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Design of a multimode interferometer-based mid-infrared multispecies gas sensor

Loïc Bodiou, Yannick Dumeige, Simone Normani, Geoffrey Louvet, Petr Němec, Virginie Nazabal, and Joël Charrier

Abstract—A 1×2 multimode interferometer beam splitter based on mid-infrared emitting chalcogenides waveguides is designed. This device multiplexes mid-infrared light in two channels whose respective passbands overlap either CO₂ or CO absorption bands, respectively between 4.20–4.32 μm and 4.50–4.86 μm . The proposed device offers a low-cost solution for monolithic combination of broadband on-chip mid-infrared light emission with dispersive spectroscopic element devoted to mid-IR multigas sensing applications. Based on restrictive interference mechanism in a 1×2 multimode interferometer, the multimode section dimensions (width and length) are engineered to increase the imbalance between the two ports for the two passbands and consequently to increase the output contrast ratio. Tolerances to variations from the optimum device design resulting from processing conditions (materials fabrication and sputtering, photolithography and dry etching steps) are assessed. In particular, the 1×2 multimode interferometer diplexer spectral transmission is investigated as a function of deposited film refractive index and multimode section dimensions (width and length) deviation from designed values. Input and output ports tapering is introduced to reduce the device insertion loss.

Index Terms—Amorphous materials, Chalcogenides thin films, Environmental monitoring, Infrared spectroscopy, Integrated circuit design, Luminescent devices, Mid-Infrared sensors, Optical strip waveguides components, Photonic Integrated Circuits, And Praseodymium

I. INTRODUCTION

MID-IR (mid-IR) integrated sensing of liquids and gases [1] has found applications as diverse as environmental monitoring and pollutant detection (smoke and greenhouse gases detection [2], emerging water pollutant identification [3]), military and homeland security (detection of drugs [4] and hazardous materials [5]) but also industrial and healthcare (food processing industry, pharmaceutical and medical products identification [6]).

Different bulk optical components (modulator, splitter or polarizer) have been transposed in photonic integrated circuits (PIC) thanks to technical advancements witnessed in the last two decades. In particular, recent advancements have associated both the mid-IR light source (Quantum Cascade Lasers or QCL) and waveguides [7]–[9] or transducer and detector [2] on the same chip. However, monolithic integration of a complete sensing platform combining a

broadband mid-IR light source, transducer and detector is still challenging [10],[11].

To improve detection capability of photonic integrated circuits, numerous works have also targeted the miniaturization of optical spectrometers. Various configurations of Fourier Transform spectrometers, namely spatial heterodyne spectrometers (SHS) and stationary-wave integrated Fourier-transform spectrometry (SWIFTS) systems have been reported using different materials platforms including silicon [12],[13], Ge rich SiGe [14],[15], silicon nitride [16] or lithium niobate [17]. Other spectroscopic or (de)multiplexing systems based on dispersive devices such as array waveguide gratings (AWG) [18]–[20] planar concave gratings (also known as echelle grating) [21]–[23] have also been demonstrated to operate in mid-IR spectral domain. Wavelength division (de)multiplexer based on multimode interferometers (MMI) have been proposed to split telecommunication wavelengths (1.3/1.55 μm [24] and 1.55/2 μm multiplexers [25]). MMI devices operating at mid-IR wavelengths have also been implemented using silicon on insulator [26],[27] suspended silicon [28] or chalcogenides [29] platforms.

As many gases, such as CH₄, CO₂, CO or NO_x have strong absorption features in the mid-IR, environmental monitoring will benefit from the development of a spectroscopic sensing platform incorporating a broadband light source operating in the 3–5 μm spectral region. Rare-earth doped chalcogenides have been shown to display broadband mid-IR luminescence in integrated waveguides [30]–[32] and fibers [33]–[36] enabling remote detection of CH₄ and CO₂ for field operations or in situ monitoring in microfluidic system [2]–[4]. Therefore, monolithic association of a broadband mid-IR light source based on rare-earth doped chalcogenides with an integrated spectroscopic system made from the same materials could help the development of multi-analyte sensor systems on a chip that are expected to have a positive impact on a myriad of applications. In particular, an integrated dual-gas sensor for the simultaneous detection of CO₂ and CO gases could be advantageously used, for example, in the aeronautic industry [37]. Indeed, environmental regulations become more stringent and require the monitoring of aircraft emission to reduce greenhouse gas emission due to incomplete kerosene combustion.

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In this paper, we report the design of a 1×2 MMI multiplexer operating in the mid-IR spectral region based on chalcogenides waveguides to develop a multispecies gas sensor. The MMI dimensions are assessed to enable the multiplexing of mid-IR broadband emission from Pr^{3+} -doped selenides to develop a dual-gas sensor allowing simultaneous detection of CO and CO_2 gases. The MMI multimode section dimensions are engineered to enlarge the operation bandwidth and to diplex mid-IR light on two spectral windows overlapping CO and CO_2 absorption bands (Fig. 1), each of them coming through one of the two MMI output channels. The design robustness is then assessed over different parameters such as refractive index change or multimode section width and length variation. Finally, tapered input and output ports are introduced to further relax fabrication tolerances and to reduce device insertion optical losses.

II. DEVICE DESIGN

A. Device operating principles

In a conventional 1×2 MMI, a single-mode input port is laterally centered in relation to the multimode section width (w_{MMI}). Multiple optical modes are thus excited by the optical mode arising from the single-mode input. Constructive interferences between these modes give rise to single or multiple replica of the input mode in the multimode section at periodic positions along the propagation direction in a well-known self-imaging effect [38].

Under restricted interferences regime, the input and output ports are shifted by $\pm w_{\text{MMI}}/6$ with respect to the center of the multimode region width (Fig. 2). In such a case, only certain optical modes will be excited in the multimode section of the MMI. Therefore, solely direct or mirrored image of the input field will be observed along the propagation direction in the multimode section. These images will, respectively, occur at even and odd integers of the so-called beat length L_{π}^{λ} defined as:

$$L_{\pi}^{\lambda} = \frac{\pi}{\beta_0 - \beta_1} \approx \frac{4n_{\text{eff},0}^2 W_{\text{eff}}^2}{3\lambda} \quad (1)$$

where β_0 and β_1 are the propagation constants for the two lowest order modes, $n_{\text{eff},0}$ is the effective refractive index of the MMI multimode region fundamental mode, λ is the wavelength and W_{eff} is the effective multimode section width which can be approximated to w_{MMI} for high contrast waveguides [38].

Based on the restricted interference mechanism in its multimode section, it is thus possible to use a MMI to separate two different wavelengths λ_1 and λ_2 incoming from the same input port into two output channels corresponding to port 1 and port 2 by forming a direct image at a given wavelength and a mirrored image at the other. To do so, the width and length of the MMI multimode section must be chosen to satisfy the following conditions [24],[25]:

$$L_{\text{MMI}} = p \cdot L_{\pi}^{\lambda_1} = (p + q) \cdot L_{\pi}^{\lambda_2} \quad (2)$$

where p is a positive integer, q is an odd integer and $L_{\pi}^{\lambda_i}$ is the beat length at the wavelength λ_i defined in (1).

In the proposed device, the MMI multimode section is designed so that the wavelengths corresponding to the absorption bands of CO_2 (black shaded region in Fig. 1) will

exit the MMI multimode section through one of the output ports whereas wavelengths corresponding to the absorption bands of CO (red shaded region in Fig. 1) will come out through the other output port.

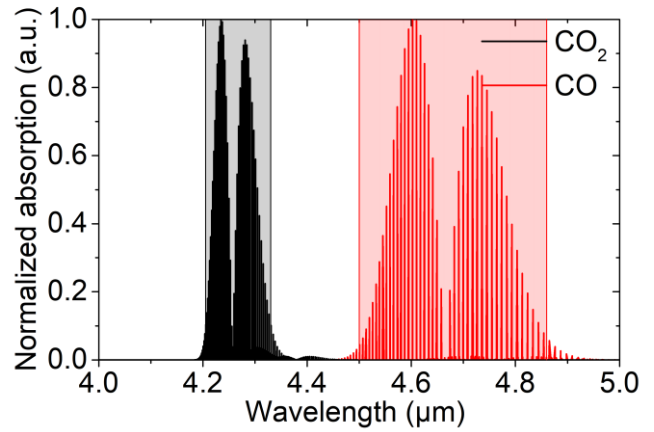


Fig. 1. Normalized absorption bands of carbon monoxide (CO) and carbon dioxide (CO_2). The two bands to multiplex are superimposed to these spectra.

B. Description of the MMI structure

The materials platform used to design the MMI follows from [30] where Praseodymium-doped selenides films ($\text{Ga}_5\text{Ge}_{20}\text{Sb}_{10}\text{Se}_{65} : 5000 \text{ ppm Pr}^{3+}$) are deposited from glass targets prepared by means of conventional melt and quenching method [39] by radio frequency (RF) magnetron sputtering on thermally oxidized ($4\text{-}\mu\text{m}$ thick SiO_2) $2''$ silicon wafer. Subsequent ridge waveguides fabrication was achieved through a classical i-line photolithographic process followed by a fluorine-based inductively coupled plasma-reactive ion etching (ICP-RIE) process. Single-mode waveguiding and photoluminescence overlapping CO and CO_2 absorption in the 4 to 5 μm spectral range (Fig. 1) was previously observed [30],[40]. Fibers of the same glass composition but codoped with Dy^{3+} and Pr^{3+} enabled simultaneous detection of CO_2 and CH_4 [36]. The linear refractive indices used in the simulations for chalcogenide and SiO_2 thin films were, respectively, obtained from the analysis of variable angle spectroscopic ellipsometry data [41] and from [42].

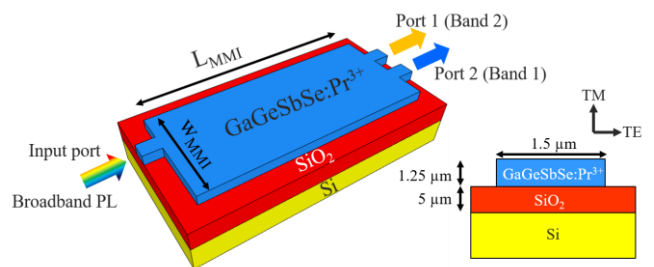


Fig. 2. Schematic representation of the multiplexing MMI structure based on GaGeSbSe:Pr^{3+} . The cross-section of the input port is displayed on the right.

C. MMI dimensions optimization

Simulations were performed using the FIMMPROP propagation module integrated with FIMMWAVE software and based on the eigenmode expansion (EME) method. These computations were undertaken with a real semi-vectorial finite difference method (FDM) mode solver in TE polarization and used a $50 \text{ nm} \times 50 \text{ nm}$ transverse grid size.

The optimization of the MMI multimode section dimensions is aimed at obtaining a direct image for

wavelengths used for sensing the first gas (band i) and a mirrored image for wavelengths at which the second gas absorbs (band j). In the simulations, the fundamental TE mode of the input waveguide corresponding to the cross-section displayed in Fig. 2 was launched at the MMI entrance. The transmitted power at both output ports was then monitored as a function of MMI multimode section width (w_{MMI}) and length (L_{MMI}) for different wavelengths corresponding to the absorption wavelengths of CO and CO₂ gases. The MMI width was scanned between 10 and 50 μm whereas MMI lengths ranged from 10 to 2500 μm (Fig. 3).

