

Photonic Band Structure: The Face-Centered-Cubic Case

E. Yablonovitch and T. J. Gmitter

Bell Communications Research, Navesink Research Center, Red Bank, New Jersey 07701-7040

(Received 25 July 1989)

We employ the concepts of band theory to describe the behavior of electromagnetic waves in three dimensionally periodic face-centered-cubic (fcc) dielectric structures. This can produce a "photonic band gap" in which optical modes, spontaneous emission, and zero-point fluctuations are all absent. In the course of a broad experimental survey, we have found that most fcc dielectric structures have "semimetallic" band structure. Nevertheless, we have identified one particular dielectric "crystal" which actually has a "photonic band gap." This dielectric structure requires a refractive-index contrast greater than 3 to 1, which happens to be readily obtainable in semiconductor materials.

PACS numbers: 42.50.-p, 41.10.Hv, 71.25.Cx, 84.90.+a

By analogy to electron waves in a crystal, light waves in a three dimensionally periodic dielectric structure should be described by band theory. Recently, the idea of photonic band structure^{1,2} has been introduced. This means that the concepts of reciprocal space, Brillouin zones, dispersion relations, Bloch wave functions, van Hove singularities, etc., must now be applied to electromagnetic waves. If the depth of refractive-index modulation is sufficient, then a "photonic band gap" could open up. This is an energy band in which optical modes, spontaneous emission, and zero-point fluctuations are all absent.

It is interesting that the most natural real-space structure for the optical medium is face-centered cubic (fcc), which also happens to be the most famous atomic arrangement in crystals. The following contrasts between electronic and photonic band structure are striking: (i) The underlying dispersion relation for electrons is parabolic, while that for photons is linear. (ii) The angular momentum of electrons is $\frac{1}{2}$, but the scalar-wave approximation is frequently made; in contrast, photons have spin 1 and the vector-wave character plays a major role in the band structure. (iii) Band theory of electrons is only an approximation due to electron-electron repulsion, while photonic band theory is essentially exact since photon interactions are negligible.

The possible applications of such a photonic band gap are rather interesting. In addition to quantum electronic applications, such as spontaneous-emission inhibition,¹ there have also been proposals^{2,3} to study mobility edges and Anderson localization within such a forbidden gap. Furthermore, Kurizki and Genack⁴ have shown that atomic and molecular physics is profoundly modified in a volume of space in which "vacuum fluctuations" are absent. In particular, the resonant interatomic potential of homonuclear diatomic molecules, as well as many other atomic physical properties, are severely modified in such a spatial region.

Since we are only at the threshold of such research, we have elected to do our initial experimental work at microwave frequencies, where the periodic dielectric structures can be fabricated by conventional machine tools.

Furthermore, this has enabled us to use sophisticated microwave homodyne detection techniques to measure the phase and amplitude of the electromagnetic Bloch wave functions propagating through the "photonic crystal."

Earlier work^{1,2} had indicated that it was desirable for the Brillouin zone in reciprocal space to be as near to spherical as possible. The lowest-order Brillouin zone for the fcc structure happens to be nearer to spherical than the Brillouin zone of any other common crystal structure. In the absence of any further theoretical guidance, we adopted an empirical, Edisonian approach. Literally, we used the cut-and-try method. Dozens of fcc structures were painstakingly machined out of low-loss dielectric materials. These structures, which we call "crystals," were roughly cube shaped and contained up to ~ 8000 "atoms." In some cases the atoms were dielectric spheres, in other cases the atoms were spherical cavities filled with air ("spherical air atoms"), the interstitial space consisting of dielectric material. The atomic volume filling fraction was varied from 11% to 86%. Refractive-index contrast was varied between 1.6 to 1 and 3.5 to 1. This tedious cut-and-try approach was very time consuming, but it tended to ensure that no possibilities were overlooked.

