Band structure of honeycomb photonic crystal slabs

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Two-dimensional (2D) honeycomb photonic crystals with cylinders and connecting walls have the potential to have a large full band gap. In experiments, 2D photonic crystals do not have an infinite height, and therefore, we investigate the effects of the thickness of the walls, the height of the slabs, and the type of the substrates on the photonic bands and gap maps of 2D honeycomb photonic crystal slabs. The band structures are calculated by the plane wave expansion method and the supercell approach. We find that the slab thickness is a key parameter affecting the band gap size, while on the other hand the wall thickness hardly affects the gap size. For symmetric photonic crystal slabs with lower dielectric claddings, the height of the slabs needs to be sufficiently large to maintain a band gap. For asymmetric claddings, the projected band diagrams are similar to that of symmetric slabs as long as the dielectric constants of the claddings do not differ greatly. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2194119]

I. INTRODUCTION

Photonic crystals have been a major research field for scientists and engineers, for their capabilities of controlling light propagation.[1] The pursuit of photonic band gaps has been a major topic in studying photonic band structure[2] because many applications of photonic crystals are based on photonic band gaps. In the band gap region, there are no optical modes and spontaneous emission. One can control the light propagation direction in the band gap more easily. That is why optimizing the size of the band gap is an interesting issue.

Chern *et al.* have recently proposed a two-dimensional (2D) honeycomb photonic crystal structure[3] (Fig. 1). The two-dimensional honeycomb photonic crystal without the walls and also its slab structure was reported earlier, in Refs. 1 and 4, respectively. There are two geometrical parameters in the two-dimensional honeycomb photonic crystal:[3] the radius of the cylinders and the thickness of the walls. The reasons to choose such a geometry are that the transverse magnetic (TM)-type band gaps are favored in an isolated high dielectric constant (ε) region and the transverse electric (TE)-type band gaps are favored in a connected lattice.[1] The cylinders are isolated dielectric medium units and the walls connect them. The full band gap can be optimized if we strike a balance between these two characteristics. Chern *et al.*[3] reported a largest full band gap of two-dimensional photonic crystals in the literature. Very recently, Fu *et al.*[5] have done some experiments on honeycomb photonic crystals. They found that the gap frequency and the gap-midgap ratio do not agree very well with the theoretical work of Chern *et al.* The underlying reasons still need further investigations.

Based on their studies, we have done some further calculations. The technique Chern *et al.* used is the finite difference multigrid method. We use plane wave expansion method as implemented in the MPB package.[6] Fully vectorial eigenmodes of Maxwell's equations with periodic boundary conditions were computed by conjugate-gradient minimization of the block Rayleigh quotient in a plane wave basis.[6] Since in experiments the photonic crystals do not have an infinite height, we investigate not only two-dimensional structures but also photonic crystal slabs. The hexagonal lattice slabs without the walls have already been studied before.[4,7] In our slab case we analyze the effects of the thickness of the walls and the height of the slabs. We also discuss the substrate impacts.

This paper is organized as follows. First, we will introduce the theoretical formulas about the theory and techniques used in our calculations, including the plane wave method, supercell technique, and the projected band diagram for photonic crystal slab calculations in the next section. Then we will present the results of our calculations for two-dimensional honeycomb photonic crystals, and honeycomb photonic crystal slabs in Sec. III. For two-dimensional systems, we will show the band structures and gap maps. For slab systems, we will show the band structures and discuss the geometric and substrate effects. Finally, we will make a brief summary of our work in Sec. IV.

II. COMPUTATIONAL METHOD

The band structures are calculated by plane wave expansion method, a frequency-domain method which expands the fields in the plane wave basis and directly solves the eigenstates and eigenvalues of Maxwell's equations, as implemented in the MPB package.[6] To analyze in an easier but exact way, we assume that light propagates in a linear, time-invariant, lossless, magnetic uniform material ($\mu=1$).

