



Design of Sub wavelength-Grating-Coupled Fano Resonance Sensor in Mid-infrared

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Abstract

By introducing the sub-wavelength grating (SWG) waveguide in the long-range surface phonon resonance (LRSPHR) device, a mid-infrared Fano resonance is formed due to the coupling between surface phonon polariton and Bloch mode. By taking advantage of strong light-matter interaction in the SWG, such Fano resonance is expected to offer improved sensing performance. Based on the rigorous coupled-wave analysis (RCWA) method, the index sensitivity and figure of merit of such a sensor reach 7496 RIU^{-1} and 46,432, respectively, which is 6 times compared with the conventional waveguide-coupled LRSPHR. The proposed SWG-coupled Fano resonance can be a promising platform for mid-infrared biochemical sensing.

Keywords Fano resonance · Mid-infrared · Long-range surface phonon resonance · Sub-wavelength grating

Introduction

Surface plasmon resonance (SPR) is a guided mode propagating along flat planar and sensitive to the changes in the environment. Under the phase-matching condition, the coupling between the incident light with the surface-guided mode can be achieved through the attenuated total reflection (ATR) mechanism [1–3]. Surface plasmon resonance (SPR)-based sensors have gained wide interests in medicine, environmental monitoring, and security [4, 5]. Over the past years, researches on SPR sensors based on noble metals such as Au and Ag have mainly limited in the visible and near-infrared (NIR) wavelength regime [6, 7]. In longer wavelength, e.g., mid-infrared (MIR), the conventional metals behave as perfect conductors with strong intrinsic loss, which limits the excitation of the SPR effect [8, 9]. To implement sensors in MIR, people have explored the use of polar dielectric materials, which supports the surface phonon

polaritons (SPhPs). The lifetime of SPhP mode could be up to picosecond order, which is one to two orders longer than that of surface plasmon polariton (SPP) mode [10–12]. With the coupling between optical photons and SPhPs, surface phonon resonance (SPHR) can be excited. Based on such characteristics, SPHR has been considered as a low loss alternative of SPR in MIR.

The SPHR effect offers a promising approach to implement the refractive index (RI) sensor in the MIR. From the viewpoint of precise sensing, the most important two parameters are the sensing accuracy and figure of merit (FOM). In order to increase the sensing accuracy, the resonance should be as narrow as possible to precisely estimate the resonance angle change. For this purpose, Fano resonance (FR) with asymmetric line shape is regarded as an effective method [13–18]. FR originates from the coupling between SPP/SPhP mode and waveguide photonic mode. In order to further enhance the sensing performance, it is desired to enlarge the contacting area between the waveguide surface and sensing medium. Recently, sub-wavelength grating (SWG) whose period is much smaller than the operation wavelength has been widely investigated. This is because the SWG can support Bloch mode with tailorable dispersion properties and low loss [19–24]. From the viewpoint of sensing, the smaller duty ratio compared with the conventional waveguide can further increase the light-matter interaction [25, 26]. It is expected that, by introducing SWG in the FR-based index sensor, the performance can be enhanced.

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In this paper, a new SWG-coupled long-range surface phonon resonance (SWG-LRSPHR) sensor operating in the MIR wavelength region is proposed. The coupling between SPhP mode and SWG Bloch mode forms the FR line shape. The overlap between the electromagnetic field and the sensing medium is enhanced due to the enlarged contacting surface of the SWG waveguide. Furthermore, to better assess the sensing performance, both the sensitivity and FOM are investigated in detail. Such configuration can be used in various bio- and chemical-sensing applications.

Materials and Methods

The structure for conventional stripe waveguide-coupled long-range surface phonon resonance (WG-LRSPHR) based on Kretschmann configuration is shown in Fig. 1a. With the homogeneous ZnSe layer replaced by the ZnSe grating, the SWG-LRSPHR sensor can be formed, as shown in Fig. 1b.