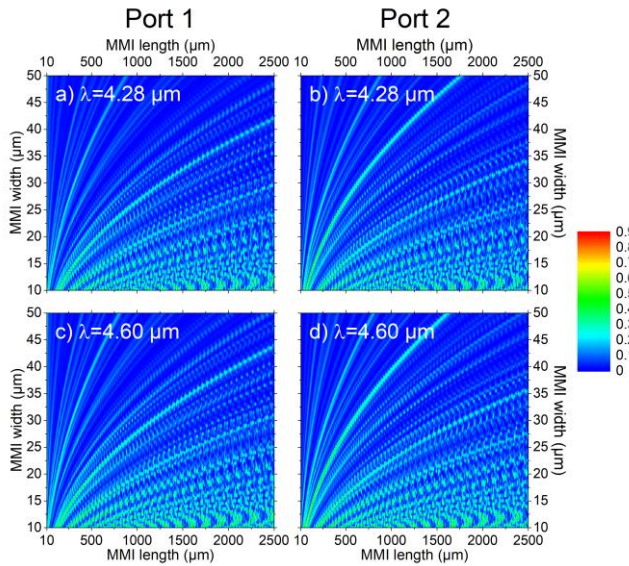


Fig. 3. Power transmission for the two output ports as a function of MMI multimode section width (w_{MMI}) and length (L_{MMI}) for two wavelengths: a), b) 4.28 μm and c), d) 4.6 μm .

Simulation results obtained for wavelengths equal to $\lambda=4.28 \mu\text{m}$ and $\lambda=4.6 \mu\text{m}$ corresponding, respectively, to the wavelengths of maximum absorption from CO₂ and CO gases are displayed in Fig. 3. From these different figures, it can be observed that, for some w_{MMI} and L_{MMI} , the imbalance between both ports can be high for two different wavelengths. However, in opposition to previously reported MMI-based multiplexers [24],[25], in this device, rather than single wavelengths, broad bands (150 to 350 nm) have to be separated. MMI transmission on both output ports was thus simulated for different wavelengths separated by 15 nm. Band 1 (corresponding to the black shaded area in Fig. 1) was sampled with 8 different wavelengths whereas 23 wavelengths were used for the broader second band (red shaded area in Fig. 1). The mean intensity on output ports 1 ($I_{Band 1, Port 1}$) and 2 ($I_{Band 1, Port 2}$) were then computed over Bands 1 and 2 for each (w_{MMI} , L_{MMI}) couple using the following expressions:

$$I_{Band 1, Port j} = \frac{\sum_{\lambda_i=1}^8 I_{Port j}^{\lambda_i}}{8} \quad (3)$$

$$I_{Band 2, Port j} = \frac{\sum_{\lambda_i=1}^{23} I_{Port j}^{\lambda_i}}{23} \quad (4)$$

where $j=1, 2$ and corresponds to output port number (Fig. 2). The sum does not contain the same number of wavelength terms for Band 1 and Band 2 because the spacing between simulated wavelengths was kept constant even if the absorption bands have different spectral widths. No

correction factors were applied to the terms of this calculation as flat-top passbands were considered to anticipate versatile device operation in terms of gas pressure or temperature resulting in absorption spectra change.

As there is no preferential output port for sensing any of the gases, the two output ports can be treated similarly. For each (w_{MMI} , L_{MMI}) couple, calculations were then performed to evaluate two different ratios defined as:

$$S_A = \frac{I_{Band 1, Port 1} \times I_{Band 2, Port 2}}{I_{Band 1, Port 2} \times I_{Band 2, Port 1}} \quad (5)$$

$$S_B = \frac{I_{Band 1, Port 2} \times I_{Band 2, Port 1}}{I_{Band 1, Port 1} \times I_{Band 2, Port 2}} \quad (6)$$

Maximization of S_A and S_B will result in the most efficient multiplexing of broadband light source over the two channels. In scheme A, for which S_A is maximal, the wavelengths devoted to CO₂ sensing (Band 1) would come out through port 1 (direct image) and wavelengths useful to detect CO (Band 2) would be transmitted through port 2 (mirror image). In scheme B, for which S_B is maximal, the application of the two channels would be opposite.

Some (w_{MMI} , L_{MMI}) couples enable the transmission of only a very small fraction of the incident light on one of the output ports. In that case, S_A and S_B can reach high values independently of the corresponding transmitted intensity through the other port. To avoid this numerical artifact, a minimum mean transmitted intensity of 35 % for the through port was added as a supplementary condition to the evaluation of S_A and S_B .

With these conditions, optimized dimensions of the MMI multimode region were found to be $w_{MMI}=10 \mu\text{m}$ and $L_{MMI}=519 \mu\text{m}$ (TABLE I).

TABLE I
LIST OF PARAMETERS OF OPTIMIZED MMI

Parameter	Value
Waveguide height h	1.25 μm
Input port width w	1.5 μm
Output ports width w	1.5 μm
Multimode section width w_{MMI}	10 μm
Multimode section length L_{MMI}	519 μm
Band 1	4.20 - 4.32 μm
Band 2	4.50 - 4.86 μm

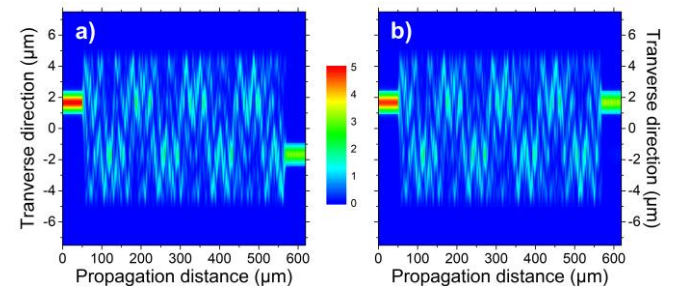


Fig. 4. Simulation of the power transmission for the MMI with optimized dimensions at a) 4.3 μm and b) 4.6 μm .

Fig. 4 shows the power transmission through the optimized MMI for wavelengths of 4.28 μm and 4.6 μm that are close to the absorption maxima of CO₂ and CO, respectively. From this Fig. 4, it can be seen that mid-IR light can efficiently be multiplexed over the two different output ports using a MMI operated in the restricted interferences regime.

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III. ROBUSTNESS TO FABRICATION TOLERANCES

As the device performances must not be altered by fabrication imperfections, it is important that tolerances are relaxed regarding the device fabrication and processing. These relaxed tolerances concern the reproducibility and the thermal variation (thermo-optic coefficient or dn/dT) of the refractive index of the sputtered Pr^{3+} -doped chalcogenides thin films but also the geometrical dimensions control during technological processing (photolithography and etching).

A. Refractive index change

Refractive index changes of the sputtered $Pr^{3+}:GaGeSbSe$ films can originate from various reasons. The most obvious is a variation related to the operating temperature, which will depend on the dn/dT coefficient not well-known in case of chalcogenide thin films. Considering values of 76 and $91 \times 10^{-6} K^{-1}$ (respectively at wavelength of 3.4 and 10.6 μm) for the thermo-optic coefficient of $Ge_{28}Sb_{12}Se_{60}$ glass and its thermal expansion coefficient of $14 \times 10^{-6} K^{-1}$, the dn/dT value of the $Ga_5Ge_{20}Sb_{10}Se_{65}$ glass composition, which displays a thermal expansion coefficient of $16 \times 10^{-6} K^{-1}$, might be slightly lower than $91 \times 10^{-6} \pm 10 \times 10^{-6} K^{-1}$ [43],[44]. If uniformity in terms of thickness and refractive index is observed over a 2" sample, there could be a ± 0.01 refractive index deviation from one film to another, due to the possible slight different composition of the target from batch to batch or wear of the target during deposition. To evaluate the impact of this effect, the wavelength dependence of the transmission through the two output ports of the optimized MMI structure (TABLE I) was simulated for different refractive index changes. Results from these simulations are displayed in Fig. 5.

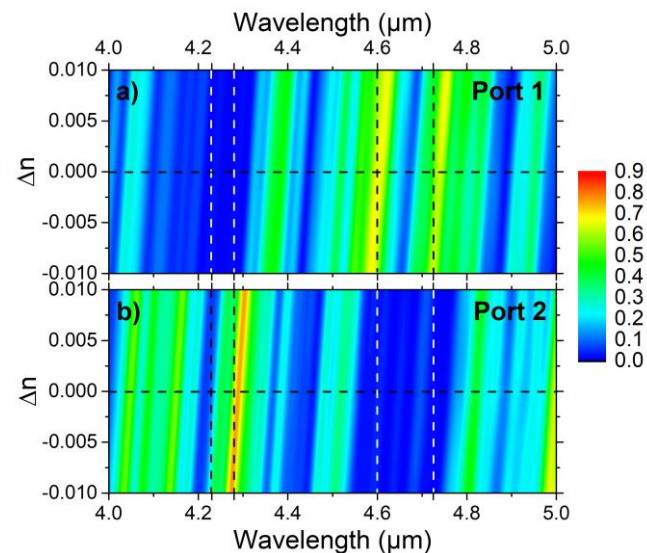


Fig. 5. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of chalcogenide film refractive index variations (Δn) for optimized MMI multimode section dimensions. Vertical dashed lines correspond to absorption maxima of CO_2 and CO .

Horizontal dashed lines in Fig. 5 correspond to the transmission through both output ports, respectively for Port 1 in Fig. 5a) and Port 2 in Fig. 5b), when the conventional refractive index of $Ga_5Ge_{20}Sb_{10}Se_{65} : 5000 \text{ ppm } Pr^{3+}$ is used in the simulations. Dashed vertical lines in Fig. 5 correspond

to the wavelengths of maximum absorption from CO and CO_2 (Fig. 1).

From this Fig. 5, it can be confirmed that the optimized MMI dimensions enable an efficient multiplexing of CO - and CO_2 related absorption bands through the two output ports. Indeed, a maximum of transmission over Band 1 or 2 on one port correspond a minimum of transmission of the same Band on the other port. Nonetheless, it can be noticed, in Fig. 5, that CO_2 second absorption band maximum is found at $\lambda=4.28 \mu m$ whereas the transmission maximum through Port 2 for MMI multimode section optimized dimensions is slightly shifted by 10 nm at $\lambda=4.29 \mu m$. The transmission through Port 2 of the optimized device (horizontal dashed line in Fig. 5) is about 65 % at $\lambda=4.28 \mu m$ and reaches 76 % at $\lambda=4.29 \mu m$. However, to ensure device operation in different environments in terms of gas pressure or temperature which will change gas absorption spectral signature, Bands have to be considered as flat-top pass-bands and consequently their respective bandwidths must be taken into account. This is the reason why MMI structure optimization procedure, through the maximization of $S_{A,B}$ (defined in Equations (5)-(6)), was targeting maximum transmission over a band whose bandwidth is more than 100 nm rather than at a specific wavelength.

From Fig. 5, it is also observed that the transmission band and bandwidth of any port are hardly affected by a moderate refractive index change up to ± 0.01 .

B. Multimode section width and length

The effect of processing imperfections must also be assessed. Indeed, lithographic (photoresist aging, thickness or exposure variation) and etching (plasma density) steps can strongly influence the geometric parameters of processed MMI. Evaluation of the designed MMI device variability on different levels scales (intra-die, die-to-die and wafer-to-wafer) must therefore be performed [45]. To this end, impact of MMI multimode section length and width variations were computed (Fig. 6 and Fig. 7).

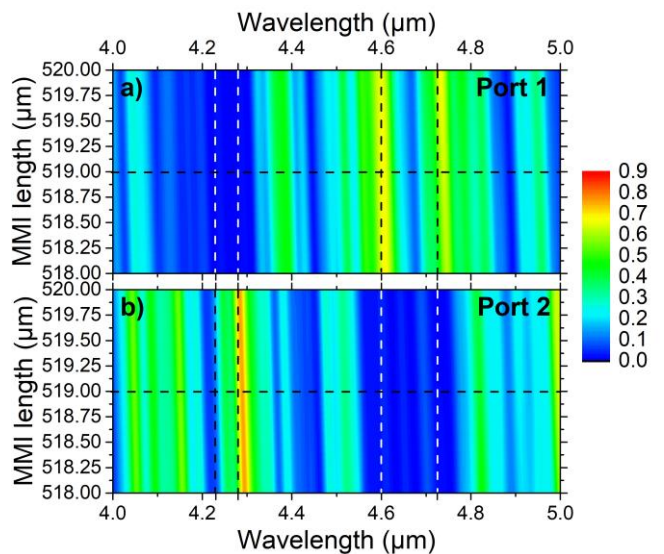


Fig. 6. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of MMI multimode section length (L_{MMI}).

