Band-gap engineering in two-dimensional periodic photonic crystals

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Abstract

A theoretical investigation is made of the dispersion characteristics of plasmons in a two-dimensional periodic system of semiconductor (dielectric) cylinders embedded in a dielectric (semiconductor) background. We consider both square and hexagonal arrangements and calculate extensive band structures for plasmons using a plane-wave method within the framework of a local theory. It is found that such a system of semiconductor-dielectric composite can give rise to huge full band gaps (with a gap to midgap ratio $\approx 2$) within which plasmon propagation is forbidden. The most interesting aspect of this investigation is the huge lowest gap occurring below a threshold frequency and extending up to zero. The maximum magnitude of this gap is defined by the plasmon frequency of the inclusions or the background as the case may be. In general we find that greater the dielectric (and plasmon frequency) mismatch, the larger this lowest band-gap. Whether or not some higher energy gaps appear, the lowest gap is always seen to exist over the whole range of filling fraction in both geometries. Just like photonic and phononic band-gap crystals, semiconducting band-gap crystals should have important consequences for designing useful semiconductor devices in solid state plasmas.
I. INTRODUCTION

Ever since the discovery of quantum Hall effect, the investigation of electronic transport in the low-dimensional systems has witnessed many important and fascinating results, both theoretical and experimental\(^1\). The ever increasing interest in these systems is attributed partly to advancement in the modern semiconductor technology (e.g., molecular beam epitaxy and electronic beam lithography) that makes it possible to fabricate the nanostructures with controllable chemical composition and geometric structures\(^2\)— quantum-wells, -wires, -dots, -rings, -crossbars, -balls are a few to name. The keystone behind the intense research interest in such systems world-wide is essentially the fact that their dimension(s) are (or have to be) comparable to the de Broglie wavelength, so as to observe the quantum-size effects.

Many novel discoveries in physics have originated from the study of wave propagation in periodic structures. Examples include x-ray and electron diffraction by crystals, electronic band structure, Bloch oscillator, and holography. Analogies between subfields of physics have also opened amazingly new fruitful avenues in research. An exciting example is the recent discovery\(^3\) of periodic dielectric structures that exhibit what is called ”photonic band gap”, by analogy with the electronic band gap in semiconductor crystals. Photons within the frequency range of the gaps are completely forbidden, so that atoms in such materials are denied to spontaneously absorb and re-emit light in this region; this has obvious implications for highly efficient lasers. Since the interesting phenomena emerging from photonic band gap structures, such as the inhibition/prohibition of spontaneous emission, the formation of localized states of light, and the photon-atom bound states, are all the consequences of the existence of the gap(s), a major part of research efforts has concentrated on the search for such photonic crystals. Within almost a decade the field has prospered much more than Eli Yablonovitch and Sajeev John could have imagined\(^4\).

It did not take long before photonic crystals aroused interest in the analogous studies in other systems as well; we refer to the ones allowing, for example, elastic/acoustic waves\(^5\), and spin waves\(^6\). The composite sytems exhibiting complete or pseudogaps, within which the respective waves are forbidden, are useful both from the practical and fundamental point of view. From the practical point of view, such systems can be used to design the filters that prohibit the propagation of respective waves at certain frequencies while allowing free propagation at others.
From the fundamental point of view, the propagation of such waves in a slightly disordered composite system can lead to the novel phenomenon concerned with the Anderson localization. It is noteworthy that the authentic seeds of classical wave localization were disseminated in a classic paper by Sajeev John in 1984\(^7\). A systematic account of the theoretical and experimental work on electronic-, phononic-, photonic-, and vibrational-band gap crystals is given in an extensive review article by the author\(^4\).

In this work we are concerned with a two-dimensional (2D) periodic system of semiconducting (dielectric) cylinders embedded in a dielectric (semiconductor) background. In fact, it could be considered a bulk-mass of semiconductor with periodically punched infinitely long thin holes. The cross-sections of these cylinders (or punched holes) are considered to be much less than the de Broglie wavelength, so as to neglect the quantum-size effects. We believe that such geometric structures should be easily realizable through the aforesaid nanostructure growth techniques. Our principal interest is the prospect of achieving a complete plasmonic band gap (PBG); this is defined to be a stop band within which the plasmon propagation is prohibited irrespective of the direction of propagation and of the polarization of the plasma wave. The existence of PBG in such composites should have important consequences for designing filters for the plasma waves and for the fundamental physics interest associated with the Anderson localization thereof. In fact, the possibility of experimental realization of the Anderson localization of plasma waves in random and incommensurate layered systems was predicted almost a decade ago\(^8\).

