Light transfer characteristics of MoS$_2$/metal one-dimensional photonic crystals

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Abstract. We present a study of the optical propagation properties of one-dimensional (1D) MoS$_2$/metal photonic crystals (PCs) formed by periodic stacking of alternating MoS$_2$ and metal layers in ambient air atmosphere. The propagation properties of light moving in such a structure are solved using the transfer matrix method. The optical properties of the MoS$_2$/metal PCs are obtained analytically as a function of the materials used, the thicknesses of the layers, and the number of units. Among Ag, Al, Ni, and Fe, Ag was the most suitable metal for constructing PCs in the visible light range. The transmission spectra of the MoS$_2$/Ag PCs exhibited periodic oscillation, with 1, 2 photonic band gaps (PBGs) in the 400–800 nm range when the thickness of the Ag film was 1–2 nm, and the optimum number of periodic units, N, was 10–20. Beyond this range, the transmittance of the structures monotonically decreased with increasing wavelength. The periodic oscillation properties of transmittance in MoS$_2$/Ag 1D PCs can be used in sensors and detectors and as real-time monitors for biological and medical technology fields.

1. Introduction
Photonic crystals (PCs) are periodic structures composed by two or three materials in one, two, or three dimensions, denoted as 1D, 2D, and 3D PCs, respectively [1-2]. Such crystals have a few photonic band gaps (PBGs) in a periodic structure, which makes it possible to manipulate the emission, propagation, and distribution of light in the structures [3]. They can thus be used to make new types of waveguides [4], micro-sized light sources [5], reflectors [6], and other optoelectronic devices. Especially, the insertion of metal layers into PCs composed of dielectric materials brings out novel optical properties and increases the width of PBGs because the metal layers have a negative refractive index and the PCs have a positive refractive index. Moreover, it presents very strong surface plasmon polaritons (SPPs) [7] at the boundary between the dielectric material and the metal layer (Au, Ag, etc.) under an electromagnetic field. The SPP effects are the result of collective oscillation of free electrons on the metal surface via light absorption, which can strongly increase the efficiency of optical processes and detection devices [8], such as nano-integrated photonic devices and biological detectors [9].

In recent years, 2D materials have attracted much research interest around the world [10]. MoS$_2$ exhibits a layered structure that is easily split into one or more layers, analogous to graphene, using the micromechanical cleavage technique [11]. It has a very high relative dielectric constant ($\varepsilon_r=10.6$, $n=3.26$) that can be used to make new optical devices by designing MoS$_2$ PCs [12]. However, there are few reports on the optical transfer characteristics of MoS$_2$/metal PCs. In this study, we fabricated MoS$_2$/metal 1D PCs using periodic stacks of alternating MoS$_2$ and metal layers in ambient air atmosphere. We analyzed the transfer properties of the nanoscale-layer-structured MoS$_2$/metal PCs by...
means of the transfer matrix method in the visible light range. The propagation properties for light in the
structures were analyzed using numerical calculations. Finally, we discuss the results and light
transfer mechanism in the MoS$_2$ PCs.

2. Principles and Structures
We consider a polarized electromagnetic wave with an electric field, $E$, perpendicular to the plane of
1D PCs formed by alternating stacks of dielectric ($d_s$) and metal ($d_m$) layers, as shown in Figure 1.
According to the thin-film optical theory, the propagation properties of electromagnetic waves moving
in each layer can be described by a characteristic matrix, $M_i$, with a rank of $2 \times 2$ [14].

$$M_i = \begin{bmatrix}
\cos \delta & i \frac{1}{\eta_i} \sin \delta \\
i \eta_i \sin \delta & \cos \delta 
\end{bmatrix}$$ [1]

where $M_1 = M_2$, $\delta = \frac{2 \pi}{\lambda} n_i d$, $\eta_i = n_i \cos \theta$, and $n_0$, $n_1$, and $n_2$ are the refractive indices of
the air, the dielectric layers, and the metal layers, respectively. $\theta$ is the incident angle of light (for
normal incidence, $\theta = 0$), and $d$ is the thickness of the layers. For the metal and medium layers, the
thicknesses are denoted as $d_m$ and $d_s$, respectively. The characteristic matrix for a periodic unit of
the 1D PCs is $M = M_1 \times M_2$. The total characteristic matrix may be the product of $N$ periodic units.

$$B = M^N = \begin{bmatrix}
m_{00} & m_{01} \\
m_{10} & m_{11}
\end{bmatrix}.$$ [2]

The total transmission coefficient of the PCs is [14]

$$t = \frac{2}{\eta_0 (m_{00} + m_{01}) + m_{10} + \eta_{11} m_{11}}$$ [3]

The transmittance of the PCs $T = |t|^2$. In the calculation, for simplicity we consider the ambient
medium is air ($n_0 = 1$).

3. Results and Discussion
First, we investigated the transmission dependence of the medium with different refractive indices, $n_i$.
The thicknesses of the Ag and dielectric layers were 1 and 10 nm, respectively, and the number of
periodic units, $N$, was 10. The results are shown in Figure 2(a). Clearly, the transmittance linearly
decreased with increasing wavelength when the dielectric layer was air ($n_i = 1$), then it periodically
changed when $n_i$ was more than 1. Also, the larger the value of $n_i$, the stronger the oscillation is.
Especially, for $n_1 = 3.26$ (MoS$_2$ material), the transmittance started to resonate, and the amplitude of the waves continually increased with increasing wavelength.

