Band-gap engineering in two-dimensional semiconductor-dielectric photonic crystals

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This paper reports the multiple band gaps in the two-dimensional semiconductor-dielectric photonic crystals of several compositions: semiconductor cylinders in the dielectric background. We consider both square lattice and hexagonal lattice arrangements and compute extensive band structures using a plane-wave method within the framework of an efficient standard eigenvalue problem for both *E* and *H* polarizations. The whole range of filling fraction has been explored to claim the existence of the lowest (the so-called acoustic) band gap and multiple higher-energy band gaps within the first 30 to 40 bands for various compositions. Such semiconductor-dielectric photonic crystals which are shown to possess huge lowest band gaps below a threshold frequency (the plasma frequency ω_p) have an advantage over the dielectric photonic crystals in the emerging technology based on the photonic crystals.

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Once in a while a research topic emerges that has a universal appeal. Such has been the case with the photonic crystals discovered in 1987. An architecural proposal of Yablonovitch [1] and a conceptual hypothesis of John [2] triggered the primary interest in photonic crystals. These are the periodic dielectric structures that (can) exhibit a photonic band gap (PBG) similar to the electronic band gap in conventional semiconductor crystals that lies at the heart of silicon technology. Since all the prominent phenomena emerging from photonic crystals, such as inhibition and/or prohibition of spontaneous emission, the formation of the localized states of light, and photon-atom bound states are all consequences of the existence of a photonic band gap, much of the research efforts has been dedicated to the search for such photonic crystals [3–13].

At the outset, it is interesting to remark that in all *artificial* periodic structures the existence of complete gaps is attributed to the joint effect of the Bragg diffraction and the Mie scattering. The destructive interference due to Bragg diffraction accompanied by the Mie resonances due to strong scattering from individual scatterer is the conceptual base of a complete gap. The latter becomes effective when the dimension of the scatterer is close to an integer multiple of wavelength [3]. A complete gap is, by definition, the one that persists independent of the direction of propagation and of the polarization of the wave. However, if the separability of the *z* (or *E*-polarized) and *x*-*y* (or *H*-polarized) modes is legitimate, as is the case with the two-dimensional (2D) PBG crystals, the term *absolute* is preferred to *complete*, just to avoid the confusion. Such a separation of the *E*- and *H*-polarized modes suggests an application as a polarization filter [3].

In order to realize the potential of truly photonic crystals as much as possible, Noda *et al.* [14] have reported a list of bona fide requirements. In the recent past, although several viable approaches, such as woodpile structure [5], 3D wire mesh [6,7], and stack-of-logs structure [14], have been proposed and investigated to design the 3D PBG crystals, it is considered exceedingly difficult for these methods to satisfy the requirements proposed in Ref. [14]. In contrast, it has been argued [4,8,9,12,15] that it is much easier to fabricate 2D PBG structures to meet the said requirements.

In this work, we consider a 2D periodic system of semiconductor cylinders embedded in a dielectric background. The cross sections of these cylinders are considered to be much larger than the de Broglie wavelength, so as to neglect the quantum-size effects. We consider both square and hexagonal arrangements and compute extensive band strcutures using augmented-block-matrix method (ABM) [15], which provides the framework of an efficient standard eigenvalue problem for both *E* and *H* polarizations on equal footing. We use the local (plasma) theory and neglect the damping effects and hence ignore the absorption. In the state-of-the-art high-quality semiconducting systems available, this is deemed to be quite a reasonable approximation. Thus, our purpose is to compute the band structures of neat and clean 2D binary periodic semiconductor-dielectric composites for legitimately separable *E* and *H* polarizations.

The present work was spurred not only by Ref. [14] but also by the recent upsurge in the design of the PBG crystals made up of the material media with *negative* effective permittvity ϵ_{eff} and permeability μ_{eff} [16]. In the nonmagnetic materials, as is the case here, we encounter at least the negative effective permittivity, while working within the local plasma theory. It so happens that as long as the actual frequency $\omega < \omega_p$, the so-called effective permittivity remains negative. This has an interesting consequence of opening up the huge lowest (the so-called acoustic) band gap (with gap to midgap ratio >1) in the semiconductor (or metal)-dielectric PBG crystals.

