## **Research Article**

# Plasmonic Effect on Broadening of Band Gaps in One-Dimensional Multilayer Metallo-Organic Photonic Crystal

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## Abstract

In this paper, we presented theoretically that the reflectance spectra of one dimensional multilayer metalorganic periodic structure (1D MOPS) can be enhanced by the addition of organic constituents. We used simple transfer matrix method (TMM) to calculate the absorption, transmittance and reflectance of the 1D MOPS. The organic component like N,N'-bis-(1naphthyl)-N,N'diphenyl-1; 1-biphenyl-4;4-diamine (NPB) absorbed the light in ultra-violet, visible and infrared electromagnetic region, this organic component with silver(Ag) also had the tendency to absorb the light by -plasmaonic action, and their refractive indexes can be calculated by Drude equation. The reflectance spectra of multilayer 1D MOPS containing Ag / (NPB) structure with a vaiable periods were calculated by taking optical constant of NPB and Ag in to account. The optical band gap and reflectance spectra of 1D MOPS were obtained in the visible and near infrared regions and varied with the thickness of metal layer or organic layer.

By TMM, the tunability in the optical band gap was examined and it was found that the tenability changed with the number of layers or incident angle. Due to optical absorption in the different regions of electromagnetic spectrum, the optical band gap of 1DMOPS showed the shifts of left ( $\lambda_L$ ) and right ( $\lambda_R$ ) band edges from ultra-violet to visible and infrared with the different optical constant.

**Keywords:** photonic crystals, dielectric and organic layer, transverse electric (TE) and transverse magnetic (TM) mode.

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## Introduction

In the last couple of decades, photonic band-gap (PBG) materials is a promising material for the various conversions like such as frequency filters, mirrors, waveguides, and frequency converters, has been made from the composite structure of dielectric or metallic blocks [1]. This is a powerful controlling capability to manipulate spectral properties of electromagnetic waves (EM). These photonic crystals possess a specific gap in the EM spectrum, in which light cannot propagate in any direction. This material shows the existence of forbidden band gaps in their transmission spectra. Due to various applications in photonic crystals (PCs), some of the important applications are optical filters, optical switches, and resonance cavities and waveguides [3, 4].

Recently, a lot of studies have been carried out on the plasma photonic crystals, and their dielectric constant can vary continuously in space with the frequency of the incident electromagnetic (EM) waves. The surface plasmon resonance (SPR) is the collective oscillations of free electrons in a metal that confines the excitation of electromagnetic surface waves at the metal-dielectric interface. Next to polariton, this surface wave propagates along the optical axis when the plasmonic crystal is set normally to the orientation of the layers. The band gap of the surface plasma (SPR) of generally lie in the UV and visible region and their strength depends upon the type of nanocrystals, stability and its existence, percentage and the morphology of the nanocomposite [5]. Plasma photonic crystal is composed from micro plasma, which controlled electromagnetic wave in millimeter or sub millimeter range of optical devices. Hitoshi Hojo [6] reported the one-dimensional plasma photonic crystals and their transmittance were studied by invariant imbedding method. The forbidden band gaps are shown the appearance in transmittance spectra, as a

function of wave frequency. The photonic band gap is being controlled by the density, frequency, width and applied magnetic field. Zhang et al, [7] studied an omnidirectional photonic band gap (OBG) of single negative index materials and plasma, which originates from Bragg gap and their problem could be solved by the transfer matrix method (TMM) by using ternary Thue–Morse a periodic structure.

Zhang et al., [8] reported the photonic band gap of three-dimensional unmagnetized dielectric plasma photonic crystals by using the modified plane wave expansion (PWE) method. Zhang [9] studied the reflectance characteristic of periodically magnetized plasma structure by using the transfer matrix method. The photonic band gap depends upon the incident angle, but a change in the large change in the magnetic field shows only small change in the band gap. The collision frequency also affects the gap location and the gap width of the PC while it makes the amplitude of reflectance and transmission decrease with an increase the magnetic field. The propagation of electromagnetic waves in one-dimensional plasma dielectric photonic crystals was studied by Laxmi [10] by using super lattice structure. The structure consists of alternating layers of plasma and dielectric layer, and the problem was solved by the transfer matrix methods. Their results showed that photonic crystals exhibit the new band gap for each angle of the incidence angles other than the normal angle of incidence where the electric plasma permittivity change the sign of nature.

