Abstract: In this paper, we applied the band structure theory to investigate the plasmonic band (PB) structures and optical properties of subwavelength metal/dielectric/metal Bragg waveguides in the near infrared range with either dielectric or geometric modulation. The Bloch wave vector, density of states, slowdown factor, propagation length and transmittance are calculated and analyzed. Both the modulations are in favor of manipulating surface-plasmon-polariton (SPP) waves. For the dielectric modulation, the PB structure is mainly formed by SPP modes and possesses a "regular pattern" in which the bands and gaps have a relatively even distribution. For the geometric modulation, due to the strong transverse scattering, the contributions of higher modes have to be considered and the gap widths have a significant increase compared to the dielectric modulation. A larger slowdown factor may emerge at the band edge; especially for the geometric modulation, the group velocity can be reduced to 1/100 of light, and negative group velocity is observed as well. While inside the bands, the slowdown factor is smaller and the bands are flat. The contribution of each eigenmode to the PB structure is analyzed.

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References and links
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1. Introduction

Subwavelength metal/dielectric/metal waveguides, as a kind of plasmonic waveguide, are currently the subject of intensive and widespread study because of their remarkable advantages, such as strong field localization, structural simplicity, convenience of fabrication and integration into optical circuits [Refs. 1–3, and references therein]. When light propagates along a metal/dielectric interface, it will excite a collective oscillation of free electrons at the surface of the metal, generating a field that decays exponentially away from the interface. This mode is called surface plasmon polariton (SPP) [4]. In a subwavelength metal/dielectric/metal waveguide, the case is somehow different, since the lowest mode is the combination of the SPP waves of the two dielectric/metal interfaces, called in-slit SPP, which decays exponentially in the metals and is flat in the dielectric [5–12]. In this paper we mainly discuss the in-slit SPP and simply call it SPP. The propagation of this mode in the waveguide structure is essential in the subwavelength optics [1–12].

Inspired by the unprecedented power of controlling the propagation of light through the band structures in photonic crystals [13–19], periodic modulations have been introduced in subwavelength metal/dielectric/metal waveguides to manipulate the propagation of SPP waves [20–31]. Due to the waveguide configuration, the periodic modulations are usually one-dimensional and along the propagation direction. These structures are named subwavelength metal/dielectric/metal Bragg waveguides, and will be called Bragg waveguides (BWGs) in short below. In a BWG, the periodical structure scatters SPP waves, and consequently the plasmonic band (PB) and plasmonic band gap (PBG) may be produced. Within the gap, the propagation of SPP is forbidden [20–31]. While within the band, the wave can propagate, but its group velocity may be slowed down [29–31]. The advantages of the PB structure facilitate designing and fabricating a variety of functional plasmonic structures [21–26], such as reflectors, mirrors, filters, and microcavities.

Several popular theoretical and numerical methods have been used to investigate the PB structures in BWGs, such as the effective index method (EIM) [20–26], characteristic impedance method [27–30], modal expansion method (MEM) [11], and finite-difference time-domain (FDTD) method [20–31]. Their accuracy, applicability, and theoretical basis have been discussed in detail and compared with each other numerically in our recent publication [12]. The advantages and disadvantages of these methods were pointed out there. It turned out that the MEM was a versatile and fast method which provided accurate results. This paper is intended to employ the band structure theory to reveal abundant information of the PB structure. This theory has been frequently used in the study of photonic crystals [13–19] and is also suitable for the physical problems in BWGs. We choose the eigenfunctions of the subwavelength metal slit as the expansion basis [11, 12] and apply the Bloch theorem in the periodic direction so as to find the PB structure with Bloch wave vectors. This method can be called the periodic version of MEM. Compared with the similar calculations in photonic crystals with the plane-wave expansion [18, 19], the eigenfunctions used here provide us a clearer picture of wave scattering within the structure and allow us to identify explicitly the contribution of each eigenmode to the PBG formation. With the PB structure, the optical properties of BWGs are discussed. Moreover, the BWGs studied here are dissipative systems because the metal is considered as a real one with permittivity having finite real and imaginary parts. Determination of the bands and gaps in a dissipative system is quite different from that in a nondissipative system. The analysis of the density of states (DOS) will reveal abundant information.

This paper is arranged as follows: Section II sets up two basic BWG structures and presents the periodic version of MEM. In Sec. III, by the analysis of DOS, transmittances and Bloch wave vectors, the proper way for determining bands and gaps in a dissipative system is pointed out; then the optical properties of BWGs are discussed, including the variation of the PBG, slow
light, negative group velocity, and propagation length. In Sec. IV, a modal analysis is carried out to reveal the role of each eigenmode in the PBG formation; by the way, the limitation and applicability of EIM are addressed. Finally, conclusions are presented in Sec. V.

2. Model and the periodic version of MEM

In this section, two kinds of BWGs and the periodic version of MEM are presented.

