Two-pattern compound photonic crystals with a large complete photonic band gap

Lin Jia1 and Edwin L. Thomas2,*

1Institute for Soldier Nanotechnologies, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139, USA
2Dean of Engineering, Rice University, P.O. Box 1892, Houston, Texas 77251, USA

(Received 13 June 2011; published 8 September 2011)

We present a set of two-dimensional aperiodic structures with a large complete photonic band gap (PBG), which are named two-pattern photonic crystals. By superposing two substructures without regard to registration, we designed six new aperiodic PBG structures having a complete PBG larger than 15% for \( \varepsilon_2 / \varepsilon_1 = 11.4 \). The rod-honeycomb two-pattern photonic crystal provides the largest complete PBG to date. An aperiodic structure becomes the champion structure with the largest PBG. Surprisingly, the TM and TE gaps of a two-pattern photonic crystal are much less interdependent than the PBGs of conventional photonic crystals proposed before, affording interesting capabilities for us to tune the TM and TE PBGs separately. By altering the respective substructures, optical devices for different polarizations (TE, TM, or both) can readily be designed.

DOI: 10.1103/PhysRevA.84.033810 PACS number(s): 42.70.Qs, 78.67.Pt, 07.05.Tp, 78.20.Bh

Photonic crystals, discovered in 1987 [1,2], have attracted great interest due to their ability to control the flow of light [3–12]. A large number of photonic band gap (PBG) structures have been developed during the past 20 years. Up to now, all PBG structures can be categorized into three types: periodic structures [1,13–24], quasicrystals (QCs) [25–27] (exhibiting higher rotational symmetries than consistent with conventional periodic lattices), and even disordered structures [28–30] with short-range order. The two-pattern photonic crystals reported here do not belong to any of these known categories and create a new fourth category: incommensurate compound crystals. Moreover, it is generally believed that high symmetry is a crucial ingredient in order to form a large PBG. The two-pattern photonic crystals exhibit an outstanding complete band gap but do not have global or even local symmetries. Physical insights to the PBG properties of these two-pattern photonic crystals are provided.

In our approach, we create a superior two-pattern photonic crystal by combining a TM substructure having discrete dielectric features that provide a large TM PBG with a TE substructure having expanded dielectric features chosen to provide a large TE PBG. The substructures can be periodic or aperiodic. Our concept is based on the rationale that the TE substructure of the two-pattern photonic crystal can be assumed to be a type of geometrical perturbation to the TM substructure and vice versa. A random perturbation of a given structure shrinks the size of the PBG, but generally, the PBG is more robust for an ordered perturbation [31]. If the TE substructure filling ratio is not high, the ordered geometrical perturbation does not strongly modify the TM PBG of the TM substructure. Furthermore, the small or zero TM PBG of the TE substructure has a trivial impact on the TM PBG of the two-pattern photonic crystal, which predominantly arises from the TM substructure. The reverse situation holds for the TE PBG of the two-pattern photonic crystal predominantly arising from the TE substructure. A two-pattern photonic crystal is composed of two superposed patterns, while previously reported photonic crystals are based on a single pattern. The TE and TM PBGs of two-pattern photonic crystals are much less interdependent than the PBGs of conventional photonic crystals. Importantly, by selectively creating defects in the different substructures, we can design photonic devices for particular polarizations (TM, TE, or both).

To analyze the PBG, we calculate the normalized density of states (DOS) via a finite-difference time-domain method [32,33]. We assign a radiating dipole near the middle of a large portion of the structure and provide a perfectly matched layer on the boundaries. Four hundred detectors are distributed near the boundary of the simulated area to collect the transmission spectra, which represents the DOS. The calculation results are tested for different radiating dipole positions and radiating sources of a group of random distributed dipoles.

