

# Mid-infrared chalcogenide slot waveguide plasmonic resonator sensor embedded with Au nanorods for surface-enhanced infrared absorption spectroscopy

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## ABSTRACT

The problem of a traditional waveguide plasmonic resonator sensor is that part of the near-field intensity enhanced area is confined in the waveguide dielectric layer, which decreases the interaction effect between light and analyte. In order to solve this problem, a novel mid-infrared (MIR) chalcogenide (ChG) slot waveguide plasmonic resonator (SWGPR) sensor embedded with Au nanorods was proposed, where Au nanorods were used as antenna for enhancing mode coupling with the waveguide through resonance at the absorption wavelength of the analyte. The antenna parameters were optimized to make the resonance wavelength align with the absorption wavelength of the analyte. The proposed waveguide structure provides a sufficient sensing area and increases the electric field enhancement factor to  $> 6400$ . Polymethyl methacrylate (PMMA) and styrene were adopted as the analyte for sensing performance evaluation. The normalized absorption reaches 23.31 when the maximum extinction coefficient of PMMA is 0.08, which is at least 7 times higher than other silicon-on-insulator (SOI) waveguide plasmonic resonator sensors. The proposed waveguide structure provides a new idea for the design of other waveguide plasmonic resonator sensors with high sensing performance and has the potential for biochemical sensing.

## Introduction

Fourier transform infrared (FTIR) spectrometer and other optical systems with discrete electrical/optical modules have been widely used for analyte measurement [1–8], but they are of large size and high cost. An on-chip optical waveguide sensor is miniature in size and shows superior performance using physical effects [9–13] or functional materials [14–16] to enhance sensitivity. Compared with the absorption in the near-infrared band, a majority of analytes has stronger absorption in the mid-infrared (MIR, 2.5–20  $\mu\text{m}$ ) band. Surface-enhanced infrared absorption (SEIRA) spectroscopy can be used for improving light field intensity and thus enhancing absorption. Therefore, using MIR

waveguide and improving the light field intensity are the two solutions to increase sensitivity.

MIR silicon-on-insulator (SOI) rib waveguide plasmonic resonator sensor has been reported with a high enhancement factor of  $> 3600$  in the optical field [17] for SEIRA sensing. However, silica ( $\text{SiO}_2$ ) with a high loss in the MIR as lower buffer layer affects the sensing performance. Compared with SOI, chalcogenide (ChG) glass with a wide transparent window (1–20  $\mu\text{m}$ ) and a high refractive index ( $> 2$ ) is a kind of suitable material for fabricating low loss MIR optical waveguide [18]. Other MIR transparent materials (e.g.  $\text{CaF}_2$  [19], sapphire [20–21]) can be used as the substrate of ChG waveguide. However, it is difficult for the light in the rectangular or rib waveguides to couple into antennas for

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SEIRA sensing and part of the near-field intensity enhanced area is confined in the waveguide dielectric layer, which cannot be adopted for sensing.

Waveguide plasmonic resonator sensor can strengthen the surface electric field to make the light-matter interaction more efficient [17,22–23], which is powerful for evanescent field sensing. Metal island structure can be used for SEIRA spectroscopy, but the enhancement factor is small and the fabrication cannot be repeatable [1]. An antenna can be a better alternative to metal island film. So far, different types of antennas, which can be integrated on optical waveguide, have been used for SEIRA spectroscopy (e.g. nanorod antenna [24–25], bowtie antenna [26–27], fan-shape antenna [28]). The size of an antenna influences the near-field intensity which can be improved by reducing the gap between antennas [29]. In 2018, Chen et al [17] demonstrated a rib waveguide sensor integrated with Au nanorods for SEIRA sensing. The gap between the nanorods was optimized to improve the sensing performance and the waveguide structure is shown in Fig. 1(a). In the same year, Mohr et al. [22] demonstrated waveguide sensors integrated with Au nanorods and Au nanoaperture for SEIRA sensing, as shown in Fig. 1(b) and (c), respectively. The major problem of these waveguide plasmonic resonator sensors is that the optical field enhancement factor and the normalized absorption are small, leading to a decrease in sensitivity.

To solve this problem, in this paper, a novel MIR ChG slot waveguide plasmonic resonator (SWGPR) sensor embedded with Au nanorods is demonstrated. The novel aspects of this sensor structure include: (1) Slot waveguide structure is used for improving the field intensity enhancement factor by making the slot overlap with the gap between the antennas, and the slot with a low refractive index provides enough sensing area for light-matter interaction. (2) Au nanorods are partially embedded in the waveguide and partially suspended in the slot, resulting in more suspended area for sensing operation. (3) The resonance wavelength of the sensor can be aligned with different absorption wavelength by changing the antenna width for the detection of any analytes. (4) The sensor length can be reduced by one or two orders by the use of the SWGPR sensing structure, which is helpful to the sensor miniaturization and high-density on-chip integration.

This paper is organized as follows. In Section 2, the structure of the SWGPR sensor and the sensing theory are presented. The structural parameters of the sensor are optimized and a feasible fabrication process is suggested. In Section 3, polymethyl methacrylate (PMMA) and styrene are used as the analyte for evaluating the sensing performance. The performances of the SWGPR sensor are compared with some reported rib and rectangular waveguide plasmonic resonator (RWGPR) sensor. The enhancement of the output absorption signal and the ability to reduce waveguide length are discussed for the SWGPR sensor. Some conclusions are reached in Section 4.

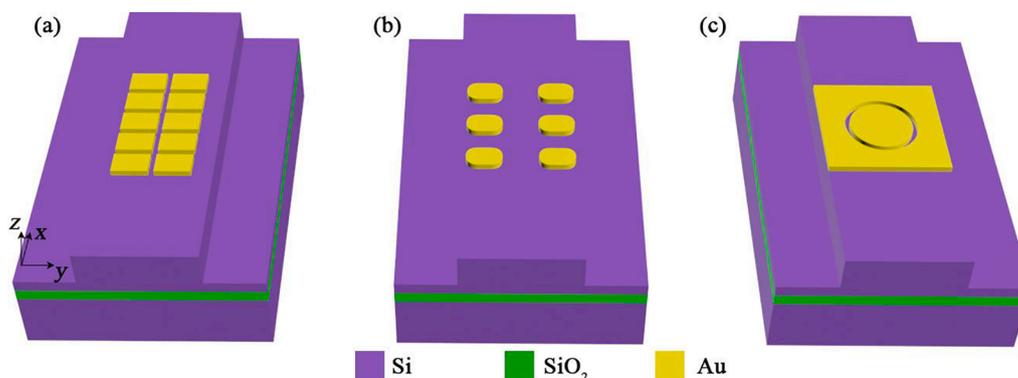


Fig. 1. The structure of rib waveguide sensor integrated with (a, b) Au nanorods, and (c) Au nanoaperture.