For the purpose of numerical computation, we specify the semiconductor-dielectric composite to be made up of doped-GaAs cylinders embedded in vacuum background. This implies that $\epsilon_L = 12.8$ (1.0) for doped GaAs (vacuum). As such the only other parameter needed to accomplish the computation is the dimensionless plasma frequency $\Omega_p = (a/2\pi c)\omega_p$; we choose to work with $\Omega_p = 0.5$ throughout. For the sake of consistency, the same set of material parameters was used for all the numerical examples presented in this work, irrespec-

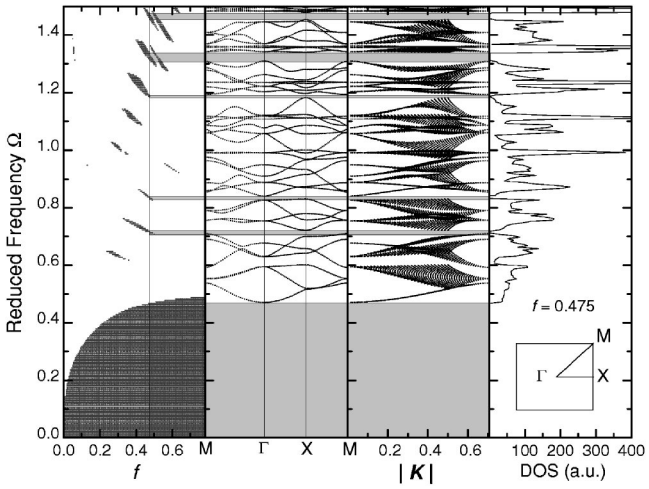

FIG. 1. Full spectrum of the multiple gap windows as a function of filling fraction, the band structure in the principle symmetry directions, the band structure in the *whole* irreducible part of the first Brillouin zone (the triangle ΓXM), and the density of states, respectively, in the first, second, third, and fourth panel, counting from the left, for the doped GaAs cylinders in vacuum background for E polarization for a square lattice. The filling fraction for the second, third, and fourth panels is $f=47.5\%$.

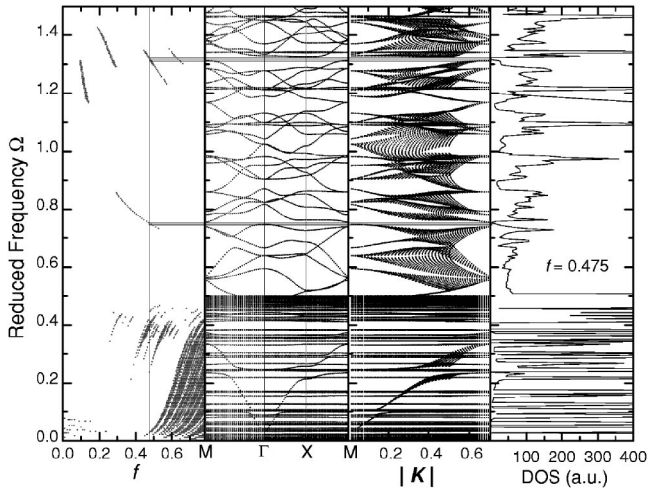

FIG. 2. The same as in Fig. 1 but for the doped GaAs cylinders in vacuum background for the H polarization.

tive of the geometry, the composition, and/or the polarization.