Both structures consist of a germanium (Ge) prism, barium fluoride (BaF₂), silicon carbide (SiC), barium fluoride, zinc selenide (ZnSe), and the sensing medium layer. For the initial investigation, the following parameters are used: the thickness of BaF₂ layer $d_1 = 4 \mu\text{m}$, SiC layer $t = 0.7 \mu\text{m}$, BaF₂ layer $d_2 = 8 \mu\text{m}$, ZnSe layer $h_g = 2.8 \mu\text{m}$, the grating period $\Lambda = 0.5 \mu\text{m}$, and the grating width $w_g = 0.25 \mu\text{m}$. In the absence of free charge carriers, the frequency-dependent complex dielectric permittivity of SiC can be given as [27–29]:

$$\epsilon_{\text{SiC}} = \epsilon'_{\text{SiC}} + i\epsilon''_{\text{SiC}} = \epsilon_{\infty} \frac{\omega^2 - \omega_{\text{LO}}^2 + i\gamma\omega}{\omega^2 - \omega_{\text{TO}}^2 + i\gamma\omega} \quad (1)$$

where the optical phonon frequency $\omega_{\text{LO}} = 972 \text{ cm}^{-1}$, the transverse optical phonon frequency $\omega_{\text{TO}} = 796 \text{ cm}^{-1}$, the damping rate $\gamma = 3.75 \text{ cm}^{-1}$, and the high-frequency

dielectric constant $\epsilon_{\infty} = 6.5$. With wavelength ranges from 10 to 15 μm , the Reststrahlen band defined by $\epsilon'_{\text{SiC}} < 0$ corresponds to $\omega_{\text{TO}} < \omega < \omega_{\text{LO}}$ that is shown in Fig. 2. With the negative dielectric constant real part, SPhP modes can be supported. At $\lambda = 10.8 \mu\text{m}$, the period of ZnSe grating $\Lambda = 0.5 \mu\text{m}$, about one-twentieth of the wavelength, matching the propagating light condition and SWG behaves as the homogeneous metamaterial [20, 23]. The corresponding refractive indexes used are $n_p = 4.0037$ for the Ge prism, $n_{\text{BaF}_2} = 1.3919$ for BaF₂, $n_{\text{ZnSe}} = 2.3950$ for ZnSe, and $n_s = 1.332$ for the sensing medium [30].

With the structure parameters mentioned above, the ATR curve of TM-polarized light calculated by rigorous coupled-wave analysis (RCWA) method [31–34] is shown in Fig. 3a. On the left side of LRSPHR, a sharp asymmetric FR arises. There are three dips with the incident angle ranging from 20 to 25°, denoted as ‘A’, ‘B’, and ‘C’, respectively, where

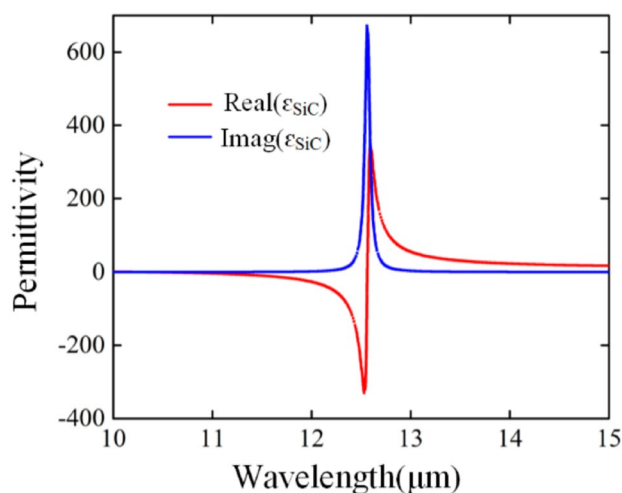


Fig. 2 The real part (red line) and imaginary part (blue line) of the permittivity of SiC, following the Drude-Lorentz model

Fig. 1 a Structure of the WG-LRSPHR sensor consisting of the Ge prism, BaF₂, SiC, BaF₂, ZnSe, and sensing medium. b Structure of the SWG sensor consisting of the Ge prism, BaF₂, SiC, BaF₂, ZnSe grating, and sensing medium