The main conclusion of this paper is that a photonic band gap can indeed be achieved in three-dimensional dielectric structures, but it requires an index contrast nearly 3.5 to 1. The early predictions had been much more optimistic, anticipating a gap opening up at index contrast 1.21 to 1 in one case¹ and 1.46 to 1 in the other.² In the experiments, all the test structures except one turned out to be "semimetals" and only one particular geometry having index contrast 3.5 to 1 gave rise to a "semiconductor" with a true photonic band gap. In semimetals, the valence band in one section of the Brillouin zone has an energy overlap with the conduction band in a different section of the Brillouin zone. A true band gap, as in a semiconductor, requires a forbidden band of energies *irrespective of the propagation direction* in reciprocal space.

Fortunately, crystalline silicon and other semiconductors are excellent infrared optical materials, providing re-

fractive indices ~ 3.5 . Therefore the optimal structure we have found in the microwave experiments can be scaled down in size to provide a photonic band gap in the near infrared.

These investigations employed the experimental arrangement shown in Fig. 1. A monopole antenna (a 6-mm pin above a ground plane) launches a spherical wave down a long anechoic chamber built of microwave-absorbing pads. The wave front becomes approximately planar by the time it reaches the "crystal" at the opposite end of the chamber, and passes onto the receiving monopole. A microwave oscillator feeds the homodyne detection system with a frequency sweep from 1 to 20 GHz. This phase and amplitude measuring system resembles an optical Mach-Zender interferometer. The relative phase shift is linearly proportional to wave vector k . In principle, it is possible to map out the full dispersion relation, i.e., frequency versus wave vector or ω vs k . Additionally we used commercial equipment such as the HP-8510 Network Analyzer, which can read out directly group velocity versus frequency.

In our most interesting crystal, the one which has a photonic band gap, the spherical atoms consist of air, while the space between the atoms is filled with a dielectric material. This commercial low-loss dielectric, Emerson & Cuming Stycast-12, has a microwave refractive index of 3.5. The material volume is only 14% while the fraction occupied by spherical air atoms is 86%. In fcc close-packed structures, the atomic volume is only 74%. Therefore the atomic spheres are actually closer than close packed; i.e., they overlap slightly. Because of the overlapping atoms, it is possible to see all the way through the crystal along certain directions.

Crystals consisting of spherical air atoms are relatively easy to fabricate. A series of hemispheres are drilled on one face of a dielectric plate by a numerically controlled

machine tool. On the opposite face of the plate an offset series of hemispheres are drilled. Then many of these plates are simply stacked up so that the hemispheres face one another, forming spherical air atoms. The volume fraction is varied by changing the hemispherical diameter.

The dielectric-atom crystals consisted of polycrystalline Al_2O_3 spheres, 6 mm in diameter with a microwave refractive index of 3.06. The volume fraction was varied by changing the sphere spacing. The dielectric spheres were supported by thermal-compression-molded dielectric foam of refractive index ~ 1.01 .

The philosophy behind our experiments is to map out the frequency-versus-wave-vector dispersion relations for a whole series of three-dimensional fcc crystals. For each crystal it becomes necessary to explore all the different angles in reciprocal space. The valence-band edge is defined by the sudden drop in microwave transmission relative to a reference frequency scan with the crystal absent. The conduction-band edge is defined by the frequency at which the transmitted signal recovers.

These two frequencies define band edges, but they do not necessarily fall at exactly the same point on the surface of the Brillouin zone. Upon transmission through the crystal surface, only the component of wave-vector momentum parallel to the surface plane is conserved. In our experiments, the external angle of incidence is held fixed as the frequency is swept. Therefore the upper and lower gap edge frequencies will appear at different Brillouin-zone positions. Because of the limitations on the external wave vector which could be attained in air, some parts of the Brillouin zone sometimes had to be accessed by transmission through a pair of giant microwave prisms on either side of the crystal. The prisms, over 15 cm square and made of polymethylmethacrylate (microwave refractive index 1.6), increased the available external wave vector.

Step by step, the angle of incidence is varied, and the frequency of the first and second band edges is mapped out on the surface of the Brillouin zone. Unfortunately, with this method it is not possible to learn much about the higher-frequency bands above the two lowest band edges. We determine only the valence-band edge where transmission is cut off, and the conduction-band edge where transmission cuts on again.