The quadripartite in Fig. 1 illustrates the full spectrum of the multiple gaps for the doped GaAs cylinders in vacuum for the E polarization. The plots are rendered in terms of dimensionless frequency Ω and Bloch vector $\vec{k}$. The frequency range $0 \leqslant \Omega \leqslant 1.5$ here covers in total 41 bands. The leftmost panel of the quadripartite, which is the most complete illustration of the existence of the gap windows, shows that there are at least 13 clearly visible gap windows, including the huge lowest (acoustic) band gap, within the whole range of filling fraction ($0 \leqslant f \leqslant f_c$). Notice that the lowest gap increases with increasing filling fraction, up to the close packing. The five of these higher-energy gaps (the shaded regions) occur at $f=47.5\%$, marked by a thin vertical line in the leftmost panel. The four parts of the quadripartite together demonstrate clearly that there are, indeed, six full gaps within the frequency range $0 \leqslant \Omega \leqslant 1.5$ at $f=47.5\%$ and we consider such calculations as essential. The lowest acoustic band gap (which is also the widest one) extends in the frequency range defined by $0 \leqslant \Omega \leqslant 0.465$ at $f=47.5\%$. The existence of this lowest gap is exclusively attributed to the semiconductor (or metal) inclusions characterized by the plasma frequency Ω_p. Notice that, whether or not the higher energy gaps exist, the lowest acoustic gap below Ω_p always persists.

The quadripartite in Fig. 2 shows a full spectrum of the multiple band gaps for the doped GaAs cylinders in vacuum for the H polarization. In the H polarization, there are at least five gap windows, above the plasma frequency Ω_p, within the first 38 bands occurring in the frequency range $0 \leqslant \Omega \leqslant 1.5$ (see the leftmost panel). At the filling fraction $f=47.5\%$, there are two full higher-energy gaps (the shaded regions) above Ω_p shared by all the four panels. A striking feature of the photonic band structure for the H polarization is the presence, in the frequency range $0 \leqslant \Omega \leqslant \Omega_p$ in which $\epsilon(\omega) < 0$, of a large number of very flat, almost dispersionless bands. This is clearly visible within the second, third, and fourth panels just below Ω_p and also correspondingly reflected in the leftmost panel. However, even within this congested part of the flat bands, there may occur some gaps; see, for instance, the gap centered at $\Omega \simeq 0.39$ existing at $f=47.5\%$ and shared by all the right panels. The number of these flat bands increases with increasing f. As the number of plane waves is increased, the flat bands start shifting upward and getting accumulated in the vicinity of the plasma frequency thereby giving rise to the lowest (acoustic) gap similar to that for the E polarization. This then requires dealing with higher-order matrices and hence a huge computational time, however.

Even though the polarization of the plasma wave into z and x-y modes is quite legitimate in the 2D PBG crystals, we explored extensively the possibility of the existence of a *complete* gap. To this end, we found that for such isotropic, semiconductor-dielectric 2D PBG crystals, it is only the second (counting from the top) gap for the E polarization in Fig. 1 that overlaps with the highest gap for the H polarization in Fig. 2, for $f=47.5\%$. This is shown in Fig. 3 where the highest gap of Fig. 2 (light gray region) lies within the next-to-highest gap of Fig. 1 (dark gray region). Thus Fig. 3 substantiates that the highest gap in Fig. 2 is a *complete* gap, which survives independent of the polarization and of the direction of propagation. We stress that we did not find any other *complete* gap for any other composition for the square geometry.

The quadripartite in Fig. 4 shows the complete spectrum of the multiple gaps for the doped GaAs cylinders in vacuum for the E polarization. There are 39 bands within the frequency range $0 \leqslant \Omega \leqslant 1.5$. The leftmost panel shows clearly visible more than ten gap windows within the whole range of filling fraction ($0 \leqslant f \leqslant f_c$). Eight of these band gaps (the shaded regions) are seen to occur at the filling fraction $f=52.5\%$, marked by a thin vertical line in the leftmost panel. The four parts of the quadripartite together demonstrate that