In two dimensions (2D), the following factors define the two-pattern photonic crystal: the morphology, the filling ratios, and the relative scale, position, and orientation of the substructures. The first design factor is the morphology of the substructures. Here, it is desirable to select one structure with a large TE PBG but a trivial TM PBG and another structure with a large TM PBG but a trivial TE PBG. Throughout, we assume that the dielectric material is GaAs with a permittivity of 11.4. We pick three candidates for the TM PBG substructure: rods on a triangular lattice (R-p6mm), [see Fig. 1(a)], the current champion structure with the largest 47.3% TM PBG [34] and no TE PBG for the 0.1 filling ratio, rods on a square lattice (R-p4mm) [see Fig. 1(b)], 37.5% TM PBG and no TE PBG for the 0.15 filling ratio, and an eightfold QC of dielectric rods generated from hyperspace projection (QC-8mm) [see Fig. 1(c)], 42.1% TM PBG and no TE PBG for the \( r / a = 0.185 \), here \( r \) is the radius of the rods and \( a \) is the QC length parameter. The two candidates for the TE PBG substructure both have \( p6mm \) symmetry: the connected honeycomb (HC) structure (HC-p6mm) [see Fig. 1(d)], the current champion TE gap structure with the largest 42.5% TE PBG [35] and no TM PBG for the 0.189 filling ratio and circular rings (CRs) on a triangular lattice (CR-p6mm) [see Fig. 1(e)], 23.4% TE PBG and TM PBG less than 10% for the 0.11 filling ratio.

The second design factor is the relative length scale of the two substructures. If we tune the scale of the TE (TM)
FIG. 1. (Color online) The set of individual substructures and their corresponding PBGs (as indicated by the gray bands in the DOS plots). Three substructures with large TM PBG (rods on a triangular lattice, rods on a square lattice, and rods decorating an eightfold QC) are shown in (a)–(c). The filling ratios \( f \) of the substructures are dependent on \( r/a \), where \( r \) is the radius of the rods and \( a \) is the appropriate lattice parameter. Two substructures with large TE PBG (the HC structure and rings on a triangular lattice) are shown in (d) and (e) along with their corresponding DOS calculations.

FIG. 2. (Color online) Tuning the PBG by altering the relative scale of substructures. (a) Two-pattern photonic crystal from the R-\( p4mm \) + CR-\( p6mm \) substructures. (b) The DOS plot for \( a(TM)/a(TE) = 0.559 \). (c) The DOS plot for \( a(TM)/a(TE) = 0.656 \).
substructure, the position of the TE (TM) PBG is shifted accordingly. The central frequency of the TE (TM) PBG is proportional to $1/a$, here, $a$ is the characteristic scale of the substructure [6]. For the TM substructure consisting of rods, the TM gap mainly comes from Mie resonance. As we increase the scale of the substructure, the radius of the rods increases, which leads to a lower Mie resonance frequency and a lower central gap frequency. An example is shown in Fig. 2(a), made from the superposition of the R-$p4mm$ and CR-$p6mm$ crystals depicted in Figs. 1(b) and 1(e). The filling ratio of the TE substructure is 0.102, and the filling ratio of the TM substructure is 0.149. The DOS plot for $a$(TM)/$a$(TE) = 0.559 is shown in Fig. 2(b). Note that the TE PBG and the TM PBG barely overlap. To maximize the complete PBG, we increase the periodicity of the TM substructure to decrease the central frequency of the TM PBG. The tuning is continued until the TE PBG and the TM PBG fully overlap, which is shown in Fig. 2(c), leading to a complete PBG of 15%.