It is noteworthy that our model theory is based on the full vectorial Maxwell’s equations. We also consider an applied magnetostatic filed oriented parallel to the axis of the cylinders (which is taken to be the z-axis). In order to calculate the band structure of such a binary composite, we employ a plane-wave method and Fourier-series-expansion of the position-dependent material parameters. It should thus be pointed out that we do not make use of any messy electromagnetic boundary conditions usually employed for inhomogeneous systems. The semiconductor medium in the inclusions and/or background is characterized by the frequency-dependent (local) dielectric function. The first hand effort of using local theory for photonic crystals has been made in the recent past\(^9\). We neglect the damping effects and hence ignore the absorption. In the state-of-the-art high quality semiconductor systems available, this is thought to be quite a reasonable approximation. Thus our purpose is to calculate the band structure of a neat and clean 2D periodic binary semiconductor-dielectric composites.
A number of investigators have calculated such dispersion characteristics of 1D periodic systems (superlattices, for example) both with and without an applied magnetic field\textsuperscript{10–12}. However, no one, to our knowledge, has ever embarked on the possibility of observing complete band gaps in the systems considered. The authors were, most of the time, interested in reporting the physical conditions leading to the existence of the bulk bands and the surface plasmons or magnetoplasmons in the infinite and semi-infinite superlattice systems. This seems to be true irrespective of the systems (compositional or doping (n-i-p-i) superlattices) considered, methodology (classical or quantal) employed, and the orientation of the magnetic field (Voigt-, perpendicular-, or Faraday-geometry) pondered. The same remark is valid for the work on the 1D lateral (quantum wire) superlattices\textsuperscript{13–14}.

The rest of the paper is designed as follows. In Sec. II we derive the secular equations required to compute the plasmon band structures of the 2D binary semiconductor composites. The extensive numerical computational results are discussed in Sec. III. This includes results both on square and hexagonal arrangements. A brief summary in Sec. IV concludes our finding in this paper.

II. METHODOLOGICAL DETAILS

We consider a 2D periodic system of semiconducting cylinders embedded in a different semiconducting background. For the sake of generality, we consider both cylindrical inclusions and the background materials to be semiconductors to be characterized by the frequency-dependent (local) dielectric functions. An external magnetostatic field ($\vec{B}_o$) is assumed to be oriented along the axis ($\hat{z}$) of the cylinders. We are interested in the nonmagnetic materials, which implies that $\vec{B} \equiv \vec{H}$ in the Maxwell equations. In the situation at hand ($\vec{B}_o \parallel \hat{z}$), the dielectric tensor $\tilde{\epsilon}$ is simplified by the symmetry requirements such that: $\epsilon_{xx} = \epsilon_{yy}$, $\epsilon_{yx} = -\epsilon_{xy}$, and $\epsilon_{zx} = \epsilon_{xz} = \epsilon_{zy} = \epsilon_{yz} = 0$.

We start with full vectorial Maxwell’s curl field equations. After eliminating the magnetic field variable $\vec{B}$, we obtain the following wave field equation for the macroscopic electric field vector($\vec{E}$):

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{E}) - q_0^2 \tilde{\epsilon} \cdot \vec{E} = 0$$ (1)
where $\tilde{\epsilon}$ is a $3 \times 3$ matrix and $q_0 = \omega/c$ is the vacuum vector; $c$ being the speed of light in vacuum and $\omega$ is the angular frequency of the wave. Eq. (1) can be written in the matrix form as follows:

$$
\begin{bmatrix}
q_0^2 \epsilon_{xx} + \partial_y^2 + \partial_z^2 & q_0^2 - \partial_x \partial_y & -\partial_x \partial_z \\
-q_0^2 \epsilon_{xy} - \partial_y \partial_x & q_0^2 \epsilon_{xx} + \partial_z^2 & -\partial_y \partial_z \\
-\partial_z \partial_x & -\partial_z \partial_y & q_0^2 \epsilon_{zz} - \partial_x^2 + \partial_y^2
\end{bmatrix}
\begin{bmatrix}
E_x \\
E_y \\
E_z
\end{bmatrix} =
\begin{bmatrix}
0 \\
0 \\
0
\end{bmatrix}
$$

(2)

Here $\partial_z \equiv \partial/\partial z$, etc. Eq. (2) can be solved for three different situations: (i) $k_z = 0$, and $\vec{k} \parallel \neq 0$; (ii) $k_z \neq 0$ and $\vec{k} \parallel = 0$; and (iii) $k_z \neq 0$ and $\vec{k} \parallel \neq 0$. We are here interested in the first case — with $k_z = 0$ but $\vec{k} \parallel \neq 0$. Here $\vec{k} \parallel$ is the 2D Bloch vector and $k_z$ is the $\hat{z}$-component of the propagation vector.