The slabs are not perfect three-dimensional photonic crystals since there is no periodicity in the z direction. We use the supercell method, which introduces defects periodically. Since the slabs are periodic only in the x-y plane, we add the original finite height cell with a sufficient amount of background region in the z direction. Now it is a three-dimensional case and takes a longer calculation time. If the

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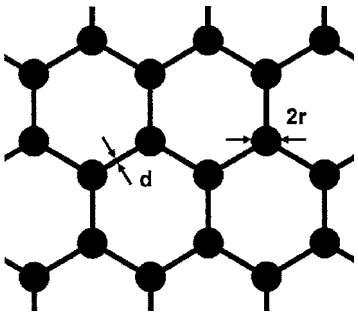

FIG. 1. The honeycomb structure: r is the radius of the cylinders and d is the thickness of the walls connecting the cylinders.

background region is large enough and the light is confined in the central region of the cell and far enough from the borders, the boundaries will not affect the result too much. In other words, this technique is very useful for the modes confined in the slab.[8]

For photonic crystal slabs, there is only two-dimensional periodicity in the x-y plane and the wave vectors are conserved in that plane, too. Since the wave vector in the z direction is not conserved, only the projected band diagrams on the plane will be plotted. That is, although we are investigating a three-dimensional system, our band structure only involves the k points in the x-y plane.

The light cone is an important feature of the projected band diagram. It is determined by the equation

$$\frac{\omega}{c} > \frac{k}{n_c}, \tag{1}$$

where n_c is the refractive index of the cladding. Equation (1) comes from the concept of total internal reflection. In the area below the light cone, light propagates within the slab. In the area in the light cone, light propagates outside the slab with a radiation loss.

In two dimensions, we always decompose the electromagnetic modes into two noninteracting modes: TE (polarization of electric field confined in the plane) and TM (polarization of magnetic field confined in the plane) mode. In slabs the modes are not purely TE or TM modes, but they can still be classified as vertically even or odd modes with respect to the horizontal symmetry plane bisecting the slab. The H_z component has a symmetrical field distribution for even modes and an asymmetrical field distribution for odd modes. Besides, for the first-order modes which have no node in the vertical direction, the field distributions within the core are very similar to the corresponding modes in infinite 2D photonic crystals. Moreover, in the mirror plane, the modes are purely TE (or TM) polarized. Therefore we can roughly regard even modes as being TE-like and odd modes as being TM-like.[9]

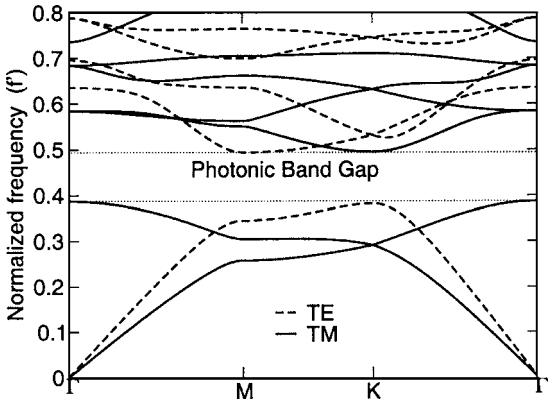

FIG. 2. Band structure for two-dimensional honeycomb photonic crystals with $\varepsilon/\varepsilon_0=13$, $r/a=0.155$, and $d/a=0.035$. The horizontal dotted lines denote the band gap region. The normalized frequency $f'=\omega a/2\pi c$.

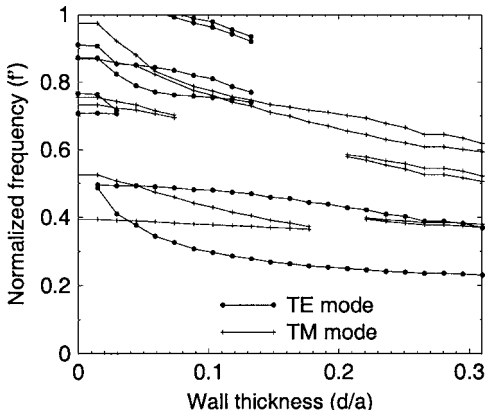

FIG. 3. Gap map for two-dimensional honeycomb photonic crystals with $\varepsilon/\varepsilon_0=13$ and $r/a=0.155$.