## MIR ChG SWGPR sensor

### Waveguide sensor structure

The 3D diagram of the MIR ChG SWGPR sensor is shown in Fig. 2(a). The sensor includes an input taper waveguide, a sensing area and an output taper waveguide.  $\text{As}_2\text{Se}_3$  and  $\text{CaF}_2$  are used as the waveguide core layer and substrate, respectively. The Au nanorods in the sensing area act as a resonator which are partially embedded in the waveguide and partially suspended in the slot. In this case, the slot with a low refractive index provides enough sensing area for light-matter interaction. Meanwhile, the Au nanorods are located in the middle of the waveguide core layer along the  $z$  direction, which improves the field intensity enhancement factor. Without sensing operation, air will be served as the cladding layer in the slot and other areas of the waveguide; whereas under sensing operation, the analyte will replace the air in the slot. A typical diagram of a measurement system based on such waveguide sensor is shown in Fig. 2(b). A broadband light source (e.g. optical parametric oscillators (OPO, M Squared, Firefly IR SW)) can be used as the light source. The light is coupled into and output from the waveguide through a fluoride optical fiber. A HgCdTe detector (e.g. Thorlabs, PDA10JT) can be used to probe the optical signal and the obtained electrical signal is sampled by a data acquisition (DAQ) card (e.g. National Instrument, USB-6211). A chopper (e.g. Thorlabs, MC1F10HP) and a lock-in amplifier (e.g. Stanford Research Systems, SR830) are used to suppress the  $1/f$  noise through the modulation of the input light and the correlation demodulation of the output sensing signal. The cross-section structure of the slot waveguide with Au nanorods and the bare slot waveguide are shown in Fig. 2(c) and (d), respectively. The width and height of the waveguide core layer are defined as  $w_1$  and  $h_1$ , respectively. The width of the slot is  $w_2$ . The structure of the Au antenna pairs is shown in Fig. 2(e). The structural parameters of the Au antenna include width  $w_3$ , length  $l_1$ , height  $h_2$ , gap width  $w_4$  and distance  $l_2$ .

The refractive index of  $\text{As}_2\text{Se}_3$  and  $\text{CaF}_2$  are  $\sim 2.8$  [31] and  $\sim 1.41$  [30] at this wavelength range, respectively. The refractive index of air is set to 1. PMMA and styrene are adopted as the analyte for evaluating the sensing performance of the sensor. The refractive index of PMMA, styrene and Au can be obtained from the refractive index database [30]. Curves of the refractive index  $n$  and extinction coefficient  $\kappa$  of the PMMA versus wavelength are shown in Fig. 3(a). As can be seen that PMMA has a strong absorption near  $3.4 \mu\text{m}$  and  $\kappa$  reaches the highest value at  $3.39 \mu\text{m}$ , mainly due to the absorption of C — H [17]. Styrene has a strong absorption near  $3.2 \mu\text{m}$  and  $\kappa$  becomes the maximum at  $3.24 \mu\text{m}$ .

### Waveguide sensing theory

The waveguide plasmonic resonator sensor obeys the temporal coupled mode theory. The Au nanorods and the analyte can be equivalent to two resonators. A principle diagram of the waveguide resonator

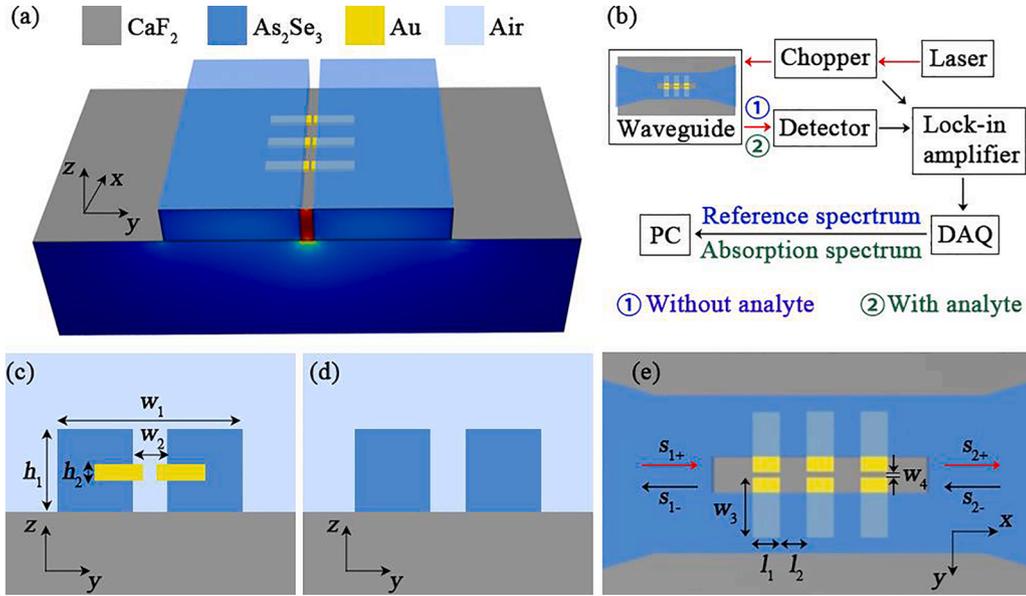


Fig. 2. (a) The 3D diagram of the MIR ChG SWGPR sensor. (b) The structure of a sensor system based on the SWGPR sensor. DAQ: data acquisition card; PC: personal computer. The cross-section structure of the (c) slot waveguide with Au nanorods and (d) bare slot waveguide. (e) The structure of the Au antenna pairs.

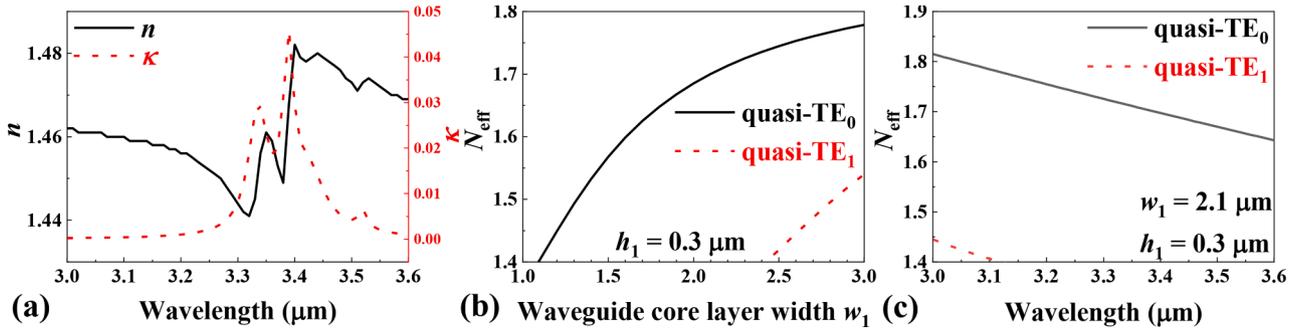


Fig. 3. (a) Curves of  $n$  and  $\kappa$  of PMMA versus wavelength. (b) Curves of the quasi-TE<sub>0</sub> mode and quasi-TE<sub>1</sub> mode effective refractive index  $N_{\text{eff}}$  of the rectangular waveguide versus core layer width  $w_1$ . (c) Curves of the quasi-TE<sub>0</sub> mode and quasi-TE<sub>1</sub> mode  $N_{\text{eff}}$  of the rectangular waveguide versus operation wavelength.