As such, eq. (2) splits in two independent sets of equations (with $k_z = 0$):

$$
\nabla^2 E_z + q_0^2 \epsilon_{zz} E_z = 0
$$

(3)

and

$$
(q_0^2 \epsilon_{xx} + \partial_y^2) E_x + (q_0^2 \epsilon_{xy} - \partial_x \partial_y) E_y = 0
$$

(4.1)

$$
(-q_0^2 \epsilon_{xy} - \partial_y \partial_x) E_x + (q_0^2 \epsilon_{xx} + \partial_z^2) E_y = 0
$$

(4.2)

where $\epsilon_{ij}$ are all functions of position. Evidently, eq. (3) represents the propagation of the plasma waves which remain independent of the magnetic field; whereas the set of eqs. (4) refers to the magnetoplasma waves. We will therefore derive two independent secular equations corresponding to the two situations. It is, however, noteworthy that both equations (3) and (4) are valid for arbitrary inhomogeneity.

2.1. Magnetic-field-independent waves

Here we are concerned with the plasma waves governed by eq. (3). We focus our attention on an inhomogeneous medium which exhibits spatial periodicity. That means that the position-dependent material parameters $\epsilon_{zz}(\vec{r})$ may be expanded in the Fourier series. We write

$$
\epsilon_{zz}(\vec{r}) = \sum_{\vec{G}} \epsilon_{zz}(\vec{G}) e^{i\vec{G} \cdot \vec{r}}
$$

(5)
where $\vec{G}$ is the reciprocal lattice vector that has the corresponding dimensionality. The $z$-component of the field vector must satisfy the Bloch theorem:

$$E_z(\vec{r},t) = e^{i(\vec{K} \cdot \vec{r} - \omega t)} \sum_{\vec{G}} E_z(\vec{G}) e^{i\vec{G} \cdot \vec{r}}$$  \hspace{1cm} (6)

Equations (5) and (6) must be substituted in eq. (3). A straightforward algebra, then multiplying the whole equation by $\exp(-i\vec{G} \cdot \vec{r})$, and integrating over the unit cell yields the following result:

$$\sum_{\vec{G}'} q_0^2 \epsilon_{zz}(\vec{G} - \vec{G}') E_z(\vec{G}') - |\vec{K} + \vec{G}|^2 E_z(\vec{G}) = 0.$$  \hspace{1cm} (7)

For binary composites every unit cell is composed of only two materials — inclusions (i) and background (b) characterized by $\epsilon_{zz}^i$ and $\epsilon_{zz}^b$. In addition, we must specify the filling fraction $f$ and $(1 - f)$, respectively, for materials $i$ and $b$. We consider $\epsilon_{zz}$ to be given by

$$\epsilon_{zz}(\vec{G}) = \begin{cases} 
\epsilon_{zz}^i f + \epsilon_{zz}^b (1 - f) \equiv \bar{\epsilon}_{zz} , & \text{for } \vec{G} = 0 \\
(\epsilon_{zz}^i - \epsilon_{zz}^b)F(\vec{G}) \equiv \Delta\epsilon_{zz} F(\vec{G}) , & \text{for } \vec{G} \neq 0 
\end{cases}$$  \hspace{1cm} (9)

where the structure factor $F(\vec{G})$ is defined as

$$F(\vec{G}) = \frac{1}{A_c} \int d^2 r e^{-i\vec{G} \cdot \vec{r}} = 2f J_1(Gr_0)/(Gr_0)$$  \hspace{1cm} (10)

where $J_1(x)$ is the Bessel function of the first kind of order one, the integration is limited to a cylinder of radius $r_0$, and the filling fraction

$$f = \pi r_0^2 / A_c = \begin{cases} 
\pi (r_0/a)^2 , & \text{for square lattice} \\
\frac{2\pi}{\sqrt{3}}(r_0/a)^2 , & \text{for hexagonal lattice} 
\end{cases}$$  \hspace{1cm} (11)

where $a$ is the period (or lattice constant) of the system. With the aid of eq. (9), one can cast eq. (7) in the form (see Appendix):

$$S \sum_{\vec{G}' \neq \vec{G}} F(\vec{G} - \vec{G}') E_z(\vec{G}') + [Q + e^2 |\vec{K} + \vec{G}|] E_z(\vec{G}) = \omega^2 \left[ R \sum_{\vec{G}' \neq \vec{G}} F(\vec{G} - \vec{G}') E_z(\vec{G}') + PE_z(\vec{G}) \right]$$  \hspace{1cm} (12)
where

\[ P = \varepsilon_i^L f + \varepsilon_b^L (1 - f) \]  
(13.1)

\[ Q = \varepsilon_i^L \omega_{pi}^2 f + \varepsilon_b^L \omega_{pb}^2 (1 - f) \]  
(13.2)

\[ R = \varepsilon_i^L - \varepsilon_b^L \]  
(13.3)

\[ S = \varepsilon_i^L \omega_{pi}^2 - \varepsilon_b^L \omega_{pb}^2 \]  
(13.4)

where \( \varepsilon_j^L \) and \( \omega_{pj} \) are, respectively, the background dielectric constant and the screened plasma frequency of the medium concerned; \( j \equiv i, b \).

