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Theoretical study of leaky-mode resonant gratings for improving the absorption efficiency of the uncooled mid-infrared photodetectors

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In this work, we studied a new theoretical approach to enhance the PbSe-based uncooled photodetector's performance in the mid-infrared (mid-IR) wavelength region. A one-dimensional grating layer was proposed to be implemented and inserted under the PbSe photosensitive layer. Due to the leaky-mode resonance tuning mechanism, this grating layer could manipulate mid-IR light-and-matter interactions in a unique way. It not only prevents the light transmission loss from the backside of the device but also tunes the destructive interference in the reflectance spectra, which consequently maximize the light absorption in the weak-absorbing energy band-tail region. By combining these two capabilities, it is possible to improve detector's sensitivity significantly. With this goal, several grating parameters including grating period, fill factor, and grating thickness were systematically investigated and optimized by using the rigorous coupled wave analysis method. Through the optimization, a 33% broadband absorption enhancement was achieved by using a Si ($n = 3.489$)/SiO₂ grating on a soda-lime glass ($n = 1.45$) substrate with the listed parameters: grating period = 2.4 μm , fill factor = 0.49, and thickness = 1.22 μm . Apparently, this simple and effective method could practically advance the uncooled mid-IR PbSe detector's performance. But more importantly, this photonic-design concept can be used in and impact many other light-matter interaction related research fields. *Published by AIP Publishing.* <https://doi.org/10.1063/1.5040373>

I. INTRODUCTION

Mid-infrared (mid-IR) detectors enable us to broaden our vision to the realm of heat which helps us to perceive the world in a different way. Built upon this technology, the thermal imaging system has developed a broad range of applications including night vision, failure analyses, infrared astronomy, and medical diagnostics.^{1,2} In comparison to thermal detectors responding to the temperature variations caused by heat, mid-IR photodetectors directly converting spectral dependent infrared radiation into electric charges are much preferable because of their intrinsic fast response advantages. However, mainly due to their thermally induced device noise and dark current limitations, the room-temperature operation of this type of detectors has been a great challenge for decades. Thus, a cooling system is generally required, which makes the imaging system bulky and expensive.² As one kind of mid-IR photodetectors, PbSe photoconductors have remained the choice for many civilian and military sensing applications in the 3–5 μm spectral region,³ simply because their uncooled functionality and superior detectivity $> 3 \times 10^9 \text{ cm Hz}^{1/2} \text{ W}^{-1}$ could satisfy many practical-use requirements.⁴

In fact, this level of performance has not been fully optimized and could be potentially improved by almost two orders of magnitude, considering that the theoretical Background-Limited Infrared Performance (BLIP) limit is at $\sim 10^{11} \text{ cm Hz}^{1/2} \text{ W}^{-1}$.⁵ In recent years, many research efforts have been focused on understanding the material physics and charge transportation behaviors in order to improve the

internal quantum efficiency and suppress the noise and dark current impacts.^{6,7} On the other hand, due to a large refractive index contrast between the PbSe material and the ambience, the overall detection efficiency is also affected greatly by reflection and transmission losses. Therefore, investigating possible methods to reduce the light coupling losses can also be an important pathway to boost the detector performance significantly.

In our recent work,⁸ an effective nanophotonic strategy has been developed to reduce the light reflection loss significantly. By using a biomimetic broadband anti-reflective nano-coating, the uncooled PbSe mid-IR photoconductor exhibited a record-high peak detectivity of $4.2 \times 10^{10} \text{ cm Hz}^{1/2} \text{ W}^{-1}$ at room temperature. This anti-reflective coating was developed to modify the light and sensor interaction on the top surface of the device. Nevertheless, considering the optical transmission loss from the bottom of the active thin film, a thick layer of the PbSe film still needs to be prepared, which unfortunately induces further issues like the increased Johnson noise.⁹ Such a problem offsets the counterpart of the advantage of enhancing the light harvesting efficiency. Therefore, to develop another solution to modify the light-matter interaction behavior at the bottom surface of the device, so that both the absorption enhancement and the device Johnson-noise suppression can be satisfied, is of great research interest to further elevate the sensor performance to a higher level.