From Fig. 6, it can be seen that the global shape of the color

maps yields almost vertical lines, which means that the wavelength dependence of the transmission on both ports is rather similar for each MMI multimode section length L_{MMI} simulated. Consequently, important variations of the MMI multimode section length hardly influences the wavelength response of the transmission. As it can be envisioned that processed devices will not suffer from such large ($\pm 1 \mu\text{m}$) length variations, this parameter change is expected not to strongly affect the device performance.

The color maps presented in Fig. 7 display a very different behavior compared to those observed in Fig. 5 and Fig. 6 where vertical shapes could be seen. For example, in Fig. 7, a 200 nm change of w_{MMI} (from 10 μm to 9.8 μm) decreases the transmission at 4.29 μm and at 4.6 μm , respectively through Port 2 and Port 1, from $\sim 80\%$ to less than 10%. This spectral dependence of the multiplexing on MMI multimode section width can be explained by the corresponding effective refractive index change, which strongly impacts the beat length and thus the transmission.

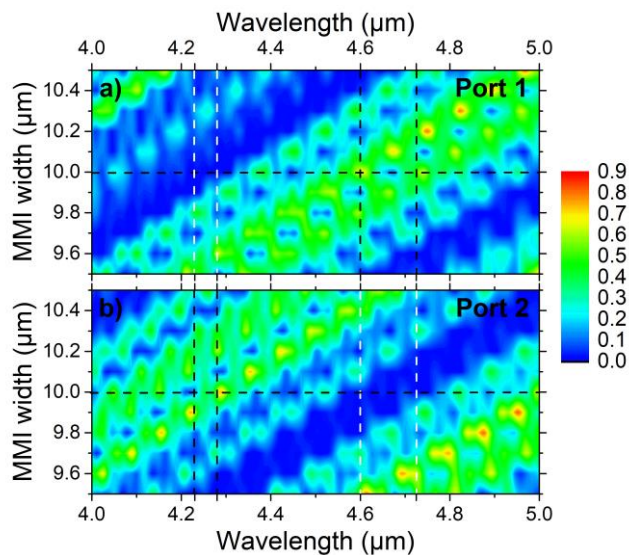


Fig. 7. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of MMI multimode section width (w_{MMI}) with straight input and output ports (ports width=1.5 μm).

C. Tapered input and output ports

Tapered port implementation was demonstrated to advantageously enable device insertion loss reduction and relax the impact of fabrication errors on MMI transmission [46],[47]. To enhance device transmission and to mitigate the detrimental effect of w_{MMI} change on spectral transmission, tapered input and output ports were then introduced in the simulations. The designed taper is identical on all ports (input and output) and consists of a 25- μm long linear tapering of the port waveguide width. Simulation results are presented in Fig. 8.

The taper width was scanned between $w_{\text{taper}}=1.5 \mu\text{m}$ to $w_{\text{taper}}=3.25 \mu\text{m}$. The former width corresponds to the single mode straight waveguides width whereas the latter is approximately equal to half of the distance between output ports. From Fig. 8, it can be noticed that the transmission increases globally as the taper width is enlarged. For large widths (above $w_{\text{taper}}=3 \mu\text{m}$), the pass bands widen and tend to shift relative to the absorption maxima of CO_2 and CO (represented by the vertical dashed lines). An optimum taper

width of 3 μm is therefore inferred from this Fig. 8. These results are in accordance with previous reports stating that the optimum taper width with regards to transmission is $3/10^{\text{th}}$ of the MMI multimode width [29].

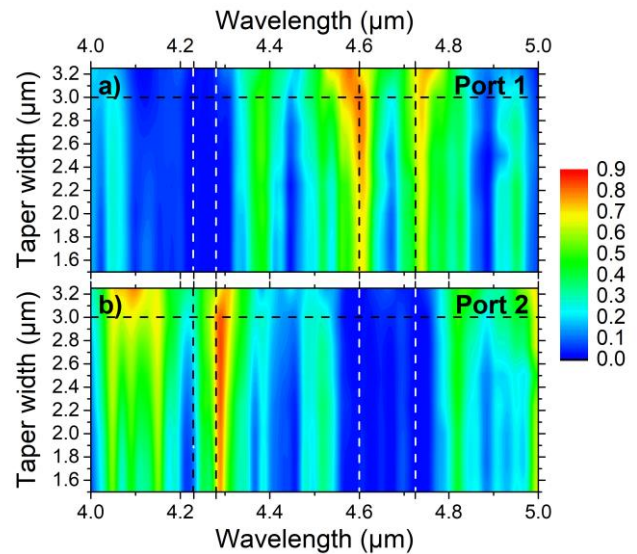


Fig. 8. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of input and output ports taper width (w_{taper}).

The spectral dependence of transmission through both ports was calculated (Fig. 9) for a taper width of $w_{\text{taper}}=3 \mu\text{m}$ (represented by the horizontal dashed line in Fig. 8). From Fig. 9, it can be confirmed that tapering the output ports increases the overall transmission. In comparison to Fig. 7, it can also be observed that fabrication tolerances are relaxed even if the device may still be sensitive to variations larger than $\pm 100 \text{ nm}$.

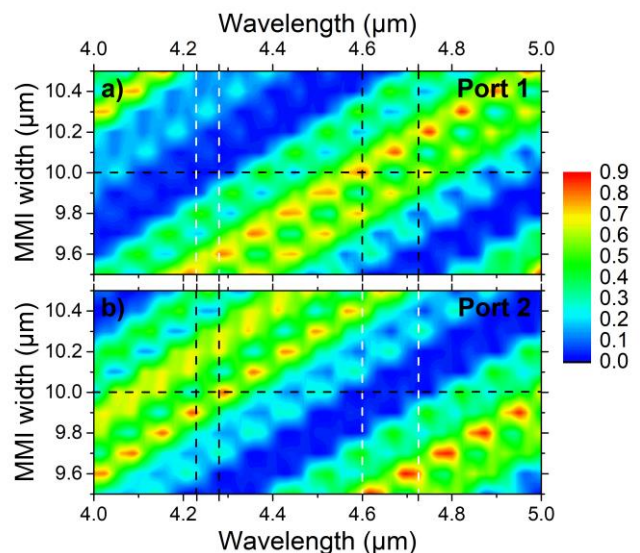


Fig. 9. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of MMI multimode section width (w_{MMI}) for an MMI with tapered input and output ports (taper width=3 μm).

IV. CONCLUSION

In this paper, a 1×2 MMI beam splitter based on luminescent Pr^{3+} -doped chalcogenides thin films and operating in the 4-5.5- μm wavelength range was investigated. This device relates on restricted interferences mechanism to multiplex Pr^{3+} luminescence on two spectral bands overlapping CO_2 and CO absorption bands. The device was

designed to be scarcely affected by imperfections occurring during processing steps (chalcogenide glass target fabrication and amorphous chalcogenide thin film deposition, photolithography, ICP-RIE etching). Optimum MMI dimensions were calculated and sensibility to refractive index, MMI multimode section width and length variations were studied. Finally, MMI ports tapering were implemented to enhance the device transmission.

The proposed combination of luminescent amorphous chalcogenides thin films with spectroscopic elements could enable the development of on-chip mid-IR multi-gas sensing devices providing low-cost solution for on-field chemical analysis.

The operating principle of the device can be extended to other gases (NO_x , CH_4 , H_2O ...) displaying mid-IR absorption overlapping the broadband luminescence of Praseodymium ions but also to other rare-earth ions. Different mid-IR emission bands may be available in order to expand the operational range of this sensing device in terms of accessible wavelengths and target gases.

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Design of a multimode interferometer-based mid-infrared multispecies gas sensor

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Abstract—A 1×2 multimode interferometer beam splitter based on mid-infrared emitting chalcogenides waveguides is designed. This device multiplexes mid-infrared light in two channels whose respective passbands overlap either CO_2 or CO absorption bands, respectively between $4.20\text{--}4.32 \mu\text{m}$ and $4.50\text{--}4.86 \mu\text{m}$. The proposed device offers a low-cost solution for monolithic combination of broadband on-chip mid-infrared light emission with dispersive spectroscopic element devoted to mid-IR multigas sensing applications. Based on restrictive interference mechanism in a 1×2 multimode interferometer, the multimode section dimensions (width and length) are engineered to increase the imbalance between the two ports for the two passbands and consequently to increase the output contrast ratio. Tolerances to variations from the optimum device design resulting from processing conditions (materials fabrication and sputtering, photolithography and dry etching steps) are assessed. In particular, the 1×2 multimode interferometer diplexer spectral transmission is investigated as a function of deposited film refractive index and multimode section dimensions (width and length) deviation from designed values. Input and output ports tapering is introduced to reduce the device insertion loss.

Index Terms—Amorphous materials, Chalcogenides thin films, Environmental monitoring, Infrared spectroscopy, Integrated circuit design, Luminescent devices, Mid-Infrared sensors, Optical strip waveguides components, Photonic Integrated Circuits, And Praseodymium

I. INTRODUCTION

MID-IR (mid-IR) integrated sensing of liquids and gases [1] has found applications as diverse as environmental monitoring and pollutant detection (smoke and greenhouse gases detection [2], emerging water pollutant identification [3]), military and homeland security (detection of drugs [4] and hazardous materials [5]) but also industrial and healthcare (food processing industry, pharmaceutical and medical products identification [6]).

Different bulk optical components (modulator, splitter or polarizer) have been transposed in photonic integrated circuits (PIC) thanks to technical advancements witnessed in

the last two decades. In particular, recent advancements have associated both the mid-IR light source (Quantum Cascade Lasers or QCL) and waveguides [7]–[9] or transducer and detector [2] on the same chip. However, monolithic integration of a complete sensing platform combining a broadband mid-IR light source, transducer and detector is still challenging [10],[11].

To improve detection capability of photonic integrated circuits, numerous works have also targeted the miniaturization of optical spectrometers. Various configurations of Fourier Transform spectrometers, namely spatial heterodyne spectrometers (SHS) and stationary-wave integrated Fourier-transform spectrometry (SWIFTS) systems have been reported using different materials platforms including silicon [12],[13], Ge rich SiGe [14],[15], silicon nitride [16] or lithium niobate [17]. Other spectroscopic or (de)multiplexing systems based on dispersive devices such as array waveguide gratings (AWG) [18]–[20] planar concave gratings (also known as echelle grating) [21]–[23] have also been demonstrated to operate in mid-IR spectral domain. Wavelength division (de)multiplexer based on multimode interferometers (MMI) have been proposed to split telecommunication wavelengths ($1.3/1.55 \mu\text{m}$ [24] and $1.55/2 \mu\text{m}$ multiplexers [25]). MMI devices operating at mid-IR wavelengths have also been implemented using silicon on insulator [26],[27] suspended silicon [28] or chalcogenides [29] platforms.

As many gases, such as CH_4 , CO_2 , CO or NO_x have strong absorption features in the mid-IR, environmental monitoring will benefit from the development of a spectroscopic sensing platform incorporating a broadband light source operating in the $3\text{--}5 \mu\text{m}$ spectral region. Rare-earth doped chalcogenides have been shown to display broadband mid-IR luminescence in integrated waveguides [30]–[32] and fibers [33]–[36] enabling remote detection of CH_4 and CO_2 for field operations or in situ monitoring in microfluidic system [2]–[4]. Therefore, monolithic association of a broadband mid-IR light source based on rare-earth doped chalcogenides with an integrated spectroscopic system made from the same materials could help the development of multi-analyte sensor systems on a chip that are expected to have a positive impact on a myriad of applications. In particular, an integrated dual-gas sensor for the simultaneous detection of CO_2 and CO gases could be advantageously used, for example, in the aeronautic industry [37]. Indeed, environmental regulations become more stringent and require the monitoring of aircraft emission to reduce greenhouse gas emission due to incomplete kerosene combustion.

