Transmission Characteristics of a 1D Photonic Crystal Sandwiched by Two Graphene Layers

Hendradi Hardhienata, Angga Ismi Aziz, Dwi Rahmawati, Husin Alatas

Theoretical Physics Division, Department of Physics, Bogor Agricultural University, Jl. Meranti, Gedung Wing S, Kampus IPB Darmaga, Bogor 16680, Jawa Barat, INDONESIA
E-mail: hendradi@ipb.ac.id

Abstract. We analyze the transmission characteristics and dispersion profile of a terahertz (THz) electromagnetic wave propagating inside a 1D dielectric photonic crystal sandwiched by two single atomic graphene sheets. We vary the thickness and number of alternating slabs of the dielectric medium as well as changing the electrical conductivities in the graphene layers and study their effects on the optical bandgap. The simulation result shows that attachment of two single atomic graphene sheets into the system will cause a decrease in the transmitted field although changes in the electrical conductivity will not alter the bandgap since the graphene layer is very thin relative to the dielectric slabs. This feature is in agreement with the results obtained from the dispersion relation curve which is unchanged by varying the electrical conductivity.

1. Introduction

The rise of modern technology is undeniably impressive and in recent times its evolution has been unprecedented in speed driven by the desire to produce not only strong but also lightweight material. Rapid progress in this field cannot be separated from the ability of physicists in manipulating at the nanoscale which is supported by mastery of solid state physics and optoelectronics. Among many important materials graphene has recently stood out as a promising candidate in shaping our future technology due to its electrical and optical properties.

Graphene is the name given to a flat monolayer of carbon atoms tightly packed into a two-dimensional (2D) honeycomb lattice, and is a basic building block for graphitic materials of all other dimensionalities. Although graphene exhibits almost uniform absorption within a large wavelength range, a single layer of graphene may absorb as much as 2.3% of the incident light.[1] Since its experimental discovery, graphene has attracted significant attention in recent years due to the richness of its optical and electronic properties. The unique band structure of graphene leads to many important potential applications in nanoelectronics, especially in the fabrication of ultrafast transistors. As an ultrathin two-dimensional semiconductor, graphene also has unique optical properties and many important potential applications, such as optical limiters and polarizers. Graphene has no band gap and very high electron mobility of about $15000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ at a temperature of $300 \text{ K}$ and about $60000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ at $4 \text{ K}$, whereas for graphene layer is about $3000–10000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$.\[2\] The special properties of graphene can be
analyzed to determine the optical conductivity of graphene as a function of energy. Without interference, the optical conductivity of graphene has a universal value or in the range of infrared energy to visible light.[3] Lately, a lot of research examines how the band gap of graphene can be opened and controlled to obtain materials in accordance with the application of modern electronic devices.

One of the open challenges is to increase the light absorption in graphene. Several mechanisms have been proposed to enhance the absorption of graphene, including putting graphene inside an optical cavity, exploiting the physics of quantum dots on graphene, using a uniaxial strain, a graphene-based grating, and surface plasmons.[4] Recently it has also been shown that inserting graphene slabs into a 1D photonic crystal can increase field absorption by a factor of four.[5] Indeed, photonic crystals has opened a new door for advanced photonic component due to its amazing properties. Photonic crystals can be found in nature and can be created artificially and possesses the remarkable feature of a forbidden band gap where light propagation is prohibited. Photonic crystals are typically classified as one, two, and three dimensional depending on the periodic layers arranged within the structure. When a defect layer is introduced in a 1D photonic crystal, the passband that occurs inside the transmission bandgap can be controlled by changing the refractive index of the defect layer.[6] However, development of optical integrated circuits has certain problems such as unavailability of such materials which can be engineered for optimal photon trapping and confinement without losses at the sharp corners of the waveguides. In this context, photonic band structures or photonic crystals are the promising one to overcome such difficulties and leading continued progress of advance optical integrated circuits. Intensive research on photonic crystals has been attempted after the pioneer works of Yablonovitch and John in 1980s.[7] This study takes understanding of the electromagnetic waves behavior in a simple photonic crystal (periodic medium bilayer). Simple photonic crystal made of two alternate transparent medium with a different refractive indices. Crystal engineering technology development has enabled the making of medium periodically with periodicity well controlled and the thickness of the layer is only a few times thickness of an atom (e.g. molecular epitaxy technique).