The result of these measurements on our 86% spherical-air-atom crystal is plotted in Fig. 2. For electromagnetic waves, two band structures must be shown, allowing for the two possible polarization states.⁵ The lines that are slanted to the right fill in the band gap for linear polarization parallel to the X plane (mostly s polarized). The left-slanted lines fill in the band gap for the orthogonal linear polarization with a partial component perpendicular to the X plane (mostly p polarized). On the high-symmetry planes, $X-U-L$ and $X-W-K$, the two linear polarizations are not expected to mix, and therefore the linearly polarized antenna excites elec-

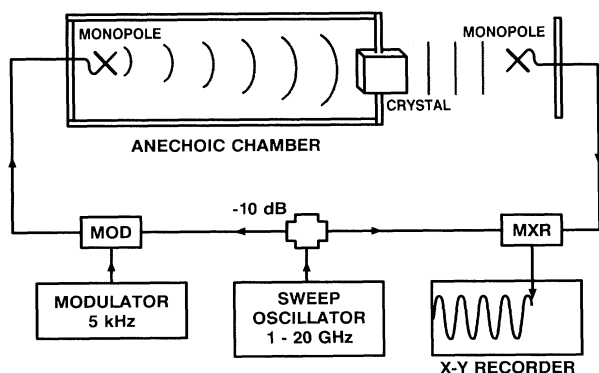


FIG. 1. A sweep oscillator feeds a 10-dB splitter. Part of the signal is modulated (MOD) and then propagated as a plane wave through a face-centered-cubic dielectric crystal. The other part of the signal is used as a local oscillator for the mixer (MXR) to measure the amplitude change and phase shift in the crystal. Between the mixer and the X-Y recorder is a lock-in amplifier (not shown).

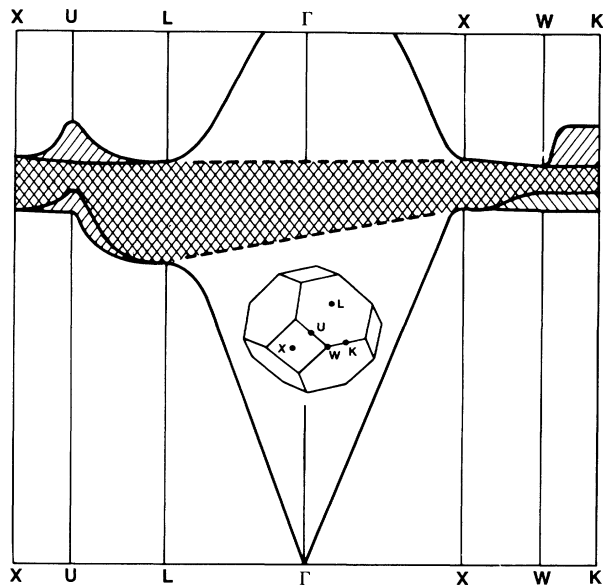


FIG. 2. The experimentally observed photonic band structure in reciprocal space of the 86% spherical-air-atom crystal. The right-sloping lines represent polarization parallel to the X plane, while the left-sloping lines represent the orthogonal polarization which has a partial component out of the X plane. The cross-hatched region where both polarizations are forbidden in all directions in k space is the "photonic band gap."

tromagnetic eigenstates of the crystal. Off the high-symmetry planes, the polarization eigenstates are no doubt complex, and some type of elliptical polarization should be expected. No absolute frequency units are given in Fig. 2, since the frequencies should all scale with the reciprocal linear size of the crystal spacing. On the actual crystal, the fcc unit cube length " a " was equal to 12.7 mm and the forbidden gap was ~ 1 GHz wide, centered at 15 GHz.

At frequencies within the forbidden gap, the wave vector is purely imaginary, and it measures the attenuation length within the crystal. Attenuation was generally very strong within the band gap, consistent with a $1/e$ attenuation length of only one or two crystal unit cells. At points where the band gap was very narrow, however, particularly for p -polarized waves at the point U , the attenuation length was much longer, ~ 10 or 20 unit cells.