In this paper, we report the design of a 1×2 MMI

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1
2 multiplexer operating in the mid-IR spectral region based on
3 chalcogenides waveguides to develop a multispecies gas
4 sensor. The MMI dimensions are assessed to enable the
5 multiplexing of mid-IR broadband emission from Pr³⁺-doped
6 selenides to develop a dual-gas sensor allowing simultaneous
7 detection of CO and CO₂ gases. The MMI multimode section
8 dimensions are engineered to enlarge the operation
9 bandwidth and to diplex mid-IR light on two spectral
10 windows overlapping CO and CO₂ absorption bands (Fig. 1),
11 each of them coming through one of the two MMI output
12 channels. The design robustness is then assessed over
13 different parameters such as refractive index change or
14 multimode section width and length variation. Finally,
15 tapered input and output ports are introduced to further relax
16 fabrication tolerances and to reduce device insertion optical
17 losses.

19 II. DEVICE DESIGN

21 A. Device operating principles

22 In a conventional 1 × 2 MMI, a single-mode input port is
23 laterally centered in relation to the multimode section width
24 (w_{MMI}). Multiple optical modes are thus excited by the optical
25 mode arising from the single-mode input. Constructive
26 interferences between these modes give rise to single or
27 multiple replica of the input mode in the multimode section
28 at periodic positions along the propagation direction in a well-
29 known self-imaging effect [38].

30 Under restricted interferences regime, the input and output
31 ports are shifted by ±w_{MMI}/6 with respect to the center of the
32 multimode region width (Fig. 2). In such a case, only certain
33 optical modes will be excited in the multimode section of the
34 MMI. Therefore, solely direct or mirrored image of the input
35 field will be observed along the propagation direction in the
36 multimode section. These images will, respectively, occur at
37 even and odd integers of the so-called beat length L_{π}^{λ} defined
38 as:

$$39 \quad L_{\pi}^{\lambda} = \frac{\pi}{\beta_0 - \beta_1} \approx \frac{4 \cdot n_{\text{eff},0} \cdot W_{\text{eff}}^2}{3 \cdot \lambda} \quad (1)$$

40 where β_0 and β_1 are the propagation constants for the two
41 lowest order modes, $n_{\text{eff},0}$ is the effective refractive index of
42 the MMI multimode region fundamental mode, λ is the
43 wavelength and W_{eff} is the effective multimode section width
44 which can be approximated to w_{MMI} for high contrast
45 waveguides [38].

46 Based on the restricted interference mechanism in its
47 multimode section, it is thus possible to use a MMI to separate
48 two different wavelengths λ_1 and λ_2 incoming from the same
49 input port into two output channels corresponding to port 1
50 and port 2 by forming a direct image at a given wavelength
51 and a mirrored image at the other. To do so, the width and
52 length of the MMI multimode section must be chosen to
53 satisfy the following conditions [24],[25]:

$$54 \quad L_{\text{MMI}} = p \cdot L_{\pi}^{\lambda_1} = (p + q) \cdot L_{\pi}^{\lambda_2} \quad (2)$$

55 where p is a positive integer, q is an odd integer and $L_{\pi}^{\lambda_i}$ is
56 the beat length at the wavelength λ_i defined in (1).

57 In the proposed device, the MMI multimode section is
58 designed so that the wavelengths corresponding to the
59 absorption bands of CO₂ (black shaded region in Fig. 1) will
60 exit the MMI multimode section through one of the output

ports whereas wavelengths corresponding to the absorption
bands of CO (red shaded region in Fig. 1) will come out
through the other output port.

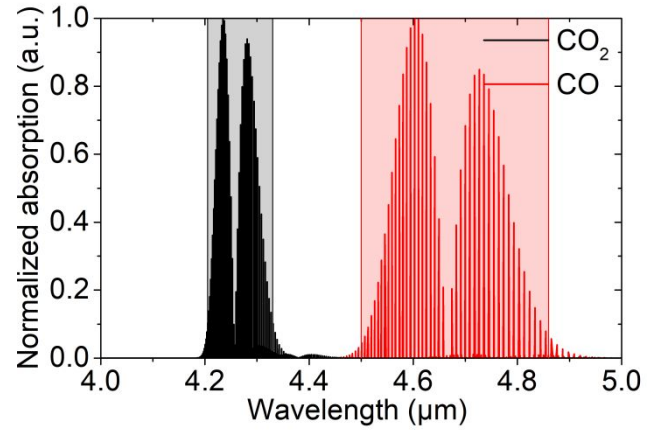


Fig. 1. Normalized absorption bands of carbon monoxide (CO) and carbon dioxide (CO₂). The two bands to multiplex are superimposed to these spectra.

21 B. Description of the MMI structure

22 The materials platform used to design the MMI follows
23 from [30] where Praseodymium-doped selenides films
24 (Ga₅Ge₂₀Sb₁₀Se₆₅ : 5000 ppm Pr³⁺) are deposited from glass
25 targets prepared by means of conventional melt and
26 quenching method [39] by radio frequency (RF) magnetron
27 sputtering on thermally oxidized (4-μm thick SiO₂) 2'' silicon
28 wafer. Subsequent ridge waveguides fabrication was
29 achieved through a classical i-line photolithographic process
30 followed by a fluorine-based inductively coupled plasma-
31 reactive ion etching (ICP-RIE) process. Single-mode
32 waveguiding and photoluminescence overlapping CO and
33 CO₂ absorption in the 4 to 5 μm spectral range (Fig. 1) was
34 previously observed [30],[40]. Fibers of the same glass
35 composition but codoped with Dy³⁺ and Pr³⁺ enabled
36 simultaneous detection of CO₂ and CH₄ [36]. The linear
37 refractive indices used in the simulations for chalcogenide
38 and SiO₂ thin films were, respectively, obtained from the
39 analysis of variable angle spectroscopic ellipsometry data
40 [41] and from [42].

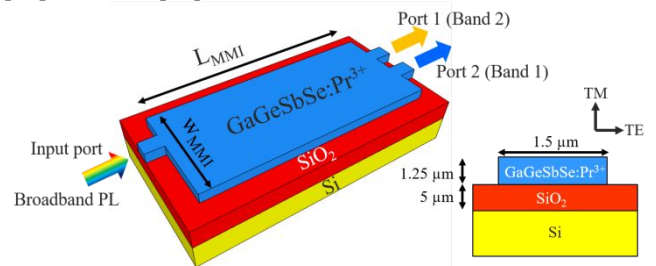


Fig. 2. Schematic representation of the multiplexing MMI structure based on GaGeSbSe:Pr³⁺. The cross-section of the input port is displayed on the right.

53 C. MMI dimensions optimization

54 Simulations were performed using the FIMMPROP
55 propagation module integrated with FIMMWAVE software
56 and based on the eigenmode expansion (EME) method. These
57 computations were undertaken with a real semi-vectorial
58 finite difference method (FDM) mode solver in TE
59 polarization and used a 50 nm × 50 nm transverse grid size.

60 The optimization of the MMI multimode section
dimensions is aimed at obtaining a direct image for
wavelengths used for sensing the first gas (band i) and a

mirrored image for wavelengths at which the second gas absorbs (band j). In the simulations, the fundamental TE mode of the input waveguide corresponding to the cross-section displayed in Fig. 2 was launched at the MMI entrance. The transmitted power at both output ports was then monitored as a function of MMI multimode section width (w_{MMI}) and length (L_{MMI}) for different wavelengths corresponding to the absorption wavelengths of CO and CO₂ gases. The MMI width was scanned between 10 and 50 μm whereas MMI lengths ranged from 10 to 2500 μm (Fig. 3).

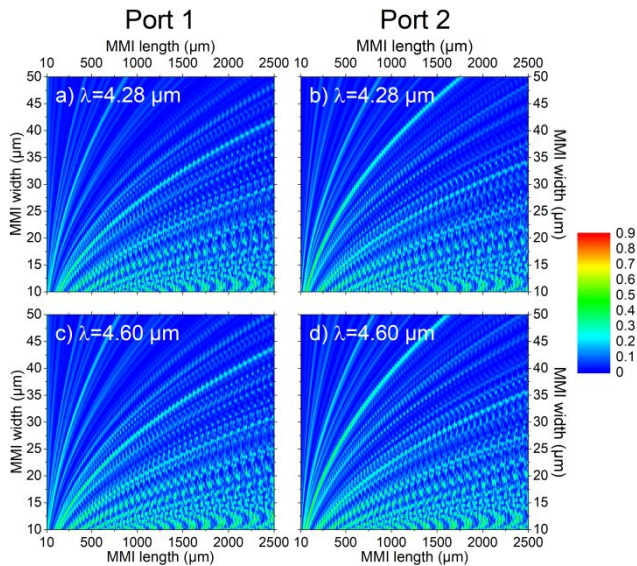


Fig. 3. Power transmission for the two output ports as a function of MMI multimode section width (w_{MMI}) and length (L_{MMI}) for two wavelengths: a), b) 4.28 μm and c), d) 4.6 μm .

Simulation results obtained for wavelengths equal to $\lambda=4.28 \mu\text{m}$ and $\lambda=4.6 \mu\text{m}$ corresponding, respectively, to the wavelengths of maximum absorption from CO₂ and CO gases are displayed in Fig. 3. From these different figures, it can be observed that, for some w_{MMI} and L_{MMI} , the imbalance between both ports can be high for two different wavelengths. However, in opposition to previously reported MMI-based multiplexers [24],[25], in this device, rather than single wavelengths, broad bands (150 to 350 nm) have to be separated. MMI transmission on both output ports was thus simulated for different wavelengths separated by 15 nm. Band 1 (corresponding to the black shaded area in Fig. 1) was sampled with 8 different wavelengths whereas 23 wavelengths were used for the broader second band (red shaded area in Fig. 1). The mean intensity on output ports 1 ($I_{\text{Band 1 or 2, Port 1}}$) and 2 ($I_{\text{Band 1 or 2, Port 2}}$) were then computed over Bands 1 and 2 for each (w_{MMI} , L_{MMI}) couple using the following expressions:

$$I_{\text{Band 1, Port } j} = \frac{\sum_{\lambda_i=1}^8 I_{\text{Port } j}^{\lambda_i}}{8} \quad (3)$$

$$I_{\text{Band 2, Port } j} = \frac{\sum_{\lambda_i=1}^{23} I_{\text{Port } j}^{\lambda_i}}{23} \quad (4)$$

where $j=1, 2$ and corresponds to output port number (Fig. 2). The sum does not contain the same number of wavelength terms for Band 1 and Band 2 because the spacing between simulated wavelengths was kept constant even if the absorption bands have different spectral widths. No correction factors were applied to the terms of this calculation

as flat-top passbands were considered to anticipate versatile device operation in terms of gas pressure or temperature resulting in absorption spectra change.

As there is no preferential output port for sensing any of the gases, the two output ports can be treated similarly. For each (w_{MMI} , L_{MMI}) couple, calculations were then performed to evaluate two different ratios defined as:

$$S_A = \frac{I_{\text{Band 1, Port 1}} \times I_{\text{Band 2, Port 2}}}{I_{\text{Band 1, Port 2}} \times I_{\text{Band 2, Port 1}}} \quad (5)$$

$$S_B = \frac{I_{\text{Band 1, Port 2}} \times I_{\text{Band 2, Port 1}}}{I_{\text{Band 1, Port 1}} \times I_{\text{Band 2, Port 2}}} \quad (6)$$

Maximization of S_A and S_B will result in the most efficient multiplexing of broadband light source over the two channels. In scheme A, for which S_A is maximal, the wavelengths devoted to CO₂ sensing (Band 1) would come out through port 1 (direct image) and wavelengths useful to detect CO (Band 2) would be transmitted through port 2 (mirror image). In scheme B, for which S_B is maximal, the application of the two channels would be opposite.

Some (w_{MMI} , L_{MMI}) couples enable the transmission of only a very small fraction of the incident light on one of the output ports. In that case, S_A and S_B can reach high values independently of the corresponding transmitted intensity through the other port. To avoid this numerical artifact, a minimum mean transmitted intensity of 35 % for the through port was added as a supplementary condition to the evaluation of S_A and S_B .

