CO_2), respectively [15,16]. These absorption lines are spectrally very far apart from one another, posing a significant challenge for the combiner.

In this manuscript, we propose the design concept of a novel on-chip 2×1 angled MMI-based duplexer operating in the NIR region. This device is devoted to optical coupling of different spectrally separated laser sources. Specifically, the device is optimized for three independent cases, namely, to combine the following wavelength pairs: (i) λ_1 and λ_2 , (ii) λ_1 and λ_3 , (iii) λ_1 and λ_4 . A rigorous evaluation of design parameters with trade-offs in CE ratios are numerically investigated for the fundamental, higher order mode profiles and using numerically calculated output beam profiles of the commercially available diode lasers. The proposed structure and design are used as broadband source for the realization of twofold-gas sensing applications.

2. Proposed structure and design

The proposed angled MMI-based duplexer, whose sketch is shown in Fig. 1, employs silicon nitride (Si_3N_4) guiding elements placed on a silicon dioxide (SiO_2) layer.

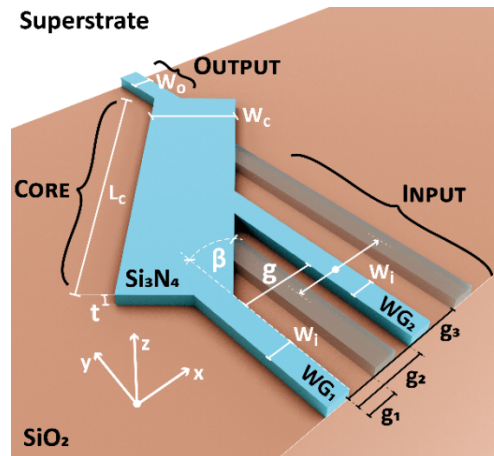


Fig. 1. Schematic diagram of angled MMI duplexer.

The Si_3N_4 on SiO_2 platform provides ultra-low loss optical propagation, relatively high refractive index contrast and a wide transparency window from 400 nm to 2350 nm [17]. The

structure can be covered with a homogenous cladding material (the choice of which will be discussed further in this work) of thickness t_c . The device is composed of three cascaded parts: an input section, a combiner (labeled as “core” in Fig. 1), and an output section. The input section consists of two waveguide ports WG_1 and WG_2 separated by a gap g , allowing the injection of two signals of different wavelengths, namely λ_i and λ_j , into the system. Specifically, λ_i will be fixed and equal to λ_1 , while λ_j will assume the value of wavelengths λ_2 , λ_3 , and λ_4 , depending on the duplexer configuration, with a different value of g for each, namely g_1 , g_2 and g_3 , as depicted in Fig. 1. It is worth noting that the position of WG_1 is fixed at the lower right corner of the combiner. Conversely, the position of WG_2 , uniquely identified by the gap g , is a function of the specific wavelength to be combined with λ_1 and will be a subject of optimization (for this reason, WG_2 is depicted with evanescent colors in Fig. 1).

These waveguides are then prolonged and connected to the multimode waveguide region, where L_C is the length and W_C is the width. This multimode region is tilted on the substrate plane forming an angle β with respect to the direction of the input and output waveguides. Within this section, interference will result in a landscape of electromagnetic field maxima and minima that is determined by geometric parameters as well as spectral parameters and the guiding properties of the structures involved. The MMI structure allows the “long side” of the core region to be exploited as the insertion point of WG_2 . The asymmetry of the structure will depend on the choice of g , which, in turn, will affect the overall transmittance. Finally, an output section consists of a single waveguide having width $W_o = W_i$, whose position mirrors WG_1 with respect to the center of the core region and to the x- and y- directions, where we expect the maximum light intensity according to the self-image principle [18].

When a single mode is injected into the multimodal region from an input port, the crossing of the discontinuity at the combiner inlet allows it to spatially disperse, resulting in the excitation of all available modes (while the total power is conserved). These modes then interfere with their own reflection from the multimodal region boundaries. According to the self-imaging principle in presence of modal dispersion, the injected mode is then regenerated along the propagation direction at specific positions, where the distance from the injection point is an integer multiple of the beating length. Here, the wavelength is inversely proportional to the length of the multimode region (L_c). Consequently, the required distance g increases with increasing wavelength separation between the two input sources [18].