sensor is shown in Fig. 2(e).  $s_{1+}$  and  $s_{1-}$  are the amplitudes of the input modes, and  $s_{2+}$  and  $s_{2-}$  are the amplitude of the output modes. The following equations are used to express the relationship among these parameters [23]:

$$s_{1-} = C_{11}s_{1+} + a\kappa_{1a} + b\kappa_{1b} \quad (1)$$

$$s_{2-} = C_{21}s_{1+} + a\kappa_{2a} + b\kappa_{2b} \quad (2)$$

Here,  $a$  and  $b$  are the plasmonic resonance mode amplitude and the analyte absorbance resonance amplitude, respectively;  $C_{ij}$  is the coupling constant between  $s_{i-}$  and  $s_{j+}$  ( $i, j = 1, 2$ );  $\kappa_{ia}$  and  $\kappa_{ib}$  are the coupling coefficients between  $s_{i+}$  and  $a, b$ , respectively. The transfer function of the waveguide can be expressed as.

$$T = \left| \frac{s_{2-}}{s_{1+}} \right|^2 \quad (3)$$

The transmission spectrum of the waveguide with analyte can be defined as the absorption spectrum (the extinction coefficient  $\kappa \neq 0$ ) and the reference spectrum ( $\kappa = 0$ ) [17].

When the input light resonates with the antenna, the electric field in the gap between the antenna pairs will be greatly enhanced, which will strengthen the absorption of analyte. The enhancement factor of the field intensity  $|E/E_0|^2$  can be used to evaluate the resonance effect between light and antenna, where  $E$  and  $E_0$  are the electric field amplitude

along the mode propagation direction and the input electric field amplitude, respectively. After spinning an analyte to the surface of the Au nanorods, the increased absorption loss will influence the mode coupling between Au nanorods and the waveguide. The normalized absorption (NA) is defined as [22].

$$\text{NA} = \frac{T_a(\lambda) - T_r(\lambda)}{T_r(\lambda)} \quad (4)$$

Here,  $T_a(\lambda)$  and  $T_r(\lambda)$  are the transmittances of the absorption spectrum and reference spectrum at  $\lambda$ . NA indicates the effect of the enhanced absorption of the analyte on the coupling efficiency of the antenna, which can indirectly characterize the influence of the antenna on the enhancement of absorption.

#### Waveguide sensor optimization

##### Simulation method

COMSOL Multiphysics was used to optimize the structure of the ChG SWGPR sensor and to analyse the sensing performances. The structural parameters and material parameters of the waveguide were set. The Electromagnetic Waves, Frequency Domain interface of the Wave Optics branch was used to obtain electric field distributions. All the optimization results are based on the parametric sweep module in COMSOL.

The frequency domain was used in the Study branch for calculating transmission spectrum of the sensor. Input port and output port were

added at the waveguide input interface and waveguide output interface to generate excitation at a specific frequency. The performance of the sensor at each wavelength can be obtained and optimized by parametric sweep. The electric field distribution and transmission spectrum can be obtained at Results branch. The wavelength and frequency of light can be transformed into each other, so the results based on wavelength can be obtained by frequency domain analysis. The excitation of the device in the frequency domain and the wavelength domain is similar, because the software calculates the response of the device when using frequency and wavelength excitation, respectively. We simulated the sensor in the frequency domain with reference to the accurate methods in other theoretical calculation work [22].

Different from the simulation of the transmission spectrum of the sensor, the mode analysis is added to the Study branch with a specific frequency for excitation instead of the frequency domain to obtain effective refractive index  $N_{\text{eff}}$ . Because the mode analysis is aimed at the waveguide cross-section structure, there is no need to add the input port and output port. The  $N_{\text{eff}}$  and electric field distribution of the waveguide mode can be obtained at Results branch.

#### Single-mode waveguide design

The structure of rectangular waveguide is optimized to satisfy the single mode condition. The quasi-TE<sub>0</sub> mode is used for producing horizontal resonance and to improve the field intensity in the gap. Curves of the quasi-TE<sub>0</sub> mode and quasi-TE<sub>1</sub> mode  $N_{\text{eff}}$  of the rectangular waveguide versus core layer width  $w_1$  are shown in Fig. 3(b), where  $h_1 = 0.3 \mu\text{m}$  and the wavelength is  $3.39 \mu\text{m}$ .  $N_{\text{eff}}$  increases with the increase of  $w_1$  and the single mode condition is satisfied when  $w_1 \leq 2.4 \mu\text{m}$ .  $w_1$  cannot be too small because the transition from rectangular waveguide to slot

waveguide reduces  $N_{\text{eff}}$  [31–32] and the slot waveguide should satisfy the condition of guiding light. So  $w_1$  and  $h_1$  are set to be  $2.1 \mu\text{m}$  and  $0.3 \mu\text{m}$ , respectively. Curves of the  $N_{\text{eff}}$  of the optimized rectangular waveguide versus the operation wavelength are shown in Fig. 3(c). The single mode condition is satisfied in the wavelength range from  $3.2 \mu\text{m}$  to  $3.6 \mu\text{m}$ , which covers the absorption peak of PMMA. The electric field distribution of the quasi-TE<sub>0</sub> mode of the rectangular waveguide at  $3.39 \mu\text{m}$  is shown in Fig. 4(a). Along the direction of optical transmission, the cross-section structure of the waveguide will become a slot waveguide, whose electric field distribution of the quasi-TE<sub>0</sub> mode at  $3.39 \mu\text{m}$  is shown in Fig. 4(b).

#### Antenna optimization

The antenna structure is optimized to make the resonance wavelength align with the absorption peak of the analyte and to improve the field intensity enhancement factor [23]. In order to obtain sufficient sensing area and ensure the interaction between the two strips of the slot waveguide,  $w_2$  is set to  $100 \text{ nm}$ . Reducing  $w_4$  can increase the electric field intensity in the gap [29]. Considering the fabrication feasibility,  $w_4$  is set to  $20 \text{ nm}$  and  $h_2$  is  $30 \text{ nm}$ . The transmission spectrum for different  $w_3$  from  $300 \text{ nm}$  to  $345 \text{ nm}$  and the curve of the resonance wavelength versus  $w_3$  are shown in Fig. 5(a) and Fig. 5(b), respectively, where  $l_1 = 100 \text{ nm}$ ,  $l_2 = 210 \text{ nm}$  and  $\kappa = 0$ . The transmission spectrum for different  $l_1$  from  $80 \text{ nm}$  to  $100 \text{ nm}$  are shown in Fig. 5(c), where  $w_3 = 335 \text{ nm}$ ,  $l_2 = 210 \text{ nm}$  and  $\kappa = 0$ . The transmission spectrum has a red shift with the increase of  $w_3$  or decrease of  $l_1$ . The resonance wavelength is aligned with the PMMA absorption wavelength when  $w_3 = 335 \text{ nm}$  and  $l_1 = 100 \text{ nm}$ . The transmission spectrum of the sensor under different  $l_2$  from  $190 \text{ nm}$  to  $230 \text{ nm}$  are shown in Fig. 5(d), where  $w_3 = 335 \text{ nm}$ ,  $l_1 = 100 \text{ nm}$

