Photonic Band Gaps in Two Dimensional Photonic Quasicrystals

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It is generally believed that long range periodic order is instrumental in the formation of a photonic band gap. Using a spectral method that scales linearly with the system size, we found that sizable spectral gaps for each polarization in 2D can be found in aperiodic arrangements of dielectrics that resemble quasicrystalline tiling. Since the aperiodic arrangement has many inequivalent sites, the defect properties of these systems are more complex and interesting than conventional photonic band gap systems. [S0031-9007(97)05157-0]

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In the past few years, there has been much research activity pertaining to photonic band gap (PBG) material, which has a spectral gap in the electromagnetic (EM) wave spectrum in which EM wave propagation is forbidden in all directions [1,2]. PBG can suppress vacuum fluctuation and spontaneous emission, and can lead to interesting quantum electrodynamics effects [3]. This is also seen as a road map to strong photon localization, itself a fascinating but elusive phenomena [4]. It has potential applications in quantum electronic devices, distributed-feedback mirror, microwave antennae substrate [5], and its unusual optical properties can be exploited to control and guide the propagation of light [6].

PBG materials are often viewed as analogs of electronic semiconductors. Only short-range order is necessary for the formation of an electronic band gap. Amorphous semiconductors exist and have band gaps that are comparable in size to those of crystalline semiconductors. However, electrons form bound states and photons do not. Most of the theoretical demonstration of the existence of an electronic band gap without periodicity is based on simplified tight-binding models, which is a reasonable description because electrons can form bound states. While it is now firmly established that a certain periodic arrangement of dielectric structures can support full photonic band gaps in 2D and 3D [2], it is not obvious whether a structure without periodic order can have complete photonic gaps or not. The photonic band gap we know of to date in 2D and 3D is the consequence of periodicity: We can define a Brillouin zone because of the periodicity; and a complete photonic gap is formed when the spectral gaps at the Brillouin zone boundary overlap in all directions. Can there be photonic gaps without periodicity and without a Brillouin zone? This is a fundamental question. Motivated by the known existence of 1D stop bands in superlattices stacked in the Fibonnaci sequence [7], and acoustic spectral gaps in nearest-neighbor coupled tuning fork arrays arranged in a Penrose tiling [8], we seek to show that sizable spectral gaps can exist a in 2D "quasiperiodic" arrangement of dielectrics.

The photonic band problem for a perfect photonic crystal can be handled well by band theoretic methods, such as the plane wave method [9], which scales typically like the third power of the size of the system. Here, we use an equation-of-motion method [10] that employs discretization of the Maxwell equations in both the spatial and time domain and the integration of the Maxwell equations in the time domain; spectral intensities are obtained by a Laplace transform. If the initial field intensities are random numbers, the spectral intensities correspond to the density of states (DOS), and thus whether a system supports photonic gaps or not can be directly determined. Local density of states (LDOS) and normal mode amplitudes can also be obtained. Its computation effort scales linearly with the number of grid points, which is proportional to the system size, and is very favorable for large scale simulations of complex systems. We will focus on quasiperiodic structures in this paper. However, our calculation is quite different from the usual tight-binding calculations for the electronic properties of quasiperiodic or disordered systems. The tight-binding Hamiltonians in those studies generally employ a minimal basis (usually single band), nearest-neighbor hopping, and each site represents an atom. Our calculation is a direct solution of the Maxwell wave equations in real space. Each cylinder (our "atom") is represented by many grid points. There is no parametrization, except for the dielectric constants of the material involved. We will use $\frac{a}{c}$ as the unit of time, and angular frequencies (ω) are measured in units of $(\frac{2\pi c}{a})$, where c is the velocity of light and a is the length of one side of the square "supercell" shown in Fig. 1 [11]. We use typically 2×10^5 time steps in the simulation, with each time step of the order of $0.00015a/c$.