The simulations were performed by the finite differences beam propagation method (FD-BPM) (BeamPROP simulation tool, provided by RSoft). Taking advantage of the monochromatic Helmholtz wave equation, FD-BPM provides an accurate yet simple computational framework for complex optical waveguide problems [19,20]. We use this method to optimize the several geometric parameters of the proposed device. After performing a convergence test, the mesh grid resolution was set to 50 nm, 100 nm, and 10 nm, along the x, y and z directions, respectively.

The material dispersion relation is introduced in simulations to account for the wavelength dependence of the refractive index and effectively manage loss and dispersion effects [21]. W_i is optimized to maximize the waveguide coupling to the mode profile of a typical diode laser, emphasizing butt coupling for efficient coupling of light [22,23]. To accomplish this, a width $W_i = 3 \mu\text{m}$ and thickness $t = 300 \text{ nm}$ are used, with SiO_2 cladding of $t_c = 1 \mu\text{m}$ thickness. The effective refractive index of fundamental mode (M00) for wavelength equal to 1530 nm, 1653.7 nm, 1684 and 2003 nm are 1.649, 1.627, 1.621 and 1.535, respectively. It is important to point out that the input waveguide can also house higher order modes M01, which have effective refractive indexes of 1.499, 1.448 and 1.38, respectively. Implementing an adiabatic mode size converter to taper the input multi-mode waveguide to single-mode dimensions, aiming to avoid higher-order modes, could increase the gap between waveguides and improve overall device performance, however, this is counter-balanced either by a decrease of the device transmittance due to tapering losses or an increase in the device footprint.

However, for the higher wavelength 2003nm, the confinement factor of the higher order mode is negligible. The corresponding mode profiles have been used to investigate the device performance. The presence of higher order modes in the system has a negative impact on the performance of the duplexer-based sensor. Higher order modes lead to increased spatial mode dispersion, decreased self-imaging fidelity, and higher crosstalk [24]. Multimode interference couplers excel in suppressing higher-order modes, thereby alleviating the performance limitations seen in comparison to alternative coupling methods. We have exclusively considered TE mode throughout our simulations, as we envisage the future integration of diode lasers operating in TE.

3. Simulation analysis

When $\beta = 0$ (i.e., “straight” MMI case), no common self-focusing positions of the two waveguides can be found for each target pairs of wavelengths. Therefore, from this point on, we consider $\beta > 0$, and commence the optimization of the duplexer for λ_1 and λ_2 , at g_1 configuration using input ports WG_1 and WG_2 . Having fixed W_i , W_o , t and t_c , the performance of the proposed duplexer was optimized by investigating the effects of varying L_c , W_c , β , and g on the total transmittance T_o . [25]. Ideally the duplexer must maximize output power T_o for both the target wavelengths, while keeping the device footprint as small as possible. A figure of merit (FOM) is defined as $T_o(\lambda_1) \times T_o(\lambda_2) / (100W_c)$ to distinguish the optimal duplexer configuration. This formula helps to identify configurations that offer superior coupling efficiencies while minimizing the footprint (L_c), which is proportional to the square of W_c . Table 1 summarises some of the best configurations in terms of FOM for the proposed duplexer, obtained in the investigated parametric space. The best configuration obtained in terms of FOM maximization is the one labelled “Case 1”. For the latter, a value of g_1 equal to 1.56 μm is deemed sufficient to prevent evanescent mode coupling between the two input waveguides [25]. The components of the output transmittance T_o obtained for $\lambda_1 = 1530 \text{ nm}$ and $\lambda_2 = 1653.7 \text{ nm}$, are equal to 86% and 88%, respectively.

Table 1. Optimized output transmittance for various duplexer configurations

Case	W_c [μm]	β [$^\circ$]	g_1 [μm]	L_c [μm]	To at λ_1 [%]	To at λ_2 [%]	FOM
1	10	4	1.56	458	86	88	7.57
2	10	4	1.16	460	70	95	6.65
3	10	5	1.86	460	82	75	6.15
4	9	4	1.28	374	80.5	80	7.15
5	11	4	1.88	547	88%	88%	7.04

Figure 2 shows the optimization process performed for Case 1 as outlined in Table 1, where T_o as a function of L_c , with W_c equal to 10 μm , for different values of g_1 . When WG_1 and WG_2 are individually excited at wavelengths $\lambda_i = \lambda_1 = 1530 \text{ nm}$ (dotted lines) and $\lambda_j = \lambda_2 = 1653.7 \text{ nm}$ (solid lines), respectively - this allows us to identify T_o depending on the excited waveguide. In particular, T_o is calculated for different values of g_1 (0.5 μm , 1 μm , 1.5 μm and 2 μm).