Conjugated polymers like Polyacetylene, polyaniline, and polythiophene is a promising material for applications in optoelectronic devices due to their lower costs, easier fabrication methods and better flexibility compared with inorganic material. The basic features of such as luminescence, electron-hole separation, or nonlinear optical response describe the electronic states as well as inter-chain interaction. In this context, the electron-electron interactions, and the strong connection between affects the electronic and geometric structures of the  $\pi$ -conjugated system. In conjugated molecules, the electron-lattice coupling affects the strong influence of the nature of optically excited states due to the presence of extra lone pair electron broadening by the charged species absorbed through out surrounding, a hole or the geometry of the molecules by the presence of the large bulky functional group. In fluorine co-oligomers, the photonic band gap changes with the addition of the different functional group or the addition of concomitant which change the energy level of the HOMO (highest occupied molecular level) and LOMO (lowest occupied molecular level). Addition of inclusion with the electron rich unit, predominantly raise the HOMO level, while electron deficient moieties reduce the LUMO level. This is due to attachment to the conjugated system [11].

One dimensional metallo-dielectric nano-films have been investigated theoretically and experimentally in the ultra-violet range [12, 13]. Zhang et al. [14] studied the optical properties of a one dimensional metallic organic photonic crystal (MOPC) with periodic Ag/N, N'-bis-(1-naphthyl)-N; N'diphenyl-1; 1'biphenyl-4; 4'diamine (NPB) layers and observed the field localization within the organic layers at the resonance wavelength. Owing to resonant tunneling through the metal layers these structures combine certain properties of bulk metal with high transparency in the desired wavelength range. The last advantage may be the most important for optical applications because it results in the tunability of both the linear and nonlinear optical properties. Especially, the broad omnidirectional stop band in the MOPC can inhibit light propagation in a certain direction for a specified frequency; therefore, PCs can modify significantly the emission characteristics of embedded optically-active materials (dyes, polymers, semiconductors, etc.) as the emission wavelengths of the active materials overlap the stop band, in the reflectance spectra of the photonic material.

The optical constant of the metal (Ag) film also depends on the wavelength [15]. The long-range mode has an asymmetric charge distribution between the top and bottom surfaces with the electric field predominantly normal to the surface in the metal. For thin metal films (usually less than 100 nm), the two single-interface surface plasmon polariton (SPPs) interact with each other and lead to form two coupled SPP, the long-range and short-range. Conversely, the short range SPP (SRSPP) has a charge distribution which is symmetric between the top and bottom surfaces with the electric field essentially parallel to the surface.

Based on these facts, in this report, we studied the enhanced reflectance spectra of the metal-organic periodic structure containing multiple layers of Ag/ NPB materials. The multiple thin layers of the various layers of periodic structure of Ag/NPB experiments were fabricated by dip coating technique. The thick organic layers were deposited on the top of the multilayer structure. TMM was used to study the reflectance spectra of the periodic structure with air substrates and we also investigated the variation of thickness of the organic layer. The variable angle spectroscopic

ellipsometer (VASE) has been used to measure the wavelength dependent optical constant of the organic film NPB on the silver surface. The wavelength dependent optical constant of the metal (Ag) film was calculated from the Drude relation in UV-visible region. The reflectance spectra of Ag/ NPB of multiple layer of the periodic structure was calculated by choosing proper thickness of Ag/PNB layers and with a variation of the thickness of the organic layer NPB.

### Formulation

As for the metal layer, the usual Drude model was employed. The temporal part of any field is assumed to be  $e^{it\omega}$ . Then the permittivity of the metal in Drude model is obtained from the following equation

$$\varepsilon_2(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + j\omega\gamma} \tag{1}$$

where  $\gamma$  the lose factor is the plasma collision frequency and  $\omega_p$  is the plasma frequency which depends upon the electron density

$$\omega_p = 2\pi f_p = \left(\frac{Ne^2}{m\varepsilon_o}\right)^{1/2}$$

Where N is the electron concentration, m the mass of free electron, e the electronic charge, and  $\varepsilon_0$  the permittivity of vacuum. The index of refraction of a metal is thus given by  $n_2 = \sqrt{\varepsilon_2}$ . For obliquely incidence of electromagnetic wave on the most left boundary of organic/metal at an angle of incidence  $\theta_0$ , the reflectance can then be calculated by using of the Abeles theory [16, 17]. A 1D PC is composed of two different media, A and B, with dielectric constants of "a and "b and thicknesses of a and b accordingly; the lattice constant (d) can be obtained by d = a + b, and the number of periods is N. The photonic band structure of a perfect photonic crystal is determined by the Eigen values of the following familiar equation [1]:

$$\vec{\nabla} \times \left[ \mathcal{E}^{-1}(\vec{r},\omega) \vec{\nabla} \times \vec{H}_{\omega}(r) \right] = \left( \frac{\omega}{c} \right)^2 \vec{H}_{\omega}(\vec{r})$$
<sup>(2)</sup>