In this work, the study of multi-layer graphene is limited to the transmittance output waveform and the analysis of the dispersion relations. The transmittance was studied using the transfer matrix methods, which have been proven to be effective in calculating the electromagnetics field propagation in dielectric and become the flexible methods for modify the dielectric layer as well as the sandwiched by two graphene layers. Electromagnetic waves are propagated in a one-dimensional photonic crystals can cause thin transmittance areas/bandpass inside the forbidden band. The position of the passband inside the photonic bandgap can also be determined from the dispersion relation.[8] The transmission properties of one dimensional graphene photonic crystals were investigated by using transfer matrix method and it was found that the structure has new type of the photonic bandgap in the terahertz (THz) region and is insensitive to the polarization. The reason we perform our simulation in the terahertz spectra is that in this region the properties of the photonic band gap depend on the optical parameters of the graphene sheets.[9] These properties of 1D photonic crystals have potential applications in tunable terahertz multiband narrow filters.[10] In the following section we describe the basic theory in obtaining the transmission profile and dispersion relation via the transfer matrix method (TMM).

2. Transfer Matrix Method

The transfer matrix method is developed based on the electromagnetic boundary conditions that Maxwells equations required. Compared with the traditional transfer matrix method, the new method can be used to calculate the optical absorption of any layer at any position in stratified media.[11] The transfer matrix method is a method used in optics and acoustics to analyze the
propagation of electromagnetic or acoustic waves through a stratified (layered) medium. The transfer-matrix method is based on the fact that according to Maxwell’s equations, there are simple continuity conditions for the electric field across boundaries from one medium to the next. If the field is known at the beginning of a layer, the field at the end of the layer can be derived from a simple matrix operation. A stack of layers can then be represented as a system matrix, which is the product of the individual layer matrices. The final step of the method involves converting the system matrix back into reflection and transmission coefficients. Figure 1 shows our model where the single atomic graphene layer structure is sandwiched near both ends of the 1D PC.

![Graphene layer model](image)

Figure 1: 1D PC structure assumed in the model. (a) The transfer matrix unit cell containing graphene layer (yellow layer) sandwiched between two dielectric materials (blue and purple slabs) with dielectric constants $\varepsilon_1$ and $\varepsilon_2$. Here the arrows to the right and left indicate the transmitted and reflected light respectively (b). Arrangement of the 1D PC and the position of the two graphene layers. The background is assumed to be air ($\varepsilon_0 = 1$).

In this study only electromagnetic waves with polarization $p$ or TM mode (Transverse Magnetic) is considered where the magnetic field is polarized in the $y$ direction and propagating in the $z$-axis, therefore the field can be written as follows:

$$H_{1y} = (a_1 e^{ik_1xz} + b_1 e^{-ik_1xz}) e^{ik_1yz} < 0,$$

$$H_{2y} = (a_2 e^{ik_2xz} + b_2 e^{-ik_2xz}) e^{ik_2yz} > 0,$$

$a_1$ and $b_1$ ($i=1,2$) is the field coefficient, $k_{iz}$ ($k_{ix}$) is the component $x$ ($z$) of the wave vector $k_{iz} = \sqrt{\varepsilon_i \omega^2/c}$ which is the angular frequency and $c$ the speed of light in a vacuum. The electric field and magnetic field at the interface of a dielectric can be connected to the boundary conditions as follows:

$$nx(E_2 - E_1)_{z=0} = 0,$$

$$nx(H_2 - H_1)_{z=0} = J,$$

Where $n$ is the normal unit of the plane and the current density of the graphene layer. From the relationship of equations (3), (4) and equations (1), (2) using boundary conditions in obtain the following matrix equations:

$$\frac{k_{iz}}{\varepsilon_1}(a_1 - b_1) - \frac{k_{2z}}{\varepsilon_2}(a_2 - b_2) = 0,$$
\[(a_1 - b_1) - (a_2 - b_2) = J_x, \]  