In general, it is possible to observe a bell-shaped trend of T_o with varying L_c . When WG_1 is solely excited at λ_1 , the change in gap value modulates the transmittance intensity, although the absolute maximum is obtained for almost the same values of L_c (i.e., in Fig. 2 the distribution of the dashed curves does not shift significantly along L_c axis), indicating that the beating length remains relatively stable with respect to g_1 . Conversely, when WG_2 is solely excited at λ_2 , changing g has only a minor effect in on the maximum transmittance intensity. Nonetheless, the beating length exhibits significant variation, spanning a range of approximately 10 microns (i.e., in Fig. 2 the distribution of the solid curves shifts toward longer L_c for increasing g). It is worth mentioning that, for a fixed value of the gap and for each different value of L_c , it is possible to identify a distinct combination of wavelength coupling ratios (i.e., T_o for pairs of the same color).

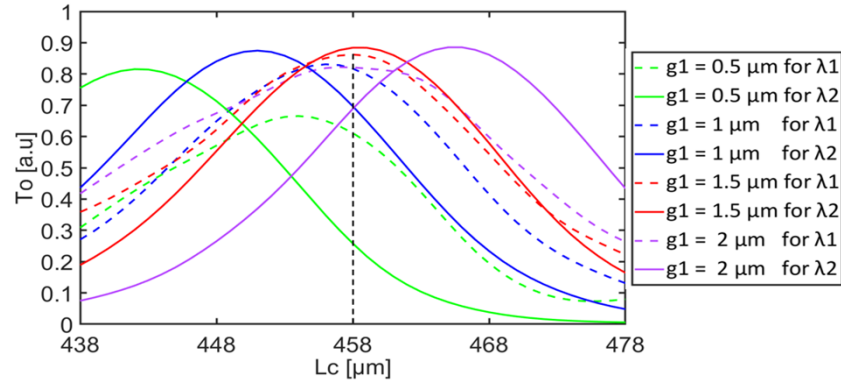


Fig. 2. Transmittance T_o as a function of L_c for different values of g_1 at fixed $W_c = 10 \mu\text{m}$ when WG_1 and WG_2 are individually excited at wavelengths 1530 nm (dotted lines) and 1653.7 nm (solid lines), respectively.

To further shed light on the behavior of the device, the transmittance has been studied by varying the angle of the core region. In particular, Fig. 3 shows T_o as a function of L_c for increasing discrete values of β (equal to 3, 4, 5, and 6, degrees respectively), when W_c , L_c and g are set as in “case 1” (see Table 1) and when WG_1 and WG_2 are individually excited at wavelengths $\lambda_i = \lambda_1 = 1530 \text{ nm}$ (dotted lines) and $\lambda_j = \lambda_2 = 1653.7 \text{ nm}$ (solid lines), respectively. The vertical line in Fig. 3 represents the $L_c = 458 \mu\text{m}$ at which maximum T_o obtained by means of figure of merit i.e., at $\beta = 4$, when wavelengths launched in their respective waveguides. The configuration referred to as “case 1” presents an excellent compromise in terms of both transmittance and compactness. For this configuration, using the mode profiles of commercially available diode laser as the input excitation leads to T_o values of 71% and 77% for wavelengths of 1530 nm and 1653.7 nm, respectively. In addition, when launching higher order modes (M01), T_o reduces to 0.5% and 9% for the same wavelengths, respectively, demonstrating a good high-order mode rejection behavior. Therefore, we set the values of W_c , L_c and β to 10 μm , 458 μm and 4°, respectively.