Traditionally, to achieve this goal, depositing a layer of metal as a mirror reflector has been the most straightforward solution. However, unlike solar cells,¹⁰ from the practical viewpoint, using the metallic reflector does not work in the PbSe detector scheme, since the thin film has to be sensitized at high temperature under active gas ambience with O₂ and

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iodine mixtures. Metal films degrade dramatically in this sensitization process and unavoidably lose their perfect reflective properties.⁷ Additionally speaking, by having a layer of metallic film laying down the PbSe thin film, the inherent short-circuit problem can also hardly be addressed. Therefore, in this work, we theoretically proposed a unique approach to fulfill the same purpose as aforementioned. A dielectric grating layer was applied to function as a broadband reflector to both enhance light absorption efficiency and suppress the intrinsic noise effect. The theory and methodology is presented in Sec. II, and the design and simulation results are presented in Sec. III in detail.

II. THEORY AND METHODOLOGY

To determine the photodetector overall performance, specific detectivity (D^*) is commonly used as the standard figure-of-merit²

$$D^* = \frac{\eta}{I_n} \left[\frac{\lambda q g (A_0 \Delta f)^{1/2}}{hc} \right], \quad (1)$$

where λ is the wavelength, η is the quantum efficiency, q is the electron charge, g is the photoconductive gain, A_0 is the optical area, Δf is the band frequency, h is Planck's constant, c is the light velocity, and I_n is the electrical noise which includes Johnson and generation-recombination noises.² According to Eq. (1), we need to generally consider two major fundamental factors, including the quantum efficiency and the electrical noise.

Quantum efficiency stands for the light-to-current conversion efficiency, which basically tells how many electrons can be collected resulting from an input photon. The expression⁹ for quantum efficiency takes the form of

$$\eta = (1 - \zeta_1 + \zeta_2 e^{-\alpha t})(1 - e^{-\alpha t}), \quad (2)$$

where ζ_1 is the Fresnel reflection on the incident surface, ζ_2 is the back-surface reflection, t is the detector thickness in the direction of propagation, and α is the absorption coefficient. One strategy to increase specific detectivity could be increasing the quantum efficiency through increasing the detector thickness. However, by increasing the thickness, the detector resistance will be decreased. So, the equivalent resistance of the load resistor and the detector resistor would be decreased. Consequently, Johnson-noise would be increased. You can see this process clearly in the following equation:⁹

$$i_J = \sqrt{\frac{4KT\Delta f}{R_{eq}}}, \quad (3)$$

in which i_J is the Johnson noise, K is the Boltzmann constant, T is the temperature, Δf is the frequency band, and R_{eq} is the equivalent resistance. Thus, inherent Johnson noise, unfortunately, offsets its counterpart of light harvesting advantage. On the other hand, the detectivity through the following equation is dependent on the detector thickness:²

$$D^* = \frac{\lambda}{hc} (1 - e^{-\alpha t}) \left[2(G + R)t^{-1/2} \right], \quad (4)$$

where λ is the wavelength, h is Planck's constant, c is the light velocity, G and R are the generation and recombination rates, t is the detector thickness, and α is the absorption coefficient. Thus, the highest detectivity will be obtained when $t = 1.26/\alpha$, where $(1 - e^{-\alpha t})t^{-1/2}$ achieves the maximum value.² This thickness is a trade-off between high quantum efficiency and low thermal generation. So, for a PbSe layer, the highest detectivity will be obtained when $t = 1.26 \mu\text{m}$, in which the average of the absorption coefficient in the range of 3–4.4 μm is 10^4cm^{-1} .¹¹ By considering all these discussions, there is a strict limitation on the detector thickness. According to Eq. (2), the other strategy to enhance quantum efficiency is minimizing Fresnel reflection, which has been conducted in previous works,⁸ resulting in a notable impact on absorption enhancement. Also, it is expected that maximizing back-surface reflection to increase the absorption length can notably improve the absorption value. To achieve this goal, a broadband reflector could be used.