Where  $\varepsilon(\vec{r},\omega)$  is the dielectric constant of the crystal and  $\vec{H}_{\omega}(\vec{r})$  is the monochromatic component (of frequency v) of the magnetic field, which satisfies the Bloch condition [1]

$$\vec{H}_{\omega}(\vec{r}) = e^{i\vec{k}_{b}\vec{r}}\vec{H}_{\vec{k}b\omega}(\vec{r})$$
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 $\vec{k}_{b}$  is the Bloch vector in the first-Brillouin zone of the crystal's reciprocal space  $H_{\vec{k}_{b},\omega}(r)$  and has the same periodicity as the underlying Bravais lattice. Considering the Eigen value for the frequency  $\omega$ , Eq. (1) has a nonlinear character because of the dielectric constant  $\varepsilon(\vec{r},\omega)$ , which acts as a scattering potential, it depends on the Eigen value  $\omega$ . In terms of the electric fields, the solution of the differential Equation is  $E = E(x/\omega)e^{i(\omega t - \beta y)}$ , where E (x/ $\omega$ ) can be taken as the superposition of the incident and reflected wave in each medium, for j<sup>th</sup> layer can be written in the form

$$E(x/\omega) = A_j e^{ik_{jx}x} + Bj e^{-ik_{jx}x}$$
<sup>(4)</sup>

$$k_{jx} = \frac{\omega}{c} \sqrt{\varepsilon_j} \cos \theta_j$$

and ɛj are the wave vector and dielectric constant in the j<sup>th</sup> layer respectively, and c is the Where speed of light in vacuum. The coefficients  $A_i$  and  $B_i$  have to be determined from the boundary condition that both electric field and its first derivative are continuous across an interface. The magnetic field vector along y-axis can be obtained by:

$$\vec{H} = \frac{\iota}{\mu\omega} \vec{\nabla} \times \vec{E} \tag{5}$$

Considering for the dielectric layer with no external current source and induced charge, the Maxwell equation becomes:

$$\vec{\nabla}.\vec{E} = 0 \quad \vec{\nabla}.\vec{B} = 0 \qquad \vec{\nabla}\times\vec{E} = -\frac{\partial B}{\partial t} \qquad \vec{\nabla}\times\vec{B} = \frac{\partial D}{\partial t} \tag{6}$$

By using the Snell's law in the above equation, the dielectric constant of the given materials is given by the following expression

$$k_d^2 = \varepsilon \frac{\omega^2}{c^2} \qquad k_{dx}^2 = \varepsilon \frac{\omega^2}{c^2} - \frac{\omega^2}{c^2} \sin^2 \theta = \frac{\omega^2}{c^2} (1 - \sin^2 \theta) \qquad \text{or} \qquad k_{dx} = \frac{\omega}{c} n_d \tag{7}$$

Where the refractive index of the taken system is given by:

$$n_d = \sqrt{\varepsilon - \sin^2 \theta} \tag{8}$$

According to this theory, the TMM is used to set the corresponding matrix of one period, which is given by the following expression:

$$M(\Lambda) = \begin{pmatrix} m_{1,1} & m_{1,2} \\ m_{2,1} & m_{2,2} \end{pmatrix} = \begin{pmatrix} \cos \beta_2 & \frac{j}{p_2} \cos \beta_2 \\ jp_2 \sin \beta_2 & \cos \beta_2 \end{pmatrix} \begin{pmatrix} \cos \beta_3 & \frac{j}{p_3} \cos \beta_3 \\ jp_3 \sin \beta_3 & \cos \beta_3 \end{pmatrix}$$
$$M(\Lambda) = \begin{pmatrix} \cos \beta_2 \cos \beta_3 - \frac{p_3}{p_2} \sin \beta_2 \sin \beta_3 & \frac{j}{p_3} \cos \beta_2 \sin \beta_3 + \frac{j}{p_2} \sin \beta_2 \cos \beta_3 \\ jp_2 \sin \beta_2 \cos \beta_3 + jp_3 \cos \beta_2 \sin \beta_3 & \cos \beta_2 \cos \beta_3 - \frac{p_3}{p_2} \sin \beta_2 \sin \beta_3 \end{pmatrix}$$
(9)

 $\beta_2 = \frac{2\pi}{\lambda_0} n_s d \cos \theta_2 \qquad \beta_3 = \frac{2\pi}{\lambda_0} n_d t \cos \theta_3 \qquad p_2 = \sqrt{\frac{\varepsilon_0}{\mu_0}} n_s \cos \theta_2 \qquad p_3 = \sqrt{\frac{\varepsilon_0}{\mu_0}} n_d \cos \theta_3 \qquad \text{for TE mode and for TM-}$   $p_2 = \sqrt{\frac{\varepsilon_0}{\mu_0}} \frac{1}{n_s} \cos \theta_2 \qquad p_3 = \sqrt{\frac{\varepsilon_0}{\mu_0}} \frac{1}{n_d} \cos \theta_3 \qquad \lambda_0 = \frac{2\pi}{k_0} = \frac{2\pi c}{\omega}$ is the wavelength in free space. The angle  $\theta_1$  and  $\theta_2$ 

determined by the Snell's law of refraction are the ray angle in layers 2 and 3 respectively. By using the above matrix, we try to construct the matrix for n-periods,

$$M(\Lambda N) = [M(\Lambda)]^{N} = \begin{pmatrix} m_{11}U_{N-1}(\psi) - U_{N-2}(\psi) & m_{12}U_{N-1}(\psi) \\ m_{21}U_{N-1}(\psi) & m_{22}U_{N-1}(\psi) - U_{N-2}(\psi) \end{pmatrix}$$
(10)