The BWG models studied in this paper are sketched in Fig. 1. In the x direction, the structures are confined between two perfectly conducting walls, and are symmetric with respect to the central lines. The propagation direction of the waveguide and the periodic modulated direction are the y direction. The basic unit consists of two layers and can be classified into two categories according to their composition: one is called dielectric modulation, see Fig. 1(a), where the slit widths are the same in all the layers but the filling materials are not; the other is called geometric modulation, see Fig. 1(b), where the filling materials are the same in all the layers but the slit widths are not. We only consider the waves with a TM polarization. The basic structural parameters are given in the caption of Fig. 1.

For the sake of convenience, the \((p-1)\)th and \(p\)th layers of the dielectric modulation shown in Fig. 1(a) are respectively called air and dielectric regions; while those of the geometric modulation shown in Fig. 1(b) are called narrower and wider regions. Please note that although the \((p-1)\)th layers in both modulations have different names, they are actually the same in our models.

The permittivity of silver as a function of the wavelength \(\lambda\) is evaluated as \(\varepsilon_{Ag} = (3.57 - 54.33\lambda^2) + i(-0.083\lambda + 0.921\lambda^3)\) [32] by fitting the experimental data [33], which is valid for \(0.6 \leq \lambda \leq 1.6 \mu m\).
Now we present the periodic version of MEM. The first step is to express the magnetic field in the $l$th layer by separating variables,

$$
H^{(l)}_z(x,y) = \sum_{n=1}^{\infty} \phi^{(l)}_n(x) \left[ e^{ik_B(\bar{x}-Q(y-1))} a_n^{(l)} + e^{-ik_B(\bar{x}-Q(y-1))} a_n^{(l)*} \right], \\
$$

where $\phi^{(l)}_n(x)$ is the eigenfunction in the $x$ direction. The corresponding derivation and information about $\phi^{(l)}_n(x)$ can be found in Ref. 11, and will not be readdressed here. Next, by applying the boundary continuum condition and Bloch theorem, we relate the magnetic and electric fields in the $(p-1)$th and $p$th layers to build the coupled equations,

$$
\begin{align*}
\left[ \begin{array}{c} e^{ik_B(p-1)q(x-1)} u_{m+1}^{(p-1)} + d_m^{(p-1)} \\ \sum_{n=1}^{\infty} I_{mn}^{(p-1,p)} u_{m+1}^{(p-1)} - d_m^{(p-1)} \\ e^{ik_B(p-1)q(x-1)} u_{m+1}^{(p-1)} \\
\end{array} \right] &= \sum_{n=1}^{\infty} K_{mn}^{(p-1,p)} \left[ \begin{array}{c} u_n^{(p)} + e^{ik_B(p)q(x)} d_n^{(p)} \\ u_n^{(p)} - e^{-ik_B(p)q(x)} d_n^{(p)} \\ e^{ik_B(p)q(x)} u_n^{(p)} + d_n^{(p)} \\
\end{array} \right], \\
\left[ \begin{array}{c} e^{ik_B(p-1)q(x-1)} u_{m+1}^{(p-1)} - e^{-ik_B(p-1)q(x-1)} d_m^{(p-1)} \\
\end{array} \right] &= \sum_{n=1}^{\infty} K_{mn}^{(p-1,p)} \left[ \begin{array}{c} u_n^{(p)} - e^{-ik_B(p)q(x)} d_n^{(p)} \\ e^{ik_B(p)q(x)} u_n^{(p)} - d_n^{(p)} \\
\end{array} \right],
\end{align*}
$$

where

$$
K_{mn}^{(p-1,p)} = \int_{L} \frac{1}{e^{ik_B(p-1)q(x-1)} - \varphi_n^{(p-1)}} \varphi_m^{(p)} dx,
$$

In Eq. (3), $\bar{\varphi}$ means the complex conjugate of $\varphi$, and $\varphi^+$ is the adjoint of $\varphi$. The factor $e^{ik_Bh}$ is introduced by the Bloch theorem. A numerical overflow may occur if $e^{ik_Bh}$ is computed directly from Eq. (2). To avoid this overflow, the eigen problem is recast, by the $S$ matrix [34], into the following form [18,19]:

$$
\begin{align*}
\left[ \begin{array}{c} S_{11}^{(p)} \\ S_{12}^{(p)} \\ S_{21}^{(p)} \\ S_{22}^{(p)} \\
\end{array} \right] \left[ \begin{array}{c} u_{(p-1)} \\ d_{(p-1)} \\
\end{array} \right] &= e^{ik_Bh} \left[ \begin{array}{c} 0 \\ -S_{12}^{(p)} \end{array} \right] \left[ \begin{array}{c} I \\ -S_{22}^{(p)} \\
\end{array} \right] \left[ \begin{array}{c} u_{(p-1)} \\ d_{(p-1)} \\
\end{array} \right],
\end{align*}
$$

where each of the four sub-matrices $S_{11}^{(p)}$, $S_{12}^{(p)}$, $S_{21}^{(p)}$ and $S_{22}^{(p)}$ contains $N \times N$ elements with $N$ being the truncation number. Equation (4) is the eigenequation for obtaining Bloch wave vector $k_B$.