(6)

With \(J\) given from Ohm’s law so the equation \(J_x\). Where \(\varepsilon_0\) is the permittivity in vacuum. From the equations (5) and (6) the field coefficients \(a_1\) and \(b_1\) can be related to the field coefficients \(a_2\) and \(b_2\) through the transmission matrix 2x2 as follows:

\[
\begin{pmatrix}
  a_1 \\
  b_1
\end{pmatrix}
= D_{1\rightarrow2}
\begin{pmatrix}
  a_2 \\
  b_2
\end{pmatrix}
\]

(7)

where \(D_{1\rightarrow2}\) is:

\[
D_{1\rightarrow2} = \frac{1}{2}
\begin{pmatrix}
  1 + \eta_p + \xi_p & 1 - \eta_p - \xi_p \\
  1 - \eta_p + \xi_p & 1 + \eta_p - \xi_p
\end{pmatrix}
\]

(8)

with parameter \(\eta_p\) and \(\xi_p\) is:

\[
\eta_p = \frac{\varepsilon_1 k_2}{\varepsilon_2 f_{12}}
\]

(9)

\[
\xi_p = \frac{\sigma k_2}{\varepsilon_0 \varepsilon_2 \omega}
\]

(10)

and the propagation matrix is:

\[
P(\Delta z) =
\begin{pmatrix}
  e^{-ik_z \Delta z} & 0 \\
  0 & e^{ik_z \Delta z}
\end{pmatrix}
\]

(11)

Thus the transfer matrix is the multiplication of the transmissi matix with the propagation matrix on the homogeneous dielectric material. With the note of the field coefficient \(a_1\) and \(b_1\) to the left of the graphene layer and the field coefficient \(a_{N+1}\) and \(b_{N+1}\) to the right of the graphene layer so that the two field coefficients are related to the transfer matrix \((\beta)\) 2x2 is:

\[
\begin{pmatrix}
  a_1 \\
  b_1
\end{pmatrix}
= \beta
\begin{pmatrix}
  a_{N+1} \\
  b_{N+1}
\end{pmatrix}
\]

(12)

with

\[
\beta = D_{1\rightarrow2} P(d_{1,2}) D_{2\rightarrow3} P(d_{2,3}) \ldots P(d_{N-1,N}) D_{N,N+1}
\]

(13)

Note that since the structure is periodic, then \(d_{1,2} = d_2\) and \(d_{2,3} = d_1\). Here \(\beta\) is a 2 x 2 matrix:

\[
\beta =
\begin{pmatrix}
  \beta_{11} & \beta_{12} \\
  \beta_{21} & \beta_{22}
\end{pmatrix}
\]

(14)

thus,

\[
\begin{pmatrix}
  a_1 \\
  b_1
\end{pmatrix}
= \beta
\begin{pmatrix}
  a_{N+1}' \\
  b_{N+1}'
\end{pmatrix}
\]

(15)

if both of segments are divided by \(d_{N+1}'\) the matrix is:

\[
\begin{pmatrix}
  a_1 \\
  a_{N+1}' \\
  b_1 \\
  b_{N+1}'
\end{pmatrix}
= \begin{pmatrix}
  \beta_{11} & \beta_{12} \\
  \beta_{21} & \beta_{22}
\end{pmatrix}
\begin{pmatrix}
  a_{N+1}' \\
  b_{N+1}'
\end{pmatrix}
= \begin{pmatrix}
  \beta_{11} & \beta_{12} \\
  \beta_{21} & \beta_{22}
\end{pmatrix}
\begin{pmatrix}
  1 & 0 \\
  0 & 1
\end{pmatrix}
\begin{pmatrix}
  a_{N+1}' \\
  b_{N+1}'
\end{pmatrix}
= \begin{pmatrix}
  \beta_{11} \\
  \beta_{21}
\end{pmatrix}
\]

(16)

The transmittance is given by:

\[
t = \left( \frac{1}{\beta_{11}} \right)
\]