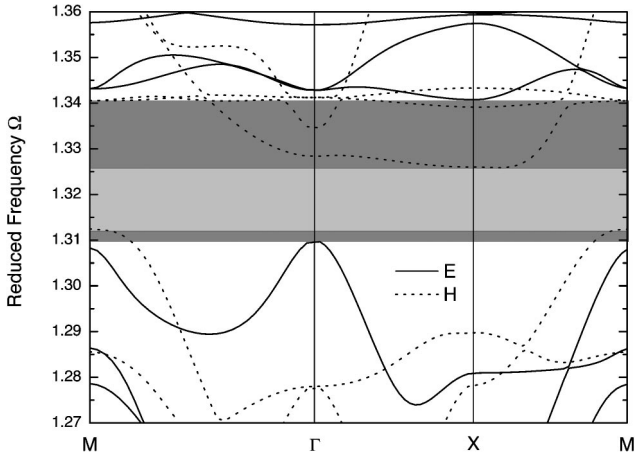

FIG. 3. Demonstration that it is only the highest gap (light gray region) for the *H* polarization in Fig. 2 that lies within the second (counting from the top) gap (dark gray region) for the *E* polarization in Fig. 1, for $f=47.5\%$. Thus the highest gap of Fig. 2 is the only *complete* gap for the doped GaAs cylinders in vacuum background for a square lattice, within the window $0 \leqslant \Omega \leqslant 1.5$.

there are, indeed, eight full gaps within the frequency range $0 \leqslant \Omega \leqslant 1.5$ at $f=52.5\%$. The lowest acoustic band gap extends in the frequency range defined by $0 \leqslant \Omega \leqslant 0.48$ at $f=52.5\%$. Contrary to the results depicted in Fig. 1, the lowest acoustic gap is always accompanied by the higher (and wider) energy gaps, for almost all values of f, except for $0.70 \lesssim f \lesssim 0.15$. From this point of view, the hexagonal geometry is deemed to be advantageous over the square one.

The quadripartite in Fig. 5 depicts the complete spectrum of the multiple gaps for the doped GaAs cylinders in vacuum for the *H* polarization. In this case the frequency range $0 \leqslant \Omega \leqslant 1.5$ covers almost 37 bands and there are at least 3

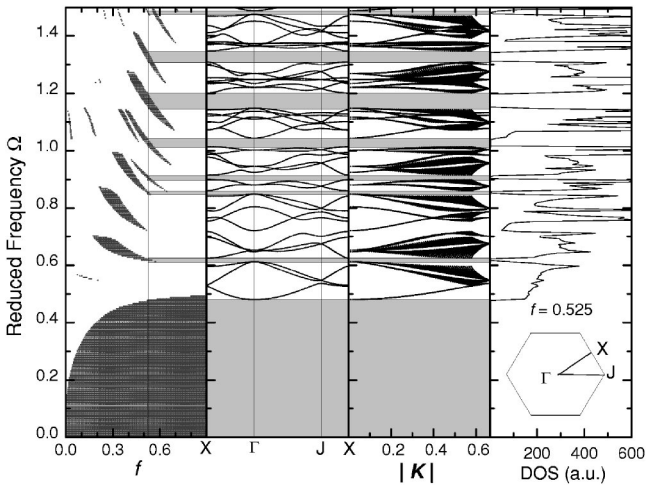

FIG. 4. Full spectrum of the multiple gap windows as a function of filling fraction, the band structure in the principle symmetry directions, the band strcuture in the *whole* irreducibe part of the first Brillouin zone (the triangle ΓJX), and the density of states, respectively, in the first, second, third, and fourth panel, counting from the left, for the doped GaAs cylinders in vacuum background for the *E* polarization for a hexagonal lattice. The filling fraction for the second, third, and fourth panels is $f=52.5\%$.

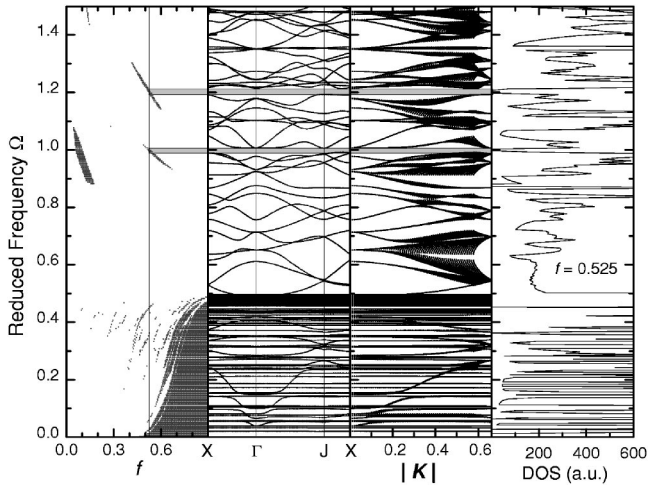

FIG. 5. The same as in Fig. 4 but for the doped GaAs cylinders in vacuum background for the *H* polarization.