Equation (12) can be cast in the form of a standard eigenvalue problem:

\[ \sum_{\vec{g}'} A_{\vec{g}, \vec{g}'} E_z(\vec{g}') = \Omega^2 E_z(\vec{g}), \]  
(14)

where the dimensionless \( \Omega = \omega(a/2\pi c) \), \( \vec{k} = \vec{K}(a/2\pi) \), and \( \vec{g} = \vec{G}(a/2\pi) \). The matrix \( \vec{A} \) is defined as follows:

\[ \vec{A} = \vec{B}^{-1} \vec{C} \]  
(15)

and the matrix elements of \( \vec{B} \) and \( \vec{C} \) are given by

\[ B_{\vec{g}, \vec{g}'} = P \delta_{\vec{g}, \vec{g}'} + RF(\vec{g} - \vec{g}')(1 - \delta_{\vec{g}, \vec{g}'}), \]  
(16.1)

\[ C_{\vec{g}, \vec{g}'} = \left[ Q' + \left| \vec{k} + \vec{g} \right|^2 \right] \delta_{\vec{g}, \vec{g}'} + S'F(\vec{g} - \vec{g}')(1 - \delta_{\vec{g}, \vec{g}'}), \]  
(16.2)

where

\[ Q' = Q(a/2\pi c)^2 = \varepsilon_i^L \Omega_{pi}^2 f + \varepsilon_b^L \Omega_{pb}^2 (1 - f) \]  
(17.1)

\[ S' = S(a/2\pi c)^2 = \varepsilon_i^L \Omega_{pi}^2 - \varepsilon_b^L \Omega_{pb}^2 \]  
(17.2)

where \( \Omega_{pj} = \omega_{pj}(a/2\pi c) \) is the normalized screened plasma frequency. Equation (14) is, in fact, performed at the computational level for both the geometries considered in the present work. The existence of matrix \( \vec{A} \) implies that its elements must be computed for every value of \( \vec{k} \), rather than for every value of \( \vec{k} \) and \( \Omega \) as implied by eq. (12). A drastic saving in computational time is achieved by transforming eq. (12) into eq. (14). The penalty one has to pay for this benefit is that one is required to invert matrix \( \vec{B} \) and perform the multiplication \( \vec{B}^{-1} \vec{C} \).
2.2. Magnetic-field-dependent waves

Now we turn to the magnetoplasma waves governed by eqs. (4). Invoking the Bloch theorem for the field components ($E_x$ and $E_y$), making Fourier expansion of the position-dependent material parameters ($\epsilon_{xx}$ and $\epsilon_{xy}$), and normalising the quantities, just as before, leads us to write eqs. (4) in the form

$$\sum_{\vec{g}'} \left[ A(\vec{g} - \vec{g}') - (\vec{k} + \vec{g}')_y(\vec{k} + \vec{g}')_y \delta_{\vec{g}' - \vec{g}} \right] E_x(\vec{g}')$$

$$+ \sum_{\vec{g}'} \left[ B(\vec{g} - \vec{g}') + (\vec{k} + \vec{g}')_x(\vec{k} + \vec{g}')_y \delta_{\vec{g}' - \vec{g}} \right] E_y(\vec{g}') = 0$$

(18.1)

$$\sum_{\vec{g}'} \left[ B(\vec{g} - \vec{g}') - (\vec{k} + \vec{g}')_x(\vec{k} + \vec{g}')_y \delta_{\vec{g}' - \vec{g}} \right] E_x(\vec{g}')$$

$$- \sum_{\vec{g}'} \left[ A(\vec{g} - \vec{g}') - (\vec{k} + \vec{g}')_x(\vec{k} + \vec{g}')_y \delta_{\vec{g}' - \vec{g}} \right] E_y(\vec{g}') = 0$$

(18.2)

where functional $A(\vec{g})$ and $B(\vec{g})$ are defined as

$$A(\vec{g}) = \begin{cases} A_i f + A_b (1 - f) \equiv \overline{A}, & \text{for } \vec{g} = 0 \\ (A_i - A_b) F(\vec{g}) \equiv \Delta A F(\vec{g}), & \text{for } \vec{g} \neq 0 \end{cases}$$

(19)

and

$$B(\vec{g}) = \begin{cases} B_i f + B_b (1 - f) \equiv \overline{B}, & \text{for } \vec{g} = 0 \\ (B_i - B_b) F(\vec{g}) \equiv \Delta B F(\vec{g}), & \text{for } \vec{g} \neq 0 \end{cases}$$