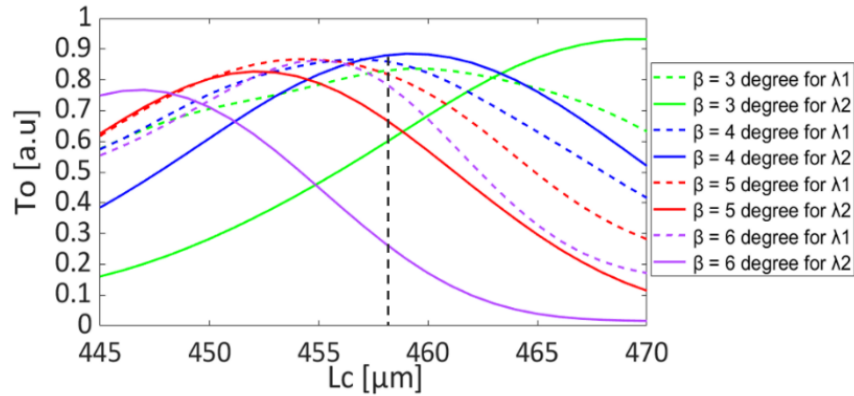


Fig. 3. Transmittance T_o as a function of L_c , for different values of β , when WG_1 and WG_2 are individually excited at wavelengths 1530 nm (dotted lines) and 1653.7 nm (solid lines), respectively.

These geometric parameters of the core region are then used to test the operation of the duplexer in the presence of other desired wavelength combinations (i.e., λ_1 - λ_3 and λ_1 - λ_4). For

each of these combinations, we optimized the corresponding gap value that maximizes the output transmittance. Table 2 summarizes the numerical results obtained for the three different wavelength pairs of interest, where λ_3 and λ_4 are launched at WG_2 .

Table 2. Values of transmittances obtained for three different pairs of excitation wavelengths when the distance between the input waveguides g is optimized

Duplexer	g [μm]	T_o for computed mode launching at [%]		T_o for laser mode profile launching at [%]		T_o for higher order mode launching at [%]	
		WG_1	WG_2	WG_1	WG_2	WG_1	WG_2
λ_1 & λ_2	$g_1 = 1.56$	86	87	68	75.5	0.5	9
λ_1 & λ_3	$g_2 = 2.03$	82	88.5	65.5	77	0	3
λ_1 & λ_4	$g_3 = 9.8$	43	84.5	30	60	30	0

Figure 4 illustrates the amplitude of electric field (TE mode) as function of x and y axis. The distribution of the propagating light in the proposed device is at $z = t_c/2 = 0.15 \mu\text{m}$. These maps provide valuable insights into the self-focusing principle and demonstrate how the gap between the two waveguides influences the focusing effect for different input waveguides targeting specific wavelengths.

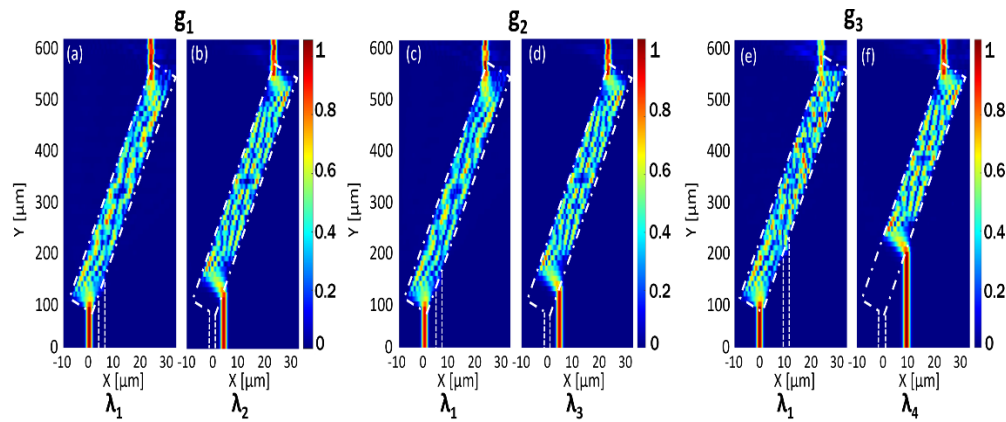


Fig. 4. Electric field distributions as a function of the x and y coordinates at $z = 0.15 \mu\text{m}$. The sole WG_1 is fed with the fundamental mode at $\lambda_1 = 1530 \text{ nm}$ (a) at $g_1 = 1.56 \mu\text{m}$ (c) $g_2 = 2.03 \mu\text{m}$ and (e) at $g_3 = 9.8 \mu\text{m}$. When WG_2 is fed with the fundamental mode at (b) $\lambda_2 = 1653.7 \text{ nm}$, at $g_1 = 1.56 \mu\text{m}$ (d) $\lambda_3 = 1684 \text{ nm}$ at $g_2 = 2.03 \mu\text{m}$ and (f) $\lambda_4 = 2003 \text{ nm}$ at $g_3 = 9.8 \mu\text{m}$.