Before going further to present our numerical results, two illustrations need to be addressed. The first is how to form the PB structure with $k_B$. As can be seen from Eq. (4), for each given frequency (or wavelength) there are $2N$ solutions of $k_B$, among which $N$ solutions have a positive sign and the other $N$ have a negative sign, representing $N$ forward and $N$ backward propagating Bloch waves. Since these two sets of $k_B$ have the same absolute values, only the set with positive imaginary parts is considered. We arrange all the $k_B$ in a way of the ascending absolute values of their imaginary parts $|\text{Im}(k_B)|$, and call the one with the smallest $|\text{Im}(k_B)|$ the first or the lowest mode, and so on. Then we find that the $|\text{Im}(k_B)|$ of the second and higher modes are larger than that of the lowest mode by at least one order of magnitude. This fact indicates that their associated Bloch waves, except the lowest mode, decay very fast so that are forbidden in the system, which is physically reasonable. Hereafter, a mode that cannot propagate in the BWG is named forbidden mode. Therefore, only the lowest mode, which has the smallest $|\text{Im}(k_B)|$, is chose to analyze the PB structure. Furthermore, the lowest mode may be forbidden for certain frequencies (or wavelengths). As a result, the PBGs are formed. Further discussion about the determination of the bands and gaps in a PB structure will be carried out with specific numerical results in the next section.
The second concerns the precision of our numerical results. In this paper, \( N = 80 \) modes are employed in the calculation that is enough to ensure the convergence, since its relative error compared to \( N = 40 \) modes is less than 1\%. However, the MEM results here are also affected by the two perfectly conducting walls. It is known that a wider confined region provides a more accurate result. Comparisons between the results of \( L = 2 \) and \( 4 \mu m \) are shown in Figs. 2(a) and 4(a). In both cases the influences introduced by the two perfectly conducting walls are negligible. Thus, \( L = 2 \mu m \) and \( N = 80 \) used in this paper are sufficient for providing trustworthy results. Although the implantation of perfectly matched layers in MEM is a better solution for this problem, it dramatically complicates the eigenmode calculation. By the way, a good agreement between the results of our calculation and FDTD can be obtain when the Yee’s cell is less than \( 1 \text{nm}^2 \) [11, 12].

3. PB structures and optical properties of BWGs

In this section, the PB structures and optical properties of BWGs are discussed in the near infrared range.

For convenience of the following discussion, we define \( f = q^{(p-1)}/h \), where \( q^{(p-1)} \) is shown in Fig. 1 and \( h = 1 \mu m \) is the unit length, as the filling factor in both modulation models. The DOS is expressed as \( D(\lambda) = \lim_{\Delta \lambda \to 0} N/\Delta \lambda = 1/\pi \times d\text{Re}(k_B)/d\lambda \). The propagation length is defined as \( L_p = 1/(2\text{Im}(k_B)) \). The group velocity is expressed as \( v_g = \partial \omega / \partial \text{Re}(k_B) = d\omega / d\lambda \times \text{Re}(k_B)/d\lambda \), and correspondingly, the slowdown factor is defined as \( c/v_g = -\lambda^2/(2\pi) \times d\text{Re}(k_B)/d\lambda \), where \( c \) is the velocity of light in vacuum. The so-called slow-light phenomena usually refer to that \( c/v_g \) is about 100. Moreover, to verify the results of the band structure calculation, we calculate the transmittance of a finitely long BWG, which is defined as the output energy divided by the input energy and calculated by the MEM developed in Ref. 11. In the transmittance calculation, a SPP source is placed in the BWG, which is defined as the output energy divided by the input energy and calculated by the results of the band structure calculation, we calculate the transmittance of a finitely long BWG.

We begin with the discussion of the dielectric modulation. The results of two cases with \( f = 0.5 \) and 0.1 are presented and analyzed below. Their DOS, transmittances, Bloch wave vectors, slowdown factors and propagation lengths are plotted in Fig. 2.

As shown in Fig. 2, we can easily recognize the bands and gaps in the DOS figures. The magnitudes of DOS are nearly zero in the gaps; at the band edges, DOS peaks are observed. It is worth emphasizing that the DOS in gaps are not zero. For a nondissipative system, such as a one-dimensional photonic crystal, see Eq. (5) or (6) below in Sec. IV, a forbidden mode usually processes a pure imaginary \( k_B \), i.e. \( \text{Re}(k_B) = 0 \). Then the gaps, if any (usually appear in the case described by Eq. (5)), should be the wavelength/frequency ranges with zero DOS since \( d\text{Re}(k_B) = d0 = 0 \). While in the present dissipative case, \( k_B \) is always a complex number, no matter whether the mode is forbidden or not. Within the gaps, as shown in Fig. 2, \( \text{Re}(k_B) \) is nearly either \( \pm \pi \) or 0, so that \( d\text{Re}(k_B) \neq 0 \), resulting a small magnitude of DOS (the abrupt changes of \( \text{Re}(k_B) \) in the gaps are caused by the periodicity of \( e^{ijk_B} \)). Moreover, this magnitude may become larger in the shorter wavelength or higher frequency range. Thus, the definition of gaps in a dissipative system is not as determinative as that in a nondissipative system.