As discussed in Sec. I using a metallic reflection mirror is not a viable method for the PbSe detectors. Alternatively, we found that the one-dimensional dielectric grating structure could offer similar broadband reflection functionality to the metallic mirrors but relying on a different physics mechanism called leaky mode resonance (LMR) in a lateral direction. Such LMR-assisted lateral grating structures have demonstrated effective broadband light manipulating capability in various fields including optical filters, displays, biosensors, and wideband reflectors.^{12,13} The LMR occurs when the incident wave is coupled with a lateral resonant mode supported by a grating structure under phase matching conditions.¹⁴ Conditions will be satisfied through optimizing grating parameters including grating period, fill factor, and grating thickness. Due to the resonance effect, the diffracted energy redistributes and manifests as transmission and reflection peaks.¹⁵ Also, electric fields of LMR modes confined to the surface evanescently could be intensively enhanced in comparison to the electric field of the excitation source.^{16,17} The leaky-mode spectral placement, their spectral density, and levels of interaction are the major factors affecting device operations and functionalities.¹⁸

In this work, a numerical simulation method called the rigorous coupled-wave analysis (RCWA) is adopted to study and design the LMR grating structures for enhancing PbSe mid-IR photodetector performance. It is a known method to solve Maxwell's equations for the electromagnetic diffraction in the grating structures.¹⁹ This method analyzes the diffracted waves from a planar grating bounded by two different media. The general approach in the RCWA method is to find solutions that satisfy Maxwell's equations in each of the three (input, grating, and output) regions and then match the tangential electric and magnetic fields. In a planar diffraction, the incident wave could have TE or TM polarization which is solved independently. Figure 1 demonstrates a schematic view of diffracted waves from a grating structure.

In this paper, we choose to work with TM-polarized modes because they have a greater Q-factor than TE modes, resulting in stronger absorption.¹⁶ Thus, we will describe the RCWA method to solve the TM polarization, although the

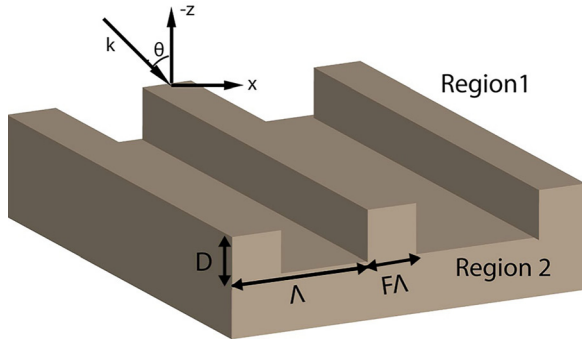


FIG. 1. Schematic view of diffracted waves from a grating structure.

general method to solve TE modes is the same. Therefore, to match tangential magnetic fields, we need to calculate the field in each region. Magnetic and electric fields in the grating region are expressed as a Fourier expansion

$$H_{g,y} = \sum_i u_{yi}(z) \exp(-jk_{xi}x), \quad (5)$$

$$E_{g,x} = j \left(\frac{\mu_0}{\epsilon_0} \right)^{1/2} \sum_i s_{xi}(z) \exp(-jk_{xi}x), \quad (6)$$

where $u_{yi}(z)$ and $s_{xi}(z)$ are the normalized amplitudes of the i th space-harmonic field and k_{xi} is driven by the Floquet condition

$$k_{xi} = k_0 \left[n_1 \sin \theta - i \left(\frac{\lambda_0}{\Lambda} \right) \right]. \quad (7)$$

By substituting Eqs. (5) and (6) into Maxwell's equations, a set of coupled-wave equations will be given. The set of coupled-wave equations is solved by calculating eigenvalues and eigenvectors of matrix \mathbf{EB} . Space harmonics of the tangential magnetic and electric fields are then given by

$$u_{yi}(z) = \sum_{m=1}^n w_{im} [c_m^+ \exp(-k_0 q_m z) + c_m^- \exp(k_0 q_m (z-d))], \quad (8)$$

$$s_{xi}(z) = \sum_{m=1}^n v_{im} [-c_m^+ \exp(-k_0 q_m z) + c_m^- \exp(k_0 q_m (z-d))], \quad (9)$$