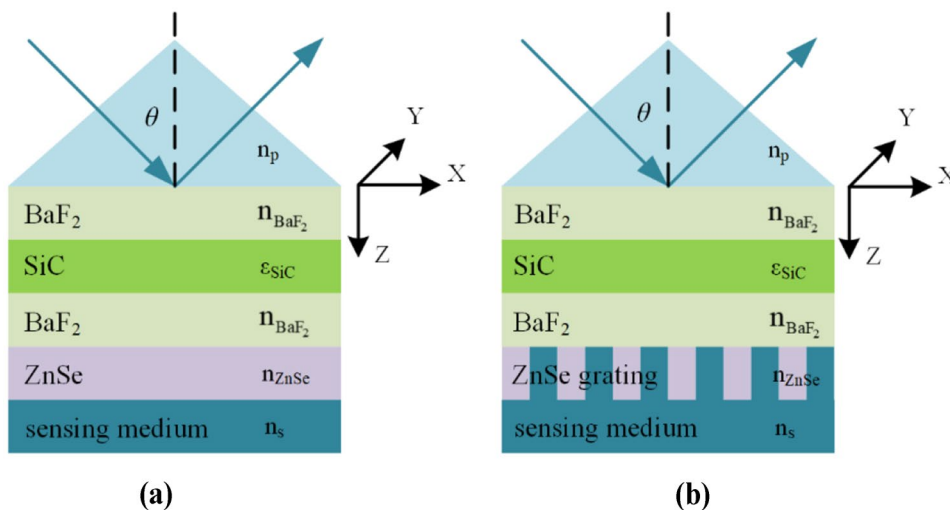
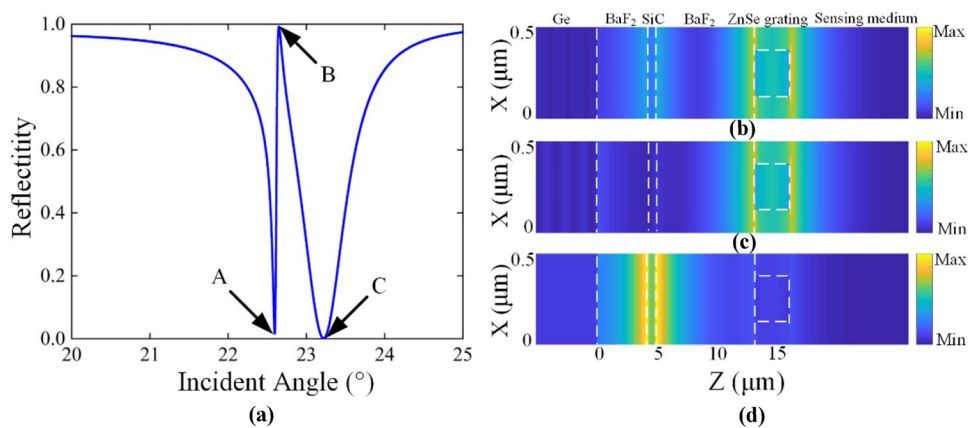


Fig. 3 **a** ATR curve of the sub-wavelength grating structure. **b–d** Electric field distributions at A, B, C in Fig. 3a with RI of sensing medium of 1.332



the value of Z-axis represents the distance from each layer to the prism surface. Fig. 3 b and c show the electric field distributions of the dip ‘A’, ‘B’ at 22.5944 and 22.6483°, respectively. It is revealed that large electric fields appear around ZnSe grating, caused by the coupling between Bloch mode and SPhP. Fig. 3 d corresponds to the dip ‘C’ at 23.2190°. Strong symmetric electric fields generated at the BaF₂-SiC-BaF₂ interface and decay exponentially away from the interface, indicating the excitation of LRSP mode.

Fano resonance exhibits a sharp asymmetric profile due to the strongly trapped resonance, where the reflectance can drop sharply from the peak to the valley of the spectra. High sensitivity can be provided to the index variations of the nearby or surrounding medium because of such a small angle change. Fig. 4 a shows that with the parameters fixed and the RI of sensing medium ranging from 1.332 to 1.333, the FR shifts to a larger angle.

The detectable change of RI determines the quality of the sensor. For evaluating the performance of the sensor, sensitivity (*S*) and FOM are given as follows:

$$S(\theta) = \lim_{\Delta n \rightarrow 0} \frac{\Delta R(\theta)}{\Delta n} = \frac{\partial R(\theta)}{\partial n} \tag{2}$$

$$FOM = \Delta R / (R * \Delta n) \tag{3}$$

where ΔR is the change of reflectivity caused by the change of index Δn , *R* denotes the reflectance in the proposed structure [30, 35]. With $\Delta n = 10^{-3}$, Fig. 4b shows the sensitivity as a function of the incident angle. The peak of the curve in Fig. 4b is defined as *S*_{max}, which is employed to compare the sensitivities to different types of sensors.