The T_o of the duplexer with g_3 configuration for λ_1 is noticeably lower ($<50\%$), due to modal dispersion, which is a consequence of the asymmetry in MMI width caused by the presence of WG_2 . A portion of the field experiences leakage at the terminus of the MMI structure, primarily due to the presence of the dielectric interface between Si_3N_4 and SiO_2 slab region.

Figure 5 represents the transmittance as a function of the wavelength within the spectra range between $1.450 \mu\text{m}$ and $2.150 \mu\text{m}$, for the three configurations reported in Table 2. In particular, the blue color corresponds the T_o for λ_1 injected in WG_1 and red, gray, and green color for wavelengths λ_2 , λ_3 , λ_4 respectively injected in WG_2 for corresponding duplexers. The vertical line corresponds to the T_o at target wavelengths.

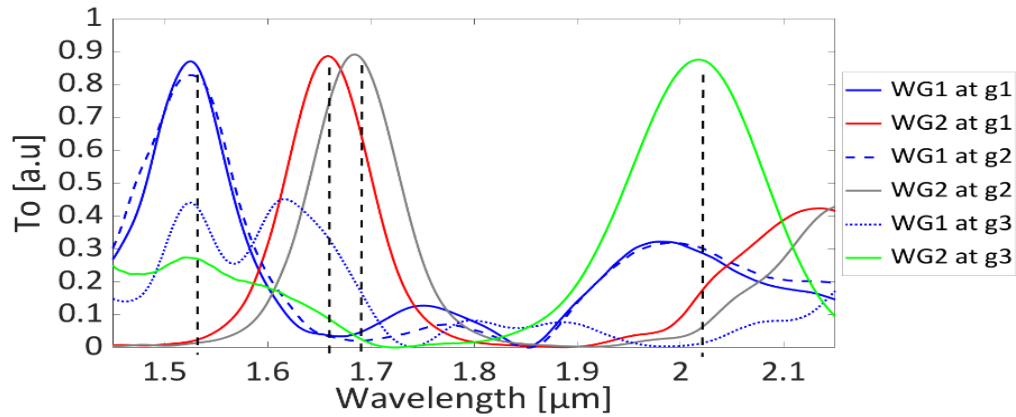


Fig. 5. Range of wavelength launched at WG_1 and WG_2 of the angled MMI.

4. Experimental results

The angled multimode interference duplexers, discussed in previous section, have been fabricated using electron beam lithography and dry etching. In order to optimize the fabrication process and transmission capabilities, various device configurations were utilized.

The fabrication process starts with the spin-coating of a 450 nm thick layer of ZEP 520A resist onto a 300 nm thick Si_3N_4 layer, which had been deposited using plasma-enhanced chemical vapor deposition (PECVD) onto a 4-inch bulk silicon wafer. This silicon wafer had a thermally oxidized (buried oxide layer) with a thickness of 2.2 μm , needed for the confinement of the optical mode in the thin Si_3N_4 layer. The devices were then patterned using electron beam lithography (EBL) at 100 kV before being developed in n-amyl acetate solution for 90 seconds and rinsed with IPA. Then, the patterns were transferred onto the PECVD Si_3N_4 layer via an inductively coupled plasma (ICP) etch step in $O_2:CHF_3$ chemistry in a 4:21 ratio (etch rate of ~ 90 nm/min). Any residual resist was removed using a bath of 1165 remover for 30 minutes and an O_2 plasma ashing step. Following SEM inspection, a 1 μm -thick SiO_2 layer was deposited using PECVD. The details of the fabricated angled MMI duplexer samples can be seen in Fig. 6. A trench with a width of 2 μm is sufficient to prevent the waveguide mode from leaking into the neighboring region. From measurements of micro-ring resonators Q-factors, fabricated using the same process, we estimate the propagation loss to be 4 dB/cm [26].