(20)

where $\vec{k}$ and $\vec{g}$ are just as defined before and

$$A_j = \left( \frac{a}{2\pi} \right)^2 q_0^2 \epsilon_{jx} = \epsilon_L^2 \left( 1 - \frac{\Omega_{yj}^2}{\Omega^2 - \Omega_{cj}^2} \right)$$

(21.1)

$$B_j = \left( \frac{a}{2\pi} \right)^2 q_0^2 \epsilon_{jy} = i \epsilon_L^2 \frac{\Omega_{cj} \Omega_{yj}^2}{(\Omega^2 - \Omega_{cj}^2)}$$

(21.2)

with sub/superscript $j \equiv i, b$. Here $\Omega_{cj} = (\omega_{cj} a / 2\pi c)$ is the normalized electron cyclotron frequency (see Appendix).

Let us now rewrite eqs. (18) symbolically as follows:

$$\hat{A}_1 E_x(\vec{g}') + \hat{A}_2 E_y(\vec{g}') = 0$$

(22.1)

$$\hat{A}_3 E_x(\vec{g}') + \hat{A}_4 E_y(\vec{g}') = 0$$

(22.2)
where the matrices $A_j; j \equiv 1, 2, 3, 4;$ are defined such that the matrix elements thereof are given by

\[
A_{1(\vec{g},\vec{g}')} = A(\vec{g} - \vec{g}') - (\vec{k} + \vec{g}')(\vec{k} - \vec{g}')\delta_{\vec{g} - \vec{g}}
\] (23.1)

\[
A_{2(\vec{g},\vec{g}')} = B(\vec{g} - \vec{g}') + (\vec{k} + \vec{g}')x(\vec{k} - \vec{g}')y\delta_{\vec{g} - \vec{g}}
\] (23.2)

\[
A_{3(\vec{g},\vec{g}')} = -B(\vec{g} - \vec{g}') + (\vec{k} + \vec{g}')z(\vec{k} - \vec{g}')y\delta_{\vec{g} - \vec{g}}
\] (23.3)

\[
A_{4(\vec{g},\vec{g}')} = A(\vec{g} - \vec{g}') - (\vec{k} + \vec{g}')z(\vec{k} - \vec{g}')z\delta_{\vec{g} - \vec{g}}
\] (23.4)

Eliminating $E_y(\vec{g}')$ from eqs. (22) leaves us with

\[
\left( A_{2}^{-1} A_{1} - A_{4}^{-1} A_{3} \right) E_x(\vec{g}') = 0
\] (24)

Nontrivial solutions of this equation are given by

\[
\begin{vmatrix}
A_{2}^{-1} & A_{1} & A_{4}^{-1} & A_{3}
\end{vmatrix} = 0
\] (25)

What is noteworthy is the fact that in this magnetic-field-dependent part of the problem, the secular equation cannot be cast in the form of a standard eigenvalue problem. That is because the eigenvalues are involved in both the diagonal and nondiagonal elements of the resultant matrix. So the only way down to the determination of the eigenvalues is to treat eq. (25) as a transcendental function and find its zeros for a given $\vec{k}_\parallel$, by inserting an additional loop over $\Omega$. Naturally, the time consumption during the computation of reliable band structures will be enormous.

It is interesting to note that one can, without much efforts, prove analytically that, in the limit of vanishing applied magnetic field ($\Rightarrow$ functional $B(\vec{g}) \to 0$), the secular equation (25) reduces to

\[
\begin{vmatrix}
A & -\Omega^2
\end{vmatrix} = 0
\] (26)

where $\hat{I}$ is a unit matrix. Eq. (26) is exactly identical to the secular equation obtained from eq. (14). This emboldens our confidence in the adequacy of the formalism presented in this work.

The last step in presenting the numerical examples is to specify the symmetry of the lattices. The specific geometrical arrangements considered in this work are the square and hexagonal lattices. Their reciprocal lattice vectors are given by

\[
\vec{G} = \frac{2\pi}{a}(n_x\hat{x} + n_y\hat{y})
\] (27)
for the square lattice and
\[ \mathbf{G} = \frac{2\pi}{a} \left[ n_x \hat{x} + \left( -n_x + 2n_y \right)/\sqrt{3} \right] \hat{y} \] (28)
for the hexagonal lattice. In this work the integers \( n_x \) and \( n_y \) were limited in the range of \(-10 \leq (n_x, n_y) \leq +10\); which implies to 441 plane waves considered. This resulted in a reliably very good convergence; at least up to the first fiftieth bands. In this paper we will confine ourselves to the waves which turn out to be independent of the applied magnetic field and hence are governed by eq. (14). The analytical and numerical details of the magnetic-field dependent waves are deferred to a forthcoming publication.