Then we studied the propagation properties of MoS$_2$ PCs with different metal layers. The thicknesses of the metal and MoS$_2$ layers were 1 nm and 10 nm, respectively, and $N = 10$. The results are shown in Figure 2(b). The visible light range of the transmittance of MoS$_2$/Al, MoS$_2$/Ni, and MoS$_2$/Fe 1D PCs decreased continually with increasing wavelength, without any periodic characteristics. However, the transmittance of MoS$_2$/Ag PCs increased initially. It reached a maximum value, and then decreased with increasing wavelength, showing vibration behavior in the 400–800 nm light range. These results indicate that MoS$_2$/Ag PCs have high transmittance in the 400–600 nm wavelength range and a wide PBG band in the 700–800 nm range. This characteristic of selective passage of light at certain wavelengths in the PCs would be useful in selecting luminescent devices, as reflectors of biological detectors, and as monitors to detect poisonous gases and toxic substances in the environment.

**Figure 2.** The transmittance spectra of the 1D PCs; (a) shows the transmittance spectra of different medium with refractive index $n_1$ increasing from 1 to 3.26; (b) shows the transmittance spectra of the different metal PCs, the metal layer is Ag, Al, Ni and Fe.

Because the optical properties of the MoS$_2$/Ag PCs exhibited such a periodic behavior in the visible light range, we further investigated the influence of the number of periodic units, $N$, on the transmittance of PCs as $N$ varies from 1 to 10. The results are shown in Figure 3(a). For $N = 1$ and 2, the transmittance curves monotonically decrease with increasing wavelength; however, they start to vibrate when $N = 5$ and 10. Therefore, for MoS$_2$/Ag PCs, it is better to use a larger $N$. Figure 3(b) shows the transmittance dependence for $N = 10$, 20, and 50. Clearly, the transmittance changes significantly, finally reaching a periodic oscillation state when $N = 20$. The number of PBGs increases from 1 to 4 when $N$ increases from 10 to 50. Also, the amplitude of the curves is strongly enhanced with increasing $N$ and increasing wavelength of light, showing that the optical transfer properties can be tuned by changing the number of periodic units and the wavelength of light.

**Figure 3.** The transmission spectra of MoS2/Ag 1D PCs with different number of metal layers; (a) the transmission spectra for $N=1$, 2, 5 and 10; (b) the transmission spectra for $N=10$, 20, and 50.
Finally, we analyzed the relationship between the thickness of the Ag layer and the optical properties; the results are shown in Figure 4. In the simulation, the thickness of the MoS$_2$ layer was 10 nm. For $N = 1$, the transmittance of all curves decreased linearly from 70% to 30% when $d_m$ increased from 1 to 10 nm. These results indicate that the thicker the Ag layer, the less light can pass through the structures. Then we investigated the transmittance dependence of the thickness of the Ag film for $N = 10$, and the results are shown in Fig. 4(b). The transmission curves no longer linearly decrease with wavelength but periodically vibrate. The amplitude of the waves decreases significantly with increasing $d_m$, showing two larger PBG bands for $d_m = 1$ and 2 nm. Figure 4(c) shows the transmission spectra for different thicknesses, $d_s$, of MoS$_2$ layer. The curves strongly vibrate with increasing $d_s$, and the amplitude of the waves gradually increased with increasing wavelength. Also, the number of PBGs increase significantly with increasing $d_s$. The results show that the light transfer characteristics can be significantly tuned by varying the thickness of the medium layers.

![Figure 4](image_url)

**Figure 4.** The transmission spectra of MoS$_2$/Ag 1D PCs with different thickness of metal and MoS$_2$ layers; (a) the transmission spectra for $N=1$ and $d_m=1, 2, 5$ and $10$ nm; (b) the transmission spectra for $N=10$ and $d_m=1, 2, 5$ nm; (c) the transmission spectra for $N=10$ and $d_s=5, 10, 20$ and $50$ nm.

4. Conclusions

We studied the optical transport properties of MoS$_2$/metal 1D PCs, especially for MoS$_2$/Ag PCs. We found that the refractive indices of the medium and metals, the thicknesses of the layers, and the number of periodic units have significant effects on the transfer properties. Among Ag, Al, Ni, and Fe, Ag was the most suitable metal for constituting PCs in the visible light range, and the optimum thickness of Ag was approximately 1-2 nm. The transmittance of MoS$_2$/Ag PCs decreased significantly at thicknesses over 5 nm. Mover it started to resonate when the number of periodic units $N$ over 10. It reaches a high transmittance in the 400–600 nm wavelength range and a wide PBG band in the 700–800 nm range. This characteristic of selective passage of light at certain wavelengths in the PCs would be useful in selecting luminescent devices, as reflectors of biological detectors, and as monitors to detect poisonous gases and toxic substances in the environment.
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