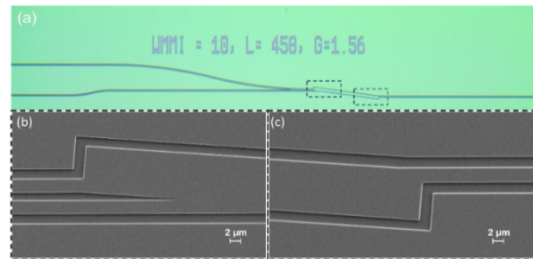


Fig. 6. Fabricated angled MMI duplexer sample under (a) microscopic imaging. SEM image (zoom) (b) between input and multimode waveguide (c) between multimode waveguide and output.

Considering optimum numerical result of case 1 from Table 1, we fabricated an array of samples having three fixed L_c for varying g_1 (1 μm , 1.5 μm and 2 μm) values, with the aim to

explore the optimum fabrication tolerances and device performance. A straight waveguide with width $W_i = 3 \mu\text{m}$ and thickness $t_c = 300 \text{ nm}$, having the same footprint of the designed duplexer (4 mm), is included in the fabricated chip for the normalization of the device performance.

The optical characterization of the fabricated samples was performed using an end-fire measurement setup similar to that shown in [27]. The input waveguides of each device are separated by $100 \mu\text{m}$ using S-bend waveguides, ultimately allowing sufficient space for bonding the diode laser to the chip. Individual alignment procedures for each wavelength are carried, considering that the optics utilized during characterization are wavelength dependent; specifically, a 60X lens to focus light into the waveguide and a 10X lens to collimate the light into the detectors. Additionally, the measurement has been performed using a TE polarizer.

The alignment process is performed using single wavelength laser (Yenista Optics TLS) for WG_1 (1530 nm) and diode laser (Eblana Photonics) for WG_2 (1653.7 nm) by maximizing the output power obtained from W_o using Thorlabs power meter. After the alignment process, the TLS was replaced with an Amonics ALS broadband light source and the diode laser with an Amonics ASLD superluminescent source. The output transmittance spectrum at W_o is collected using an Yenista Optics optical spectrum analyzer (OSA).

We employed two normalization processes for our measurements. One using the transmittance collected from a blank waveguide integrated into the fabricated chip, while the other uses the output spectra of the sources under the same conditions as those applied to the chip. Table 3 shows the calculated CE for each sample obtained by normalizing the duplexer transmittance spectrum with respect to the transmittance spectrum obtained from the reference straight waveguide.

Table 3. The normalized transmittance of the duplexer configurations

Sample	L_c [μm]	g_1 [μm]	CE at λ_1 [%]	CE at λ_2 [%]	FOM
1		1	58	66.5	8.45
2	456	1.5	61	62	8.29
3		2	60	39.2	5.15
4		1	54.4	70	8.31
5	458	1.5	63	57	7.84
6		1.56	62	67	9.06
7		2	60	40	5.24
8		1	59.5	71.5	9.24
9	460	1.5	53.5	55	6.39
10		2	75.8	52.6	8.66

Results exhibit a favorable trade-off in CE concerning variations in the geometric parameters L_c and g . Samples configurations 6 and 8 (Table 3) are specifically highlighted due to their notable performance in terms of the figure of merit (FOM). However, other samples do exhibit good performance, and their CE trends align with the simulation data concerning variations in L_c and g (see Table 3). The drift from optimized L_c and g values causes a decrease in the CE values for λ_1 and λ_2 . Sample 6 has adopted the same device configuration of as the optimized angled MMI duplexer with L_c value of $458 \mu\text{m}$ and $g_1 = 1.56 \mu\text{m}$ (case 1 from Table 1). Considering the FOM in CE, Sample 6 shows promising CE values of 62%: 67%. Nevertheless, Sample 8 shows the most promising performance, where $L_c = 460 \mu\text{m}$ and $g_1 = 1 \mu\text{m}$ having CE 59.5% and 71.5%, for λ_1 and λ_2 , respectively.