With these conditions, optimized dimensions of the MMI multimode region were found to be $w_{\text{MMI}}=10 \mu\text{m}$ and $L_{\text{MMI}}=519 \mu\text{m}$ (TABLE I).

TABLE I
LIST OF PARAMETERS OF OPTIMIZED MMI

Parameter	Value
Waveguide height h	1.25 μm
Input port width w	1.5 μm
Output ports width w	1.5 μm
Multimode section width w_{MMI}	10 μm
Multimode section length L_{MMI}	519 μm
Band 1	4.20 - 4.32 μm
Band 2	4.50 - 4.86 μm

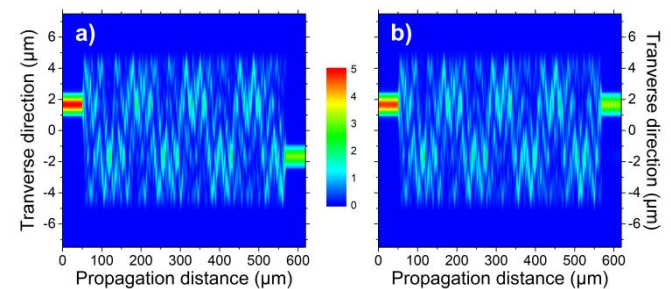


Fig. 4. Simulation of the power transmission for the MMI with optimized dimensions at a) 4.3 μm and b) 4.6 μm .

Fig. 4 shows the power transmission through the optimized MMI for wavelengths of 4.28 μm and 4.6 μm that are close to the absorption maxima of CO₂ and CO, respectively. From this Fig. 4, it can be seen that mid-IR light can efficiently be multiplexed over the two different output ports using a MMI operated in the restricted interferences regime.

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III. ROBUSTNESS TO FABRICATION TOLERANCES

As the device performances must not be altered by fabrication imperfections, it is important that tolerances are relaxed regarding the device fabrication and processing. These relaxed tolerances concern the reproducibility and the thermal variation (thermo-optic coefficient or dn/dT) of the refractive index of the sputtered Pr^{3+} -doped chalcogenides thin films but also the geometrical dimensions control during technological processing (photolithography and etching).

A. Refractive index change

Refractive index changes of the sputtered $Pr^{3+}:GaGeSbSe$ films can originate from various reasons. The most obvious is a variation related to the operating temperature, which will depend on the dn/dT coefficient not well-known in case of chalcogenide thin films. Considering values of 76 and $91 \times 10^{-6} K^{-1}$ (respectively at wavelength of 3.4 and 10.6 μm) for the thermo-optic coefficient of $Ge_{28}Sb_{12}Se_{60}$ glass and its thermal expansion coefficient of $14 \times 10^{-6} K^{-1}$, the dn/dT value of the $Ga_5Ge_{20}Sb_{10}Se_{65}$ glass composition, which displays a thermal expansion coefficient of $16 \times 10^{-6} K^{-1}$, might be slightly lower than $91 \times 10^{-6} \pm 10 \times 10^{-6} K^{-1}$ [43],[44]. If uniformity in terms of thickness and refractive index is observed over a 2" sample, there could be a ± 0.01 refractive index deviation from one film to another, due to the possible slight different composition of the target from batch to batch or wear of the target during deposition. To evaluate the impact of this effect, the wavelength dependence of the transmission through the two output ports of the optimized MMI structure (TABLE I) was simulated for different refractive index changes. Results from these simulations are displayed in Fig. 5.

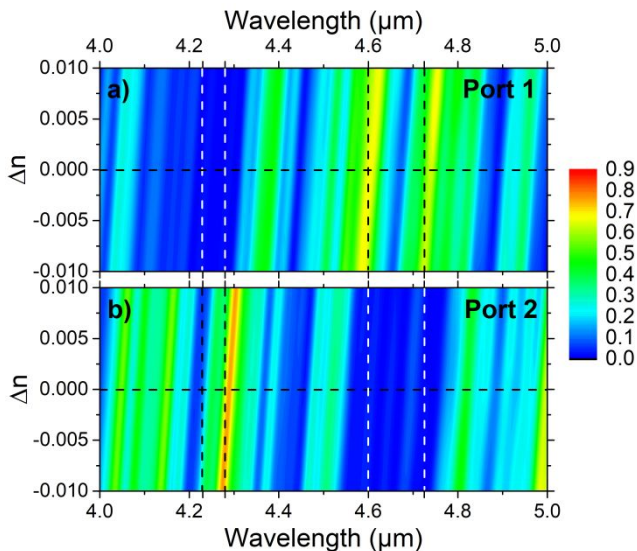


Fig. 5. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of chalcogenide film refractive index variations (Δn) for optimized MMI multimode section dimensions. Vertical dashed lines correspond to absorption maxima of CO_2 and CO.

Horizontal dashed lines in Fig. 5 correspond to the transmission through both output ports, respectively for Port 1 in Fig. 5a) and Port 2 in Fig. 5b), when the conventional refractive index of $Ga_5Ge_{20}Sb_{10}Se_{65} : 5000 \text{ ppm } Pr^{3+}$ is used in the simulations. Dashed vertical lines in Fig. 5 correspond

to the wavelengths of maximum absorption from CO and CO_2 (Fig. 1).

From this Fig. 5, it can be confirmed that the optimized MMI dimensions enable an efficient multiplexing of CO- and CO_2 related absorption bands through the two output ports. Indeed, a maximum of transmission over Band 1 or 2 on one port correspond a minimum of transmission of the same Band on the other port. Nonetheless, it can be noticed, in Fig. 5, that CO_2 second absorption band maximum is found at $\lambda=4.28 \mu m$ whereas the transmission maximum through Port 2 for MMI multimode section optimized dimensions is slightly shifted by 10 nm at $\lambda=4.29 \mu m$. The transmission through Port 2 of the optimized device (horizontal dashed line in Fig. 5) is about 65 % at $\lambda=4.28 \mu m$ and reaches 76 % at $\lambda=4.29 \mu m$. However, to ensure device operation in different environments in terms of gas pressure or temperature which will change gas absorption spectral signature, Bands have to be considered as flat-top pass-bands and consequently their respective bandwidths must be taken into account. This is the reason why MMI structure optimization procedure, through the maximization of $S_{A,B}$ (defined in Equations (5)-(6)), was targeting maximum transmission over a band whose bandwidth is more than 100 nm rather than at a specific wavelength.

From Fig. 5, it is also observed that the transmission band and bandwidth of any port are hardly affected by a moderate refractive index change up to ± 0.01 .

B. Multimode section width and length

The effect of processing imperfections must also be assessed. Indeed, lithographic (photoresist aging, thickness or exposure variation) and etching (plasma density) steps can strongly influence the geometric parameters of processed MMI. Evaluation of the designed MMI device variability on different levels scales (intra-die, die-to-die and wafer-to-wafer) must therefore be performed [45]. To this end, impact of MMI multimode section length and width variations were computed (Fig. 6 and Fig. 7).

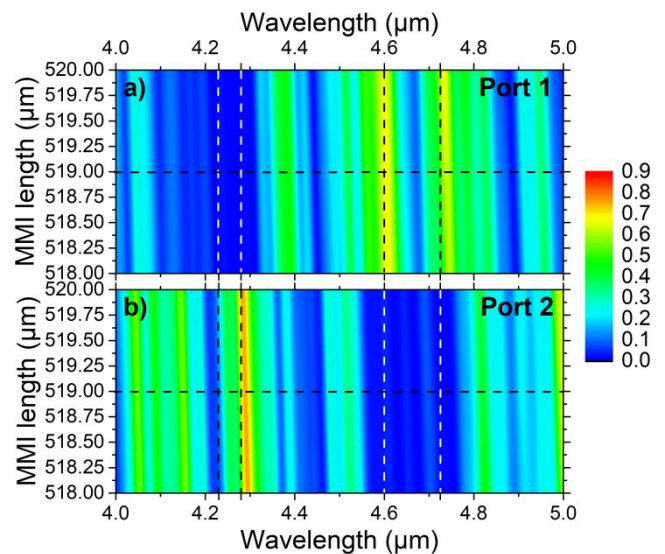


Fig. 6. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of MMI multimode section length (L_{MMI}).

From Fig. 6, it can be seen that the global shape of the color

maps yields almost vertical lines, which means that the wavelength dependence of the transmission on both ports is rather similar for each MMI multimode section length L_{MMI} simulated. Consequently, important variations of the MMI multimode section length hardly influences the wavelength response of the transmission. As it can be envisioned that processed devices will not suffer from such large ($\pm 1 \mu\text{m}$) length variations, this parameter change is expected not to strongly affect the device performance.

The color maps presented in Fig. 7 display a very different behavior compared to those observed in Fig. 5 and Fig. 6 where vertical shapes could be seen. For example, in Fig. 7, a 200 nm change of w_{MMI} (from 10 μm to 9.8 μm) decreases the transmission at 4.29 μm and at 4.6 μm , respectively through Port 2 and Port 1, from $\sim 80\%$ to less than 10%. This spectral dependence of the multiplexing on MMI multimode section width can be explained by the corresponding effective refractive index change, which strongly impacts the beat length and thus the transmission.

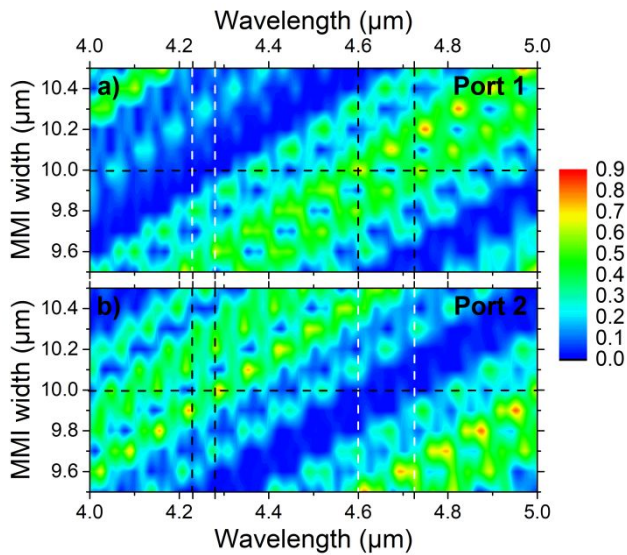


Fig. 7. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of MMI multimode section width (w_{MMI}) with straight input and output ports (ports width= $1.5 \mu\text{m}$).

C. Tapered input and output ports

Tapered port implementation was demonstrated to advantageously enable device insertion loss reduction and relax the impact of fabrication errors on MMI transmission [46],[47]. To enhance device transmission and to mitigate the detrimental effect of w_{MMI} change on spectral transmission, tapered input and output ports were then introduced in the simulations. The designed taper is identical on all ports (input and output) and consists of a 25- μm long linear tapering of the port waveguide width. Simulation results are presented in Fig. 8.

The taper width was scanned between $w_{\text{taper}}=1.5 \mu\text{m}$ to $w_{\text{taper}}=3.25 \mu\text{m}$. The former width corresponds to the single mode straight waveguides width whereas the latter is approximately equal to half of the distance between output ports. From Fig. 8, it can be noticed that the transmission increases globally as the taper width is enlarged. For large widths (above $w_{\text{taper}}=3 \mu\text{m}$), the pass bands widen and tend to shift relative to the absorption maxima of CO_2 and CO (represented by the vertical dashed lines). An optimum taper

width of 3 μm is therefore inferred from this Fig. 8. These results are in accordance with previous reports stating that the optimum taper width with regards to transmission is $3/10^{\text{th}}$ of the MMI multimode width [29].

