Photonic Crystal Optics and Homogenization of 2D Periodic Composites

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We study the long-wavelength limit for an arbitrary photonic crystal (PC) of 2D periodicity. Light propagation is *not* restricted to the plane of periodicity. We proved that 2D PC's are uniaxial or biaxial and derived compact, explicit formulas for the effective ("principal") dielectric constants; these are plotted for silicon-air composites. This could facilitate the custom design of optical components for diverse spectral regions and applications. Our method of "homogenization" is not limited to optical properties, but is also valid for electrostatics, magnetostatics, dc conductivity, thermal conductivity, etc. Thus our results are applicable to inhomogeneous media where exact, explicit formulas are scarce. Our numerical method yields results with unprecedented accuracy, even for very large dielectric contrasts and filling fractions. [S0031-9007(98)08154-X]

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Photonic crystals (PC's) are arrays of dielectric materials with one-, two-, or three-dimensional periodicity. Since the suggestion [1] that PC's may be useful for controlling light emission, their properties have been researched intensively [2,3]. Recently, it was proposed that PC's could advance photonic information technology [4–6]. These ideas rely on the existence of a photonic band gap—a frequency region in which light propagation is forbidden. The region well below the gap received much less attention [7–12]. Here the wavelength is much greater than the lattice period; hence light "sees" a homogeneous medium. This situation is analogous to light propagation in natural crystals, whose optical properties like birefringence are described in crystal optics [13]. We studied analytically, for the first time, propagation in an arbitrary direction in space for a 2D PC.

In general, a PC supports two distinct propagation modes. Independently of the existence of a band gap, for sufficiently low frequencies ω, the dispersion relations ω versus the vector of propagation $\mathbf{k}$ are linear for the two modes. The slopes ω/k define two effective dielectric constants $\epsilon_{\rm eff} = (ck/\omega)^2$ [7–12]. Thus, in this long-wavelength limit the composite may be treated as if it were homogeneous. At the same time $\epsilon_{\rm eff}$ does depend on the direction of propagation ($\mathbf{k}/k$), implying that the effective medium is anisotropic [7,9,10,12]. An electrostatic calculation ($\omega = 0$) must yield the same values for the $\epsilon_{\rm eff}$ as the previously described quasistatic approach ($\omega \to 0$). In fact, the *homogenization* of composites [14] has been studied for many years by means of both the static [15–23] and the quasistatic [7,24,25] methods. The homogenization of 1D structures has been accomplished a long time ago [23]. Solution for 3D photonic crystals was given in Ref. [7].

The object of our investigation is a periodic, 2D array of infinitely long cylinders. The cross section of a cylinder can have an arbitrary shape, and the unit cell is in general a parallelogram. These rods are assumed to be made of a homogeneous material (dielectric constant ϵ_a), as is the interstitial material (ϵ_b). The cylinders occupy a fraction f of space. For propagation of light parallel to the plane of periodicity there are two independent modes: the $E(H)$ mode has its electric (magnetic) field parallel to the cylinders [2–4,26–28]. In a preliminary work we have examined the in-plane behavior of these modes in the low-frequency limit [12]. We also note that homogenization has been performed for the E mode in the case of metallic cylinders modeled with $\epsilon_a = 1 - \omega_p^2/\omega^2$ [29]. In this Letter we achieve a homogenization of our photonic crystal for an arbitrary direction of propagation in space; namely, we take a 3D approach to composites of 2D periodicity. We are aware only of a single, numerical study (p. 66 of Ref. [2]) of out-of-plane propagation.

Crystal optics [13] is the product of homogenization of the periodic atomic structure. In the same way photonic crystal optics is the result of homogenizing a periodic composite with macroscopic inhomogeneities. Hence it should be possible to give a complete description of this structure in terms of a dielectric tensor, which becomes diagonal in the principal set of axes, embedded in the crystal. In this system of coordinates the dielectric response is simply $D_i = \epsilon_i E_i$ $(i = 1,2,3)$, the ϵ_i being the *principal dielectric constants* of the composite. Now there is a simple, but crucial, consideration that for the (in-plane) E mode the displacement vector $\mathbf{D}$ must be parallel to the cylinders at every point. Then the coordinate axis parallel to the cylinders (say, z) must be a *principal axis*. Moreover, it is well known [14] that if $\mathbf{E}$ is parallel to *all* the dielectric interfaces, then $\epsilon_{\rm eff}$ is equal to the weighted average of the dielectric constants of the constituents. This gives immediately one of the principal dielectric constants,

$$\epsilon_3 = \bar{\epsilon} = \epsilon_a f + \epsilon_b (1 - f). \quad (1)$$

The principal axes x and y must be parallel to the plane of periodicity, and the corresponding dielectric constants ϵ_1 and ϵ_2 must be calculated from an $\omega \to 0$ expansion of the wave equation. If the three ϵ_i are known then, for an arbitrary direction of $\mathbf{k}$, the indices of refraction along with the displacement vectors of the two propagating modes are found with the help of the normal ellipsoid [13] whose z axis is parallel to the rods [30].