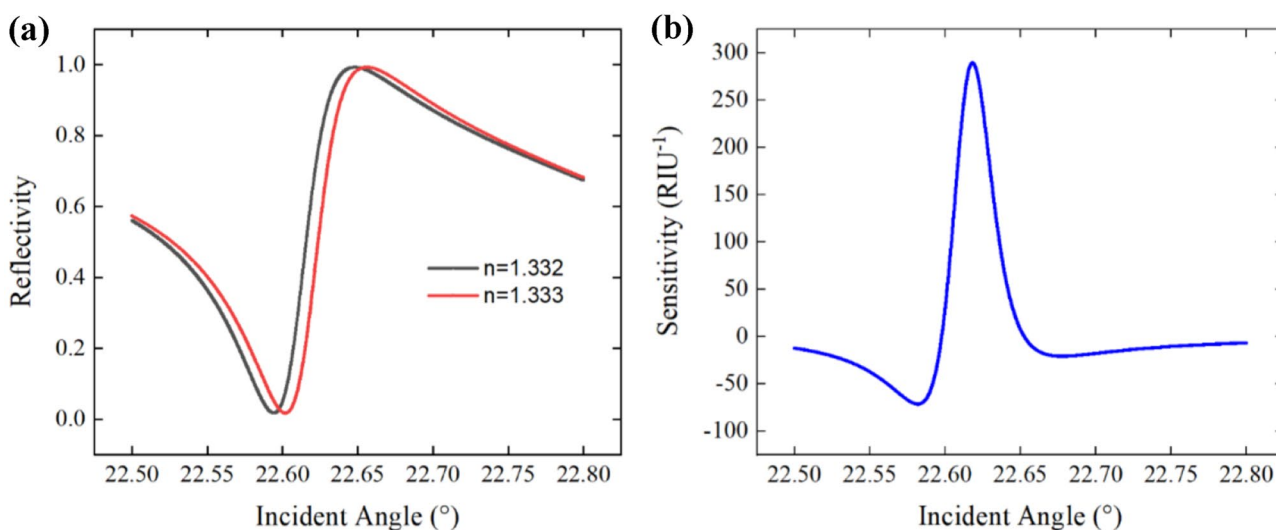


Fig. 4 **a** Variation in ATR curves with respect to the RI of sensing medium ranging from 1.332 to 1.333. **b** Sensitivity as a function of incident angle with $\Delta n = 0.001$

Results and Discussions

For further optimization, we investigate the sensing performance as function of period, duty ratio, height of grating layer, and thickness of BaF₂, respectively. Fig. 5 a demonstrates the variation of ATR curves with the thickness of the BaF₂ layer varying from 8.0 to 12.0 μm. Apparently, with a thicker BaF₂ layer, the coupling between Bloch mode and SPhP is weaker, resulting in a narrower FR. Also, it is obvious that narrower resonance makes a sharper FR curve, leading to higher sensitivity and FOM. Variations of the sensitivity and FOM as functions of BaF₂ thickness are shown in Fig. 5 b and c, respectively. The sensitivity and FOM keep increasing with the increment of the thickness of BaF₂. With $d_2 = 12.0$ μm, they are 5675 RIU⁻¹ and 70,586, respectively.

ATR curves under different grating height are calculated and plotted in Fig. 5d, with d_2 fixed at 12 μm. It is clearly shown that with the increment of grating height, the resonant angle of FR keeps increasing, but the resonant shape remains almost unchanged. Fig. 5 e and f show the variations of sensitivity and FOM with ZnSe grating height ranging from 2.55 to 3.5 μm. Both sensitivity and FOM experience sharp fall before maximizing at $d_3 = 3.4$ μm and 3.25 μm, respectively. This can be attributed that when the resonant peaks of Bloch mode and SPhP get too close, the two modes interact with each

other drastically. The FR becomes more like symmetric electromagnetic induced transparency (EIT) shape with a broader resonant angle.

Fig. 6 a shows the variation of ATR curves with various periods of ZnSe grating. When the period is in the range from 0.5 to 2.5 μm, the LRSPHR angle remains almost unchanged. However, according to Fig. 6 b and c, with the increment of the period, both sensitivity and FOM increase exponentially. This is because a larger period offers a larger contacting area for the sensing medium.

Fig. 6 d shows the variation of ATR curves with duty ratio ranging from 40 to 60%. The resonant angles of FR keep increasing from the left side to the right side of SPhR. Fig. 6 f illustrates the FOM of the proposed SWG sensor maximized with a duty ratio of 57.5%.