We consider an array of dielectric cylinders with circular cross sections of $\epsilon = 10$ positioned at the vertices of an octagonal quasiperiodic tiling [12], shown schematically in Fig. 1. The background has $\epsilon = 1$. A periodic boundary condition was imposed on the square supercell of 164 cylinders (Fig. 1), discretized by a 616×616 grid. The cylinders occupy about 30% of the total volume. The solid line in Fig. 2 is the corresponding DOS for the TM

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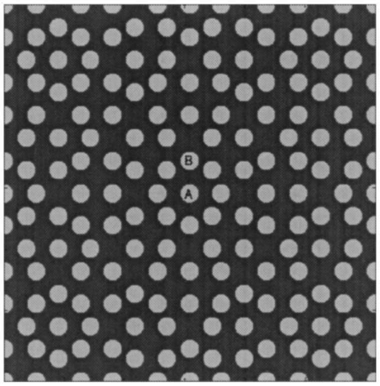

FIG. 1. "Octagonal tiling" arrangement of dielectric cylinders with $\epsilon = 10$.

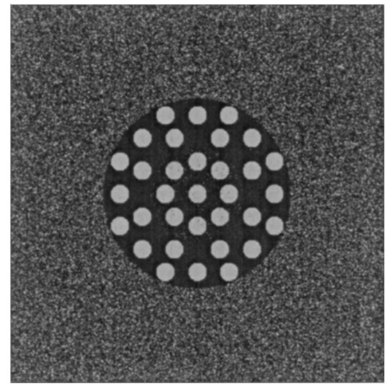

FIG. 3. A small circular segment of Fig. 1.

modes, with E field parallel to the cylinders. The DOS has a multiple of spectral gaps inside which TM mode propagation is forbidden. These spectral gaps are the intrinsic property of the aperiodic arrangement. If the gaps are an artifact of the periodic boundary condition, the position and size of the gaps should depend sensitively on the size of the supercell chosen. We found that the opposite is true. The dotted line shown in Fig. 2 is the TM mode DOS of a bigger realization (274 cylinders) of the octagonal aperiodic structure, and the frequency and size of the first two dominant gaps are virtually identical to the smaller 164-cylinder cell [13]. These cylinder arrays are not periodic, but the structure is generated from a simple deterministic algorithm. We now consider a structure shown in Fig. 3, which contains only a small portion (a circular cluster of 33 cylinders) of the quasiperiodic structure. The rest is replaced by an effective medium of equal average dielectric constant for the TM mode (i.e., $\epsilon = 0.7 \times 1 + 0.3 \times 10$). We sample the photon LDOS at grid points up to half of the radius [14] of the circular cluster, and the DOS is shown in Fig. 4. Comparing with Fig. 2, we see that the gaps have almost the same midgap frequency and size as the complete structure. This shows that these TM-mode gaps are not an artifact of the boundary condition, and the short-range environment governs the existence of the gaps.

We next consider the TE modes, with the H field parallel to the z axis. We found that, for TE modes to have sizable spectral gaps, the structure should be a connected network. One possible configuration is shown in Fig. 5, in which the high dielectric "veins" of $\epsilon = 10$ occupy about 25% of the volume. The TE mode DOS is shown in Fig. 6, showing a spectral gap at just below five frequency units. The fact that isolated cylinders are good for photonic gaps for the TM mode and a connected network is good for the TE mode has been demonstrated for periodic structures [15]. We found that quasiperiodic arrangements behave in a similar manner, and the structures that have sizable spectral gaps for TE and TM are different. This is not a serious limitation since these two polarizations are decoupled in 2D.

The study of defects in PBG material is at least as important as the study of the perfect PBG materials. It is because many plausible applications of PBG materials in laser, LED, frequency selective filters, and waveguides

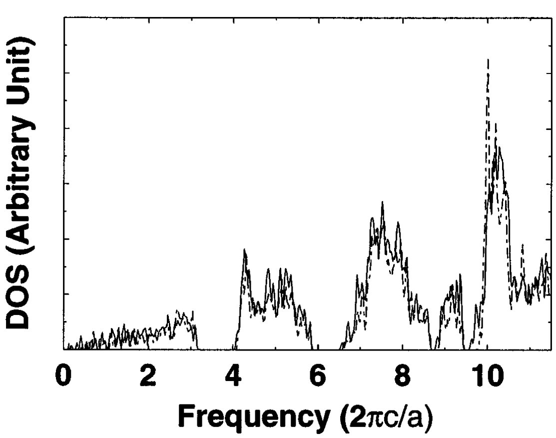

FIG. 2. Solid line: the density of states for TM modes for the structure shown in Fig. 1. Dotted line is the DOS for a larger square supercell. See text and Ref. [11] for the definition of a.