### III. NUMERICAL EXAMPLES

For the purpose of numerical computation, we specify the semiconductor–dielectric composite to be made up of doped GaAs–intrinsic GaAs or doped GaAs–vacuum. This implies that \( \epsilon_L = 12.8 \) (1.0) for doped or undoped GaAs (vacuum). As stated above, we confinir ourselves to the waves which are independent of the applied magnetic field. As such the only other parameter needed to accomplish the computation is the dimensionless plasma frequency \( \Omega_p \); two specific values used in this work are \( \Omega_p = 0.5 \) and 0.75. We will discuss a variety of illustrative numerical results. This includes exchanging materials in the cylindrical inclusions and the background medium; in addition to the two values of \( \Omega_p \). The whole range of filling fraction is explored in order to discuss the regime of at least first ten bands of the respective composites in both square and hexagonal lattices (see Fig. 1).

#### 3.1. Square lattice

Figure 2 illustrates the band structure (BS) and density of states (DOS) for a square lattice of doped GaAs cylinders in vacuum for a filling fraction \( f = 10\% \). The plots are rendered in terms of the dimensionless frequency \( \Omega \) versus Bloch vector \( \mathbf{k} \). The left part of the triptych represents the BS in three principal symmetry directions, letting \( \mathbf{k} \) scan only the periphery of the irreducible part of the first Brillouin zone (see the inset on the right). The middle part is the result of an extensive scanning of \( |\mathbf{k}| \) in the irreducible triangle \( \Gamma XM \) of the Brillouin zone — the interior of this zone and its surface, as well as the principal directions shown in the left part of this figure.
Each curve here corresponds to some direction of $\vec{k}$. The DOS in the right part of the triptych has been calculated on the basis of the scanning in the middle part, which corresponds to 1326 $\vec{k}$ points. The three parts of the triptych together demonstrate that there is, indeed, a genuine full gap in the frequency range defined by $0 \leq \Omega \leq 0.320$ and we consider such calculations as essential.

Extensive computation of the BS for the same composite as considered in Fig. 2 reveals that one can also achieve some higher energy gaps within the first ten bands for certain values of the filling fraction. For instance, for $f = 30\%$, there are three full gaps within the first ten bands — the first one is analogous to the one shown in Fig. 2, the second one exists between the third and fourth bands, and the third one opens between the ninth and tenth bands. For $f = 40\%$, the third gap exists between the sixth and seventh bands, whereas the second gap, although differs in magnitude and frequency range, still persists between the third and fourth bands. For $f = 50\%$, there are only two gaps — the first one exists below the first band and the second one opens between the sixth and seventh. We find that, whether or not the higher energy gaps exist, the lowest gap below a threshold frequency $\Omega_t$ (which varies with $f$) defined as the minimum of the first band at the $\Gamma$ point, always persists. It has been noted that, for $f \geq 60\%$, only the lowest gap exists. This is true even for the close-packing value ($f = 0.7853$) where the cylinders just touch each other.

The dependence of the gap-widths of the lowest (which is also the widest) gap on the filling fraction for diversely designed composites in square lattice is summarized in Fig. 3. The curves designated as AS$j$, SA$j$, IS$j$, and SI$j$ refer, respectively, to the composites made up of cylindrical holes in doped GaAs background, cylindrical doped GaAs in vacuum, cylindrical intrinsic GaAs in doped GaAs background, and cylindrical doped GaAs in intrinsic GaAs background; $j = 1(2)$ correspond to $\Omega_p = 0.5(0.75)$. The important points one can notice at glance are the following. The composites made up of doped semiconductor inclusions in the dielectric background give rise to the lowest gap (below $\Omega_t$) whose width increases with increasing filling fraction (see, for example, the curves SA$j$ and SI$j$; $j = 1, 2$). On the other hand, the composites made up of dielectric cylinders in the doped semiconductor background give rise to the lowest gap which decreases as the filling fraction increases (see, for example, the curves AS$j$ and IS$j$). Comparing the curves AS$j$ with IS$j$ (or SA$j$ with SI$j$) leads us to infer that the larger the dielectric mismatch (between the inclusions and the background), the wider is the gap-width. Similarly, comparing
the respective curves for j=1 with those for j=2 reveals that the gap-width becomes larger as the plasma frequency increases. It is also noteworthy that the maximum gap-width (of the lowest gap) one can achieve is, empirically, defined by $0 \leq \Omega_t \leq \Omega_p$. This implies that the largest gap to midgap ratio (GMR) one can achieve is exactly two. This abides by the fact that in order to obtain GMR $\geq 1$, $\Omega_2$ should be $\geq 3\Omega_1$; $\Omega_2$ ($\Omega_1$) being the frequency of the top (bottom) of the existing gap.