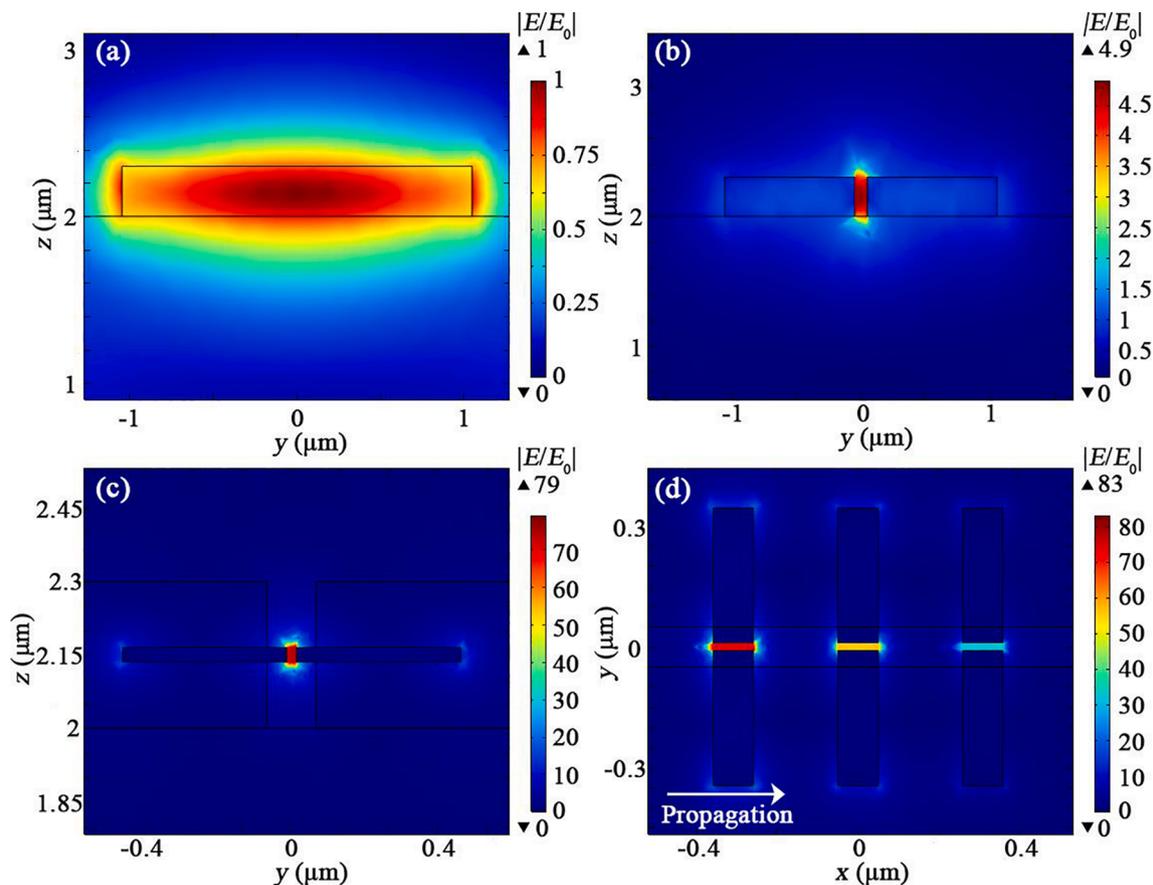
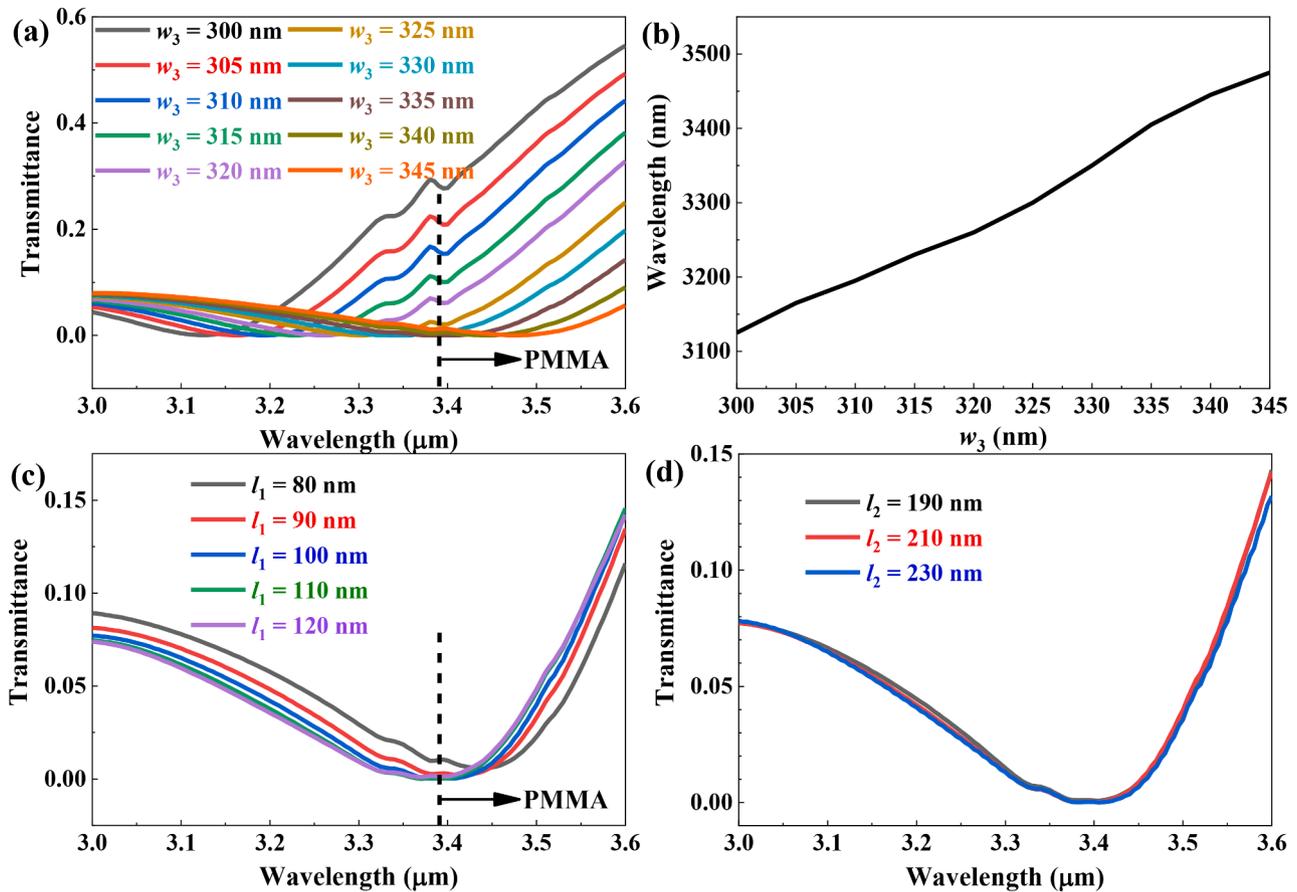