where $w_{i,m}$ and q_m are elements of the eigenvector matrix \mathbf{W} and the positive square root of eigenvalues of the matrix $\mathbf{EB} = \mathbf{K}_x^2 - \mathbf{I}$, respectively. \mathbf{K}_x is a diagonal matrix, where the i, i element is equal to k_{xi}/k_0 , and \mathbf{I} is the identity matrix. Quantities $v_{i,m}$ are elements of the product matrix $\mathbf{V} = \mathbf{E}^{-1} \mathbf{W} \mathbf{Q}$, where \mathbf{Q} is a diagonal matrix in which diagonal elements q_m , c_m^+ , and c_m^- are constants and are determined by the boundary conditions. Then, by matching tangential electric and magnetic-field components at the boundaries, the amplitude of diffracted waves will be calculated (R_i is the diffracted reflected wave in region 1, and T_i is the transmitted wave in region 2). Diffraction efficiencies are defined as¹⁹

$$DE_{ri} = R_i T_i^* \operatorname{Re} \left(\frac{k_{1,zi}}{k_0 \cos \theta n_1} \right), \quad (10)$$

$$DE_{ti} = T_i T_i^* \operatorname{Re} \left(\frac{k_{2,zi}}{n_2^2} \right) / \left(\frac{k_0 \cos \theta}{n_1} \right), \quad (11)$$

where

$$k_{l,zi} = \begin{cases} k_0 \left[n_l^2 - \left(\frac{k_{xi}}{k_0} \right)^2 \right]^{1/2} & k_0 n_l > k_{xi} \\ -jk_0 \left[\frac{k_{xi}}{k_0} - n_l^2 \right]^{1/2} & k_0 n_l < k_{xi} \end{cases} \quad l = 1, 2.$$

Therefore, to design a grating structure which reflects the light in the considered region, the grating parameters, the incident angle, and the refractive index are critical.

III. DESIGN, SIMULATION, AND DISCUSSION

In this study, the LMR grating layer is embedded underneath the PbSe ($n_{\text{PbSe}}=4.95$) photo-sensitive layer in the device. The schematic view is presented in Fig. 2. As shown, the grating structure consists of a periodically distributed dielectric material of silicon ($n_{\text{silicon}}=3.489$) and SiO_2 ($n_{\text{SiO}_2}=1.45$), which is the same material used for the substrate. The design parameters include the grating layer thickness d_1 , PbSe thickness d_2 , fill factor F , and grating period Λ . Meanwhile, the incident wave, reflectance, and transmittance are denoted as \mathbf{I} , \mathbf{R} , and \mathbf{T} , respectively.

By investigating the impacts of these parameters as mentioned, a broadband and strong mid-IR reflection of the grating layer is intended to be achieved. In this way, the backside transmission loss of the PbSe thin film would be strongly suppressed, and the light absorption could be enhanced consequently. The optimization of the grating period and fill factor has been conducted through investigating transmission patterns. As shown in Fig. 3, a broadband suppression of transmission has been realized when the fill factor and period are in the range of 0.5–0.6 and 2.3–2.5, respectively. It is also necessary to mention that our design in this study focuses on the wavelength range from 3 to 4.4 μm , considering the fact that the uncooled PbSe photodetector can only detect the photons up to $\sim 4.4 \mu\text{m}$ due to the energy bandgap limitation. Therefore, its wavelength dependent absorption coefficient values have been included in our simulation model as well.²⁰

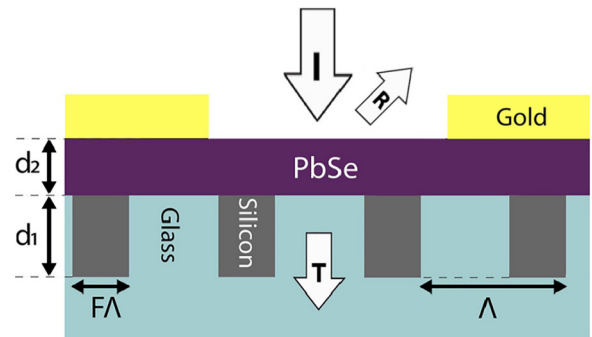


FIG. 2. Schematic view of a PbSe photoconductive detector with the integration of the grating structure under normal incidence.