It is advantageous to solve the wave equation for the magnetic field $\mathbf{H}(\mathbf{r})$. In addition to being continuous across the interfaces and giving rise to a Hermitian eigenvalue problem [2], it has the added benefit that $\mathbf{H}(\mathbf{r})$ vanishes in the static case. The static dielectric constants ϵ_1 and ϵ_2 are calculated by taking the limit $\mathbf{k} \to 0$ in the wave equation written in the k representation and using the l'Hôpital rule for the ratio ω/k. The proof will be given elsewhere, and here we state only the final result. This involves the reciprocal dielectric constant $\eta(\mathbf{r}) = 1/\epsilon(\mathbf{r})$ and its Fourier coefficient $\eta(\mathbf{G})$, where $\mathbf{G}$ is a reciprocal vector of the general (oblique) 2D lattice. Defining the matrix $M(\mathbf{G},\mathbf{G}') = \mathbf{G} \cdot \mathbf{G}' \eta(\mathbf{G} - \mathbf{G}')$, the principal dielectric constants can be written as

$$\begin{aligned} \epsilon_1 &= [\overline{\eta} - A_{xx} \sin^2\theta - A_{yy} \cos^2\theta - A_{xy} \sin 2\theta]^{-1}, \\ \epsilon_2 &= [\overline{\eta} - A_{xx} \cos^2\theta - A_{yy} \sin^2\theta + A_{xy} \sin 2\theta]^{-1}, \\ A_{ik} &= \frac{1}{2} \sum (G_i G_k' + G_i' G_k) \eta(\mathbf{G}) \eta(-\mathbf{G}') M^{-1}(\mathbf{G},\mathbf{G}'). \end{aligned} \tag{2}$$

Here $\overline{\eta}$ is the weighted average of $\eta(\mathbf{r})$, and the summation is performed over all *nonzero* components of $\mathbf{G}$ and $\mathbf{G}'$ (in the crystal axes system). For high-symmetry unit cells ($A_{xy} = 0$), the principal axes coincide with the crystal axes. Otherwise, the principal axes system is rotated about the axis z by an angle $\theta = -(1/2) \tan^{-1}[2A_{xy}/(A_{xx} - A_{yy})]$. Equations (2) and (1) are the exact and explicit results of homogenization for a 2D PC with arbitrary unit cell. The values of the ϵ_i depend only on the structure of this cell and on ϵ_a and ϵ_b.

An oblique or a rectangular lattice gives rise to $\epsilon_1 \neq \epsilon_2$. This also occurs for a square or a hexagonal lattice if the cylinders have a cross section of sufficiently low symmetry. Also, according to the Wiener bounds [14] $\epsilon_i < \overline{\epsilon}$; therefore the effective dielectric constant must be largest when the electric field is parallel to all interfaces. Then, for anisotropy in the xy plane, $\epsilon_1 \neq \epsilon_2 < \epsilon_3$. This situation results in a *biaxial crystal* [13]; namely, there are two specific optical axes or directions of $\mathbf{k}$, for which the two wave modes have equal refractive indices. We have computed $\epsilon_{1,2}(f)$ for a rectangular array of circular silicon rods in air, and for the conjugate case—cylindrical holes in a silicon host, Fig. 1(a). A test on the accuracy of our numerical results is provided by the generalized Keller theorem [17], which states that $r \equiv \epsilon_1(\epsilon_a, \epsilon_b)\epsilon_2(\epsilon_b, \epsilon_a)/\epsilon_a \epsilon_b = 1$ for any f. Because $\epsilon_2 < \epsilon_1 < \epsilon_3$ (for air cylinders) the optical axes lie in the zy plane, forming equal angles with the cylinders [13].