### 3.2. Hexagonal lattice

Figure 4 illustrates the band structure and DOS for a hexagonal lattice of doped GaAs cylinders in vacuum for a filling fraction $f = 10\%$. The plots are rendered in terms of the dimensionless frequency $\Omega$ versus Bloch vector $\vec{k}$. The left part of the triptych represents the BS in three principal symmetry directions, letting $\vec{k}$ scan only the periphery of the irreducible part of the first Brillouin zone (see the inset on the right). The middle part is the result of an extensive scanning of $|\vec{k}|$ in the irreducible triangle $\Gamma JX$ of the Brillouin zone — the interior of this zone and its surface, as well as the principal directions shown in the left part of this figure. The DOS in the right part of the triptych has been calculated on the basis of the scanning in the middle part, which corresponds to 1275 $\vec{k}$ points. The three parts of the triptych together demonstrate that there is a genuine full gap in the frequency range defined by $0 \leq \Omega \leq 0.329$. In addition, there is another band-gap opening up between the first and second bands — defined by the maximum (minimum) of the first (second) band at $J$ ($X$) point.

Extensive computation of the BS for the same composite as represented by Fig. 4 reveals that there are some other higher energy gaps opening up within the first ten bands for certain values of $f$. For instance, for $f = 20\%$, there are three more full gaps, apart from the lowest one that opens below $\Omega_t$ — the first one exists between the first two bands, the second one opens between the third and fourth bands, and the third one exists between the eighth and ninth bands. For $30\% \leq f \leq 60\%$, we obtain two more full gaps, apart from the lowest one, with varying frequency range and magnitudes. At $f = 70\%$, we left with only two full gaps — the first one is the same that exists below the minimum (at $\Gamma$ point) of the lowest band and the second one opens between the third and fourth bands. For $f \geq 70\%$, there are no more full gaps except the lowest one. The semiconductor-dielectric composites in the hexagonal lattice, just as in the square lattice,
are always seen to give rise to the lowest gap persisting below a threshold frequency $\Omega_t$.

The dependence of the lowest gap-width on the filling fraction for diversely designed composites in the hexagonal lattice is depicted in Fig. 5. Comparing Fig. 5 with Fig. 3 clearly reveals that the gap-widths (of the lowest gap) for the respective composites in the hexagonal lattice, over almost the whole common range of filling fractions, are larger than those in the square lattice. The rest of the discussion related to Fig. 3 is still seen to be valid. It should be pointed out that this trend of achieving larger gaps in the hexagonal lattice as compared to the square lattice is the same as has been noted earlier in the cases of photonic as well as phononic crystals$^4$. This seems to be physically quite a reasonable result, because the constant energy surfaces in the hexagonal lattice are closer to the circular shape than those of a square lattice.

**IV. CONCLUDING REMARKS**

In summary, we have demonstrated that the simple 2D periodic binary semiconductor- dielectric composites can give rise to full plasmonic band-gaps. Although we consider an applied magnetic field oriented along the axis of the cylindrical inclusions, two independent polarizations of the waves have been obtained — $E_z \parallel \hat{z}$ axis and $H_z \parallel \hat{z}$ axis, just as in the absence of an applied magnetic field. Only the waves in the latter polarization are magnetic-field dependent. The numerical results presented in this work correspond to the former polarization. As such the term "full" should be reserved with respect to this polarization. In principle, the band structures computed separately for the two polarizations should be superimposed — one over the other — to check and claim whether or not the band-gaps are independent of the polarization. This is the task aimed at in a future publication.

Our theoretical results on achieving full band-gaps must be accompanied by a word of warning. Apart from the fact that both polarizations need to be considered, we have here also assumed the $z$-component of the wave vector ($k_z$) to be zero. Considering $k_z$ finite would give a better insight into the problem. We have also ignored the damping effects and the interaction of the charge carriers with the optical phonons. The latter could be taken into account by considering the frequency-dependence of the background dielectric constants. Additional work addressing the effect stemming from the cylinders of different cross-sections and orientation of the external magnetic field would be worthwhile. Considering the cylindrical inclusions of finite lengths should
be of more practical interest.

Attractive possibilities exist for the experimental observation of such plasmonic band-gaps, both with and without an applied magnetic field, in the semiconductor- dielectric composites as investigated here. Resonant Raman scattering, as employed to study plasmons in quantum wire superlattices, may be one option worth attempting.

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**APPENDIX**

The dielectric tensor components employed in this work are defined as follows:

\[
e_{xx} = e_{yy} = e_L \left[ 1 - \frac{\omega_p^2(\omega + i\nu)}{\omega(\omega + i\nu)^2 - \omega_c^2} \right]
\]  

(29.1)

\[
e_{yx} = -e_{xy} = -i e_L \frac{\omega_p^2\omega_c}{\omega(\omega + i\nu)^2 - \omega_c^2}
\]  

(29.2)

\[
e_{zz} = e_L \left[ 1 - \frac{\omega_p^2}{\omega(\omega + i\nu)} \right]
\]  

(29.3)

where \(e_L\) is the background dielectric constant, \(\nu\) is the free carrier collision frequency, \(\omega_p\) is the screened plasma frequency, and \(\omega_c\) is the electron cyclotron frequency.