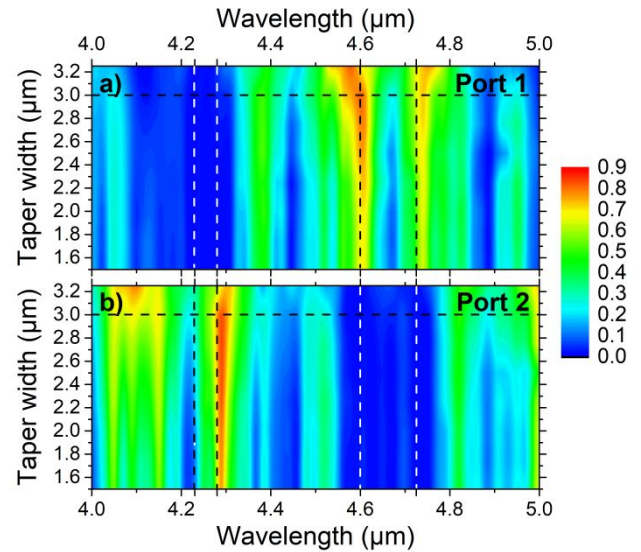


Fig. 8. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of input and output ports taper width (w_{taper}).

The spectral dependence of transmission through both ports was calculated (Fig. 9) for a taper width of $w_{\text{taper}}=3 \mu\text{m}$ (represented by the horizontal dashed line in Fig. 8). From Fig. 9, it can be confirmed that tapering the output ports increases the overall transmission. In comparison to Fig. 7, it can also be observed that fabrication tolerances are relaxed even if the device may still be sensitive to variations larger than $\pm 100 \text{ nm}$.

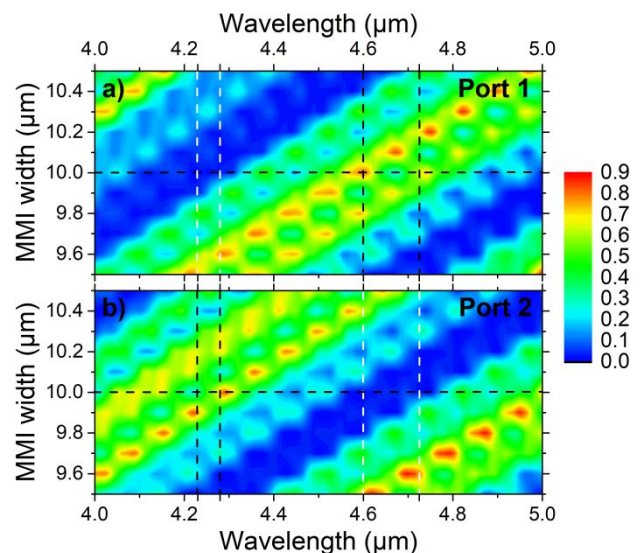


Fig. 9. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of MMI multimode section width (w_{MMI}) for an MMI with tapered input and output ports (taper width= $3 \mu\text{m}$).

IV. CONCLUSION

In this paper, a 1×2 MMI beam splitter based on luminescent Pr^{3+} -doped chalcogenides thin films and operating in the 4-5.5- μm wavelength range was investigated. This device relates on restricted interferences mechanism to multiplex Pr^{3+} luminescence on two spectral bands overlapping CO_2 and CO absorption bands. The device was

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designed to be scarcely affected by imperfections occurring during processing steps (chalcogenide glass target fabrication and amorphous chalcogenide thin film deposition, photolithography, ICP-RIE etching). Optimum MMI dimensions were calculated and sensibility to refractive index, MMI multimode section width and length variations were studied. Finally, MMI ports tapering were implemented to enhance the device transmission.

The proposed combination of luminescent amorphous chalcogenides thin films with spectroscopic elements could enable the development of on-chip mid-IR multi-gas sensing devices providing low-cost solution for on-field chemical analysis.

The operating principle of the device can be extended to other gases (NO_x , CH_4 , H_2O ...) displaying mid-IR absorption overlapping the broadband luminescence of Praseodymium ions but also to other rare-earth ions. Different mid-IR emission bands may be available in order to expand the operational range of this sensing device in terms of accessible wavelengths and target gases.

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4
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19 She received in 2010 a bronze medal of CNRS and a Pollutec-
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22 **Joël Charrier** received the Ph.D. degree from the
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25 nanostructured waveguides. Since 2000, he has been with the
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27 Rennes 1. He is interested in photonic integrated circuits for
28 optical communication and sensing applications. He is
29 currently the head of the Guided Optics and Sensors research
30 group (OGC-Optique Guidée et Capteurs) of FOTON
31 Institute.
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Table I

Parameter	Value
Waveguide height h	1.25 μm
Input port width w	1.5 μm
Output port width w	1.5 μm
Multimode section width w_{MMI}	10 μm
Multimode section length L_{MMI}	519 μm
Band 1	4.20 - 4.32 μm
Band 2	4.50 - 4.86 μm