 $\psi = \frac{1}{2}(m_{11} + m_{22})$  and UN are the Chebyshev polynomials of the second kind defined by

$$U_{N}(\psi) = \frac{\sin[(N+1)\cos^{-1}\psi]}{\sqrt{1-\psi^{2}}}$$
(11)

By using the above relation, the matrix elements are given by the following formula:-

$$M_{11} = (\cos \beta_2 \cos \beta_3 - \frac{p_3}{p_2} \sin \beta_2 \sin \beta_3) U_{N-1}(\psi) - U_{N-2}(\psi)$$
$$M_{12} = j(\frac{1}{p_3} \cos \beta_2 \sin \beta_3 - \frac{1}{p_2} \sin \beta_2 \cos \beta_3) U_{N-1}(\psi)$$
$$M_{12} = j(p_2 \sin \beta_2 \cos \beta_3 + p_3 \cos \beta_2 \sin \beta_3) U_{N-1}(\psi)$$
$$M_{11} = (\cos \beta_2 \cos \beta_3 - \frac{p_2}{p_3} \sin \beta_2 \sin \beta_3) U_{N-1}(\psi) - U_{N-2}(\psi)$$
(12)

The reflection and transmittance of the multilayered structure can be determined from Eq (12) and given as follows

$$\tilde{r} = \frac{(M_{11} + M_{12}p_s)p_0 - (M_{21} + M_{22}p_s)}{(M_{11} + M_{12}p_s)p_0 + (M_{21} + M_{22}p_s)} \quad \text{and} \quad \tilde{t} = \frac{2p_0}{(M_{11} + M_{12}p_s)p_0 + (M_{21} + M_{22}p_s)} \quad (13)$$

Here p<sub>0</sub> and p<sub>s</sub> are the first and the last medium of the considered structure and given by,  $p_0 = \sqrt{\frac{\varepsilon_0}{\mu_0}} n_0 \cos \theta_0$ 

$$p_{s} = \sqrt{\frac{\varepsilon_{0}}{\mu_{0}}} n_{s} \cos \theta_{s}$$
 and for TE-mode and for TM-mode  $p_{0} = \frac{1}{n_{0}} \sqrt{\frac{\varepsilon_{0}}{\mu_{0}}} \cos \theta_{0}$ ,  $p_{s} = \frac{1}{n_{s}} \sqrt{\frac{\varepsilon_{0}}{\mu_{0}}} \cos \theta_{s}$ . Both the media

$$R = \left| \tilde{r} \right|^2$$
 and  $T = \frac{p_s}{p_0} \left| \tilde{t} \right|^2$ 

are taken to be a free space. The reflectivity and transmittance are given by

## **Results and discussion**

The theoretical reflectance spectra of the multilayer structure were calculated by solving the Maxwell equations, the optical constants of Ag was calculated from the Drude model and the linear refractive index of the NPB film was measured using an ellipsometer covering the visible and near infrared spectral range. The chemical formula of the NPB is given in **Figure 1** in which two naphthyl groups attached to the nitrogen atom along with biphenyl group. This is especially used for the molecular design of amorphous molecular materials.



Figure 1 N,N'-bis (1-naphthyl)-N,N'-diphenyl-1,1'-biphenyl-4,4'-diamine (NPB)

Especially this molecules are often characterized by a preferential arrangement of the conjugated framework in molecular aggregates, i.e., in the bulk crystal structure. This may lead to a coplanar alignment of the  $\pi$ -electron system with the possibility to enhance the intermolecular coupling, causing remarkable electronic and optical properties. Electrical properties of molecular materials are determined, among other factors, by the energies of levels (bands) allowed for electrons and holes in these materials. The electrical energy gap molecular materials is then the difference of the two latter parameters, being a measure of the energy difference between the energies of levels allowed for non-interacting electrons and holes. Molecular organic materials like NPB function as holes transporting between the highest occupied molecular orbital (HOMO) and the lowest un-occupied molecular orbital (LUMO) electron-transporting or emitting materials, mainly depending upon their ionization potentials and electron affinities. HOMO and LUMO are also called the frontier orbital, and their difference in energy  $E_{LUMO} - E_{HOMO} = Egap$  is sometimes called an electronic band gap, although strictly speaking, bands do not occur until a spatially extended solid is formed. The majority of typical non-substituted low-molecular weight materials like acenes, phenylenes, thiophenes, phthalocyanines, behave like as p-type semiconducting (hole-conducting) materials.