(17)
3. Dispersion Relation for Simple 1D Photonic Crystals

In general, wave propagation in periodic media can be described in terms of Bloch waves. For a determination of the dispersion of a periodic crystal, it is necessary only to integrate the wave-field through a periodic media. Periodicity requires that the Bloch wave must obey the translation symmetry $z = z + i \Lambda$, where $i$ is an integer. Here we follow the derivation of the dispersion relation in accordance with Yariv and Yeh.[12] According to the Bloch theory, the electric field vector which propagate on a line to the $z$-axis (component $k_y = 0$) in the form of periodic photonic crystals:

$$E = E_k(z) e^{i K_z}$$

(18)

where the $K$ subscript here indicates that the function of $E_k$ depend on Bloch wave vector $K$. The problem that needs to be solved is how to determine $K$ as a function of $\omega$, or otherwise. The relation between the variables $\omega$ and $K$ is called the dispersion relation. Mathematically it can be written as:

$$\omega = \omega(k)$$

(19)

In matrix notation the equation would be:

$$\begin{pmatrix} A_N^{(1)} \\ B_N^{(1)} \end{pmatrix} = e^{i k z} \begin{pmatrix} A_{N-1}^{(1)} \\ B_{N-1}^{(1)} \end{pmatrix}$$

(20)

whereas $A_N$ is the amplitude of the electric field that is passed on to the $K$ $N$-layers, while $B_N$ is reflected electric field amplitude. Eq. (20) can be combined with eq. (18) to produce:

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} A_N^{(1)} \\ B_N^{(1)} \end{pmatrix} = e^{i k z} \begin{pmatrix} A_{N-1}^{(1)} \\ B_{N-1}^{(1)} \end{pmatrix}$$

(21)

A phase factor $e^{i K \Lambda}$ and the matrix components $(A_N, B_N)$, the equation (21) satisfies the seeuler equation:

$$\begin{pmatrix} A - e^{i k \lambda} & B \\ C & D - e^{i k \lambda} \end{pmatrix}$$

(22)

The seeuler equation can be obtained easily from linear algebra because $M x = \lambda x$ (with $\lambda = e^{i K \Lambda}$) is an Eigen equation, then $(M - \lambda I)x = 0$ or in other words det $(M - \lambda I)$ should be zero. Then the seeuler equation takes the form[12]:

$$e^{i K \Lambda} = \frac{1}{2} (A + D) \pm \left[ \left( \frac{1}{2} (A + D) \right)^2 - 1 \right]^{1/2}$$

(23)

Equation (23) is the dispersion relation between $\omega$, $k_y$ and $K$ for the Bloch wave. The equation consists of real and imaginary components. By taking the real components the following is obtained:

$$K(k_y, \omega) = \frac{1}{\lambda} \cos^{-1} \left[ \frac{1}{2} (A + D) \right]$$

(24)

In areas where $\left[ \frac{1}{2} (A + D) \right] < 1$ the $K$ value is real while for $\left[ \frac{1}{2} (A + D) \right] > 1$ the $K$ value is complex and for the latter case Bloch wave disappears hence no photon with momentum $\hbar k$ can propagate and we observe a forbidden band or band gap. The edges of forbidden band occurs at $\left[ \frac{1}{2} (A + D) \right] = 1$. Changing the refractive index $n_1$ and $n_2$ as well as the distance layer, $a$ and $b$
will change the value of transfer matrix elements $A$ and $D$ therefore changing the width of the forbidden band. Applying the notation convention in eq. (14) the dispersion relation takes the form:

$$\cos K\Lambda = \left( \frac{\beta_{11} + \beta_{22}}{2} \right)$$

Eq. (25) will be used in generating the dispersion relation in the simulation.

4. Results and Discussions
In the following section we describe the transmission profile for variation of the dielectric medium thickness, number of layers, and electrical conductivity.