Figure 1

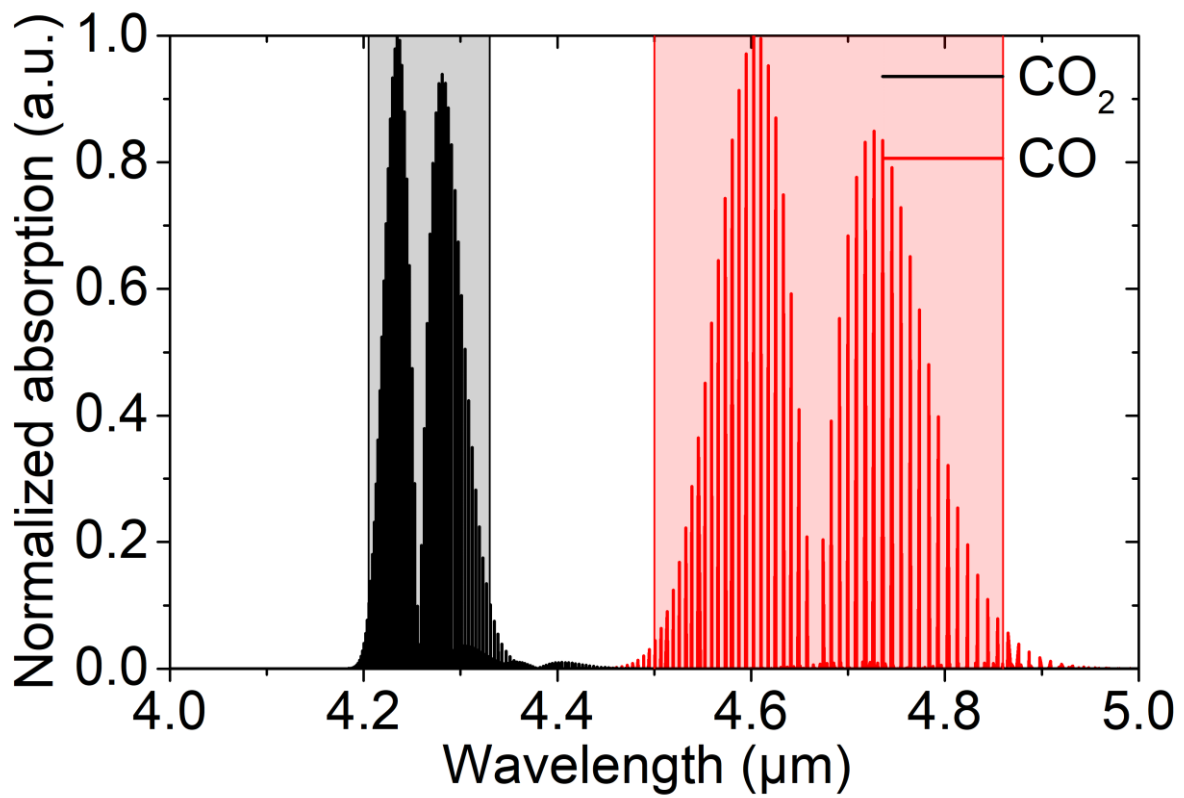


Figure 2

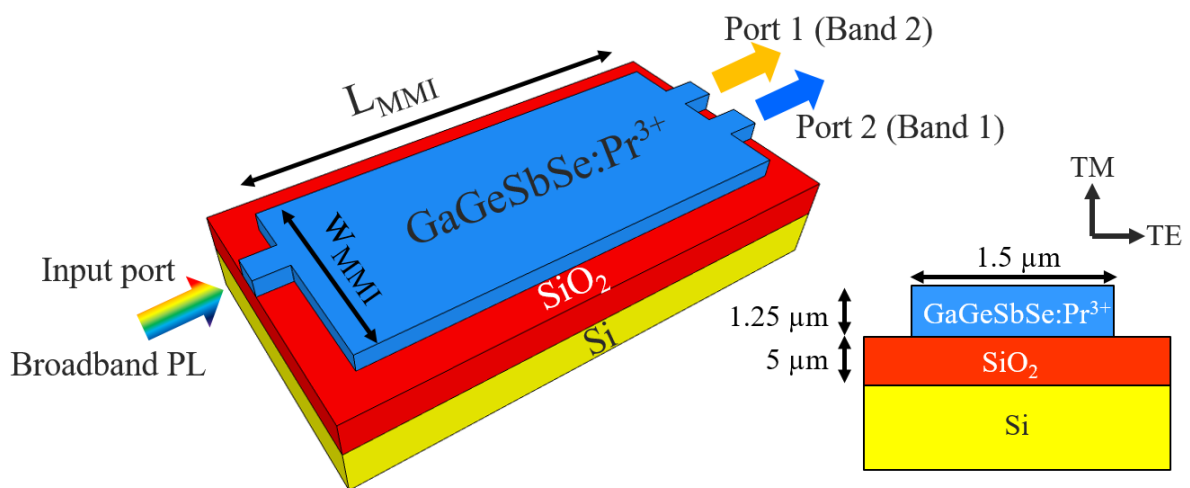


Figure 3

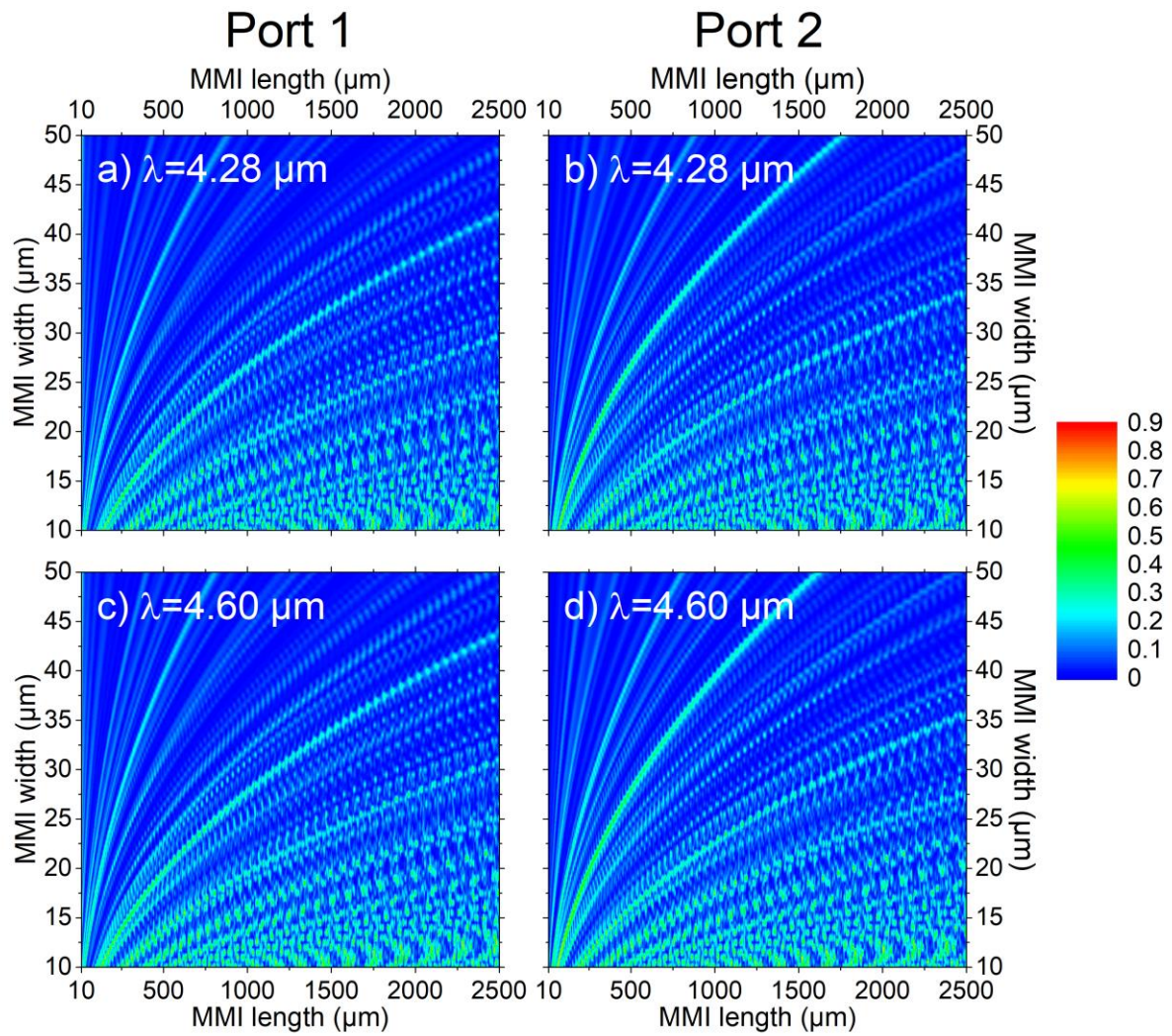
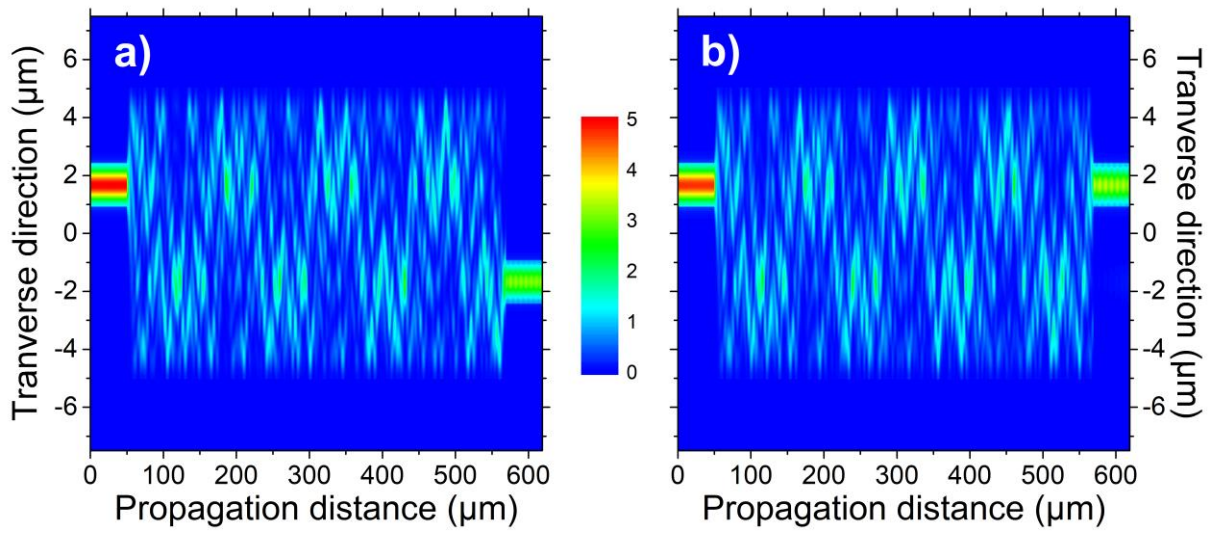