clearly visible higher-energy gap windows (see the left-most panel) above the plasma frequency Ω_p. Note that there is no higher-energy gap-window opening up for $f \gtrsim 65\%$. Unlike the square lattice (see Fig. 2), there are no appreciable gaps within the flat bands below Ω_p. At $f=52.5\%$, there are two full gaps (the shaded regions) shared by all the four panels and hence both of these are, indeed, absolute gaps persisting independent of the direction of propagation. The top of the flat-band region containing pseudogaps is seen to become more and more congested with increasing f thereby turning the pseudogaps into absolute ones as discussed in relation with Fig. 2. The pseudogaps are characterized by the (i) low density of states and/or (ii) small but nonzero transmission coefficient; and they are mostly direction dependent (i.e., they may exist in one direction but not in the other).

Extensive efforts made to search a *complete* gap in the

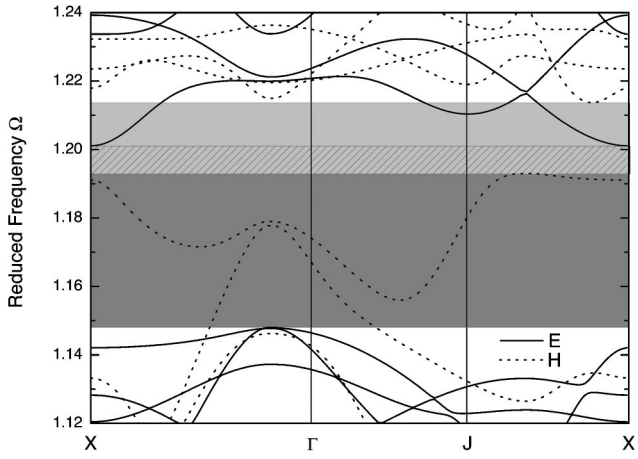

FIG. 6. Demonstration that it is only the highest gap (light gray region) for the *H* polarization in Fig. 6 that slightly overlaps with the third (counting from the top) gap (dark gray region) for the *E* polarization in Fig. 5, for $f=52.5\%$. The hatched region represents the only *complete* gap for the doped GaAs cylinders in vacuum background for a hexagonal lattice, within the window $0 \leqslant \Omega \leqslant 1.5$.

hexagonal geometry led us to find that it is only the third (counting from the top) gap for the *E* polarization in Fig. 4 that slightly overlaps with the highest gap for the *H* polarization in Fig. 5 for $f=52.5\%$. This is shown in Fig. 6 where the lower part of highest gap of Fig. 5 (light gray region) overlaps with the upper part of the third next-to-highest gap of Fig. 4 (dark gray region). Thus the hatched region indicates the *complete* gap that persists independent of the polarization and of the direction of propagation. Again, we stress that for the set of material parameters used here no other *complete* gap was found for any other composition for the hexagonal geometry.

In summary, we have demonstrated that the 2D periodic semiconductor-dielectric PBG crystals can give rise to multiple *absolute* photonic band gaps for both (*E* and *H*) polarizations. In principle, the band structures computed separately for the two polarizations should be superimposed to check and claim whether or not the band gaps are *complete*. The extensive efforts made in the search for such *complete* gaps led us to infer that only a *single* small *complete* gap can exist for a specific filling fraction that is independent of the polarization in both geometries (see Figs. 3 and 6). However, the legitimacy of the polarization of the plasma wave (into *E* and *H*) in such 2D PBG crystals implies that both *z* and $x-y$ modes can be excited independently of each other; and hence the *absolute* gaps demonstrated for each polarization make sense.

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