As a test of our DOS curves, the transmission through a finitely long BWG is calculated. As shown in Fig. 2, the light is able to transmit in the bands and is not in the gaps. Our computation also reveals that a finite BWG with 5 periods is sufficiently long to exhibit clearly the photonic crystal effect and the ones with 15 periods shows the gaps accurately.

The imaginary part of \( k_B, \text{Im}(k_B) \), can be use to determine the PB structure as well. As shown in Fig. 2, the drastic changes of \( \text{Im}(k_B) \), corresponding to the peaks in DOS, indicates the locations of band edges. Then the larger \( \text{Im}(k_B) \) regions, standing for fast decaying waves,
Fig. 2. Numerical results of the dielectric modulation with (a) $f = 0.5$ and (b) $f = 0.1$. In each figure, the 1st (top) panel is the DOS; the 2nd panel is the transmittances of BWGs containing 5, 10 and 15 periods; the 3rd panel is the real part (left, green) and imaginary part (right, yellow) of Bloch wave vector $k_B$; and the 4th (bottom) panel is the slowdown factor $c/v_g$ (left, green) and propagation length $L_p$ (right, yellow). In the bottom panels, the green dotted horizontal lines are $c/v_g = 1$, and the green circles represent the divergences caused by the abrupt changes of the real parts of $k_B$.

are the gaps, and the smaller $\text{Im}(k_B)$ regions, representing long propagating waves, are the bands. According to our calculation, $\text{Im}(k_B)$ is of order of magnitude of $10^{-1}$ (the magnitude of $\text{Im}(k_{SPP})$ in the dielectric region) or less within the bands, and is larger with one or two orders within the gaps. Moreover, the bands in the shorter wavelength ranges always possess larger $\text{Im}(k_B)$, resulting in small transmittances. For example, in Fig. 2(b), among the three transmittance curves, only the one with 5 periods can be used to confirm the existence of bands in the wavelength range between 0.6 and 0.7 μm, despite of its small value. This is another major difference from the nondissipative system—even in the bands waves may decay fast. The propagation length $L_p$ is inverse to $\text{Im}(k_B)$, and its value reflects the attenuation of the wave. Within the gaps, $L_p$ is very small.

Other important information provided by $\text{Re}(k_B)$ concerns the group velocity $v_g$ and slowdown factor $c/v_g$. From the definitions of slowdown factor and DOS, it is known that the curves of these two physical quantities should have a similar shape, so that the slowdown factor also have the ability to determine the bands and gaps like the DOS. In the bands, the group velocities are slowed down with $c/v_g$ being $3 \sim 10$. Usually, $c/v_g$ and its changing rate become smaller as the wavelength moves from the band edge to band center. Thus, it is expected that the $c/v_g$ curve is comparatively smooth around the band center, where signals may travel without dispersion. For instance, the wavelength range $1.27 - 1.37 \mu m$ of the $c/v_g$ curve in Fig. 2(a) can be considered as a flat band. On the other hand, $c/v_g < 1$ is observed in the gaps, which means that the group velocity is superluminal. However, since the superluminal group velocity does not mean superluminal signal velocity [35], this phenomenon is not a matter of our concern.

All the results in Fig. 2 are for the confined width $L = 2 \mu m$ except those marked by crosses “×” that are for $L = 4 \mu m$. Since the crosses fit the solid lines perfectly, our results are reliable.

The variations of the corresponding curves in Fig. 2 for the two $f$ values are similar, except that with the $f$ value decreasing, the widths of both bands and gaps become narrower. It is seen
from Fig. 2 that the PB structure of $f = 0.1$ consists of more and narrower bands and gaps. In order to give an intuitionistic view of how $f$ influences the PB structures and optical properties of BWGs, we plot in Figs. 3(a) and 3(b) the variation of slowdown factor and propagation length as functions of $f$ and $\lambda$, respectively.

![Diagram](image)

**Fig. 3.** Variation of (a) slowdown factor $c/\nu_g$ and (b) propagation length $L_p$ with $f$ and $\lambda$ in the dielectric modulation. The structural parameters were given in Fig. 1.