Fig. 4. (a) The electric field distribution of the quasi-TE<sub>0</sub> mode of the rectangular waveguide at  $3.39 \mu\text{m}$ . (b) The electric field distribution of the quasi-TE<sub>0</sub> mode of the slot waveguide at  $3.39 \mu\text{m}$ . (c) The electric field distribution in the  $yz$  plane at the center of the first antenna pair in the  $x$  direction. (d) The electric field distribution in the  $xy$  plane at the center of the antenna pairs in the  $z$  direction.



**Fig. 5.** (a) Transmission spectrum of the SWGPR sensor at different  $w_3$  from 300 nm to 345 nm, where  $l_1 = 100$  nm,  $l_2 = 210$  nm and  $\kappa = 0$ . (b) Curve of the resonance wavelength of the SWGPR sensor versus  $w_3$ , where  $l_1 = 100$  nm,  $l_2 = 210$  nm and  $\kappa = 0$ . (c) Transmission spectrum of the SWGPR sensor at different  $l_1$  from 80 nm to 100 nm, where  $w_3 = 335$  nm,  $l_2 = 210$  nm and  $\kappa = 0$ . (d) Transmission spectrum of the SWGPR sensor at different  $l_2$  from 190 nm to 230 nm, where  $w_3 = 335$  nm,  $l_1 = 100$  nm and  $\kappa = 0$ .

and  $\kappa = 0$ . The transmission spectrum hardly shifts with  $l_2$ , which is set to 210 nm in the design. Therefore, the variation of  $l_2$  on the resonance wavelength can be ignored, and the resonance peak and the absorption peak can be aligned by adjusting  $w_3$  and  $l_1$ . So the optimization results of antenna are  $w_3 = 335$  nm and  $l_1 = 100$  nm and  $l_2 = 210$  nm. The final optimized ChG SWGPR sensor parameters are listed in Table 1. The electric field distribution in the  $yz$  plane at the center of the first antenna pair in the  $x$  direction is shown in Fig. 4(c). The electric field distribution in the  $xy$  plane at the center of the antenna pairs in the  $z$  direction is shown in Fig. 4(d). The area where the significantly enhanced electric field intensity is concentrated near the gap and the enhancement factor  $|E/E_0|$  reaches 83. Sufficient sensing area and enhanced electric intensity ensure a good sensing performance.

**Table 1**

The optimized parameters of the ChG SWGPR sensor.

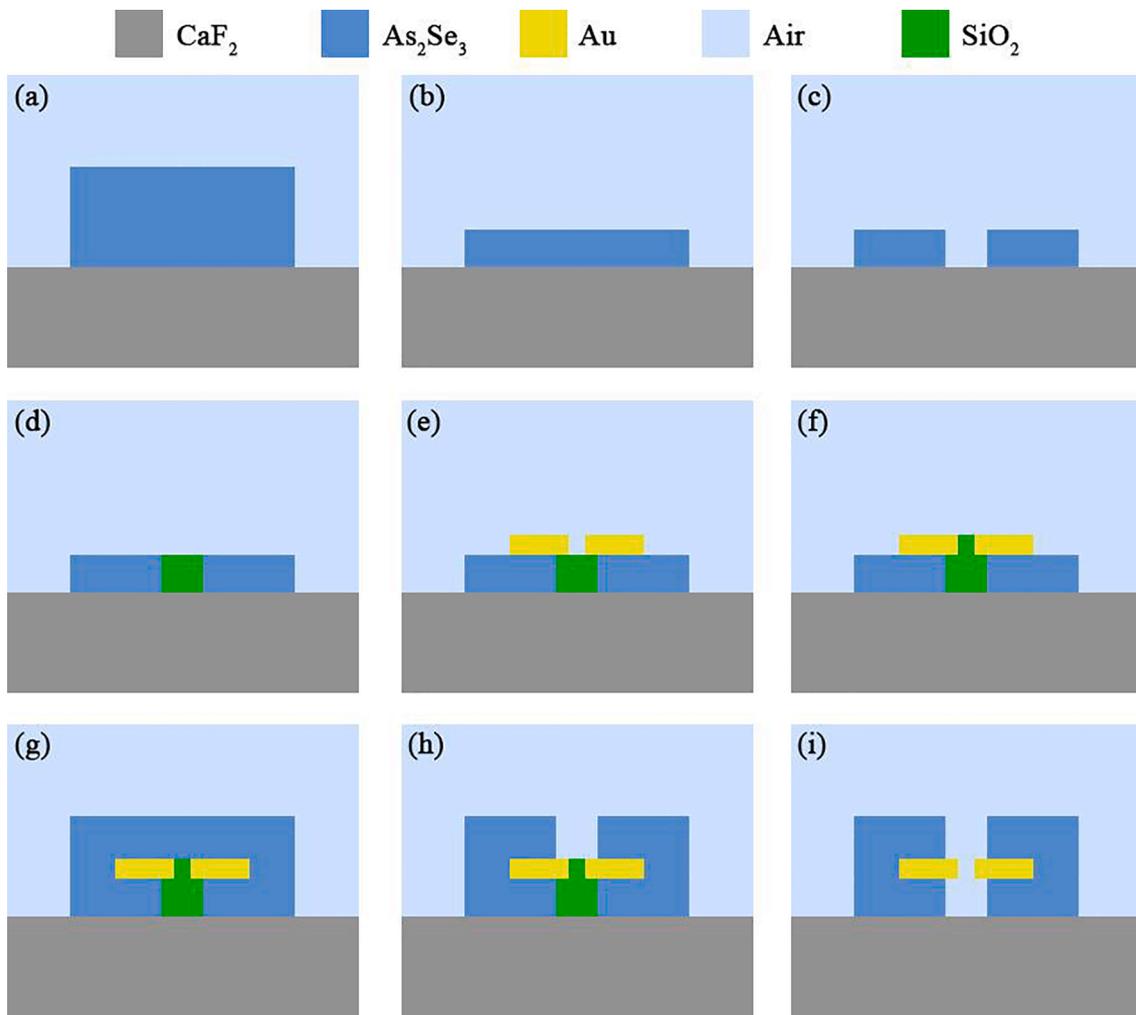
Sensor structural parameters	Value
Waveguide core layer width, $w_1$	2.1 $\mu\text{m}$
Slot width, $w_2$	100 nm
Antenna width, $w_3$	335 nm (for PMMA) 318 nm (for styrene)
Gap width, $w_4$	20 nm
Waveguide core layer height, $h_1$	0.3 $\mu\text{m}$
Antenna height, $h_2$	30 nm
Antenna length, $l_1$	100 nm
Antenna distance, $l_2$	210 nm