All the ~ 20 other crystal structures that were fabricated and tested in our experiments produced "semimetals" rather than "photonic band gaps." Most frequently, the conduction band at the point L in the Brillouin zone generally tended to overlap in energy with the valence band at the points W and U . Inevitably if band gaps at the X and L points were inadequate, band overlap would develop at peripheral points between facets, such as U , W , or K .

We found that the X -point center frequency was a good extrapolation of the low-frequency dispersion out to

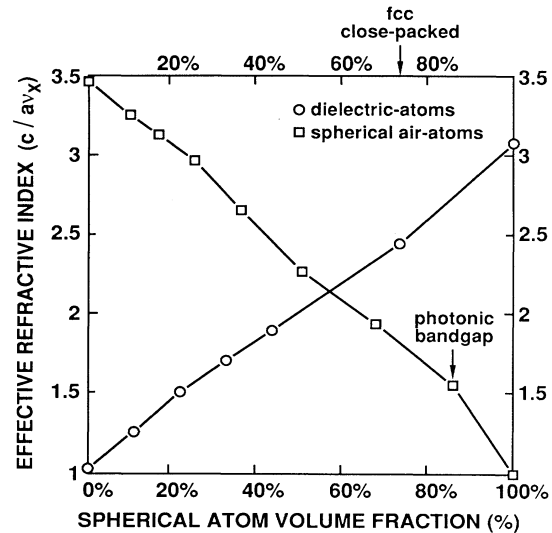


FIG. 3. The effective long-wavelength refractive index of two basic crystal structures at various volume fractions. Spherical dielectric atoms are represented by \circ and spherical air atoms are represented by \square . fcc close packing occurs at 74% volume fraction. Of all these structures, only the one marked "photonic band gap" has a forbidden frequency band for all directions in reciprocal space.

the X point, making c/av_X a good approximation to the long-wavelength refractive index. The experimental indices in Fig. 3 are modeled by a simple linear interpolation of refractive index with volume fraction. Only the one structure marked "photonic band gap" had a forbidden gap all the way around the Brillouin zone.

The measured gap width normalized to v_X is plotted against spherical-air-atom volume fraction in Fig. 4. We believe that the null X gap at 68% volume fraction is a node at which the $\langle 200 \rangle$ Fourier component of dielectric modulation changes sign. This sign change is simply due to a shift of material density from the interstitial layers to the cube faces as the spherical-air-atom radius goes up. Accordingly, we plotted the 86% X -gap point as a negative quantity. The L gaps were all positive, however.

The gap widths for spherical dielectric Al_2O_3 atoms in Fig. 5 are all rather feeble. The L -plane gap exhibited a polarization dependence even at the center of the hexagonal L plane, where s and p polarizations are degenerate. The X -plane gap was stronger. The index contrast was 3.03 to 1, somewhat less than the spherical-air-atom case, but that does not explain the semimetallic behavior. Instead it must be attributed to the smallness of the L -plane gap at all tested volume fractions.

Our dielectric structures represent the classic⁶ muffin-tin potential. Nevertheless, we have analyzed our data in terms of the "nearly free-photon model" which is appropriate so long as the wave functions are weakly perturbed plane waves. The widest relative gap width, which measures the strength of perturbation, occurred at