The black regions in Figs. 3(a) and 3(b) represent the PBGs. As can be seen, the bands and gaps have a relatively regular and even distribution as $f$ and $\lambda$ vary. This kind of pattern is a distinguishable feature of the dielectric modulation, and is regarded as “regular pattern”. In Sec. IV, we will show that this “regular pattern” is mainly formed by the SPP modes under a weak transverse scattering. When $f$ and $\lambda$ are small, see, the lower left corner of Figs. 3(a) and 3(b), both bands and gaps have comparatively smaller widths, showing a denser distribution; in the bands, the slowdown factor is larger but the propagation length is smaller. As $f$ and $\lambda$ become larger, towards the higher right corner of the figure, the widths of both bands and gaps gradually increase. As mentioned before, although the slowdown factor in the bands becomes smaller, its variation also becomes smoother so as to form a flat band. Especially in a broader band, a flat band may be observed. For example, when $f = 0.79$, the wavelength range $1.35 - 1.55 \mu m$ is a flat band. Moreover, the propagation length increases with $f$ significantly, which is less than $5 \mu m$ for a small $f$ but is nearly $50 \mu m$ when $f$ closes to 1. The main cause of this significant increase is that the air regions have a smaller absorption of the wave than the dielectric regions,
thus the increase of their weight in the unit cells leads to a smaller absorption and a longer propagation.

Next, we discuss the numerical results of the geometric modulation. The DOS, transmittances, Bloch wave vectors, slowdown factors, and propagation lengths as functions of wavelength for \( f = 0.5 \) and 0.1 are plotted in Fig. 4.

![Fig. 4. Numerical results of the geometric modulation with (a) \( f = 0.5 \) and (b) \( f = 0.1 \). The gray areas in (b) represent the wavelength ranges for “local modes”. Other captions are the same as those in Fig. 2.](image)

Compared with the dielectric modulation, the geometric modulation has a stronger scattering of SPP waves, resulting in wider PBGs. For example, many gaps in Fig. 4 are broader than those in Fig. 2 in the corresponding PB structures. Moreover, the real and imaginary parts of \( k_B \) are no longer smooth when \( f \) closes to 0. As shown in Fig. 4(b) for \( f = 0.1 \), the \( \text{Im}(k_B) \) curve has four dips at 0.662, 0.690, 0.812 and 1.116\( \mu m \). At first glance, it seems that they are caused by numerical error. To verify the correctness of the results, we enlarge the transmittance figure at the corresponding wavelength range in the inset of Fig. 4(b). It is seen that the first two dips do correspond to two small transmission peaks. As for the latter two dips, no transmission peak is observed (not shown in the inset). This is because these modes, as will be proved in the next section, are composed of both symmetric and anti-symmetric modes, thus the SPP source used in the transmittance calculation cannot excite them. As a testing, we adopt \( N = 120 \) modes in the modal expansion to check the precision of \( N = 80 \) modes result, and the two calculated curves fit each other very well. Thus \( N = 80 \) modes are trustworthy. Again, the results of \( L = 4\mu m \) are plotted in the third panel of Fig. 4(a) to confirm that the influence brought by the two perfectly conducting walls is negligible.

The abrupt changes of \( k_B \) cause severe oscillations of the DOS and slowdown factor. It is noticed that Fig. 4(b) shows the slow-light phenomena and negative group velocity. But what surprised us more is the gray areas labeled in Fig. 4(b), where both large DOS and large \( \text{Im}(k_B) \) are observed. It seems that the DOS and transmittance curves show contradiction. The large DOS definitely means the modes are allowed in the system; while the large \( \text{Im}(k_B) \) indicates the wave decay quickly. Let us recall the birth of photonic band gaps in photonic crystals, where the gaps are designed to efficiently forbid the atomic spontaneous emission [13, 14]. For the gray areas in Fig. 4(b), although the modes attenuate quickly, their atomic spontaneous emissions actually are accelerated, rather than forbidden, because of the large DOS. Thus, we
take these regions as bands, and call the associated modes as “local modes”. Actually, in Fig. 2(b), we have already encountered this situation as the bands had small transmittances, but the concept of “local modes” have not been mentioned there, because we think their propagation lengths and transmittances are relatively large, compared with the ones here. To identify and clearly observe the “local modes”, a reference, with the propagation length and transmittance being much smaller than 1, should be used.

The variation of the slowdown factors in the bands is similar to that in the dielectric modulation, where larger values are observed at the band edges than in the bands, and they vary smoothly within the bands. Generally speaking, the slow-light phenomenon in a periodic structure is originated from the interference between the forward and backward propagating Bloch waves. However, for the geometric modulation, waves can also engender a transverse resonance in the x direction, raising the value of the slowdown factor. Here the width of the wider regions is 0.6μm. Increasing the width will further raise the slowdown factor. Besides, the propagation length here is also larger than that in the dielectric modulation. This is partly because the two regions are both air-filled which corresponds to small absorption, and partly because a wider air region corresponds to a smaller absorption.

In Figs. 5(a) and 5(b) we plot the slowdown factor and propagation length in the geometric modulation as functions of $f$ and $\lambda$, respectively.