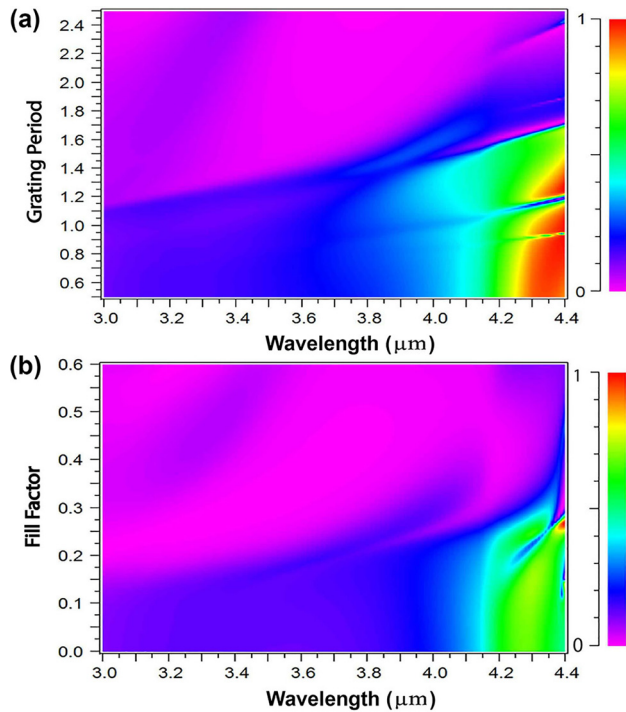


FIG. 3. (a) Changing pattern of transmission according to the manipulation of the grating period and (b) changing pattern of transmission according to the manipulation of the fill factor.

As follows, we present the theoretical optimization efforts by studying the reflectance and transmittance patterns in response to the grating period, fill factor, and the grating thickness. As shown in Fig. 4(a), a strong transmission attenuation effect is achieved by applying a grating structure having the period of $2.4 \mu\text{m}$, fill factor of 0.49, and thickness of $1.22 \mu\text{m}$. It is also noted that the top PbSe layer in this design is of the optimized thickness value at $1.26 \mu\text{m}$. Obviously, Fig. 4(a) demonstrates a strong suppression of the transmission spectrum in a broadband wavelength range from 3 to $4.4 \mu\text{m}$. What is notable close to the bandgap region is that the intensity reduces significantly from 65% down to $\sim 15\%$. The broadband reflection is achieved as shown in Fig. 4(b), which clearly makes this grating structure behaves like a mirror in the mid-IR region. The underlying physics is due to the multi-mode coupling effect by two LMRs in this wavelength range, which is presented as the transmission spectrum dips in Fig. 4(b).

Figure 5 shows the enhanced absorption due to the grating structure. As can be seen, there are two peaks at $4.1 \mu\text{m}$ and $3.4 \mu\text{m}$. These peaks are the product of suppression of transmitted waves by LMR and destructive interference of reflected waves at the same time. The calculation of the area under the curve demonstrates that total absorption enhanced from 0.49 to 0.65. This means that for a thin layer of PbSe ($1.26 \mu\text{m}$), implanting the grating structure enhances the absorption value by nearly 33%.

Moreover, we also discovered another unique advantage of using this LMR grating layer to enhance the light absorption for the PbSe mid-IR device, which is the ability to control the interference peak positions. That is to say, besides