Generally, organic materials have low ionization energy together with low electron affinities, they usually function as hole-transporting materials by accepting holes carriers with a positive charge and transport holes depending upon the concentration of the dopant in the matrix. While materials having high electron affinities and high ionization potentials usually function as electron-transporting materials by accepting negative charges, those materials can move an electron through the molecules between the  $\pi$ -electron in the aromatic ring. Other reason for its popularity is that sublimed NPB can be manufactured readily and is thus abundantly available even through its T<sub>g</sub> at 98°C, which may affect its morphological stability at high operating temperature. The materials possess high hole drift mobility and are capable of swiftly transporting the hole through them. The following approaches to design the complex organic molecules can be roughly categorized into biphenyl diamine derivatives, the  $\pi$ - starburst amorphous molecular glass, spiro-linked biphenyl diamine and miscellany which is similar to NPB. Molecular structures of these three types of hole-transporting materials are shown in **Figure 2**.

Another one of the most widely used electron-transporting materials is 2-biphenyl-4-yl-5-(4-tert -butyl phenyl) - 1, 3, 4-oxadiazole and its branched, Spiro-linked derivatives. In all these molecules, there are aromatic rings either attached to nitrogen atoms or jointed each other. By the irradiation from the electromagnetic wave, the charge is excited from the nitrogen to  $\pi$ -electron of aromatic rings. With the addition of the functional group either with N /or N' sides or attached to the large bulky functional group with the benzene ring (as shown in Figure2) they affect the optical absorption in different region of the electromagnetic spectrum. Due to the presence of the various functional groups in aromatic compounds, the absorption occurs in different regions. Due to variable permittivity, the layer of plasma along with any dielectric materials in PC, the plasmonic layer can act as dispersive medium. In the first order approximation, where, we suppose that the damping frequency tends to be zero, the propagation of the wave s characterized by the frequency  $\omega_{p}$ . At the higher frequency, the plasmonic layer is transplants due to positive permittivity and electromagnetic wave easily propagate inside the multiple layers. On the other hand, the propagation is completely prohibited if the frequency of the plasma is higher than the incident wave. This type of the presentation is studied in this investigation.







N,N'-bis(1-phnathrene)-N,N'-diphenyl-1,1'-biphenyl-4,4'diamine (PPD)



N,N'-bis(1-naphthyl)-N,N'-diphenyl-1,1'-biphenyl-4,4'diamine (NPB)



N,N'-tetra(1-biphenyl)-N,N'-diphenyl-1,1'-biphenyl-4,4'diamine (TBPB) (1.6-1.8)



N,N'-bis(1-biphenyl)-N,N'-diphenyl-1,1'-biphenyl-4,4'diamine (PBPD)



Figure 2 Molecular structures of various types of electron transport organic materials

In the metal-organic periodic structure, a large absorption in 320-1000 nm region has been observed, and it presents the presence of the organic layer. The organic layer is the alternate layer along with the metal. This layer shows the maximum absorption at 320, 380 and 800 nm. The optical band gap was determined from the absorption edges and using the Tauc-relation [18]:

$$Ah\nu = \left(h\nu - E_g\right)^n$$

where n is  $\frac{1}{2}$  for allowing, 2 for allowed and 3 for forbidden indirect transition, A is the absorption coefficients,  $E_g$  is the band gap corresponding to a particular absorption occurring in the film and h-v is the photon energy. The direct optical band gap was obtained from the extrapolation of the straight-line portion of the absorption versus h v curves. By utilizing the following relationship, the refractive index of the thin film is directly calculated by

$$\frac{n^2 - 1}{n^2 + 2} = 1 - \sqrt{\frac{E_g}{20}}$$

However, metals are not optically transparent and the dielectric constant is a complex quantity and a function of frequency. The metallic layer is taken to be silver (Ag) with the plasma frequency  $\omega_p$  is defined by:

$$\omega_{p}^{2} = \frac{Ne^{2}}{\mu_{0}m_{eff}} = 2\pi x 2.175 x 10^{15} \text{ rad/s}$$

and the damping frequency is  $\gamma^{\circ} = 2\pi x 4.35 x 10^{12}$  rad/s [19] where N is the electron density, m<sub>eff</sub> is the effective mass of the electron, e is the electronic charge and the permittivity of the vacuum is  $\varepsilon_0$ . It is clear that changing N will cause the plasma frequency to be varied, which, in turn, leads to a variation in the permittivity of a plasma system. The dielectric of the layer can be expressed as a complex function  $\mathcal{E} = \mathcal{E}' - j\mathcal{E}''$ . The real part of the permittivity is negative and describes the dielectric properties. The positive imaginary part defines the intrinsic material absorption, which leads to an evanescent mode of propagating EM wave incident on the surface the metal from a dielectric medium. With a variable permittivity, a plasma system can be regarded as a dispersive medium. **Figure 3** shows the optical constant of Ag versus wavelength calculated from the Drude model. The real part (Re) increases drastically with the frequency between 0.75 x10<sup>16</sup> and 1.5 x 10<sup>16</sup> but after that it becomes constant. The imaginary part (Im) of the refractive index is also known as extension coefficients (k) of metal, given by