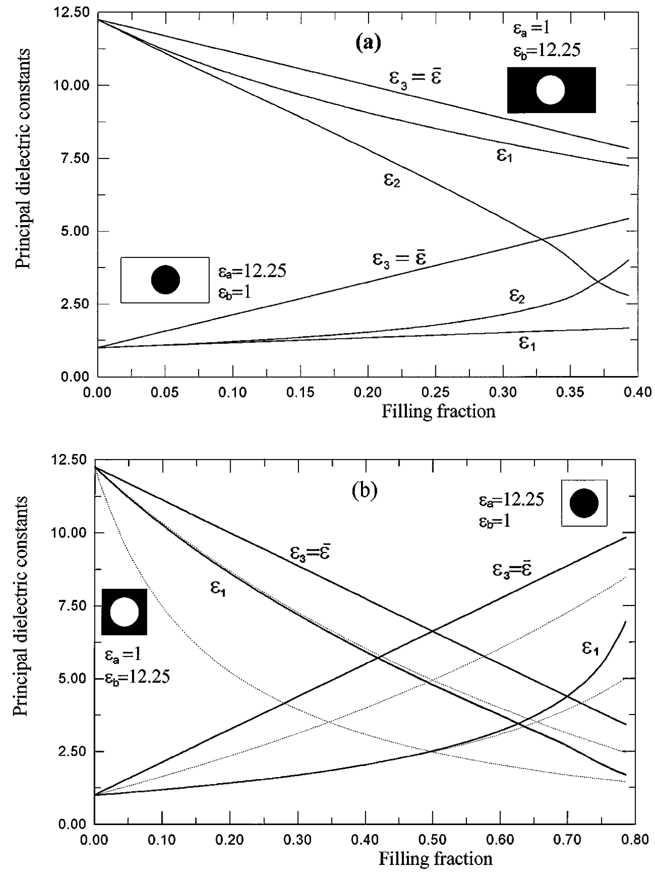

FIG. 1. Principal dielectric constants of arrays of circular Si rods in air and of cylindrical holes in a Si host as a function of the filling fraction. For a rectangular lattice (a), $\epsilon_1 \neq \epsilon_2$ and the crystal is biaxial. In this case we used 1130 $\mathbf{G}$ values in the computation, giving rise to a precision factor $r = 0.98$. If the lattice is square (b), $\epsilon_1 = \epsilon_2$ and the crystal is uniaxial. Note that $\epsilon_1(f)$ falls within the Hashin-Shtrikman bounds (dashed). Here we employed only 1028 $\mathbf{G}$ values; however, the precision was greatly increased by taking the geometric average referred to in the text.

For a square lattice of circular or square cylinders with the sides of the rods either parallel to the lattice or rotated by 45° we proved analytically that $\epsilon_1 = \epsilon_2$. We also checked numerically that this equality holds for a hexagonal lattice of circular or triangular cylinders with the sides of the rods parallel to three sides of the hexagon. Isotropy in the plane of periodicity is a consequence of a third- or higher-order rotation axis z [31]. These five photonic crystals are then uniaxial, with their optical axis coinciding with the cylinder axes. This is then the only direction for which the *ordinary* and *extraordinary* waves become degenerate and have the same index of refraction, $\sqrt{\epsilon_1} = \sqrt{\epsilon_2}$. For off-axis propagation the ordinary mode still has the same index of refraction, its electric field being parallel to the (isotropic) plane of periodicity. The extraordinary mode has its electric field parallel to the plane formed by $\mathbf{k}$ and z, and its refractive index depends on the angle between these two vectors. Figure 1(b) shows the principal dielectric constants of a square lattice of circular Si

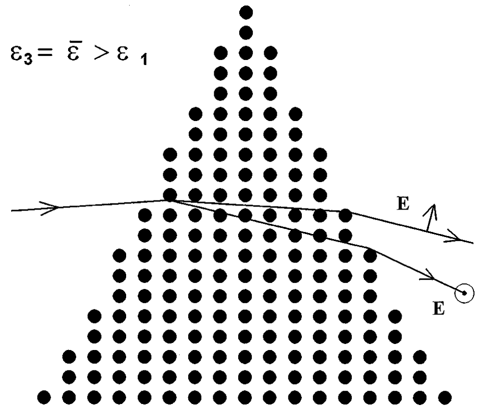

FIG. 2. Design of a prism using a 2D photonic crystal. The circular dots represent cylinder cross sections. The birefringent prism polarizes the outcoming light.

cylinders and of the conjugate crystal. We also plot the Hashin-Shtrikman bounds [15] as a check of consistency. It is interesting to note that for $f \lesssim 0.5$ the upper (lower) bound is a reasonable approximation for the Si (air) cylinders. We stress that Fig. 1(b) provides a complete characterization of this PC in the low-frequency limit. Note that the ratio ϵ_3/ϵ_2 can be greater than 2(3) for the uniaxial (biaxial) crystal. Such anisotropy is substantially larger than that occurring in natural crystals. In fact, unlike 3D PC's [7], 2D PC's cannot be isotropic because $\epsilon_3 = \overline{\epsilon}$ is always greater than ϵ_1 and ϵ_2.