III. RESULTS AND DISCUSSION

A. Two-dimensional honeycomb photonic crystals

Figure 2 is the band structure of 2D honeycomb photonic crystals, calculated by plane wave expansion method. This figure agrees well with the results calculated by multigrid method (Fig. 4 in Ref. 3). Here normalized frequencies ($f'=\omega a/2\pi c$) and wave vectors are applied. From this figure we can see that for both TE and TM modes, no light within $f'=0.388$ to $f'=0.492$ are allowed in this structure. This means that there is a complete band gap in this system. We define a gap-midgap ratio (ratio between band gap width and midgap frequency) to measure how large the photonic band gap is. Even if the scale of the system is changed, this quantity remains the same.

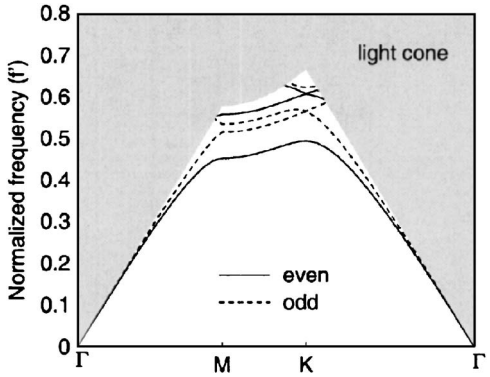

FIG. 4. Band structure for air-bridged honeycomb photonic slabs with $\varepsilon/\varepsilon_0=11.9$, $r/a=0.155$, $d/a=0.035$, and $h/a=0.4$.

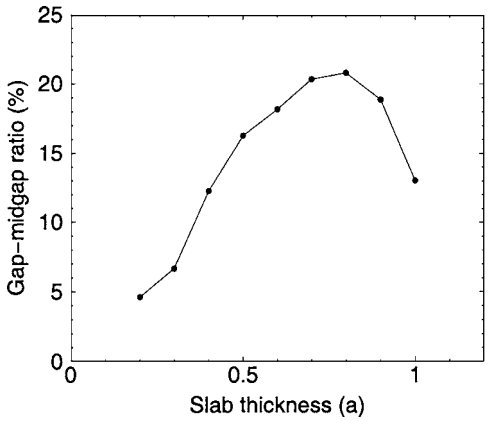

FIG. 5. Even mode gap size (as the percentage of midgap frequency) vs slab thickness of air-bridged honeycomb photonic slabs with $\varepsilon/\varepsilon_0=13$, $r/a=0.155$, and $d/a=0.035$.

We plot a gap map by plane wave method to see the effect of the wall thickness. Figure 3 is the relationship between gap-midgap ratio and wall width d (with fixed $r/a=0.155$). First, we notice that as d/a increases, the frequencies decrease. This is because of a larger dielectric fraction and average index.[1] Moreover, in some frequency ranges, the TE mode gaps and the TM mode gaps overlap with each other and form complete band gaps. Near $d/a=0.035$ the complete band gap is the largest. From gap map we can find out the optimal wall thickness easily.

B. Geometric effects on honeycomb photonic crystal slabs

Figure 4 shows the band structure of air-bridged honeycomb photonic crystal slabs. The slab thickness is one of the key parameters in determining the band gap size in photonic crystal slabs. For too thin slabs, the slabs do not provide sufficiently strong perturbation to the background. The modes can propagate outside the slabs easily and therefore the guided modes will be very close to the light cone. For too-thick slabs, higher-order modes with horizontal nodal planes lie slightly above the lowest-order mode because of a little more energy. Therefore no gaps exist.[7] Figure 5 shows

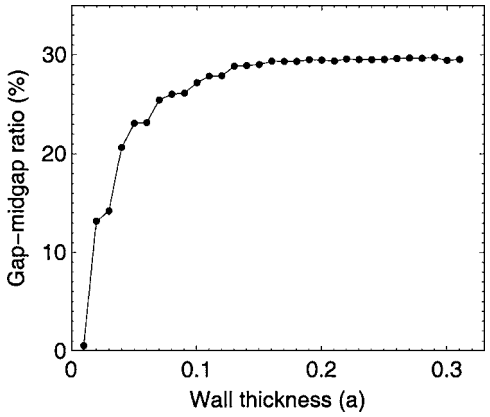

FIG. 6. Even mode gap size (as the percentage of midgap frequency) vs wall thickness for air-bridged honeycomb photonic slabs with $\varepsilon/\varepsilon_0=13$, $h/a=0.8$, and $r/a=0.155$.