4.1. Variation of dielectric slab thickness
In the simulation we set the 1\textsuperscript{st} and 2\textsuperscript{nd} dielectric medium refractive index to 1 and 3 respectively and set $\sigma = 0$. Here $d_1$ is the thickness of the 1\textsuperscript{st} dielectric medium, $d_2$ is the thickness of the 2\textsuperscript{nd} dielectric medium where their dimension is in accordance with the condition $n_i d_i \approx \lambda_0$ where $\lambda_0$ is the Bragg wavelength. Here, $N$ is the number of alternating layers (double layers). Assuming no graphene layer, variation of $N$ and dielectric thickness results in changes of the bandgap width as presented in Fig. 4. This result is not new and is indeed well-known, but here we also plot the dispersion relation profile (green curve) to see how the bandgap changes accordingly.

Fig. 2. Variation of dielectric slab thickness on the transmission profile (a) $d_1=0.4$ mm, $d_2=0.6$ mm, $N=30$, $\sigma = 0$, (b) $d_1=0.6$ mm, $d_2=0.6$ mm, $N=30$, $\sigma = 0$, (c) $d_1=0.6$ mm, $d_2=0.8$ mm, $N=30$, $\sigma = 0$
From figure 4(a), 4(b), and 4(c), it can be inferred that assuming no graphene layers, the effect of adding more dielectric layers will increases the number of bandgaps for a similar bandwidth range. Applying the dispersion relation in eq. (25) shows that increasing the number of layers will increase the wave number of the cosine function where the region near the cosine peaks exceed $\pm 1$ thus resulting in a complex value to $K$ and in this frequency region ($\cos K \Lambda > \pm 1$) the photon cannot propagate hence we observe an optical bandgap.

4.2. Variation of number of dielectric layers
Keeping the dielectric medium refractive index to have a value of $n_1 = 1$ and $n_2 = 3$ respectively and setting $\sigma = 0$ we vary the number of dielectric layers and observe the field transmission profile. The simulation result is depicted in Fig. 5.

As expected increasing the number of dielectric alternating layers will sharpen the bandgaps but has the same bandwidth and increase the number of ripples. Again this result is already well-known, and this can directly be inferred from the dispersion relation curve which stays unchanged.
4.3. Variation of graphene layer conductivity

In the following subsection we keep the 1\textsuperscript{st} and 2\textsuperscript{nd} dielectric medium refractive index 1 and 3 respectively and set the number of dielectric layers \( N = 10 \). The thickness of the 1\textsuperscript{st} and 2\textsuperscript{nd} dielectric medium is chosen to be 0.5 mm and 0.8 mm respectively.

(a)

(b)

(c)

Fig. 4. Variation of Graphene layer conductivity for (a) \( \sigma_1 = 10, \sigma_2 = 10 \) (b) \( \sigma_1 = 100, \sigma_2 = 100 \) and (c) \( \sigma_1 = 1000, \sigma_2 = 1000 \)

Fig. 5. Graphene layer conductivity variations on the transmission profile shown here by combining Fig. 4 (a)-(c). Red, blue, and black lines corresponds to Fig. 4 (a), 4(b), and 4(c) respectively whereas the green line corresponds to the dispersion curve which is independent of the graphene conductivity. It is clear that increasing the imaginary part of the graphene conductivity results in higher attenuation due to higher absorption but the bandgap width is unaltered.
From figure 4(a), 4(b), and 4(c) by using the variation of the graphene layers conductivity, changing the imaginary part of the graphene electrical conductivity changes the transmittance peak dramatically. This effect can be explained due to the absorption of the field by the graphene slabs along the vertical axis since it was assumed that the thickness of the graphene layer along the propagation direction can be neglected. It is interesting to infer from the dispersion relation curve that although the field is attenuated due to absorption, the bandgap width does not change. Further investigation into the dispersion formula reveal that the effect of changing the electrical conductivity does not affect eq. (25). Only if we attribute certain length for the graphene slab the dispersion relation formula will be altered and thus also the band gap width will change. This feature can neatly be seen in Fig. 5.

5. Conclusion

We have shown that attachment of two very thin graphene layers in a one dimensional photonic crystal alter the transmission profile significantly. Increasing the graphene layer imaginary electrical conductivity value will result in a decrease of the transmission peak although the photonic band gap width remains unaltered. These features can be well explained by the dispersion relation formula which is non sensitive upon changes in the graphene electrical conductivity if the layer thickness is very thin.

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