![Fig. 5. Variation of (a) slowdown factor $c/v$ and (b) propagation length $L_p$ with $f$ and $\lambda$ in the geometric modulation. The structural parameters were given in Fig. 1.](image-url)
Compared with the “regular pattern” shown in Fig. 3 for the dielectric modulation, the PB structure in Fig. 5 presents an irregular distribution, which is mainly resulted from the strong transverse scattering of the SPP and higher modes. The formation of this PB structure will be analyzed in Sec. IV. Also because of this strong transverse scattering, the gaps become much wider compared to the dielectric modulation.

In Fig. 5(a), $c/v_g$ merely covers $-10 \sim 20$, where the minus sign means negative group velocity. For $c/v_g$ out of this range, no matter positive or negative, their magnitudes have the same order as those shown in the insets of Fig. 4(b). For example, in Fig. 5(a), the magnitude of the bright narrow bands is between 40 and 150, while one of the black curves is between $-100$ and $-30$ (Please note that these black curves are bands). However, as revealed from the comparison of Figs. 5(a) and 5(b), these bright narrow bands and black curves that possess very large $|c/v_g|$ appear at the band edges or in the gaps and have small propagation lengths, usually smaller than 1μm, which means that they are the “local modes”. For the modes with larger propagation lengths, their $c/v_g$ curves have similar distributions with those in the dielectric modulation, but have an increase in magnitude. Unlike the $L_p$ distribution of the dielectric modulation in Fig. 3(b), Fig. 5(b) shows an even distribution within the bands, because both the two air-filled regions have a small absorption of waves.

4. PBG formation: modal analysis

In this section, the reason of the PBG formation and the contribution of each mode to the PB structure are discussed by modal analysis. By the way, the applicability of EIM is demonstrated.

Before going to the modal analysis, we give a brief outline of the properties of eigenmodes in a subwavelength metal slit as a preparation. Their details can be found in Ref. 11. The first is that the eigenmodes can be classified according to the field distribution along the $x$ direction into two groups: guided modes, of which the fields oscillate in the slit but decay in the metal, and radiation modes, of which the fields oscillate in both the slit and metal. The second is that if the eigenmodes are arranged according to the absolute values of the imaginary parts of their wave vectors $|\text{Im}(k_y)|$ (a greater $|\text{Im}(k_y)|$ means a faster attenuation), the symmetric and anti-symmetric modes appear alternatively. The SPP mode is always the lowest one, which is a guided and symmetric mode. In the case where the structure and light source are symmetrically arranged, the anti-symmetric modes are forbidden [11]. In the present calculation, there is no prescription for the source, thus all the modes may contribute in Eq. (4). The third is that the eigenmodes can also be classified as propagation and evanescent modes according to their propagation properties along the $y$ direction. The former has very small $|\text{Im}(k_y)|$ so that can propagate for a long distance; while the latter has large $|\text{Im}(k_y)|$ and decays quickly. In the present paper, the SPP modes are always propagation ones. For the higher order modes, the statement that “the slit width should be equal to an integer multiple of half the wavelength” can be used as an approximate criterion of determining whether they can propagate or not [10]. For example, the narrower region with $w(p^{-1}) = 0.1\mu$m only allows the SPP mode to propagate. While for the wider region with $w(p) = 0.6\mu$m, the second mode (the first anti-symmetric mode) can also propagate when the wavelength is in the range of $0.6 - 1.2\mu$m.

Now we proceed to take modal analysis. First we investigate the case of $f = 0.1$ in the dielectric modulation. For comparison, the $k_0$ shown in Fig. 2(b), calculated by MEM with $N = 80$, is redrawn in Fig. 6, along with the results of EIM and the single-mode MEM. As can be seen, the three curves agree with each other well, which indicates that the latter two approximation methods also give relatively accurate results. We would like to take a look at their theoretical basis. The EIM transfers a BWG into an equivalent one-dimensional photonic crystal according to the propagation properties of the SPP mode in each layer by $n_{eff}^{(l)} = k_{SPP}^{(l)}/k_0$, where $k_0 = 2\pi/\lambda$ is the wave vector in vacuum. Without loss of generality, the dispersion relation of
a one-dimensional photonic crystal is expressed by the well known Kronig–Penney relation:

\[
\cos(k_b h) = \cos\left(\frac{(p-1)}{k_{\text{SPP}}} q(p-1)\right) \cos\left(\frac{(p)}{k_{\text{SPP}}} q(p)\right) - \frac{1}{2} \left(\frac{k_{\text{SPP}}[(p-1)]}{k_{\text{SPP}}[(p)]} \frac{\tilde{\varepsilon}[(p-1)]}{\tilde{\varepsilon}[(p)]} + \frac{k_{\text{SPP}}[(p)]}{k_{\text{SPP}}[(p-1)]} \frac{\tilde{\varepsilon}[(p)]}{\tilde{\varepsilon}[(p-1)]}\right)
\times \sin\left(\frac{(p-1)}{k_{\text{SPP}}} q(p-1)\right) \sin\left(\frac{(p)}{k_{\text{SPP}}} q(p)\right),
\]