We propose that PC's could be useful not only as photonic *band-gap* materials, but also as *optical* materials. They could be custom designed for applications in desirable spectral regions—for instance, the far infrared employing nanofabricated arrays, and in the microwave for macroscopic structures. As an example, in Fig. 2 we show a birefringent prism constructed of suitably shaped 2D photonic crystals (square arrays of circular cylinders). It is apparent that PC's could also be designed to exhibit optical activity [32], conical refraction, dichroism, etc.

Next we put the accuracy of our calculations to a tough test. While Eq. (2) is exact, the computation necessitates cutting down the matrix $M(\mathbf{G}, \mathbf{G}')$ to finite size. This happens to underestimate the values of ϵ_i. On the other hand, a similar solution of the wave equation for $\mathbf{D}$, derived for the special case of a uniaxial crystal, overestimates the ϵ_i. If $A_{xy} = 0$ (symmetric unit cell), this alternative formula for ϵ_i is given by the denominator in Eq. (2), however, with all of the η replaced by ϵ. *Our numerical simulations show that the geometric average of the two expressions for ϵ_i is almost independent of the size of M (the number of $\mathbf{G}$ vectors).*

In Table I we present results for a square array of prismatic rods in air. Dielectric contrasts as large as 50 and 100 have been selected. Our values are compared with those of Refs. [19,21] and are also tested by the Keller theorem [16], according to which the product of the effective dielectric constants of the crystal (ϵ) and of the conjugate crystal (ϵ^*) is equal to $\epsilon_a \epsilon_b$. The last column demonstrates that the theorem is obeyed with great precision (we give only significant figures). This has been achieved with an array of only 1812 $\mathbf{G}$ values and modest computational effort. So our method gives practically exact results even for very large dielectric contrasts ϵ_a/ϵ_b.

The important formula Eq. (2) has direct analogies in other areas of transport properties of inhomogeneous media. Thus all the ϵ's may be replaced by the corresponding μ's, σ's, or K's, and one gets useful formulas for the effective static magnetic permeability, the conductivity, or the thermal conductivity, respectively. This is because the validity of Eq. (2) rests only on the equations $\nabla \cdot \mathbf{D} = 0$, $\nabla \times \mathbf{E} = 0$, and $\mathbf{D} = \epsilon \mathbf{E}$, and the basic equations of magnetostatics, electric transport, and heat transport have the very same structure.

TABLE I. Comparison of our results for the effective dielectric constant ϵ with Refs. [19,21] for a square array in air. The penultimate column gives our results (ϵ^*) for the corresponding conjugate composite. The last column demonstrates that the Keller theorem is obeyed with extremely high precision.

	Ref. [21]	Ref. [19]		Present Work	
f	ϵ	ϵ	ϵ	ϵ^*	$\epsilon\epsilon^*/\epsilon_a\epsilon_b$
			$\epsilon_a = 50$		
0.1	1.2339	1.29 ± 0.01	1.239 010	40.354 793	0.999 999
0.2	1.5377	1.63 ± 0.04	1.511 636	33.076 744	0.999 999
0.3	1.9662	2.2 ± 0.1	1.971 824	25.357 226	0.999 999
0.4	2.683	3.0 ± 0.2	2.644 923	18.904 143	1.000 000
0.5	7.07	8.87 ± 0.01	7.071 068	7.071 068	1.000 000
			$\epsilon_a = 100$		
0.1	1.2402	1.34 ± 0.05	1.249 889	80.007 121	1.000 000
0.2	1.5548	1.7 ± 0.1	1.569 954	63.696 132	0.999 999
0.3	2.0039	2.4 ± 0.3	2.000 515	49.987 129	1.000 000
0.4	2.775	3.3 ± 0.5	2.935 262	34.068 509	1.000 000
0.5	10.	15.4 ± 0.2	10.000 000	10.000 000	1.000 000

We have added the technologically promising 2D PC's to the brief list of inhomogeneous systems for which exact homogenization has been previously accomplished. This has been achieved for an arbitrary structure of the PC and with unprecedented numerical precision. Because of the linearity of the dispersion curves below the gap, Eqs. (1) and (2) are applicable even for frequencies ω close to the value c/a, where a is the lattice constant. These ideas could lead to the homogenization of *phononic* crystals (elastic composites) and could also have implications for random composites.

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