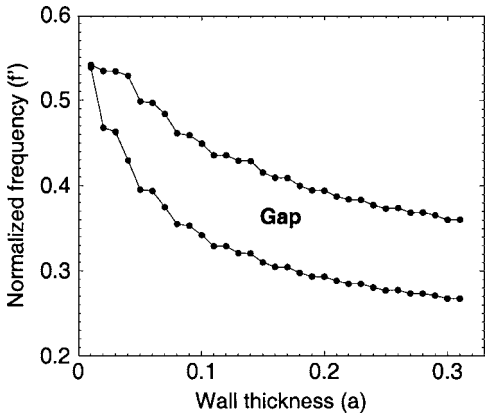

FIG. 7. Even mode gap map vs wall thickness for air-bridged honeycomb photonic crystal slabs with $\varepsilon/\varepsilon_0=13$, $h/a=0.8$, and $r/a=0.155$.

the gap size as a function of slab thickness. The gap-midgap ratio is optimized when the slab thickness is equal to $0.8a$.

Figure 6 is the gap size figure of honeycomb photonic crystal slabs and Fig. 7 is the gap map of various wall thicknesses of slab structures. It is noticeable that when the wall thickness is larger than $d/a=0.13$, the gap size remains the same while the frequency range of gap differs. We know that the key parameter affecting the band gap size is the slab thickness, not the wall thickness. This reveals that the tolerance of wall thickness fabrication can be very large. Band gap size is not sensitive to wall thickness. With the same gap size, we can obtain different band gap frequencies by tuning the wall thickness.

C. Substrate effects on honeycomb photonic crystal slabs

Both symmetric and asymmetric triangular lattices of circular air cylinders in dielectric slabs have been studied before.[7,10,11] Here we focus on honeycomb photonic crystal slabs. We consider two examples for symmetric photonic crystal slabs: air-bridged photonic crystal slabs and weak-confinement symmetric photonic crystal slabs.

Air-bridged photonic structures consist of a thin 2D photonic crystal in a high-index membrane (for example, silicon) surrounded by air [Fig. 8(a)]. Here the index contrast between the core and the cladding is very high so the light is strongly confined in the slab. However, it is not easy to integrate into a chip and this is the major disadvantage of this system.[12]

Figure 8(b) is an example of weak-confinement symmetric photonic crystal slabs. It consists of a silicon core and silicon dioxide claddings. If we compare Fig. 9 to Fig. 4, we can see that if we want to obtain the same order of band gap

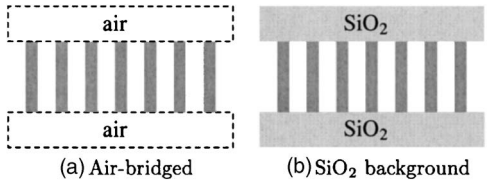

FIG. 8. Side view of symmetric photonic crystal slabs with $\varepsilon/\varepsilon_0=1$ for air and $\varepsilon/\varepsilon_0=2.1$ for SiO_2.

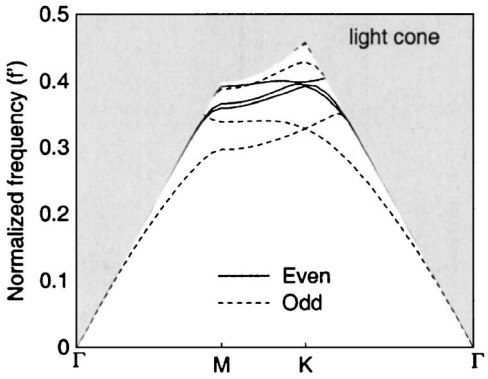

FIG. 9. Band structure of weak-confinement symmetric honeycomb photonic crystal slabs with $h/a=2.0$, $\varepsilon/\varepsilon_0=1$ for air, $\varepsilon/\varepsilon_0=2.1$ for SiO_2, and $\varepsilon/\varepsilon_0=11.9$ for silicon.