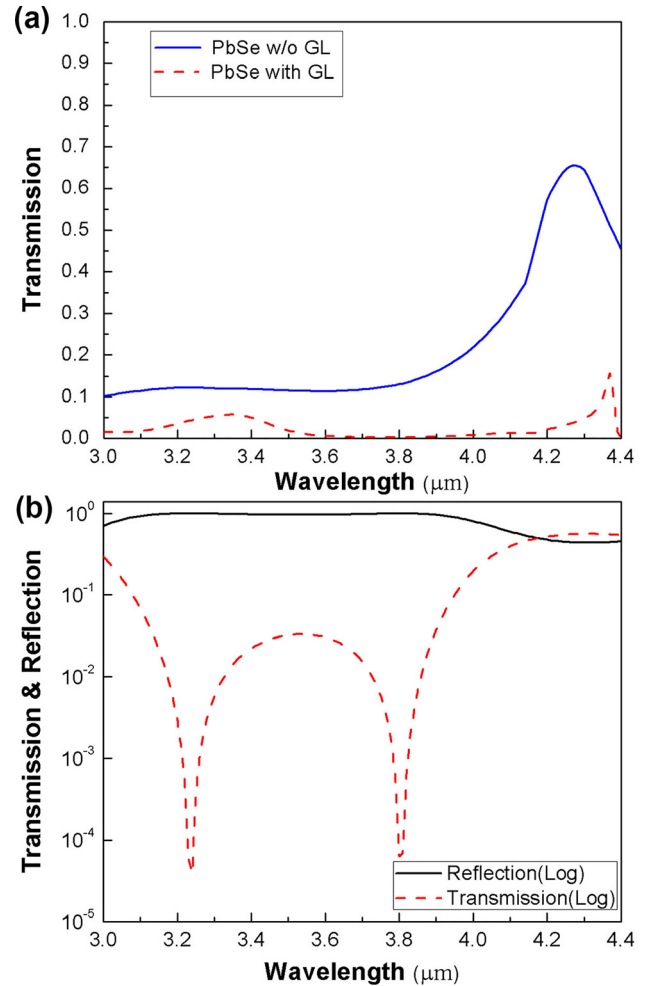


FIG. 4. (a) Transmission comparison of the mid-IR photodetector device with and without the optimized grating structure under the PbSe thin film. (b) Reflection and transmission spectra of the grating reflector on the logarithmic scale. (Note: the simulated light is of TM polarization.)

benefiting the transmission loss suppression from the LMR coupling effect, we could also minimize the reflection loss by controlling the vertical interference effect. The reason is explained in the following part.

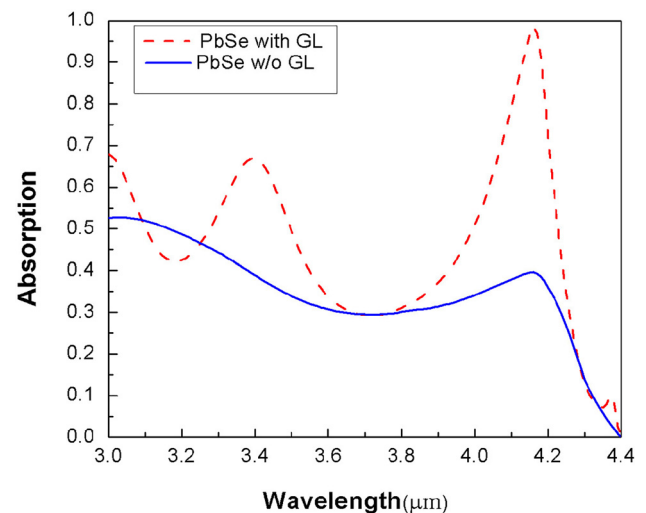


FIG. 5. A comparison between absorption values with and without the grating structure as the reflector (PbSe thickness = $1.26 \mu\text{m}$).

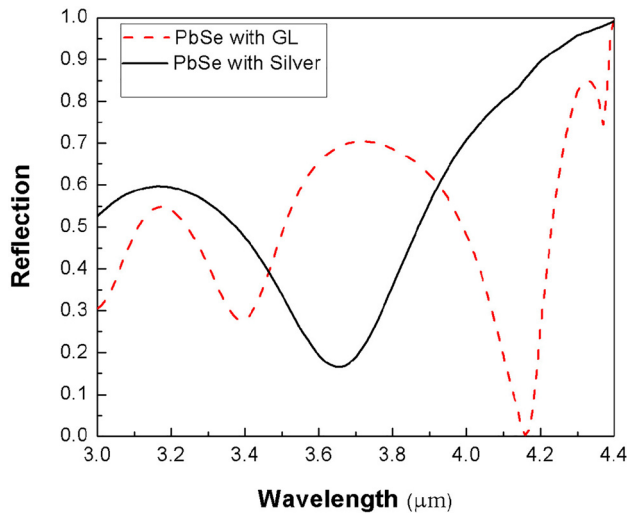


FIG. 6. A comparison between reflection values when we use the grating structure and silver as the reflector (PbSe thickness = $1.26 \mu\text{m}$); normal incidence.