Moreover, in order to compare the performances between the SWG-LRSPHR sensor and conventional WG-LRSPHR sensor, sensitivity and FOM have been calculated with BaF₂ thickness ranging from 8.0 to 12.0 μm, as shown in Fig. 7a–d. Noted that with the height of the ZnSe layer of WG-LRSPHR sensor fixed at 1.7 μm, 1.8 μm, 1.9 μm, and 2.0 μm, we adjust the grating height of SWG-LRSPHR sensor to ensure the same resonant angle for comparison. Also, in order to track the sharp slope within the dynamic regime, the change of RI Δn and angle resolution $\Delta\theta$ have been resized. As shown in Fig. 7a–d, the SWG-LRSPHR sensor has good monotonicity and better performance than

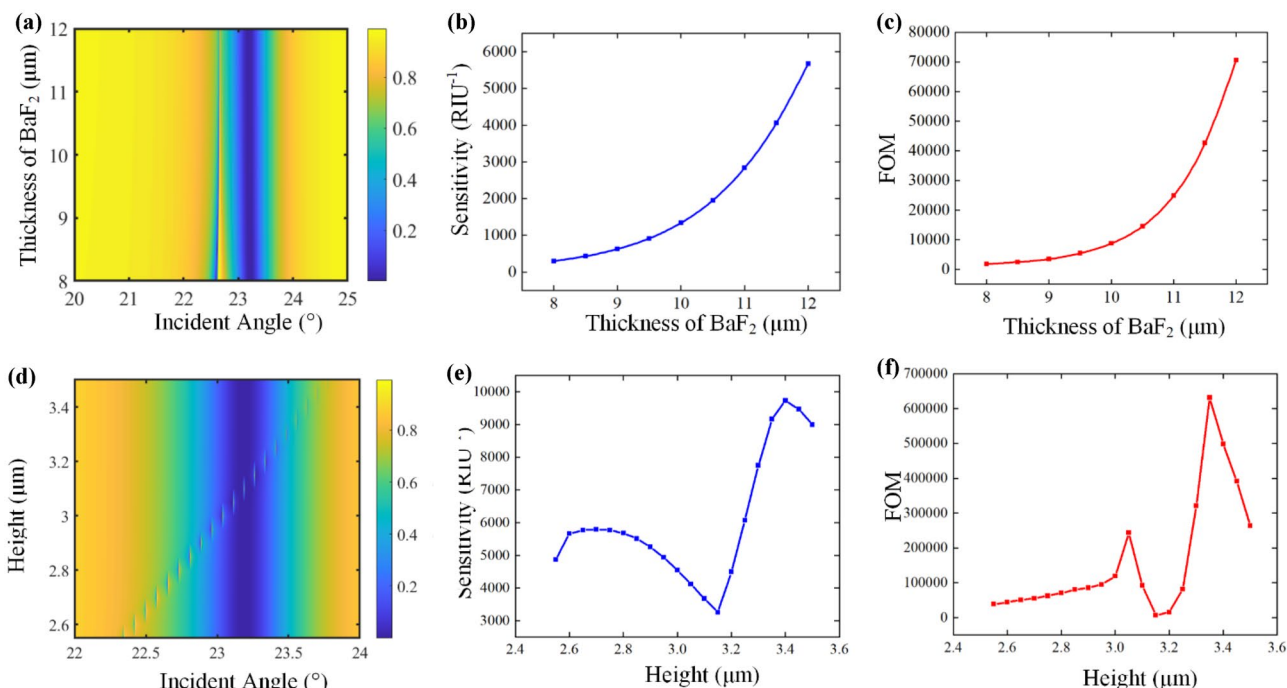


Fig. 5 Angle-resolved density plots of the reflectance with various **a** BaF₂ thickness and **d** height of ZnSe grating. **b**, **e** Sensitivity and **c**, **f** FOM as functions of BaF₂ thickness and height of ZnSe grating, respectively