Figure 4



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Figure 5

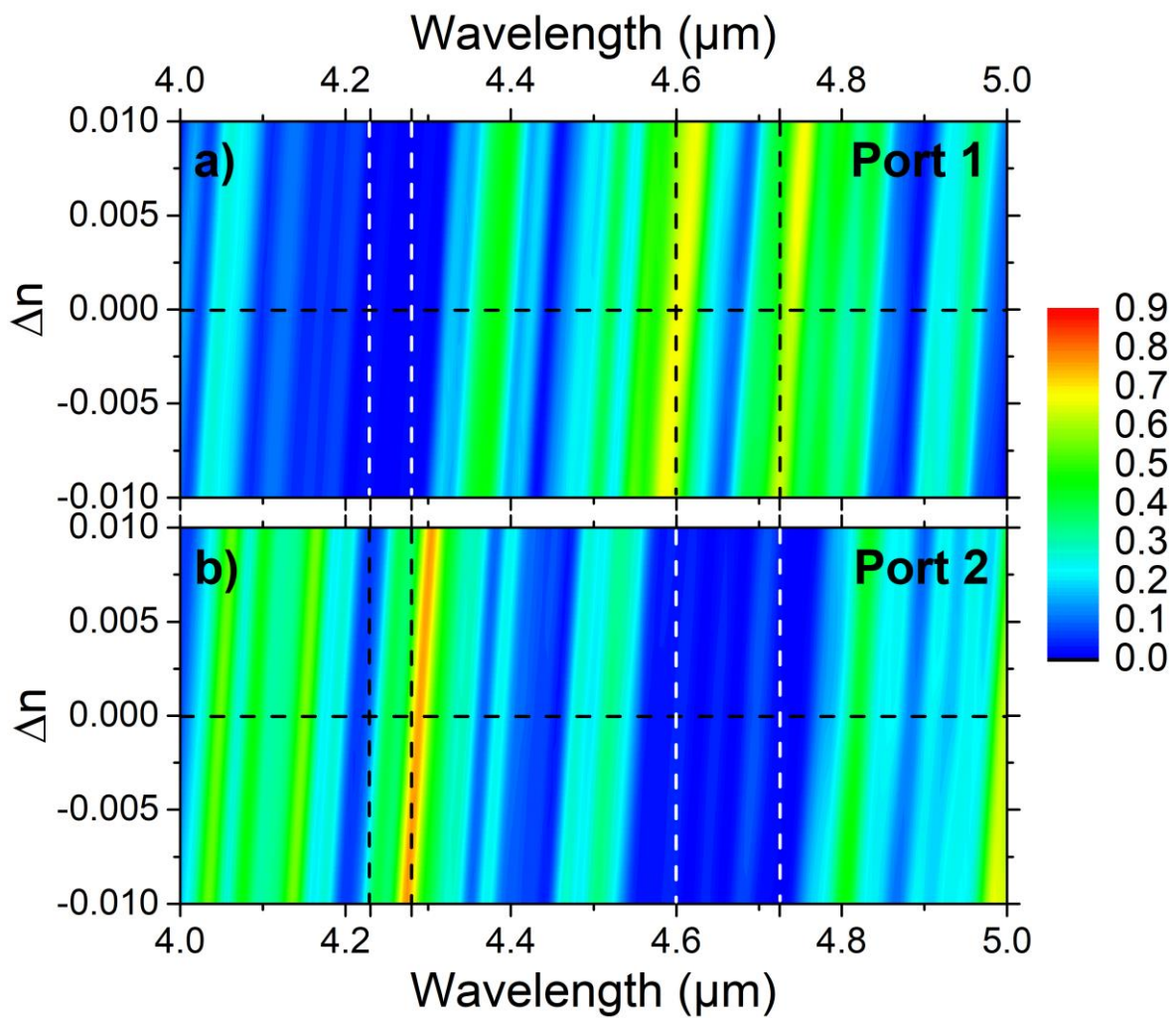


Figure 6

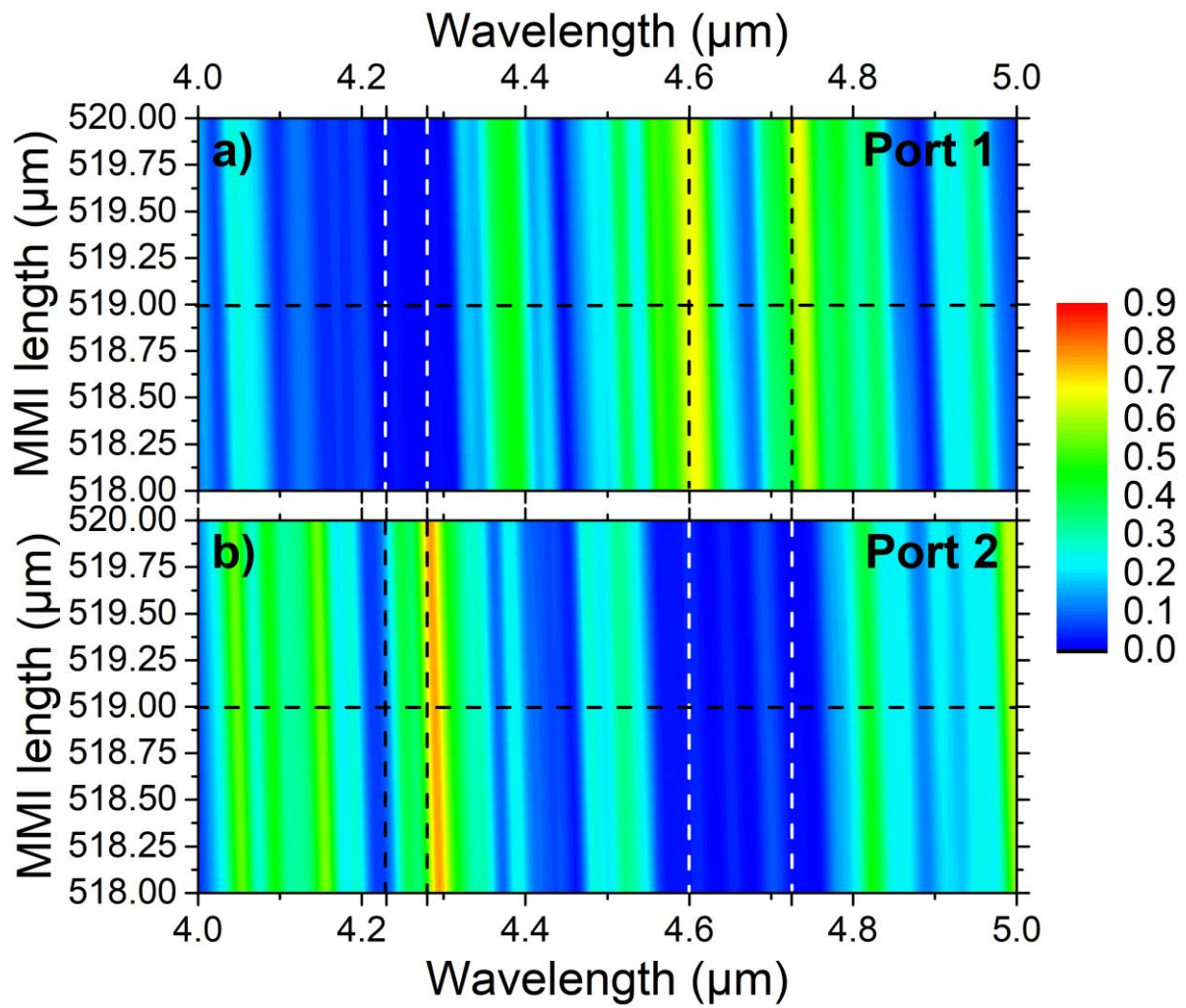


Figure 7

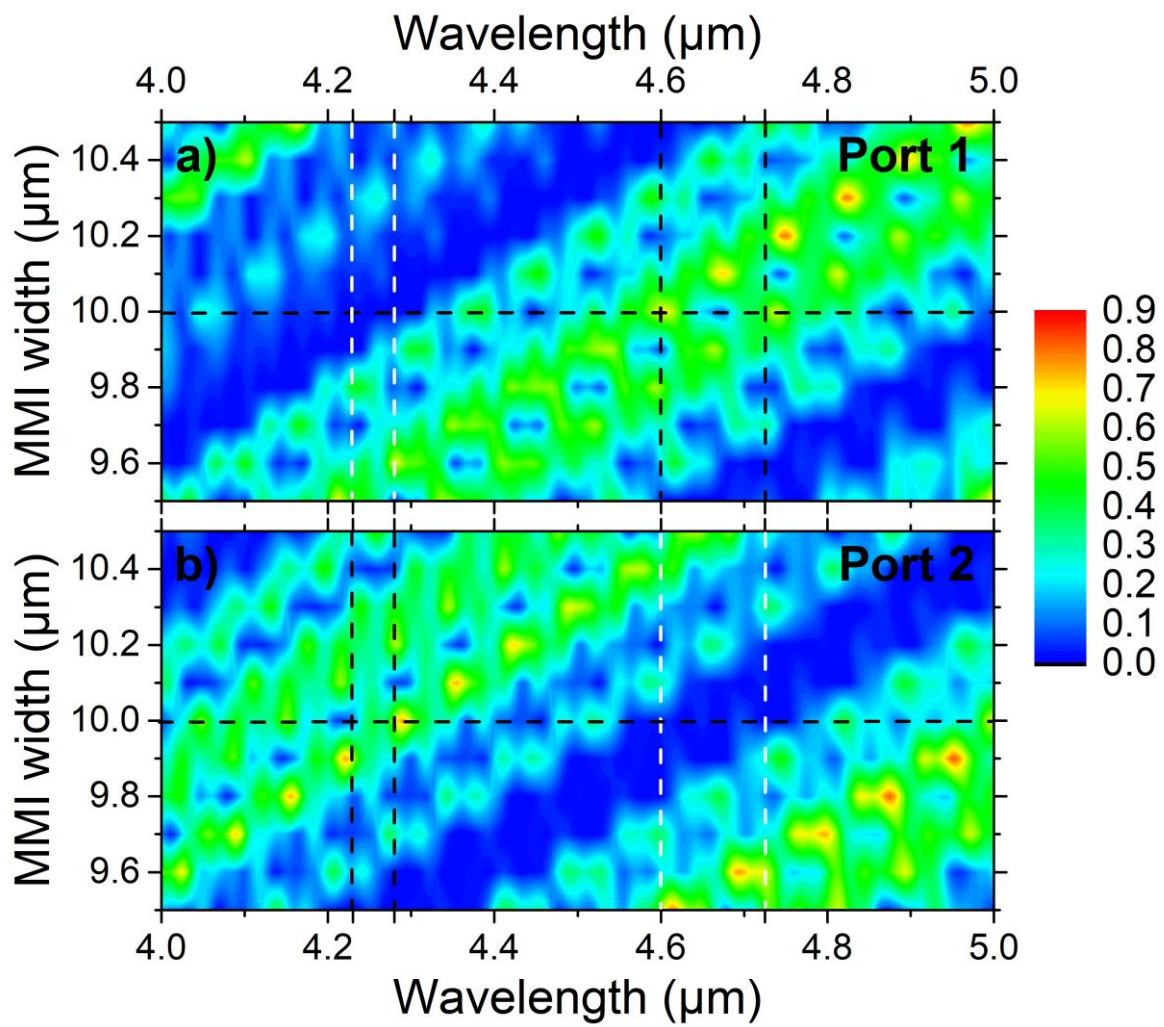


Figure 8

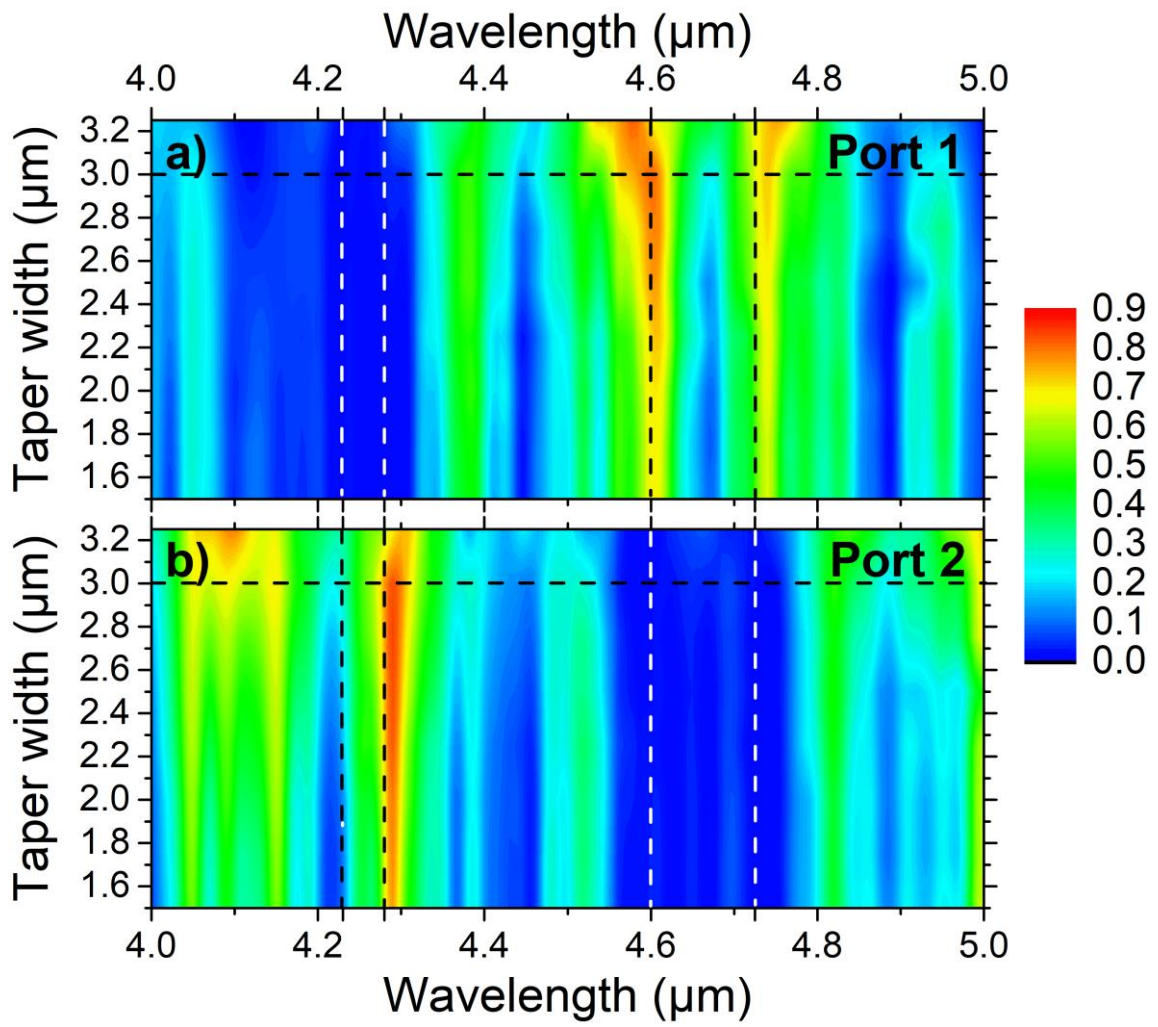
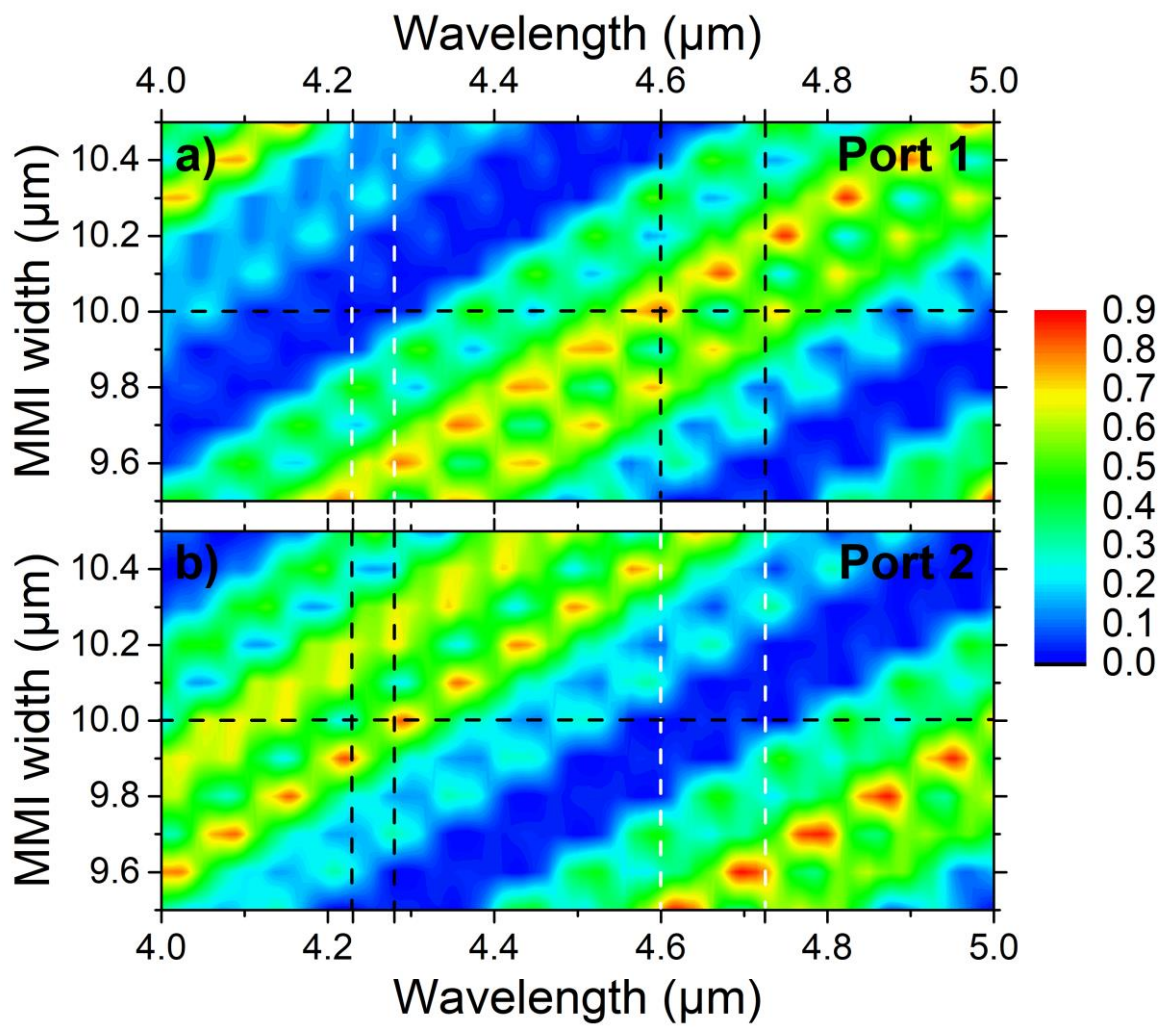


Figure 9



Figures captions

Fig. 1. Normalized absorption bands of carbon monoxide (CO) and carbon dioxide (CO₂). The two bands to multiplex are superimposed to these spectra.

Fig. 2. Schematic representation of the multiplexing MMI structure based on GaGeSbSe:Pr³⁺. The cross-section of the input port is displayed on the right.

Fig. 3. Power transmission for the two output ports as a function of MMI multimode section width (w_{MMI}) and length (L_{MMI}) for two wavelengths: a), b) 4.28 μm and c), d) 4.6 μm .

Fig. 4. Simulation of the power transmission for the MMI with optimized dimensions at a) 4.3 μm and b) 4.6 μm .

Fig. 5. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of chalcogenide film refractive index variations (Δn) for optimized MMI multimode section dimensions. Vertical dashed lines correspond to absorption maxima of CO₂ and CO.

Fig. 6. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of MMI multimode section length (L_{MMI}).

Fig. 7. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of MMI multimode section width (w_{MMI}) with straight input and output ports (ports width=1.5 μm).

Fig. 8. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of input and output ports taper width (w_{taper}).

Fig. 9. Wavelength dependence of a) Port 1 and b) Port 2 transmission as a function of MMI multimode section width (w_{MMI}) for an MMI with tapered input and output ports (taper width=3 μm).

Table captions

TABLE I:
LIST OF PARAMETERS OF OPTIMIZED MMI

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