### Fabrication process

The suggested fabrication process of the sensing area for the SWGPR sensor is shown in Fig. 6, which can be used for future experimental verification. First,  $\text{As}_2\text{Se}_3$  rectangular waveguide is fabricated on  $\text{CaF}_2$  substrate by lift-off method (Fig. 6(a)). The input taper waveguide and the output taper waveguide are also fabricated in this step. Then the thickness of the rectangular waveguide in the sensing area is reduced by lithography and inductively coupled plasma (ICP) etching (Fig. 6(b)). Next, the slot structure is obtained by electron beam lithography (EBL) and ICP etching (Fig. 6(c)). Under the protection of a photoresist mask,  $\text{SiO}_2$  is deposited into the slot by chemical vapor deposition (CVD) (Fig. 6(d)). Then Au nanorods are fabricated by another lift-off processing (Fig. 6(e)). Next,  $\text{SiO}_2$  is deposited into the gap also by CVD under the protection of the photoresist mask (Fig. 6(f)). Then  $\text{As}_2\text{Se}_3$  previously removed by etching (Fig. 6(b)) is fabricated again by lift-off method (Fig. 6(g)). The slot at the top of the waveguide is obtained by EBL and ICP etching (Fig. 6(h)). Finally,  $\text{SiO}_2$  is removed by HF etching (Fig. 6(i)).

### Waveguide sensing performance

In this Section, PMMA and styrene are adopted as two analytes for the performance evaluation of the waveguide sensor. A key figure of merit is to observe the enhancement factor in terms of infrared absorption due to the use of the waveguide resonator structure.



**Fig. 6.** Waveguide fabrication process in the sensing region for the MIR ChG SWGPR sensor. (a)  $\text{As}_2\text{Se}_3$  rectangular waveguide fabrication on  $\text{CaF}_2$  substrate by lift-off method. (b) Lithography and ICP etching of the rectangular waveguide. (c) EBL and ICP etching of the lower slot. (d)  $\text{SiO}_2$  deposition into the slot by CVD. (e) Au nanorods fabrication by lift-off method. (f)  $\text{SiO}_2$  deposition into the gap by CVD. (g)  $\text{As}_2\text{Se}_3$  fabrication by lift-off method. (h) EBL and ICP etching of the upper slot. (i)  $\text{SiO}_2$  removal by HF etching.

#### SEIRA sensing based on ChG SWGPR sensor

Take PMMA as analyte. During sensing operation of the ChG SWGPR sensor, PMMA is required to wrap around each Au antenna pair. The width, height and length of the PMMA area are 100 nm, 120 nm and 180 nm, respectively. The cross-section structure of the Au antenna pair is shown in the inset of Fig. 7(a). The reference spectrum and absorption spectrum of the ChG SWGPR sensor are shown in Fig. 7(a). The transmission is greatly reduced at the wavelength of 3.39  $\mu\text{m}$  due to absorption. Curve of  $|\text{NA}|$  versus the operation wavelength is shown in Fig. 7(d). It can be seen that  $|\text{NA}|$  reaches the maximum value of 15.37 at 3.39  $\mu\text{m}$ .

Then, the PMMA under the nanorods is removed to simulate the situation that the waveguide dielectric layer occupies the sensing area. The cross-section structure in the  $yz$  plane of the Au antenna pair wrapped in partial PMMA is shown in the inset of Fig. 7(b). The reference spectrum and absorption spectrum are shown in Fig. 7(b). Curve of  $|\text{NA}|$  versus wavelength is shown in Fig. 7(d). In this case, NA only reaches 10.43 at 3.39  $\mu\text{m}$ . Therefore,  $|\text{NA}|$  can be increased by  $\sim 50\%$  when the sensing area at the bottom of the Au antenna pair is utilized for sensing.

The resonance wavelength of the sensor can be changed with the variation of  $w_3$  (Fig. 5(b)). In order to illustrate the advantage of the ChG SWGPR sensor structure, another analyte, styrene is used to evaluate the

sensing performance, which is listed as a kind of class 2B carcinogens by the World Health Organization's International Agency for Research on Cancer. Curves of  $n$  and  $\kappa$  of styrene versus wavelength are shown in Fig. 8(a).  $w_3$  is set to 318 nm to make the resonance wavelength align with the absorption peak wavelength of styrene at 3245 nm. The width, height and length of the sensing area filled with styrene are 100, 34 and 104 nm, considering the thickness of the self-assembled monolayer liquid molecule of  $\sim 2$  nm [22]. The reference spectrum, absorption spectrum and NA of styrene are shown in Fig. 8(b), respectively. The obtained NA at the absorption peak is 3.32, which is smaller than that of PMMA because of a lower  $\kappa$  of 0.018.

#### SEIRA sensing based on ChG RWGPR sensor

In order to further show the effect of the bottom area of the Au antenna pairs on sensing performance, we investigate the ChG RWGPR sensor whose 3D diagram is shown in the inset of Fig. 7(c). The width and height of the rectangular waveguide are the same as the slot waveguide sensor. The width of the antenna is changed to 380 nm to make the resonance wavelength aligned with the PMMA absorption wavelength. The height of the PMMA analyte is reduced to 75 nm, and the cross-section structure in the  $yz$  plane of the Au antenna pair wrapped in PMMA is shown in the inset of Fig. 7(c). The reference spectrum and absorption spectrum are shown in Fig. 7(c). It can be