$$\varepsilon'' = \frac{\omega_p^2}{\omega^3} \gamma$$

decreases linearly with the increasing of wavelength. The reason of enhanced absorption in MDPC with a large thickness of the Ag layer and increasing periods was due to the existence of a wide PBG, which had already been explained by Yu et al [20]. As an example of such 1D photonic crystal, let us consider a stack of Ag/NPB. The typical response of the interference peak due to presence of the organic layer/ or dielectric materials with silver was calculated from the thickness d of the peak position of the longest wavelength

$$d = \frac{m\lambda_p^{(m)}}{4\sqrt{n_{org}^2 - 1}} \tag{14}$$



Figure 3 Optical constant of silver (Ag) calculated from the Drude model in UV-visible region



Figure 4 Reflection spectra of one-dimensional binary photonic crystals normally incident on a surface calculated by TMM methods

where m is the order of the maxima interference ( in this calculation, m= is taken to be 1 for the longestwavelength band);  $\lambda p$  is the longest wavelength of the m<sup>th</sup> absorption peak; and n<sub>org</sub> is the refractive index of the organic layer.

The optical constants like refractive index (n) and extinction coefficients (k) of Ag and NPB are observed n= 0:815, k= 0:526 and n = 1:7, k = 0:12 respectively at 320 nm. [19]. Figure 4 shows the reflectance and transmittance of metallo-organic periodic structure containing a variable number of periods of Ag/ NPB with thicknesses of 50 nm Ag and 100 nm of the NPB layers. The reflectance of the 1D MOPS are 64.59 % (peak values  $\lambda$ =508.67nm) at N=2

layer, 96.16 % (peak values  $\lambda$ =450.22nm) at N=5 layers and 99.88 % at N=10 layers in the visible region spectrum respectively. With the increasing number of the layer, the obtained spectrum becomes much denser and peak position becomes flat. It is clearly observed that the absorption of MOPS with the least number of the periods is larger than its reflectance in the visible regions. As the number of the periodic layer augment, the reflectance increases, but the absorption decreases. Such property of the MOPC makes it have many potential applications. Although the spectral position is determined by the total optical thicknesses of the high and low index layers, the lowest transmission occurs when optical thicknesses of the respective layers are the quarter wavelength of the ones ( $\lambda/4n_h$ ,  $\lambda/4n_l$ ).

In case of non-absorbing materials, the low transmission directly gives the higher reflectivity. The difference among the refractive indexes of organic materials ( $\Delta n=1.7 - 0.815 = 0.885$ ) is double of the Ag. At normal incidence, it was found that in the binary photonic crystals, there were a wide PBG within visible region and the bandwidth was 178.3 nm and it is located between short wavelength at  $\lambda_1=373$ . 53 nm and long wavelength at  $\lambda_2=511.83$  nm. This wide band gap in MOPC may be explained due to high index contrast between organic and metallic components. The significant increase in PBG of MOPC is ascribed to the metallic layer which can be characterized by the plasma frequency, and calculated from Drude relationship. The thickness of the metallic layer in 1D MDPCs is set as equal to or smaller than the metal's skin depth. Due to presence of the multiple layer in binary PC, the flat band are existed because of presence of surface Plasmon mode wich shows the coupling effect from the interface of the binary layer. In this flate band region, the group velocity is very slow. To further investigate the effect of the metallic layer on the PBG, we studied the reflectance spectra at the different thicknesses of the metallic layer. As increase of the thickness of the metallic layer from 100 to 500 nm the reflection spectra split into a number of pass band with large amplitude as shown in **Figure 5**.



Figure 5 Reflection spectra of one-dimensional binary photonic crystals at the different thicknesses of metallic layers (a) 50nm, (b) 100 nm, (c) 200nm, (d) 300nm, (e) 400nm, and (f) 500nm

The edges of PBG of MOPC are shifted from the ultra-violet region to the visible region. At the thickness of the metallic layer is 50 nm (see Figure5: Gray region indicates the width of the band gap), the bandwidth is 130.79 nm but as the thickness is 500 nm, the bandwidth is around 472.14 nm. This frequency region may be highly useful for the designing of the plasma functional devices. The thickness of the organic layer in MOPC also provides the tune-

ability in the reflectance spectra. As the thickness of the organic layer is increased from 50 to 500nm, the magnitude of PBG is enlarged from 139.7 to 362 nm as shown in Figure 6. It is evident that the peak position is also shifted from the visible to infrared regions and large band gap is observed in the near infrared region as shown in **Figure 6**. Based on the analytical expression, the effective plasma frequency can be expressed by the following expression

$$f_{p,eff} = \frac{\omega_{p,eff}}{2\pi} = \frac{\phi^{1/2}\omega_p}{2\pi\sqrt{\varepsilon_A + \phi(1 - \varepsilon_A)}}$$