The third design factor is the individual substructure filling ratio. The filling ratio of each type of substructure controls the respective TE or TM gap but also modifies the strength of the ordered geometrical perturbation on the PBG of the other substructure. Therefore, altering the TE substructure, in general, can shrink the size of the TM PBG, and the shrinkage increases with the filling ratio of TE substructure while the reverse situation holds for varying the filling ratio of the TM substructure. Also, the above effect has been observed in a disordered system [30]. An example of the effect of the filling ratio on the band gap is evident from the superposition of the R-$p6mm$ and HC-$p6mm$ crystals shown in Fig. 3(a). In Fig. 3(b), we fix the filling ratio of the TM substructure at 8.6% and increase the filling ratio of the TE substructure. If the filling ratio of the TE substructure is too high (above 14%), the TM PBG is destroyed, and the complete PBG closes. If the filling ratio of the TE substructure is too low (below 3%), the TE PBG of the two-pattern photonic crystal is low or even closes, which obviously, also is obviously disadvantageous. Therefore, the filling ratios of the substructures need to be carefully adjusted to maximize the complete PBG. In Fig. 3(c), the TE PBG is smaller than the TM PBG, and the complete PBG size is determined by the TE PBG. To maximize the complete PBG, it is necessary to increase the TE PBG size. Therefore, we increase the filling ratio of the TE substructure. Although the TM PBG shrinks because of this tuning, as shown in Fig. 3(b), the complete PBG size increases. We increase the filling ratio until the TE PBG and TM PBG match, which is shown in Fig. 3(d). The complete PBG is maximized because, if the filling ratio of the TE substructure increases further, as shown in Fig. 3(e), the TM PBG is smaller than the TE PBG, and the complete PBG is determined by the TM PBG, which is relatively smaller than the complete PBG in Fig. 3(d).

The fourth and fifth design factors are the relative position and orientation of the substructures. Interestingly, it turns out that these factors essentially have no influence on the PBG since the changes in the relative location of the TE pattern, as an ordered geometrical perturbation for the TM pattern, should not substantially vary the TM PBG of the two-pattern photonic crystal with the same reasoning for the behavior of the TE PBG by the presence of the TM pattern. Therefore, the relative position and orientation of the TE and TM substructures only
FIG. 4. The PBG for the R-6mm + HC-6mm structure is robust for different superposition positions. (a) Four two-pattern photonic crystals corresponding to different relative positions of the substructures are shown. The relative position causes a trivial impact on the complete PBG, which is shown in (b).
cause a minor impact on the complete PBG, as confirmed in Figs. 4 and 5. The above fact is advantageous for the fabrication of the two-pattern photonic crystals because it is not necessary to precisely adjust the relative position or orientation of the two patterns.