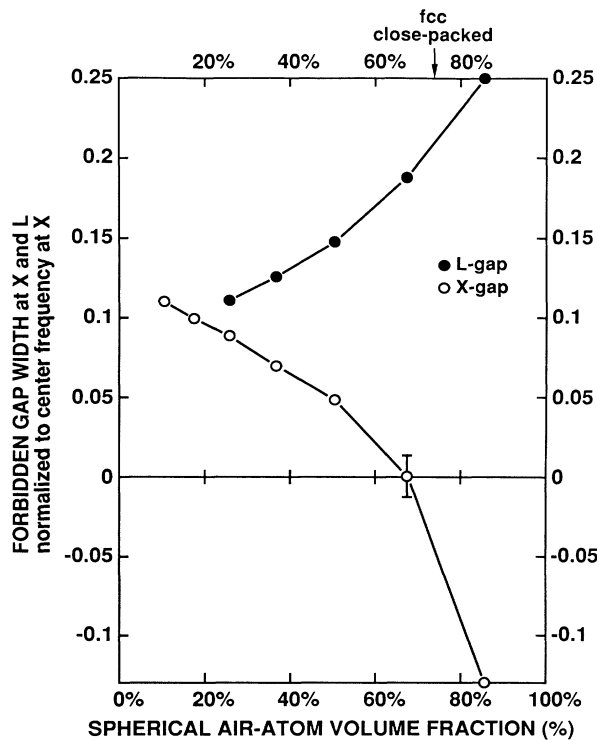


FIG. 4. The forbidden gap width normalized to ν_X observed at the L point (●) and at the X point (○) for a series of spherical-air-atom fcc crystals of varying atomic volume fraction. The interstitial dielectric material has a refractive index of 3.5. We have elected to plot the 86% X -gap width as a negative number since the $\langle 200 \rangle$ Fourier component has opposite sign on either side of the null point at 68% volume fraction.

the L point in the 86% spherical-air-atom crystal and was only $\sim \frac{1}{4}$. All other gap widths were at least a factor of 2 smaller, lending credence to the model.

At the point W , four different plane waves are degenerate. The $\langle 111 \rangle$ and $\langle 200 \rangle$ dielectric Fourier components split the modes, but two remain degenerate. This is no accident, nor is it specific to the nearly free-photon model. It arises directly from the group-theoretical properties of the W point in the fcc structure. In the character tables given by Callaway,⁷ the W_3 representation is doubly degenerate. If the ordering of energy levels was unfavorable, then valence and conduction bands would touch at the degeneracy. Fortunately, the sign and strength of the $\langle 111 \rangle$ and $\langle 200 \rangle$ Fourier components prevent this from happening in the 86% spherical-air-atom crystal.

In calculating the split level structure at the points W and U in terms of the measured X - and L -gap widths, it

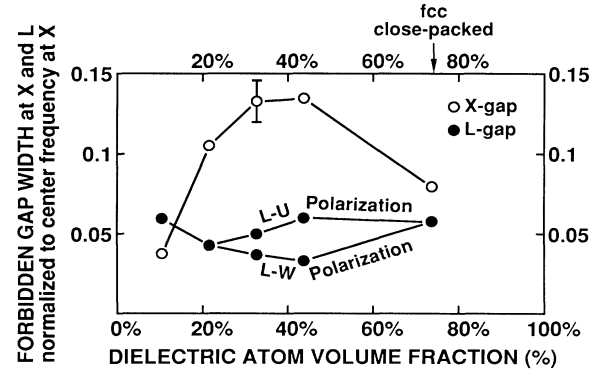


FIG. 5. The forbidden gap width normalized to ν_X observed at the L point (●) and at the X point (○) for a series of fcc crystals made of Al_2O_3 spherical dielectric atoms (refractive index 3.06). The atomic volume fraction was varied by changing the size of the unit cube. In all cases, the L -point gap width was too feeble for the existence of a "photonic band gap."

is necessary to take polarization into account. Fortunately, in the high-symmetry planes $X-U-L$ and $X-W-K$, there exist two orthogonal linear polarizations which are not expected to mix. The calculations⁸ are in reasonable agreement with experiment for both polarization components of the measured band structure at the point U in Fig. 2. However, a similar calculation (requiring more trigonometry) at the W point leads to gap widths that are significantly larger than observed in Fig. 2.

We would like to thank Professor S. John for numerous discussions and Professor Gene Mele for help with the group theory.

¹E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).

²S. John, Phys. Rev. Lett. **58**, 2486 (1987).

³S. John, Comments Condens. Matter Phys. **14**, 193 (1988).

⁴G. Kurizki and A. Z. Genack, Phys. Rev. Lett. **61**, 2269 (1988).

⁵S. John and R. Rangarajan, Phys. Rev. B **38**, 10101 (1988).

⁶N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders, Philadelphia, 1976), pp. 171 and 172.

⁷J. Callaway, *Quantum Theory of the Solid State, Part A* (Academic, New York, 1974), Appendix C.

⁸E. Yablonovitch, in "Analogies in Optics and Microelectronics," edited by W. van Aeringen and D. Lenstra (Kluwer, Hingham, MA, to be published).