If we also consider the effect of phonons, which, in a way, incorporates the coupling of the plasmons (or magnetoplasmons) to the optical phonons, then the background dielectric constant \(e_L\) has to be replaced by its frequency dependent expression:

\[
e_L(\omega) = e_\infty \frac{\omega_{LO}^2 - \omega^2 - i\Gamma\omega}{\omega_{TO}^2 - \omega^2 - i\Gamma\omega}
\]  

(30)

where \(e_\infty\) is the high-frequency dielectric constant, \(\Gamma\) is the optical-phonon damping frequency, and \(\omega_{LO}\) and \(\omega_{TO}\) are, respectively, the longitudinal and transverse optical phonon frequencies at the zone center of the Brillouin zone.
REFERENCES

1 See, e.g., Proceedings of the 11th International Conference on Electronic properties of Two-Dimensional Systems (EP2DS), Surf. Sci. 361/362 (1996).

2 See, e.g., P. Rai-Chaudhry, Editor, The Handbook of Microlithography, Micromachining, and Microfabrication (SPIE, 1996).

3 E. Yablonovitch, Phys. Rev. Lett. 58, 2059 (1987); S. John, ibid. 58, 2486 (1987).

4 For a recent extensive review, see M.S. Kushwaha, Int. J. Mod. Phys. B10, 977 (1996).

5 M.S. Kushwaha, P. Halevi, L. Dobrzynski, and B. Djafari-Rouhani, Phys. Rev. Lett. 71, 2022 (1993); M.S. Kushwaha, Appl. Phys. Lett. 70, 3218 (1997); and references therein.

6 J.O. Vasseur, L. Dobrzynski, and B. Djafari-Rouhani, Phys. Rev. B 54, 1043 (1996).

7 S. John, Phys. Rev. Lett. 53, 2169 (1984).

8 A. Kobayashi and R.E. Prange, Phys. Rev. Lett. 56, 1280 (1986).

9 A.R. McGurn and A.A. Maradudin, Phys. Rev. B48, 17576 (1993); see also V. Kuzmiak and A.A. Maradudin, Phys. Rev. B 58, 7427 (1997).

10 R.F. Wallis and J.J. Quinn, Phys. Rev. B 38, 4205 (1988).

11 M.S. Kushwaha, Phys. Rev. B 42, 5602 (1990).

12 B.L. Johnson and R.E. Camley, Phys. Rev. B 43, 6554 (1991).

13 R. Strenz et al. Phys. Rev. Lett. 73, 3022 (1994).

14 M.S. Kushwaha and P. Zielinski, Europhys. Lett. (to be published).
Figure captions

**Fig. 1.** Schematics of a few units cells of square (a) and hexagonal (b) lattices investigated in this work. The cylindrical inclusions are oriented along the \( \hat{z} \) axis. The propagation is confined to the \( \hat{x} - \hat{y} \) plane. An external magnetic field field is oriented parallel to the cylinders.

**Fig. 2.** Band structure (BS) and density of states (DOS) of a square lattice of cylindrical (GaAs) semiconductor inclusions of circular cross-section in a vacuum background. The filling fraction is \( f = 10\% \). The triptych is comprised of three parts. In the left panel, we plot the BS in three principal symmetry directions, letting \( \vec{k} \) scan only the periphery of the irreducible part of the first Brillouin zone (see inset on right). The middle panel demonstrates a novel way of plotting the eigenvalues as a function of \( |\vec{k}| \); i.e., the distance of a point in the irreducible part of the Brillouin zone from the \( \Gamma \) point. The right panel illustrates the DOS. We call attention to the full gap below a threshold frequency \( \Omega_t = 0.320 \) and extending down to zero.

**Fig. 3.** Dependence of the gap-widths (of the lowest gap) on the filling fraction for diversely designed composites in a square lattice. The curves designated as AS\( j \), SA\( j \), IS\( j \), and SI\( j \) refer, respectively, to the composites made up of cylindrical holes in doped GaAs background, cylindrical doped GaAs in vacuum, cylindrical intrinsic GaAs in doped GaAs background, and cylindrical doped GaAs in intrinsic GaAs background. The horizontal dashed lines stand for the plasma frequencies \( \Omega_{p1} = 0.50 \) and \( \Omega_{p2} = 0.75 \).

**Fig. 4.** The same as in Fig. 2, but for the hexagonal lattice. The threshold frequency for the lowest gap that extends down to zero is \( \Omega_t = 0.329 \). Notice a small second full gap (hatched region) existing between the first two bands.

**Fig. 5.** The same as in Fig. 3, but for the hexagonal lattice.
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