Ultra-high green light transparency coating on 1D photonic crystal structure

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Abstract. The anti-reflective (AR) coatings were regarded as one of the promising options to improving the efficiency of light transmission in optical-based devices. In this work, we designed an ultra-high anti-reflective layer based on a 1D photonic crystal structure. By using the specific properties of the 1D photonic crystal on a particular filtering wavelength, a high transmission enhancement was achieved. The periodic stack of tantalum pentoxide (Ta\textsubscript{2}O\textsubscript{5}) and molybdenum disulfide (MoS\textsubscript{2}) in borosilicate glass (BK7) layers was modified with a graphene as a defect layer to investigate the effect of the modification on the optical transmission factor. The FDTD simulations showed an extremely 99.8255\% transparency at the wavelength of 505.263 nm. The result was consistent with the analytical results obtained from a transfer matrix calculation. The proposed design can be applied to the coated narrow linewidth thin film as used for example in integrated optical systems.

1. Introduction

The performance of optoelectronics devices with the lossless transmission enhancement of anti-reflective (AR) coatings has played an important role for various photonics applications [1]. Recently, the most effective designs of AR coating has been considered on the results of constructive and destructive interference which are provided by the stack layer of high and low dielectric materials [2]. The AR values can also be reduced, in which low-refractive index material is neglected due to the controllable dielectric layers and their thicknesses [3]. Moreover, the presence of AR structure designs has been developed to improve AR coatings hardness and high thermal resistance [4] for the better quality of optoelectronics and optical devices, potentially useful to high-temperature applications [5].

Previous studies, for example, have examined how periodic surface modulations can decreases the degree of reflection [6]. Additionally, 1D photonic crystal (PhC) structures given in terms of periodic stacks in several materials have been used with the aim to minimising the transmitting power when the number of stack elements is increased appropriately [7]. Moreover, homogeneous coatings as for example produced by the sol-gel technique have faced some problems. Due to changes in the temperature, cracks can form in the coatings and can reduce the performance [8]. Also, the reflective index of sol-gel can easily be temperature dependent [9].

In this work, we will present an AR coating design for the blue-green spectral region that is based on a 1D PhC structure. The design consists of a stack of tantalum pentoxide (Ta\textsubscript{2}O\textsubscript{5}) and molybdenum disulfide (MoS\textsubscript{2}) which is embedded in borosilicate glass (BK7) layers. This stack is used as the 1D PhC to achieve a low optical reflectance. In this context, one of the MoS\textsubscript{2} layers will be replaced into a graphene layer. This modification may give rise to the promising design for ultra-low anti-reflective coatings. The hope is that the embedded graphene layer increases the flexibility of AR coatings such that the coatings are less subjected to crack formation due to changes in temperature.
2. Structure Design

The basic design of proposed AR coating is displayed in the top left of Fig.1. Accordingly, the AR coating was based on a 1D PhC structure which was arrayed by a periodic 50 nm thick Ta2O5 layers and 50 nm thick MoS2 layers with 100 nm thick BK7 layers in between. As shown in the middle panel on the left of Fig. 1, a 13 layer structure (including a substrate layer) was selected for this investigation because it exhibited the lowest reflectance. Subsequently, the same structure was divided into three alternative designs with the different positions of graphene layer as displayed to the right of Fig 1.

Reasonably, this modification would prevent the preferable anti-reflective enhancement even though this replaced defect layer has minimised the local refractive index (MoS2 around 4.5 – 5.5 in a visible range) lower than the BK7 (~1.52) which breaks the periodic low and high dielectric order. However, the potential property of 1D PhC provides the photonic band gap (PBG), in which the identical transverse electric (TE) and magnetic (TM) modes have been formed. These modes appear the guided mode coupling in a waveguide for the superior optical transmission.

In addition to the defect properties, the graphene layer width has been estimated from the stack of graphene sheets for the single thickness [10]. Importantly, the significant advantage of graphene in this work is their ability to reinforce glass with the absorbing capability on their interface contacts [11], and self-healing phenomenon [12]. This improvement may increases the flexibility of the AR coating. We also hope that the improvement makes that the temperature-dependency of the refractive index is reduced. If so, our proposed design would be a promising coating for high-temperature applications.