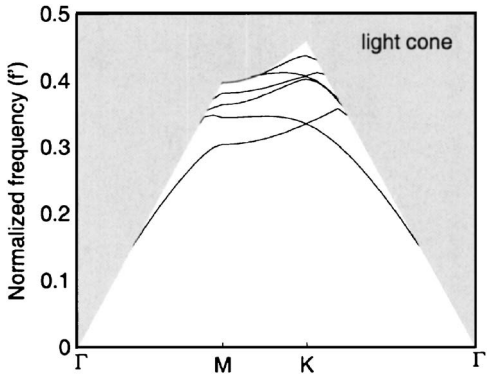

FIG. 11. The band structure of asymmetric honeycomb photonic crystal slabs with $h/a=2.0$, $\varepsilon/\varepsilon_0=1$ for air, $\varepsilon/\varepsilon_0=2.1$ for SiO_2, and $\varepsilon/\varepsilon_0=11.9$ for silicon.

size, the height of the structured slab should be larger. This is because with the same height of air-bridged structures, the perturbation photonic crystal provided is not strong enough and we will not obtain any band gap in this case. On the other hand, we should provide more perturbation to the background by adding the height of the slabs.

As for the asymmetric photonic crystal slabs, we consider the silicon-on-insulator (SOI) systems. In a SOI system, the lower cladding usually consists of an oxide layer and the upper cladding consists only of air (Fig. 10). This structure is easier to integrate onto a chip than a membrane, but the asymmetry of the structure leads to additional losses when ε of one of the claddings is lower.

Since the slab is not symmetric anymore, the modes cannot be identified as pure even or odd modes. But if we compare Fig. 11 to Fig. 9, we can see that although there are some slight differences, we can still distinguish them as evenlike or oddlike modes. The reason is that the $\varepsilon/\varepsilon_0$ of upper cladding does not vary a lot in these two cases. Therefore the modes do not vary very much in the symmetric [Fig. 8(b)] and asymmetric (Fig. 10) structures. The SOI system behaves in a way similar to the asymmetric one.

IV. CONCLUSIONS

Tuning the frequency range of photonic crystal band gap is a very important issue in photonic crystal applications. We have done further studies of the honeycomb photonic crystal that Chern *et al.* proposed in 2003. This structure has the potential of a large complete photonic band gap. Two geometric parameters, namely, the radius of the cylinders and the thickness of the walls, provide more flexibilities of designing photonic crystals. For two-dimensional honeycomb photonic crystals, we have calculated the gap map for both TM and TE modes and optimize the complete band gap. The band structure tells us that the complete band gap is large, as reported before.[3]

The main topic of this paper is, however, the photonic bands and gap maps of honeycomb photonic crystal slabs. For honeycomb photonic crystal slabs, projected band diagrams have been calculated. We focus on the guided modes below the light cone boundary. We find that the band gaps of two independent polarizations do not overlap with each other anymore. Our results show that the slab thickness is the key parameter of the band gap size and we have also determined the optimal slab thickness. On the other hand, the wall thickness does not affect the gap size very much. We obtain a saturated gap size when the wall thickness is above a certain value. This means that the tolerance for slab thickness fabrication is small, but large for wall thickness. We have also discussed about the effects of slab cladding, including the symmetric and asymmetric ones. For symmetric claddings, those slabs with weak-confinement claddings should be higher to provide stronger perturbation to the background. For asymmetric claddings, as long as the dielectric constants do not differ a lot, the guided modes are much like the modes of symmetric slabs. We can use the asymmetric slab structures instead of the symmetric ones since asymmetric structures are more commercially available.

In short, this work reveals various properties of honeycomb photonic crystal slabs. Hopefully, the optimized parameters would provide useful tips for experimentalists.

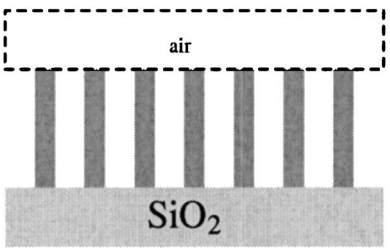

FIG. 10. Side view of a silicon-on-insulator system with $\varepsilon/\varepsilon_0=1$ for air and $\varepsilon/\varepsilon_0=2.1$ for SiO_2.

ACKNOWLEDGMENTS

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