Controlling electromagnetic waves at terahertz and gigahertz frequencies is important, and the fabrication of two-pattern photonic crystals at the associated length scales (micrometers and millimeters) is easy. Experimental techniques that can be used to fabricate two-pattern photonic crystals for the visible and near-IR frequency regimes include nanoimprint lithography [36], electron-beam lithography [37], and focused ion-beam lithography. The two-pattern photonic crystals are reasonably tolerant to possible experimental errors, including the variations of air gaps between dielectric regions. For example, for the structure shown in Fig. 6(a), we introduced a 40% random variation in the diameter of the rods \( r = r_0 + \Delta r_0 \), here \( \Delta r_0 \) is a random value in \([0.4r_0, 0.4r_0] \) and a 40% random variation in the thickness of the HC walls \( h = h_0 + \Delta h_0 \), here \( \Delta h_0 \) is a random value in \([0.4h_0, 0.4h_0] \), and the complete PBG is still large, 16%. Furthermore, we also introduced 30% random variation in the positions of the rods \( \mathbf{s} = \mathbf{s}_0 + \Delta \mathbf{s}_0 \), here \( |\Delta \mathbf{s}_0| \) is a random value in \([0.3a(TM), 0.3a(TM)] \), and the complete PBG is 15%.
FIG. 6. (Color online) Optimized two-pattern photonic crystals with large complete PBGs. (a) Champion structure based on the R-\( p6mm \) + HC-\( p6mm \) substructures with \( f(TE) = 0.086 \) and \( f(TM) = 0.086 \) and \( a(TM)/a(TE) = 0.7157 \). The discrete Fourier transform (DFT) of the two-pattern photonic crystal and the corresponding DOS calculation are shown below. (b) The two-pattern photonic crystal from the R-\( p4mm \) + HC-\( p6mm \) substructures with \( f(TE) = 0.08, f(TM) = 0.14, \) and \( a(TM)/a(TE) = 0.67 \). (c) The two-pattern photonic crystal from the QC-8\( mm \) + HC-\( p6mm \) substructures with \( f(TE) = 0.11 \) and \( r/a = 0.22 \). (d) The two-pattern photonic crystal from the R-\( p6mm \) + CR-\( p6mm \) substructures with \( f(TE) = 0.121, f(TM) = 0.102, \) and \( a(TM)/a(TE) = 0.7258 \). (e) The two-pattern photonic crystal from the R-\( p4mm \) + CR-\( p6mm \) substructures with \( f(TE) = 0.108, f(TM) = 0.149, \) and \( a(TM)/a(TE) = 0.6563 \). (f) The two-pattern photonic crystal from the QC-8\( mm \) + CR-\( p6mm \) substructures with \( f(TE) = 0.084 \) and \( r/a = 0.189 \).
For the three selected TE substructures and the two TM substructures shown in Fig. 1, six two-pattern photonic crystals can be constructed. For each combination, we maximize the complete PBG size by tuning the filling ratios and the relative scale of the substructures. The optimized structures with their DFTs and the associated DOS calculations are shown in Fig. 6. The six optimized two-pattern photonic crystals all have a complete PBG above 15%, although as composite structures, they do not possess any 2D symmetry. The aperiodic structure depicted in Fig. 6(a) has the best complete PBG (20.4%), which is highest reported complete PBG for 2D structures. Surprisingly, an aperiodic structure now becomes the champion PBG structure. The optimized structures generally have almost equal substructure filling ratios (around 0.1), and the length scales of the substructures need to be similar.

Because the TM and TE PBGs of the two-pattern photonic crystals each arise from one of the two patterns, by purposely introducing defects into the substructures, different types of photonic devices for different polarizations (TE, TM, or both) can readily be designed. For example, the waveguide in Fig. 7(a) is created by removing features from the TE substructure without modifying the TM substructure. This waveguide only allows the propagation of TE waves and stops the propagation of the TM waves. The waveguide in Fig. 7(c) is created by only removing features from the TM substructure, allowing the propagation of TM waves and stopping TE waves.

To summarize, a set of aperiodic PBG structures named two-pattern photonic crystals, consisting of two substructures, has been investigated. They do not belong to any of the known PBG structure categories and create a new category: incommensurate compound photonic crystals. Surprisingly, these new photonic crystals do not possess any symmetry, but they exhibit a large complete PBG. Our paper opens a wide range of future opportunities. First, a rich variety of different two-pattern photonic crystals can be developed using the large inventory of existing photonic crystals with sizable TM or TE gaps. We anticipate that our method will become a useful tool for designing photonic crystals with large complete PBGs, which is essential for the associated photonic devices. Second, our paper shows that the impact of symmetry on the PBG needs further investigation. Here, we show that structures without any global crystallographic symmetry can have a complete PBG size larger than any of the present highly symmetric 2D photonic crystals or QCs. Finally, we demonstrate that the TE and TM PBGs of a two-pattern photonic crystal can be tuned much more independently than conventional photonic crystals. By introducing defects into the substructures, photonic devices for TM and TE polarizations can be realized to achieve functionality not possible or highly challenging for conventional photonic crystal devices.

We thank Professors J. Joannopoulos, E. Yablonovitch, L. Kimerling, S. Johnson, and Dr. M. Maldovan for their helpful
advice. This research is partially supported by the U.S. Army Research Office through the Institute for Soldier Nanotechnologies under Contract No. W911NF-07-D-0004 and by the National Science Foundation Grant No. DMR 0804449.