3. Analytical and Simulation Results

The reflectivity of 1D PhC structure, with Ta2O5 and MoS2 arrays on BK7 layers, was determined by means of FDTD simulations (Lumerical Solutions, Inc.). The results were compared with analytical results obtained from a transfer matrix method. The proposed structure was examined in different stack sizes of Ta2O5, MoS2, and BK7 with 9, 13, and 17 layers of the 1D PhC, respectively. The analytical results with transfer matrix model [13] were calculated numerically as,
\[ M_T = M_H \cdot M_L \cdot M_H \cdot M_L \cdots M_H \] (1)

where \( M_T \) is the transfer matrix, \( M_H \) is the Ta\(_2\)O\(_5\) or MoS\(_2\) refractive index \( (n_H) \) matrix, \( M_L \) is the BK7 refractive index \( (n_L) \) matrix, and \( M_D \) is the graphene refractive index \( (n_C) \) matrix which can be replaced with \( M_H \) if a defect is neglected from the system. The refractive index matrix was described by

\[
M_H = \begin{bmatrix}
\cos \left( \frac{2\pi}{\lambda} n_H t \right) & \frac{i \sin \left( \frac{2\pi}{\lambda} n_H t \right)}{n_H \sqrt{\varepsilon_0 \mu_0}} \\
\frac{i n_H \sqrt{\varepsilon_0 \mu_0} \sin \left( \frac{2\pi}{\lambda} n_H t \right)}{\cos \left( \frac{2\pi}{\lambda} n_H t \right)} & \cos \left( \frac{2\pi}{\lambda} n_H t \right)
\end{bmatrix}
\]

\[
M_L = \begin{bmatrix}
\cos \left( \frac{2\pi}{\lambda} n_L t \right) & \frac{i \sin \left( \frac{2\pi}{\lambda} n_L t \right)}{n_L \sqrt{\varepsilon_0 \mu_0}} \\
\frac{i n_L \sqrt{\varepsilon_0 \mu_0} \sin \left( \frac{2\pi}{\lambda} n_L t \right)}{\cos \left( \frac{2\pi}{\lambda} n_L t \right)} & \cos \left( \frac{2\pi}{\lambda} n_L t \right)
\end{bmatrix}
\] (2)

where \( t \) is the layer thickness, \( \varepsilon_0 \) and \( \mu_0 \) is the permittivity and permeability of free space, and \( \lambda \) is a broadband wavelength from the plane-wave input. First, we determined the optimal number of both layers and wavelength. The FDTD and the analytical method produced consistent results. As the results, the best reflectivity of 0.6454% was achieved at the wavelength of 505.263 nm for 13 layers design as shown in Fig. 2. This number was subsequently used for the embedded graphene designs.

![Figure 2](image-url)

Figure 2. The number of Ta2O5, MoS2, and BK7 layers, including a substrate, in a proposed 1D PhC structure for the lowest reflectance investigation. The FDTD simulations and analytical results showed that the maximum AR value for three different stack numbers emerges at the wavelength 505.263 nm.

Furthermore, the modification of structure with a replaced graphene in three different positioning layer was examined by the same approaches which showed similar results. Accordingly, the structure of a graphene at layer \( N = 8 \) produced the dramatic drop of reflectance from 0.6454%, in the non-defect system, to 0.1745% (FDTD) and 0.1951% (analytical method) as depicted in Fig.3(b). In contrast, the defect at layer \( N = 12 \), in which located as the interface between 1D PhC and a substrate,

![Figure 3](image-url)

Figure 3. The FDTD and analytical results of 13 layers at the wavelength 505.263 nm with an embedded graphene at the layer (a) \( N = 4 \) (b) \( N = 8 \) (c) \( N = 12 \), note that FDTD provides the reflectivity more than the analytical results.
and N = 4 as a periodic surface have increased the reflectance up to 0.9039% and 27.8650%, respectively see Figs. 3(a) and 3(c). These significant results are clearly confirmed that only the perfect conditions of defect position in a PhC can cause the interesting results in a proposed design.

4. Summary
The ultra-high anti-reflective coating 1D PhC structure has been designed and simulated. The most effective transparency of Ta2O5 and MoS2 stacking has been observed by the 13 arrayed layer. We also found that a replaced graphene on MoS2 layers in three different positions can vary the reflectivity to be higher or lower value than a non-defected structure. By locating a graphene in the middle periodic position of MoS2 (layer N = 8), the transparency value increased by about 0.5% to approximately 99.9% within the blue-green spectral region. We speculate that the transparency increase of about 0.5% improves significantly the quantum efficiency of optical devices. We also conjecture that the use of graphene allows for high-temperature applications and can reduce the crack mechanisms in AR coatings for optoelectronic devices.

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