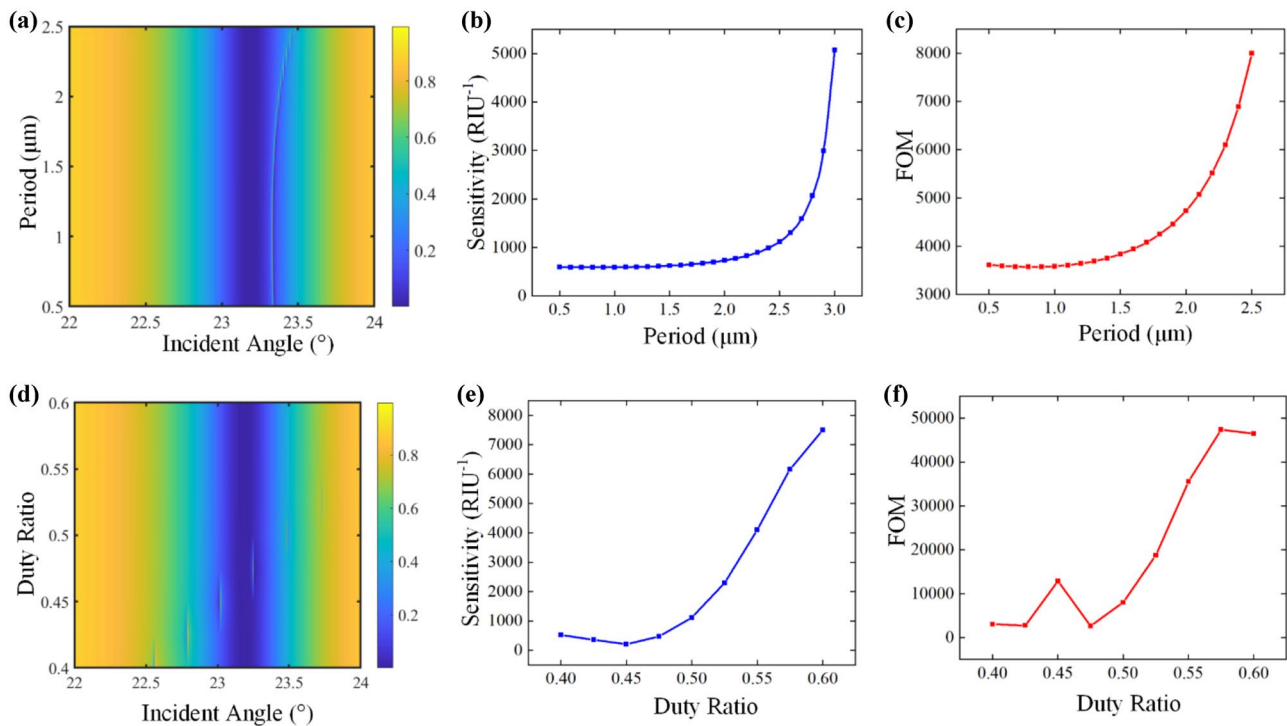


Fig. 6 Angle-resolved density plots of the reflectance with various **a** period and **d** duty ratio. **b**, **e** Sensitivity and **c**, **f** FOM as functions of period and duty ratio of ZnSe grating, respectively

its counterpart. With thicker BaF₂, the advantages of SWG-LRSPHR are more pronounced.

Discussion and Conclusion

Over the past years, researchers have made great efforts to develop the SPR-based sensors' unique advantages such as high sensitivity and miniaturization [36–41]. The devices reported in the above-mentioned references are mainly working in the visible or near-infrared (NIR) wavelength regime. Thus, the footprints are much smaller than the one in our manuscript, which operates in the mid-infrared (MIR) wavelength regime. To further reduce the size, materials supporting surface wave in the MIR, e.g., graphene and transition-metal dichalcogenide (TMDC), can be employed. In the future, optimizing the structure to produce more Fano resonances in single device [42] and introducing two-dimensional materials for enhancing the light-matter interaction are considered to improve the sensor performance [43].

In conclusion, a SWG-LRSPHR-coupled FR sensor has been proposed in MIR. RCWA method has been employed to optimize the structure parameters. Sensitivity and FOM have been employed to assess the sensing performance of RI. Numerical results have demonstrated clearly that the sensitivity and FOM of such a structure can reach 7496 RIU⁻¹

and 46,432, respectively, which shows 6 times enhancement compared with the conventional WG-LRSPHR sensor. With such an excellent performance, the configuration can be a promising platform for biochemical sensing in the MIR.

Authors' Contributions

Tianye Huang and Xiangli Zhang directed the project; Dianhong Wang and Yuhan Wang designed the structure; Xiang Zhao analyzed field distribution; Yuhan Wang made the simulations; Yuhan Wang and Tianye Huang wrote the manuscript in consultation with Dianhong Wang, Xiangli Zhang, and Shuwen Zeng.