The normalized output transmittance spectra of the duplexer collected from W_o with respect to the source are shown in Fig. 7(a) and (b) for the selected samples (6 and 8). Figure 7(a) corresponds to the wavelength launched at WG_1 and Fig. 7(b) at WG_2 . The vertical line in the figures indicates the target wavelengths λ_1 and λ_2 .

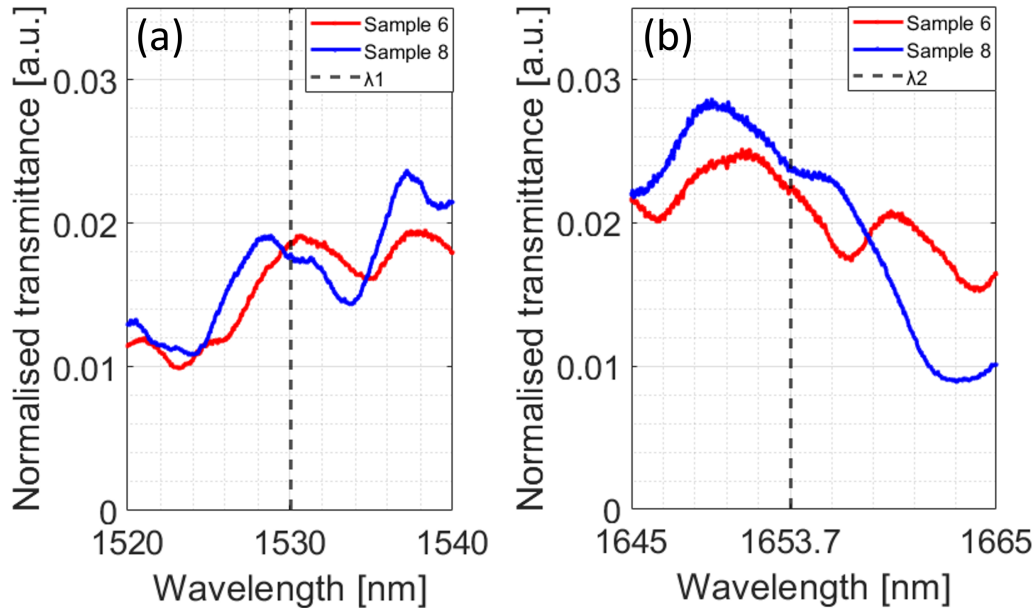


Fig. 7. Experimental results for launching a range wavelength (a) at WG1 (b) at WG2.

This normalization process facilitates accurate and meaningful comparisons across different samples and experimental conditions. These findings indicate that the designed device exhibits an optimal performance within a spectral range of approximately 10 nm centered around these specific wavelengths. Notably, these results demonstrate a satisfactory agreement with the corresponding simulation outcomes. A duplexers at 1684 nm was also tested, as this wavelength is at the limit of that provided by the super luminescent diode, the signal to noise was low and we estimated the CE to be 32% and 8% for samples 6 and sample 8, respectively. Optical losses in the measurement are attributed to several practical factors, including challenges in properly coupling the light to the chip's input port (free-space end-fire setup using lenses to resize the optical fiber mode to match the waveguide mode), fabrication imperfections, parasitic reflections within the waveguide structure due to cleaved facets, or the filtering of higher-order modes within the MMI region. These factors collectively contribute to the reported losses measured.

5. Conclusion

We have presented results for a high-performance duplexers based on, on-chip angled MMI configuration, for wavelengths 1530 nm - 1653.7 nm, 1530 nm - 1684 nm, 1530 nm - 2003nm. The coupling efficiencies are numerically verified for various modes of operation, including the fundamental, higher-order, and realistic diode lasers mode profiles, for all target wavelengths. The experimental results show significant enhancement in measured coupling efficiency of the duplexers with 57% and 68% for target wavelengths of 1530 nm and 1653.7 nm, respectively. Following similar design and fabrication principles, duplexers can be designed for operation at other wavelengths such as 1684 nm 2003nm amongst others and be utilized for customized applications in multi-gas sensing and telecommunication fields.

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Disclosures. The authors declare that there is no conflict of interest.

Data availability. Data implicit in the results submitted in this report are not publicly accessible at this time but may be obtained from the authors upon reasonable request.

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