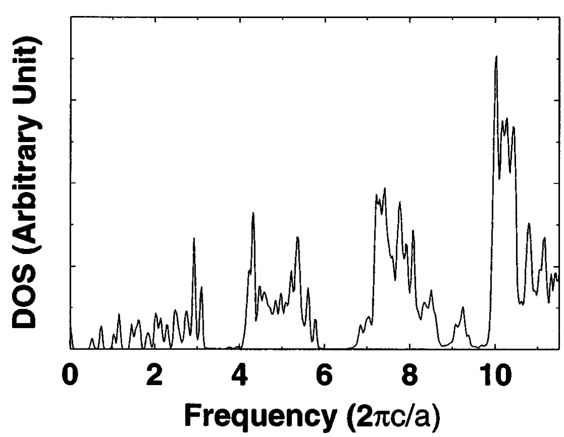

FIG. 4. TM mode DOS for the structure shown in Fig. 3 (see text).

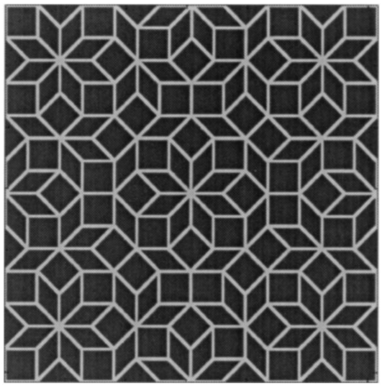

FIG. 5. The structure with spectral gaps in TE modes.

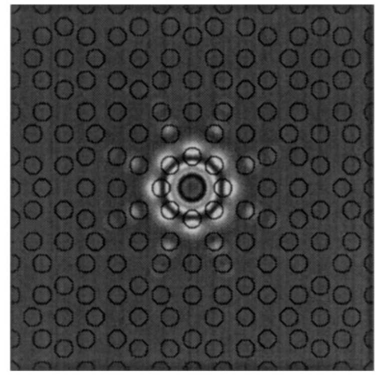

FIG. 7. E-field intensity of the defect mode in the first gap, created by removing a cylinder marked as A in Fig. 1.

are based on the highly localized defect states in the photonic gap. We first remove a cylinder from the center of our cylinder array (labeled A in Fig. 1). This defect site is surrounded by eight cylinders. We found that defect modes are introduced at $\omega = 3.96$ (first gap), 5.96 (second gap), and 9.57 (fourth gap). Since these defect modes have frequencies that are not allowed in the system, the mode has to be localized around the defect. This is confirmed in Fig. 7, where we show the E_z^2 for the defect state in the first gap projected onto the 2D plane. If we remove one of the cylinders surrounding the central cylinder, labeled B in Fig. 1, the defect mode frequency and patterns are very different. There is no defect mode in the first gap, and one defect mode is observed deep inside the second gap at $\omega = 6.3$, and the mode distribution is shown in Fig. 8. This mode is more localized than the mode shown in Fig. 7, consistent with the fact that it is farther away from the band edges and deeper into the spectral gap.

The behavior of defects of these systems is more interesting, and possibly more useful than the defect states in periodic PBG material. Removing one cylinder from a periodic array would produce one fixed set of localized defect modes. However, for a quasicrystalline arrangement of cylinders, each cylinder is located in a different environment, so that removing one cylinder from a different location can produce defect states with different frequencies and mode patterns as illustrated by the example given. Even if we focus on local nearest-neighbor environments near a particular cylinder, there are six types of sites with coordination numbers ranging from three to eight. It is of course also possible to "tune" the defect mode properties in periodic PBGs by changing the nature and size of the defects [16], but the "photonic quasicrystals" allow for a higher degree of flexibility and tunability for defect mode properties.

