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Enhancement of absorption of molybdenum disulfide monolayer on low-index contrast dielectric grating in the visible regions

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ABSTRACT

A design consists of low-index contrast grating is proposed to achieve the narrow absorption response for two-dimensional (2D) materials such as a MoS_2 monolayer in the visible wavelength regime. High absorption occurs at the wavelength of Fano resonance for both transverse dielectric (TE) and transverse magnetic (TM) polarizations. It is proved that by manipulating related structural parameters and the incident angle, the peak wavelengths of MoS_2 absorption can be tuned in a wide range. In addition, an improved structure with MoS_2 ribbons is proposed to further boost the light-MoS_2 interaction. The relationships between the absorptance and the period and width of MoS_2 ribbons are discussed. The proposed optical devices could be efficiently exploited as tunable absorbing structures for optoelectronics and photovoltaic devices in the visible region.

1. Introduction

In recent years, two-dimensional (2D) materials [1–8], such as graphene [9–13], hexagonal boron nitride (hBN) [5,14], and transition-metal dichalcogenides (TMDCs) [15–18] have received burgeoning amount of interest due to their promising properties including tunability, high thermal conductivity, and high electron mobility. Owing to special direct band gaps and internal amplification, monolayer TMDCs have been considered as more preferable atomically thin materials for photodetection, photoluminescence, the field-effect transistors as well as photovoltaic devices [17–26].

MoS_2 becomes as a direct-bandgap semiconductor when it is transformed from the bulk to monolayer [27]. Monolayer MoS_2 has a direct band gap around 1.8 eV for electronic transition [28]. However, due to the thickness of monoatomic, the absorptance of monolayer MoS_2 is usually very low within the visible wavelength [29], which limits its further applications in optoelectronic devices. Efforts of promoting the interaction between the monolayer MoS_2 and the incident light have been made to enhance the absorption rate of light [30,31]. Ansari [32] et al. proposed a three-layer stack structure consisting of monolayer MoS_2 which reaches to be 65% absorption for internal reflection and polarization. Long et al. [33] investigated the absorption of the structure formed by a metal grating structure covered with a monolayer MoS_2, the absorptance can reach to near-unity at the resonance wavelength. Lu et al. [34] theoretically increased the absorptance of monolayer MoS_2 to 70% at work wavelength by laying MoS_2 layer sandwiched between the top and bottom chirped distributed Bragg reflector (DBR). However, in the studies related with the boost absorption of MoS_2, the enhancement is usually induced with additional metal layers and multilayer MoS_2, which is more difficult to be fabricated for practical application.

In this paper, a low-index contrast dielectric grating structure of Fano resonance with MoS_2 monolayer and ribbons covered on is proposed to realize the tunable high absorption of light. The operation principle of the structure is analyzed by using the rigorous coupled wave analysis (RCWA). It is demonstrated that the enhancement of the interaction between MoS_2 and light can be realized for TE and TM polarizations in the visible wavelength range. The resonant positions of absorption peaks can be tuned effectively by varying the structural parameters. In addition to MoS_2, the principle can be introduced to improve the absorption in monolayer $MoSe_2$, WS_2, and WSe_2.

2. Structure model and physical mechanism

Fig. 1 shows the schematic diagram of the structure consisting of a monolayer MoS_2. The dielectric grating is composed of two different

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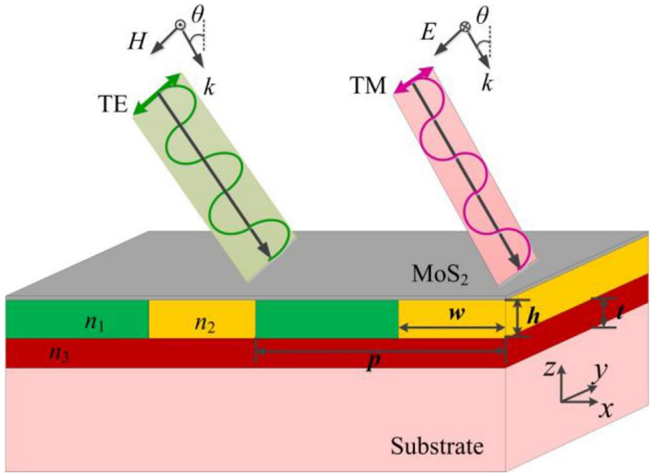

Fig. 1. Schematic of the proposed multilayer absorber with low-contrast index grating covered by a MoS_2 monolayer. Optical waves (TE or TM) are incident with angle of θ. The structural parameters as chosen as: $n_1 = 1.78$, $n_2 = 2.03$, $n_3 = 3.96$, $p = 0.4$ µm, $w = 0.16$ µm, $h = 0.18$ µm and $t = 0.04$ µm.