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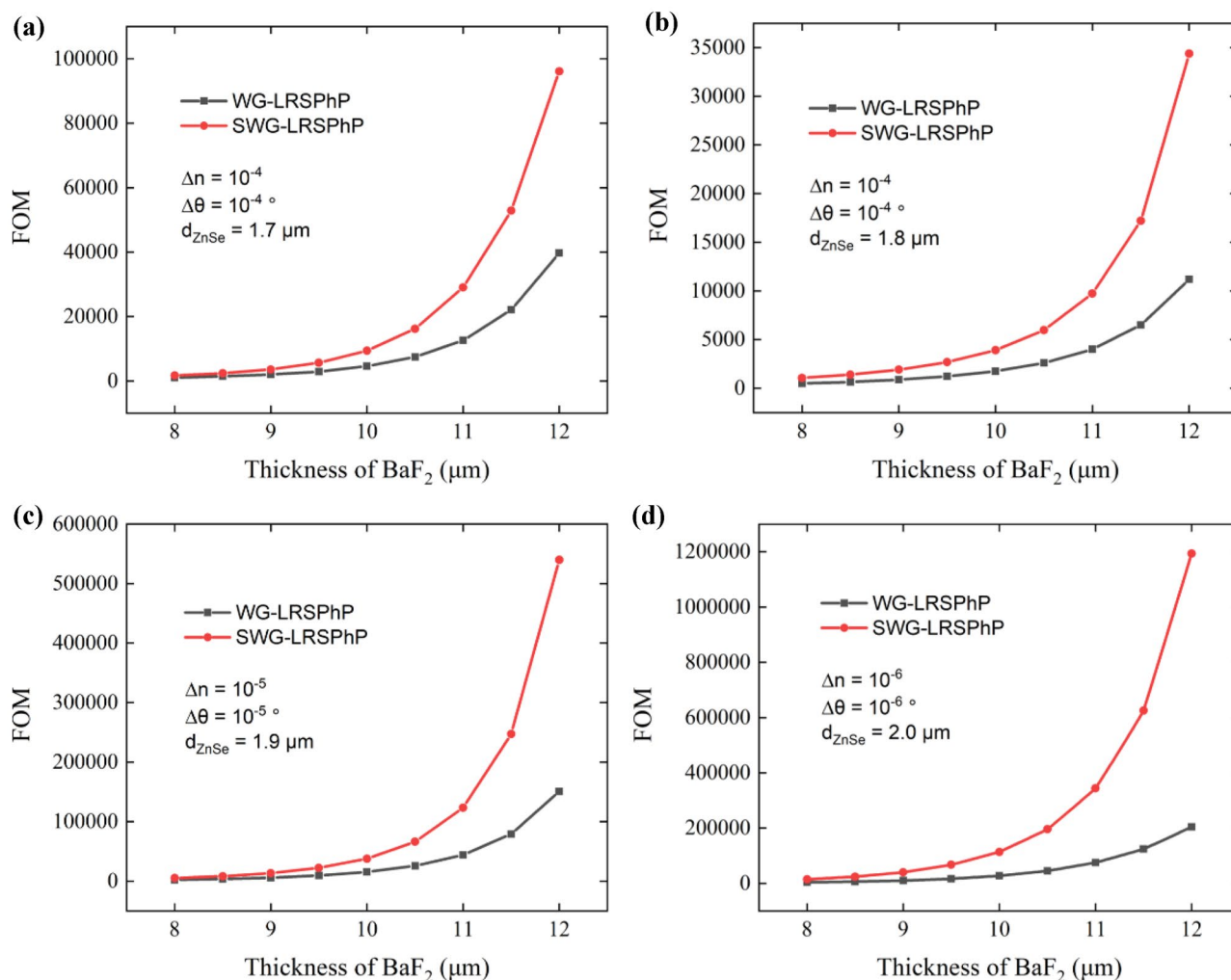


Fig. 7 Comparison of FOM between WG-LRSPhR and SWG-LRSPhR with different thicknesses of the BaF₂ layer

Data Availability The datasets used or analyzed during the current study are available from the corresponding author on reasonable request.

Compliance with Ethical Standard

Conflict of Interest The authors declare that they have no conflict of interest.

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