Photon localization is an effect of fundamental interest and has motivated the introduction of the concept of photonic band gap [4]. Up to now, the realization of photon localization is based on periodic order and is facilitated by the introduction of either defect or disorder in an otherwise perfect periodic photonic crystal. On the other hand, it is known from tight-binding models and force-and-spring models that quasicrystalline arrangements have nonextended eigenstates in 1D and 2D. Figure 9 shows the H_z^2 of a TE mode with frequency near the upper edge of the photonic gap shown in Fig. 6 (marked by an arrow). This state is strongly peaked about the central eightfold

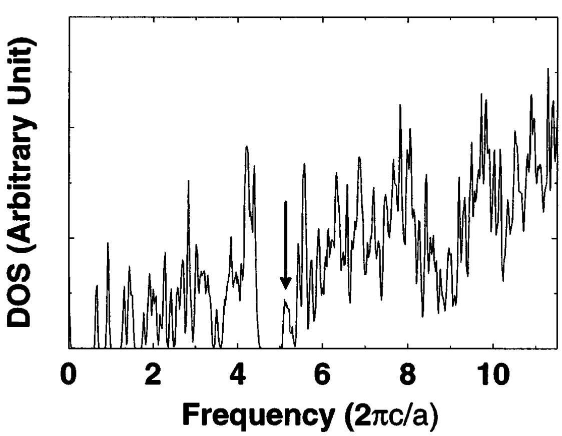

FIG. 6. The TE mode DOS for the structure shown in Fig. 5.

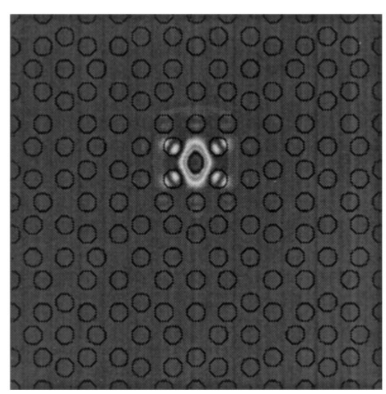

FIG. 8. E-field intensity of the defect mode in the second gap, created by removing a cylinder marked as B in Fig. 1.

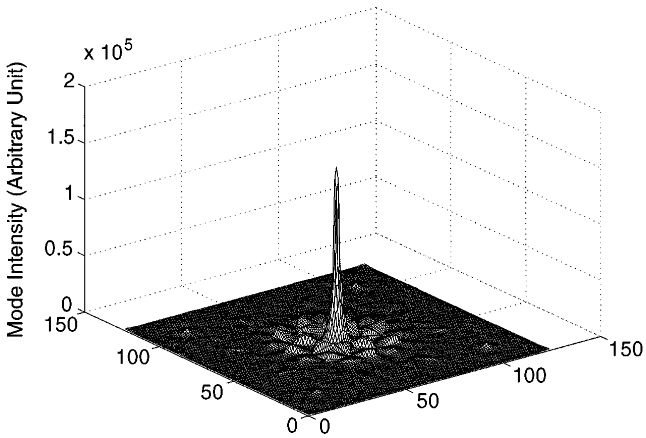

FIG. 9. The H_z^2 of a TE mode near the band edge. High frequency oscillations have been filtered out to show the envelope function.

coordinated cylinder. States with slightly different frequencies are found to be localized about other eightfold sites in the structure. States that are in the "pass band" far away from the band edge look extended relative to the size of our sample. Although our system is too small for a quantitative characterization of the localization property of these states, the results show that photonic "quasicrystals" can open another possibility of realizing the localization of photons, and the localization behavior may be qualitatively different from that of disordered media. We note that these highly localized states have nothing to do with defect or disorder.

More attention has been focused on 2D photonic crystals recently [17], probably because fabricating photonic band gap materials in 3D can be a major technological challenge [18], but it is more manageable in 2D [19]. In the microwave regime, the quasiperiodic arrangement (Fig. 1) can be realized by putting some dielectric rods in a predefined pattern, and experiments can be performed similar to the crystalline arrangement [20]. Scaling down to infrared or optical wavelengths would require defining (say by lithography) and etching a 2D pattern vertically downwards into a substrate. This should not be too difficult with current technology.

In summary, we showed that spectral gaps exist in a 2D quasiperiodic arrangement of dielectrics, and that periodicity is not required for the opening of photonic gaps. Since the quasiperiodic arrangement has many inequivalent local environments, the properties of defects are more complex and interesting then those created in photonic crystals, and may offer more flexibility in tuning the defect state properties. Photonic quasicrystals also offer new platforms for realizing and investigating the localization of light. It would be interesting to see if the same effects can be found in 3D, but it is dangerous to extrapolate current results to higher dimensions unless explicit calculations are performed.

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