materials which are glass (SF11, n_1) and Si_3N_4 (Silicon nitride, n_2) with refractive indices (RI) of $n_1 = 1.78$ and $n_2 = 2.03$ [35], respectively. Since the index ratio of the ridge and the groove n_2/n_1 is just 1.14, such a grating of the structure can be called as a "low-contrast grating" [36]. The period of the dielectric grating is $p = 0.4$ µm. The ridge width of the grating is $w = 0.16$ µm. The thicknesses of the grating and the spacer layer are $h = 0.18$ µm and $t = 0.04$ µm, respectively. The spacer layer is set as silicon (Si) and the substrate is chosen as SiO_2. The optical constants of them are referred from Ref. 35. The grating structure is sensitive with the polarization by its nature of one-dimensional (1D) periodicity. The real and imaginary parts of the complex refractive index of monolayer MoS_2 as a function of wavelength are taken from Ref. 37. Several models have been proposed to describe the dielectric functions of MoS_2 [16,37,38]. In this study, a hybrid Lorentz-Drude-Gaussian model [33,37] is employed, where the dielectric function of a monolayer MoS_2 consists of Lorentz-Drude (LD) and Gaussian (G) terms, i.e.,

$$\varepsilon_{MoS2} = \varepsilon_{MoS2}^{LD} + \varepsilon_{MoS2}^{G} \tag{1}$$

The Lorentz-Drude part of the frequency dependent permittivity is given by

$$\varepsilon_{MoS2}^{LD} = \varepsilon_{\infty} + \sum_{j=0}^{5} \frac{a_j \omega_P^2}{\omega_j^2 - \omega^2 - i\omega b_j}, \tag{2}$$

Where $\omega_P = 4.3 \times 10^{13} rad/s$ indicates the plasma frequency, $\varepsilon_{\infty} = 4.44$ represents the DC permittivity, ω_j , a_j and b_j are the j-th oscillator's resonance frequency, oscillator strength, and damping coefficients, respectively.

For the Gaussian component, we first define it as

$$\mathrm{Im}[\varepsilon_{MoS2}^{G}] = \alpha \exp\left(-\frac{(\hbar\omega - \mu)^2}{2\sigma^2}\right), \tag{3}$$

$$\mathrm{Re}[\varepsilon_{MoS2}^{G}] = -\frac{1}{\pi} PV \int_{-\infty}^{\infty} \frac{\mathrm{Im}[\varepsilon_{MoS2}^{G}]}{\omega' - \omega} d\omega', \tag{4}$$

where the mean $\mu = 2.7723$, standard deviation $\sigma = 0.3089$, and maximum value $\alpha = 23.224$. The real part of the Gaussian component is defined by utilizing Kramers-Kronig relation [39].

The refractive index of the MoS_2 monolayer is $RI_{MoS2} = n + ik$ [40], where

$$n = \sqrt{\frac{\sqrt{\varepsilon_{real}^2 + \varepsilon_{imag}^2} + \varepsilon_{real}}{2}}, \tag{5}$$

$$k = \sqrt{\frac{\sqrt{\varepsilon_{real}^2 + \varepsilon_{imag}^2} - \varepsilon_{real}}{2}} \tag{6}$$

are the real and imaginary parts of the complex refractive index of monolayer MoS_2 at a temperature of 300 K and Fermi energy of 0 eV depicted in Fig. 2(a). The thickness of monolayer MoS_2 layer is used as 0.65 nm. From Fig. 2 (b), it can be seen that the absorption of monolayer MoS_2 is mainly attributed to the imaginary part of the complex refractive index. Incident plane waves with E-field polarization along and perpendicular to the grating bars are referred to as TE and TM polarizations, respectively.

3. Results and discussions

Fig. 3 shows the calculated reflection, transmission and absorption spectra of the proposed grating structure by the RCWA method. RCWA is usually uased for modeling the diffraction of electromagnetic waves on the periodic grating array. It solves Maxwell's equations corresponding to the light scattering problem by using a Fourier expansion to represent the optical property at periodic grating region based on the Floquet's theorem [41]. The convergence is ensured by including sufficient total number of diffracted orders of 103. When there is no MoS_2 layer coated, the spectra of the grating structure show a Fano-like line type for both two polarizations. Specifically, a total reflection occurs at the resonant wavelength of 0.59 µm for TE-polarized wave and 0.69 µm for TM-polarized wave. It is interesting to find that the absorptance of the proposed structure increases sharply to about 80% for TE polarization and about 90% for TM polarization at the resonant wavelengths

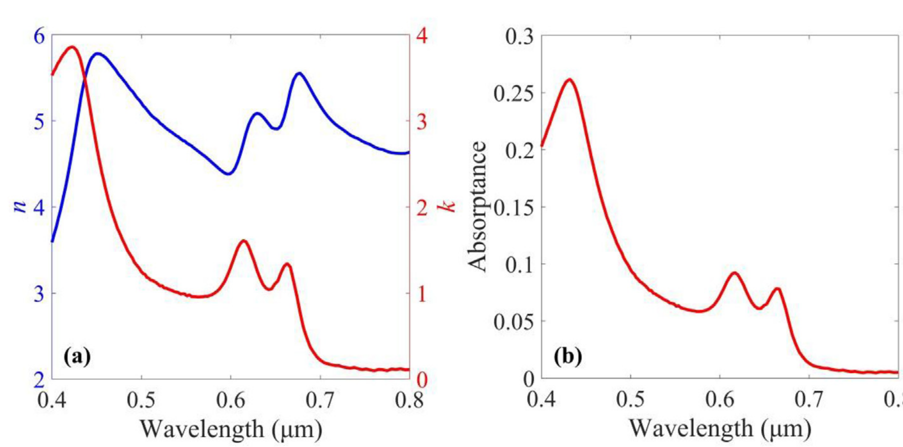

Fig. 2. (A) Complex refractive index of MoS_2 in the visible wavelength region. (b) absorptance of a suspended MoS_2 monolayer.