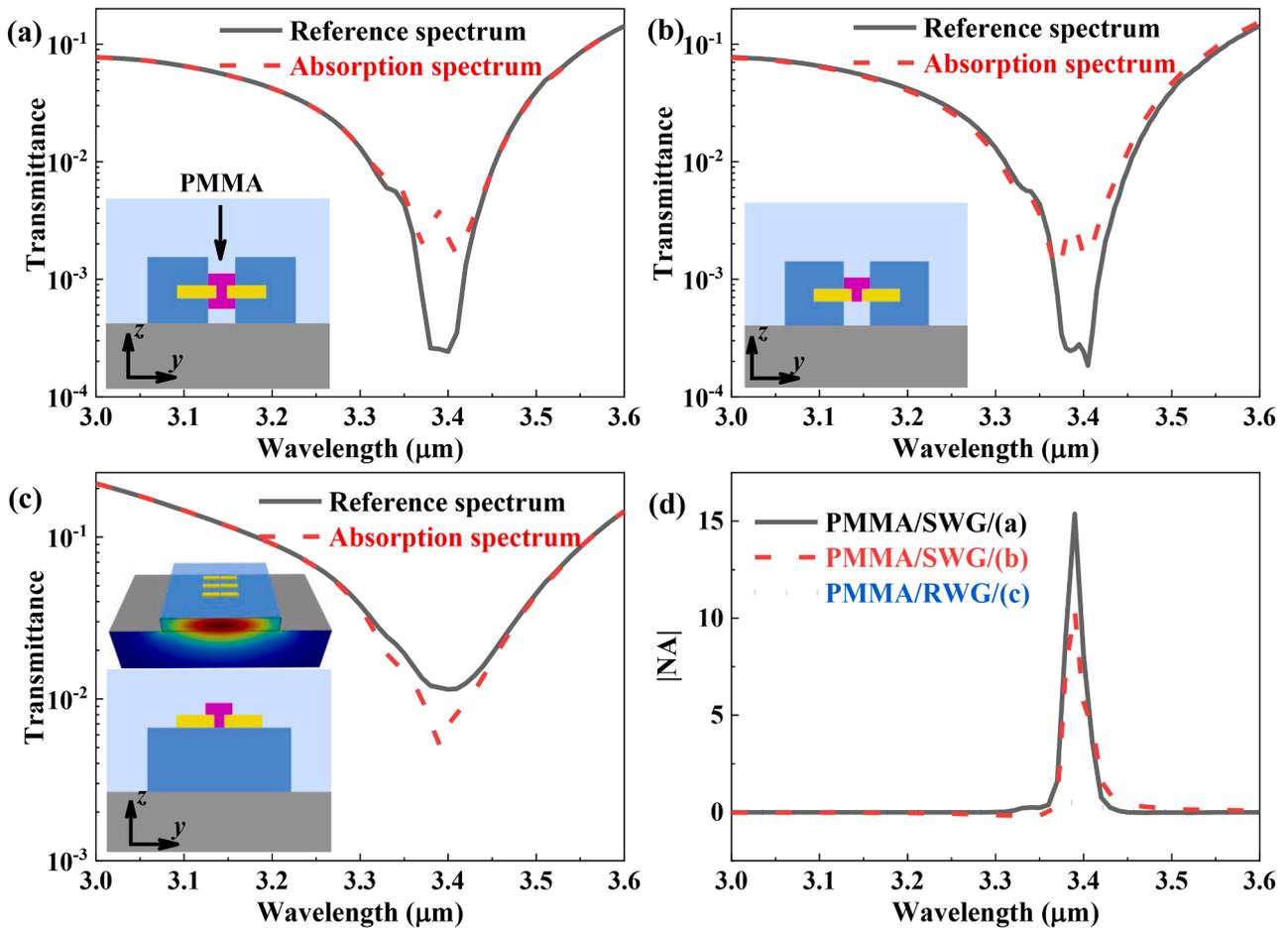


Fig. 7. (a) The reference spectrum and absorption spectrum of the ChG SWGPR sensor when the Au antenna pairs are wrapped in PMMA. Inset: the cross-section structure in the  $yz$  plane of the Au antenna pairs wrapped in PMMA. (b) The reference spectrum and absorption spectrum of the ChG SWGPR sensor when the Au antenna pairs are wrapped in partial PMMA. Inset: the cross-section structure in the  $yz$  plane of Au antenna pairs wrapped in partial PMMA. (c) The reference spectrum and absorption spectrum of the ChG SWGPR sensor. Inset: the 3D diagram of the sensor and the cross-section structure in the  $yz$  plane of Au antenna pairs wrapped in PMMA. (d) Curves of  $|NA|$  of the ChG SWGPR sensor versus wavelength when the Au antenna pairs wrapped in PMMA and partial PMMA, and the  $|NA|$  of the ChG RWGPR sensor versus wavelength when the Au antenna pairs wrapped in PMMA.

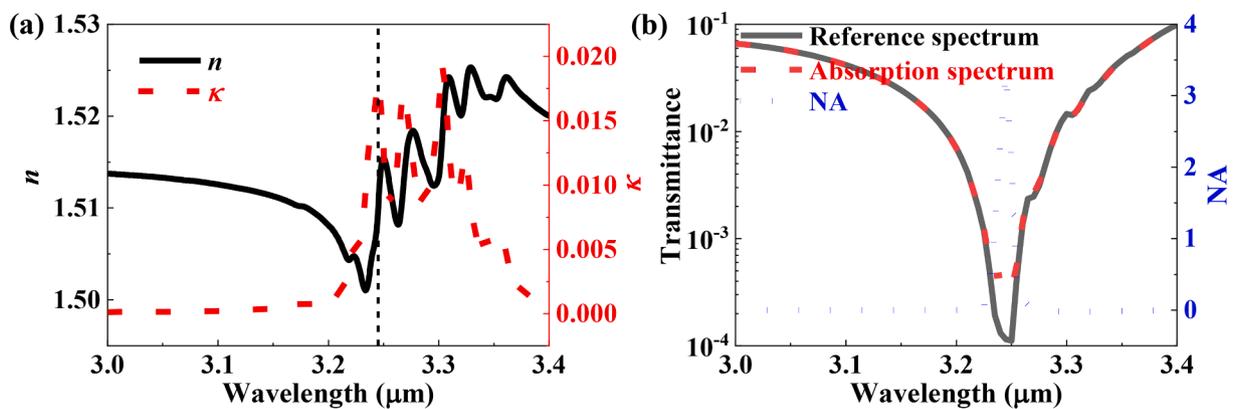


Fig. 8. (a) Curves of  $n$  and  $\kappa$  of styrene versus wavelength. (b) The reference spectrum, absorption spectrum and NA of styrene using the SWGPR sensor.

found that  $T_a(\lambda)$  is smaller than that of the  $T_r(\lambda)$ , resulting in a negative NA. Curve of  $|NA|$  for the ChG RWGPR sensor versus the operation wavelength is shown in Fig. 7(d). The obtained  $|NA|$  is  $< 1$ , because the bottom area of the Au antenna pair is filled with  $As_2Se_3$ , and PMMA has less effect on the light coupled into the antennas, which weakens the effect of the Au nanorods on PMMA.

#### Absorption enhancement

As a clear evidence of the sensor for absorption enhancement, the performances of some other reported waveguide plasmonic resonator sensors using PMMA as analyte with the same absorption wavelength range are compared with those of the proposed ChG SWGPR sensor, as shown in Table 2. The maximum  $\kappa$  of PMMA in other reports is  $> 0.08$ ,

**Table 2**  
Comparison among the proposed ChG SWGPR sensor and other reported waveguide sensors.

Refs.	Waveguide material	Waveguide type	Antenna type	$ E/E_0 $	NA
23	SOI	Rib	Nanorod	40	3.3 ( $\kappa > 0.08$ )
22	SOI	Rib	Nanorod	15	0.02 ( $\kappa > 0.08$ )
22	SOI	Rib	Nanoaperture	33	0.07 ( $\kappa > 0.08$ )
This paper	ChG	Rectangular	Nanorod	52.7	-0.56 ( $\kappa = 0.046$ )
This paper	ChG	Slot	Nanorod	83	15.37 ( $\kappa = 0.046$ )
					23.31 ( $\kappa = 0.08$ )

which is larger than the maximum  $\kappa$  ( $\kappa = 0.046$ ) in this paper. In order to make the comparison more reasonable,  $\kappa = 0.08$  is also taken into account in this comparison. The NA of the ChG SWGPR sensor rises to 23.31 when  $\kappa = 0.08$ . Compared to other SOI rib waveguide sensors, the ChG SWGPR sensor has the largest  $|E/E_0|$  and NA, and NA is at least 7 times higher than other SOI rib waveguide sensors. Therefore, the presented waveguide sensor structure will be beneficial to increase measurement sensitivity due to a large signal variation.