When we use a layer of silver as a metallic mirror, it prevents the light penetration into itself and reflects the transmitted light completely, and the only destructive wave is made at $3.66 \mu\text{m}$ (Fig. 6) according to the following equation:²¹

$$2nd = \left(m - \frac{1}{2}\right)\lambda, \quad (12)$$

where n , d , m , and λ are the refractive index of PbSe, thickness of PbSe, diffracted index (integer), and wavelength, respectively. Thus, the only way to change the position of destructive interference is changing the thickness of PbSe. However, as described in Sec. II the PbSe thickness should be set at a fixed value for achieving the best D* performance. Comparing with the metallic mirror, this LMR grating layer can be treated as an imaginary uniform layer with a constant effective reflective index, which allows a fraction of transmitted waves to go into the layer. Therefore, combining with

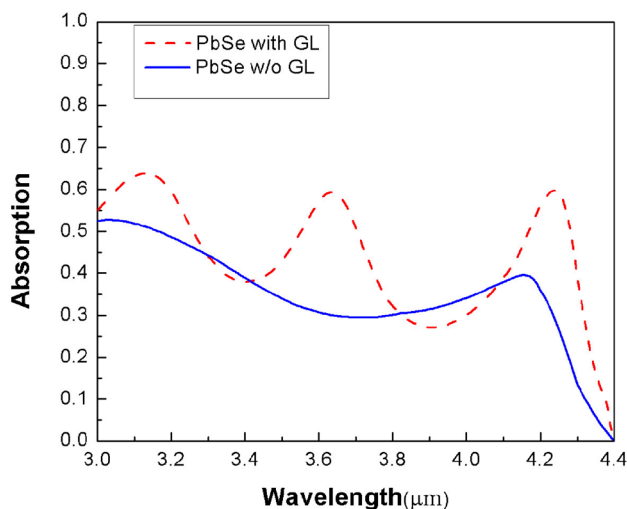


FIG. 7. A comparison between absorption values with and without the grating structure ($\Lambda = 2.4$, $F = 0.49$, $d_1 = 1.48 \mu\text{m}$, and $d_2 = 1.26 \mu\text{m}$); TM polarization under normal incidence.

the PbSe layer on top, the multilayer wave interference effect can be achieved. With this advantage, we could solely adjust the thickness of the grating layer and then be able to tune the reflection dip position to the energy band tail region where the weak absorption typically locates. The importance of this can be clarified in some imaging purposes, in which covering a broader range without a cooling system is critical. Figure 6 shows the comparison between the reflected wave from the surface of PbSe when we use a layer of silver and the grating structure as the reflector.

Without changing the PbSe thickness and just by manipulating the grating parameters, we could make two destructive interferences in this range of wavelength. With that, implanting a grating structure at the bottom of the PbSe not only strongly attenuates transmitted waves but also suppresses the reflected waves through the destructive interference as well. To provide a demonstration, as shown in Fig. 7, using the grating structure of $\Lambda = 2.4 \mu\text{m}$, $F = 0.49$, $d_1 = 1.48 \mu\text{m}$, and $d_2 = 1.26 \mu\text{m}$, we would be able to modulate the absorption performance in the energy band tail region and the total absorption can be enhanced significantly between 4.2 and $4.4 \mu\text{m}$, and the overall enhancement is by $\sim 24\%$.

IV. CONCLUSION

In conclusion, we presented a new theoretical approach to enhance PbSe-based uncooled photodetectors in the mid-IR wavelength region. To avoid increasing the device noise by using a thick PbSe film, we proposed a unique solution by using a broadband LMR grating reflector to enhance the device performance. Such structures behave like a metallic mirror and could prevent the light transmission loss from the backside of the device significantly, from 65% to less than 15%. Consequently, the total absorption enhanced nearly 33% by designing the grating layer. Moreover, simply by tuning the grating thickness, it also enables us to adjust the interference pattern and minimize the reflection loss in the interested area. For example, this strategy could help us compensate the decreased absorption near the band-gap range. In this way, the device could deliver decent performance at its cut-off band-edge area without cooling the material to move the band-edge into the higher wavelength region. This offers advantages including low-cost, low-power consumption, and smaller foot-print. They are critical for civilian and military applications, like gas sensing and thermal imaging. In our future research, we will explore an integrated solution to enhance absorption for both TM and TE polarized light at the same time, e.g., a two-dimensional grating layer.

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