Figure 6 Variation of reflectance with different the thicknesses of organic layers at normal incidence on the surface (a) 50 nm, (b) 100 nm, (c) 200nm, (d) 300nm, (e) 400nm, (f) 500nm,

$$\phi = \frac{d_B}{d_B}$$

*a* is defined the plasma filling factor in one unit cell. However the band-edges are very sensitive to Where the incident angle  $\theta$ . In order to calculate, the angle dependence of the Bragg gap, the reflectance spectra are calculated with different the incident angles in the range from 0°-82°, by TE and TM polarizations. In the case of oblique incidence, as illustrated in Figure 7 (Gray Box: just visualize the size of the band gap), the region of the PBG is expanded slightly with the wavelength increasing. PBG is enhanced as the angle increase from  $15^{\circ}$  to  $78^{\circ}$ . If the angle of the incidence changes from 0 to  $\pi/4$ , the reflectance spectra are not shifted towards the higher or the lower frequency i.e., it maintains the omni-directional reflection. The small increment in the corresponding reflectance amplitudes and reflectance bands because of the plasma density is due to shifting of the right band edges towards the higher wavelength. When the angles of incidence changed from 0 to 32° the PBG increased toward the shorter wavelength regions. Further increasing the angle of incidence, the PBG increase is still maintained. The bandwidth shifts towards the blue region when the angle of the incidence is increased to 74°. The magnitude of the PBG of MOPC is invariable as changes from 74°-80°. But the shifting of the bandwidth towards blue shift is still remained beyond 80°. At  $\theta$ =69°, the upper and lower band edges are  $\lambda_1$ =414.29 and  $\lambda_2$ =637.95 nm respectively, and the bandwidth is extended with  $\Delta\lambda$ =223.66 nm but as  $\theta$ =32° the bandwidth is centralized between  $\lambda_1$ =334.87 and  $\lambda_2$ =528.43 nm and width is  $\Delta\lambda$ =183 nm.



**Figure 7** Variation of reflectance with different incident angle (100nm metallic layer and 100 nm layer of the organic thickness are considered in this calculation) (1)  $\theta$ =0 (2)  $\theta$ =32 (3)  $\theta$ =47 (4)  $\theta$ =59 (4)  $\theta$ =69 (5)  $\theta$ =82°

**Figure 8** shows the reflectance of the MOPC at the different angle of the incidence with thicknesses of 200 nm Ag and 100 nm of the NPB layers. The position of the left and right band edges are not varied with the increase of the incident angle from 0° to 69°. The bandwidth of the PBG materials is affected by the change of the incident angle and the positions of left and right band edges are observed at  $\lambda_L$ =533.44 nm and  $\lambda_R$ =866.22 nm. With the variation of the incident angle, the PBG is expanded from the visible region to infrared region and there is a small bandwidth in the visible region. The width is about 332.78 nm and the reflection height is only 98.36%. The reflectance spectra splits into a number of pass band below 69° incidence angle.

The multilayer film of the organic layer with NPB also has absorption in the visible region, and the optical constant of organic NPB layer has high n and k in the wavelength ranges of 350 -420 nm, and the optical constant of silver layer has high n and low k in the 250 -380 nm wavelength. Now the optical constants of Ag and NPB are taken n = 0.178, k = 1.86 and n = 1.966, k = 0.115 respectively at 380 nm. For the metal, the refractive index depends upon the interaction of the plasma electron with electromagnetic waves. With increase the wavelength of the electromagnetic waves interacting with silver, the refractive index continuously decreases. Most of the organic components are characterized by attaching functional group to the parent's molecules. Each functional group can also change the absorbing characteristics of the electromagnetic waves that is to say it can change the refractive index of the exiting organic materials. The reflectance of the MOPC is changed with the varying the refractive index from 1.7 to 1.966. Figure 9 shows the reflectance spectra of the MOPC at normal incidence and the number of the periods are taken from N=2 to 15. To increase the refractive index of the NPB from 1.7 to 1.966, the reflectance spectra splits into a number of distinct pass band. The different number of pass band not only arises from a change in refractive index, but also depends upon the number of the periodic layer. The number of pass band increases with increases the number of the periodic layer as shown in Figure 9. At N=2, the 1<sup>st</sup> enlarge band starts at 396.91 to 735.06 with a gap of 698.15nm and the next enlarge band is observed at 759.153to 1392.74nm with PBG of 633.62. Only one bandwidth is observed between the wavelength 393.88 to 579.36 nm of small gap of 185.48 nm. The flatness of the

width becomes sharp with an increasing the number of layer from N=2 to N=15. The maximum flatness is obtained at n=15 and it is desirable to study of the other effect.