(5)

where \(k_{\text{SPP}}^2 + k_x^2 = \bar{k}_0^2 \varepsilon(p)\). The notation “\(\sim\)” on is added in order to avoid the symbol of dielectric constant in the models. When \(k_x = 0\), Eq. (5) is simplified into the following form that is commonly used in the EIM:

\[
\cos(k_b h) = \cos\left(\frac{(p-1)}{k_{\text{SPP}}} q(p-1)\right) \cos\left(\frac{(p)}{k_{\text{SPP}}} q(p)\right) - \frac{1}{2} \left(\frac{n_{\text{eff}}[(p-1)]}{n_{\text{eff}}[(p)]} + \frac{n_{\text{eff}}[(p)]}{n_{\text{eff}}[(p-1)]}\right)
\times \sin\left(\frac{(p-1)}{k_{\text{SPP}}} q(p-1)\right) \sin\left(\frac{(p)}{k_{\text{SPP}}} q(p)\right).
\]

(6)

The EIM curves in Fig. 6 are calculated by Eq. (6). Taking \(k_x = 0\) means that the information of the transverse scattering is completely omitted. This negligence is reasonable in the case of dielectric modulation because the slit widths of all the layers are the same, and consequently the transverse scattering is very weak [11]. This is the reason why the EIM can be applied in the case of dielectric modulation. However, omitting the transverse scattering will cause a slight difference on the magnitude of scattering amplitude and phase from the precise ones, and this difference will be amplified as the ratio of wavelength and slit width becomes smaller [11]. Therefore, as can be seen in Fig. 6(a) the EIM curve slightly deviates from the MEM curve at shorter wavelengths. On the other hand, considering the feasibility of one mode approximation in the weak transverse scattering, we may as well use SPP modes to perform a modal calculation since MEM can provide more scattering information. Letting \(N = 1\) in Eq. (2), then the dispersion relation of the one mode MEM can be obtained analytically, which has the same expression as Eq. (5) but with \(\tilde{\varepsilon}[(p-1)] = \left(f_{11}[(p-1)]\right)^{-1}\) and \(\tilde{\varepsilon}[(p)] = \left(k_{11}[(p-1)]\right)^{-1}\). Since the effect of the transverse scattering is included in \(\tilde{\varepsilon}[(p-1)]\) and \(\tilde{\varepsilon}[(p)]\), compared to EIM results from Eq. (6),
the $N = 1$ MEM produces more accurate results, which also manifests that the PB structure in the dielectric modulation is mainly formed by the interference of forward and backward SPP modes. By the way, the slight deviation of EIM results from FDTD simulation has been mentioned in our previous work [20]. The discussion above provides a clear explanation of this deviation.

Next, we turn to discuss the PBG formation in the geometric modulation. In contrast to the dielectric modulation, the EIM is inappropriate for the geometric modulation since the slit widths in the unit cell are not the same. Then taking $k_x = 0$ to neglect the transverse scattering may result in imprecise results. Actually, for the given structural parameters in the present model, the effective refractive indexes in different layers are too close to form a PBG. On the other hand, as we have demonstrated in Ref. 11, in the geometric modulation the contributions from higher modes to the scattering cannot be neglected. Compared with the dielectric modulation, the transverse scattering here is stronger, which admits that one mode approximation is inapplicable. Thus in the following only the MEM is used to discuss the PBG formation in the cases of $f = 0.5$ and 0.1.

Fig. 7. Bloch wave vectors $k_B$ in the cases of (a) $f = 0.5$ and (b) $f = 0.1$ in the geometric modulation.

For the case of $f = 0.5$, Fig. 7(a) shows the convergence with the increasing modes, which manifests that the higher modes have more or less contributions to the PBG formation. The lower modes lay down the basic PB structure, and the higher modes “correct” it gradually.
Moreover, as can be seen from Fig. 7(a), the curves of $N = 1$ and $N = 2$ are almost identical, indicating that the second mode (the first anti-symmetric mode) has little contribution to the formation. This is because the necessary condition for a mode to participate in the PBG formation is to form a Bloch wave. For a narrower region with $w = 0.1\mu m$, all the higher modes are evanescent except the SPP mode; and $q = 0.5 \times 1\mu m = 0.5\mu m$ is a sufficiently long layer length for the higher modes to attenuate to negligible values. Therefore, all the anti-symmetric modes are forbidden by the narrower slit (Please keep in mind that the symmetric and anti-symmetric modes are decoupled in our symmetric model, which means the SPP mode cannot excite the anti-symmetric modes). The higher symmetric modes, although evanescent in the narrower slit, participate the scattering and “correct” the PBG formation since the boundary conditions demand the SPP mode to excite them for fulfilling the continuum at the waveguide junctures. For example, the third mode (the second symmetric mode) is excited and cause the big difference between the results of $N = 2$ (or $N = 1$) and $N = 3$, because the SPP mode only is insufficient to link smoothly the fields between the layer boundary. This point consists with the conclusion that the one mode approximation is inapplicable for the geometric modulation.