### Sensing length reduction and miniaturization

A traditional waveguide sensor based on evanescent field absorption (Fig. 9(c)) and a sensor based on bulk material absorption (Fig. 9(b)) can be used for absorption measurement of an analyte, which generally obeys the Lambert-Beer law. For a dielectric waveguide, power confinement factor (PCF) in the sensing area determines the absorption of the analyte [31]. The PCF of an evanescent field based waveguide sensor is generally  $< 1$  and the PCF of a sensor using bulk material absorption is equal to 1. Therefore, for achieving the same absorbance, a traditional waveguide sensor simply based on evanescent field absorption will have a longer length. Compared to the sensing scheme simply based on bulk material absorption (i.e. light propagates through the analyte) and the scheme based on evanescent field absorption, in order to illustrate the advantage of the SWGPR sensor (Fig. 9(a)) in waveguide length reduction, the effective sensing lengths for achieving the same absorbance of the proposed sensor are compared for the three schemes. Curves of sensor length versus absorbance are shown in Fig. 9(d) and the comparison results are shown in Table 3. The absorbance of the proposed sensor with an effective sensing length of  $L_1$  is  $1 \mu\text{m}$ . The effective path length based on bulk material absorption  $L_2$  ( $=21.52 \mu\text{m}$ ) is  $> 21$  times larger than  $L_1$  to achieve the same absorbance as this sensor. For the evanescent field based waveguide sensor, the effective sensing length is equal to  $L_2/\text{PCF}$ . Normally, the PCF of a bare slot waveguide sensor is 30%, so  $L_3$  ( $=L_2/30\% = 71.73 \mu\text{m}$ ) is  $> 70$  times larger than  $L_1$ .

**Table 3**

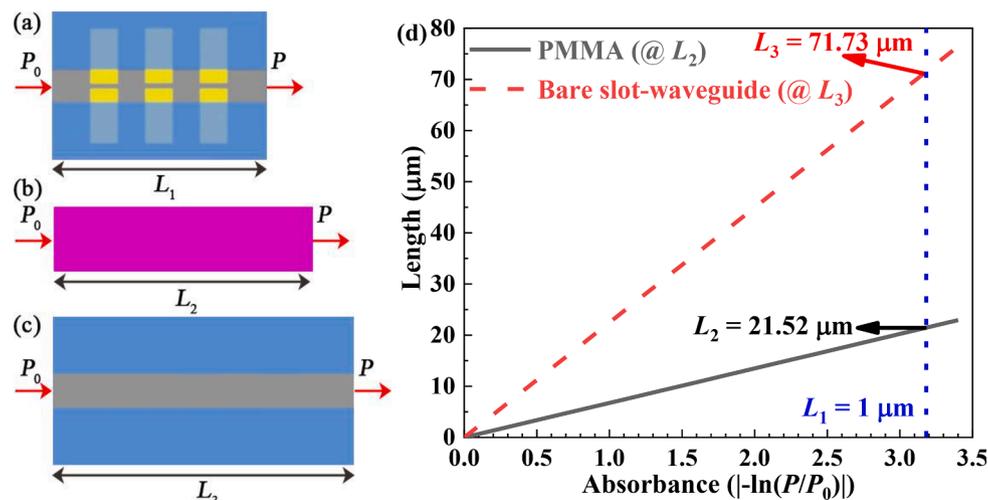
Comparison of the sensor length with the same absorbance for the three schemes.

Sensing scheme	Sensor type	Length ( $\mu\text{m}$ )
SEIRA	SWGPR	1
Bulk material absorption	Bulk PMMA	21.52
Evanescent field absorption	Bare slot waveguide	71.73
	Bare rectangular waveguide	$> 107.60$

For example, a bare rectangular waveguide is widely used for evanescent field sensing with a PCF of  $< 20\%$ , so  $L_1$  can be reduced at least 100 times ( $>L_2/20\% = 107.60$ ) than the bare rectangular waveguide. Therefore, the proposed SWGPR is of great significance to sensor miniaturization. Microring resonator can also reduce the device length with large interaction length through resonance, but the ring waveguide occupies a large area and the resonance wavelength is difficult to align with the absorption peak considering unavoidable fabrication errors [32].

### Conclusions

A novel MIR ChG SWGPR sensor was proposed for SEIRA sensing. PMMA and styrene were adopted as the analytes for sensing performance evaluation. The antenna parameters were optimized to make the resonance wavelength align with the absorption wavelength of the two analytes. The novel ChG slot waveguide structure increased the electric field enhancement factor and provided a sufficiently large sensing area. The  $|E/E_0|$  and NA reach 83 and 23.31 when the maximum  $\kappa$  of PMMA is 0.08, which is at least 7 times larger than other SOI waveguide plasmonic resonator sensors. The proposed sensor reduced the device length by at least two orders of magnitude than other evanescent field based rectangular waveguide sensors, which is of great significance to the miniaturization of the device. The resonance wavelength can be aligned



**Fig. 9.** The schematic diagrams of the (a) SWGPR sensor with a length of  $L_1 = 1 \mu\text{m}$ , (b) the bare PMMA with a length of  $L_2$ , and (c) the bare slot waveguide sensor with a length of  $L_3$ .  $P$ : the output power.  $P_0$ : the input power. (d) Curves of the sensor length ( $L_2, L_3$ ) versus the absorbance.

with different absorption wavelength by changing the antenna width for the detection of different analytes. The styrene measurement shows that the proposed sensor has the potential for biochemical sensing.

#### CRedit authorship contribution statement

**Mingquan Pi:** Conceptualization, Methodology, Investigation, Writing – original draft. **Huan Zhao:** Investigation, Validation, Writing – review & editing. **Chunguang Li:** Investigation, Writing – review & editing, Funding acquisition. **Yuting Min:** Investigation, Validation. **Zihang Peng:** Investigation, Validation. **Jialin Ji:** Investigation. **Yijun Huang:** Investigation. **Fang Song:** Writing – review & editing. **Lei Liang:** Writing – review & editing. **Yu Zhang:** Writing – review & editing. **Yiding Wang:** Resources, Funding acquisition. **Frank K. Tittel:** Writing – review & editing. **Chuantao Zheng:** Conceptualization, Investigation, Writing – review & editing, Funding acquisition.

#### Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

#### Data availability

Data will be made available on request.

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