Figure 8 Reflection spectra of one-dimensional binary photonic crystals incident at a different angle on the surface and calculated by TMM methods where d<sub>1</sub>=200 nm (metallic layer) and d<sub>2</sub>=100 nm (organic layer)



Figure 9 Variation of the reflectance spectra with the number of the layer incident normally on the surface (the refractive index of the organic layer  $n_2=1.966$ )



Figure 10 Reflection spectra of one-dimensional binary photonic crystals incident normally on the surface versus wavelength at the different thicknesses of the metallic layers (1) 50 nm, (2) 100 nm, (3) 200 nm, (4) 300 nm, (5) 400 nm, and (6) 500nm

**Figure 10** shows the reflectance spectra of the multilayer MOPC with varying thickness of the metallic layer in the different optical absorption region. It is evidently found from Figure 10, that band gap becomes wide with the increasing the thickness of the metallic layer in MOPC. Figure 11 shows the variation of reflectance of MOPC with different thicknesses of the organic layer. The red shift is observed from 100 to 300 nm thickness of the organic layer, but from 300 nm to 500 nm, the position of the left and right band edges are not changed shown by the gray box with red liners in **Figure 11**. The positions of left and right band edges are linearly changed from slightly ultraviolet to infrared region with the increase of the thickness of the organic layer. Whereas optical bandwidth is up to 400nm as the thickness is between 50-400nm, but as thickness of the organic layer is beyond 400nm, the optical bandwidth starts decrease. Now the optical constants of Ag and NPB are also changed with the wavelength of the applied electromagnetic waves for the calculation of the band gap, the following parameter is taken: n = 0.144, k = 5:33 and n = 1:859, k = 0:0097 respectively at 800nm. **Figure 12** shows the reflectance spectra of the MOPC at 100 nm thickness of the organic layer. The refractive index of the Ag and organic layer depends upon the wavelength of the EM waves. The refractive index of the metal layer is varied from n = 0:815, to 0.144 and organic layer n = 1:7, to 1.859 by varying the wavelength from 320 to 800nm. For further calculation in the infrared region, the optical constants of Ag and n = 1:859, k = 0:0097 respectively at 800 nm.

The reflectance of MOPC is plotted in Figure 12 at the different thickness of the metallic layer. The optical band gap also continuously increases with the thickness of the metallic layer up, the optical band gap becomes enhanced at d=500nm.Due to tunability of the refractive index with applied frequency/or wavelength, the enhancement of reflectance spectra in the Ag-NPB periodic system may lie in the peculiar photonic band gap of metallo-organic photonic structure which has no tendency to give the propagating modes in the particular frequency region. Widen band gap is obtained at the less number of the periods, but wideness decreases with increase the number of the periods in the PC. The maximum number of band gap splitting is more observed at the higher of periods in the system. More and more number of states of Ag-NPB has been concentrated over a frequency range of the photonic band structure.



Figure 11 Reflection spectra of one-dimensional binary photonic crystals incident normally on the surface versus wavelength at the different thickness of the organic layer (1) 100 nm, (2) 200 nm, (3) 300 nm, (4) 400 nm, and (6) 500 nm



Figure 12 Reflection spectra of one-dimensional binary photonic crystals incident normally on the surface versus wavelength at the different thicknesses of the metallic layers (with refractive index of organic layer, n=1.895) (1) 50nm, (2) 100nm, (3) 200nm, (4) 300nm, (5) 400nm, and (6) 500nm

# Conclusion

- In the metal-organic photonic structure, plasmonic response plays a very important role for the broadening of the band gap. Wide reflection has been observed in 500 nm-1000nm region due to presence of the organic layer. Maximum number of periods affects the density of the reflectance.
- The optical band increase with increasing the thickness of the metallic layer and also shows the maximum band gap of 500nm due to plasmonic response in the uv-visible region.
- The maximum effects of the plasma are found in uv-visible region, while in IR region, they show less effect. Their response is changed with increased the attenuation constant.
- Since metal-organic periodic structures show the multiple Bragg scatterings which play an important role leading to the formation of photonic band gaps like metal-dielectric photonic crystals.
- The study of reflectance spectra of the same structure versus the thickness of the NPB layer at different incidence wavelengths also found the enhanced the optical band gap, but less compared to the metallic layer when the attenuation of the metal is too low. In uv-visible region, plasmonic actions are enhanced due to association from the functional group of the organic molecules.
- The attenuation of organic and metallic layers is important criteria which gives maximum band gap due to the variation of the thickness of either organic layer or metallic layer. It means that the absorption can be enhanced in a periodic structure due to the metal and organic layers; even the attenuation of the metal is too low in certain frequency region.

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