The curves of $f = 0.1$ shown in Fig. 7(b) are quite different from those in Fig. 7(a). The length of the narrower region is $q = 0.1 \times 1\mu m = 0.1\mu m$. Since it is too short, some higher modes may pass through this region in evanescent forms. Among all possible Bloch waves, only the one with the smallest positive $\text{Im}(k_B)$ can form the band (see the discussion about the selection of $k_B$ at the end of Sec. II). That is to say, at least one mode is able to propagate through the wider regions because the Bloch wave composed of evanescent waves in both layers cannot provide the smallest $|\text{Im}(k_B)|$. Apparently, the SPP modes satisfy this condition since they are able to propagate through both layers. The second mode becomes propagating when the wavelength is within $0.6 \sim 1.2\mu m$ as mentioned above. Thus when $\lambda > 1.2\mu m$ the anti-symmetric modes have no contribution to the PB structure; this is verified by Fig. 7(b) where the curves of $N = 1$ and 2 are identical when $\lambda > 1.2\mu m$. However, within the range $0.6 < \lambda < 1.2\mu m$ where the second mode could participate in forming the Bloch wave, the two curves are also basically identical. This is because the $\text{Im}(k_B)$ of the Bloch wave formed by the symmetric modes is smaller in this wavelength range. But around $\lambda = 0.77$ and $1.064\mu m$, the $\text{Im}(k_B)$ curve with $N = 2$ has dips while the $N = 1$ curve has not, so that these dips are mainly introduced by the second mode. The “correction” by the higher modes makes the $N = 80$ curve have abrupt changes around $\lambda = 0.81$ and $1.116\mu m$. Moreover, the comparison between the $\text{Im}(k_B)$ curves of $N = 1, 2$ and 3 reveals that the dips at $\lambda = 0.662$ and $0.690\mu m$ are mainly caused by the third mode. Our numerical calculations confirm that it needs up to $N = 5$ modes to determine the basic PB structure, and the details have to be “corrected” by the higher modes, which needs at least $N = 20$ modes to get trustworthy results.

5. Conclusion

In this paper, we have studied the optical properties of two BWG models. The band structure theory usually used in photonic crystals is applied to the BWGs. The fields are expanded by the eigenfunctions of the BWGs and related by the Bloch theorem, which can be called the periodic version of MEM. By this method, we investigated their optical properties in the near infrared range, including the PB structure, DOS, transmittance, slowdown factor, and propagation length. The contributions of eigenmodes to the PBG formation are analyzed.

So far, a class of technologies has been demonstrated to produce slow light [36], such as quantum interference effects or electromagnetically induced transparency, stimulated Brillouin scattering or stimulated Raman scattering, photonic crystal waveguides, and coupled resonance optical waveguides. However, only the subwavelength metal slit structures are able to make the devices as small as possible so as to easily integrate into the compact optical circuit. Further-
more, the introduction of periodical structures in the subwavelength slit generates the energy
gaps and smooth energy bands. Compared with the conventional plasmonic waveguides that
suffer from dispersion and losses [37-39], the BWG process PBGs and broad bands almost
without dispersion, which is very important for practical utilities.

For dielectric modulations, since the transverse scattering in a slit with an unvaried width
is weak, the contribution from the SPP modes is dominant, and those of the higher modes are
negligible. This one-mode-formed PB structure has a “regular pattern” in which the widths of
the bands and gaps become larger as the wavelength and filling factor increase. Therefore, one
can design narrow band multi-channel devices with small filling factors, or achieve broad bands
and gaps when the filling factor is large. For the model we studied, the slowdown factor in the
band is between $3 \sim 15$. A slowdown factor larger than 10 is observed at the band edge; while
near the band center, the slowdown factor and its variation become smaller so that the band is
flat. In short, when the filling factor is large a broad band is comparatively flat. The propagation
length here is mainly affected by the dielectric layers, since they have a larger absorption of
waves. When the dielectric layer gets longer the propagation length will become shorter. For
the mode with propagation length larger than $5 \mu m$, its slowdown factor is between $2 \sim 8$.

For geometric modulations, since the transverse scattering within the BGW is strong and
the contributions of higher modes are not negligible, the PB structure is not of the feature of
the “regular pattern” and the gap widths increase significantly, which provides us more spaces
to design flat bands and defect modes for controlling the output signal. “Local modes” that
have large DOS but small propagation length are observed. As for the slowdown factor and
propagation length, the conclusion with respect to the dielectric modulation is still suitable
here, but they are larger in magnitudes; especially at the band edges, the slowdown factor can
be nearly $\pm 100$ while the corresponding propagation length is comparatively shorter. For the
mode with propagation length larger than $5 \mu m$, its slowdown factor is between $3 \sim 15$.

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