Photonic band structure: the face-centered-cubic case

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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" that actually has a "photonic band gap." This dielectric structure consisting of 86% empty space, requires a refractive-index contrast of greater than 3:1, which happens to be readily obtainable in semiconductor materials.

INTRODUCTION

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 so-called 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 contrasts between electronic and photonic band structures are striking:

(i) The underlying dispersion relation for electrons is parabolic, while that for photons is linear.

(ii) The angular momentum of electrons is 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 quite tantalizing. In addition to quantum-electronic applications, such as spontaneous emission inhibition,¹ there have also been proposals^{2,3} for studying 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 zero-point electromagnetic 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 research at microwave frequencies, for which the periodic dielectric structures can be fabricated by conventional machine tools. Furthermore, this has enabled us to use sophisticated microwave homodyne detection techniques for measuring the phase and amplitude of the electromagnetic Bloch wave functions propagating through the photonic crystal.

Earlier research^{1,2} had indicated that it was desirable for the Brillouin zone in reciprocal space to be as near to spherical as possible. Among possible three-dimensional periodic structures, this had suggested that face-centered-cubic (fcc) dielectric geometry would be optimal for achieving a photonic band gap. The lowest-order Brillouin zone for the fcc structure happens to be closer 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 might be called 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 1.6:1 and 3.5:1. The propagation of electromagnetic waves through these structures was then carefully investigated. This tedious cut-and-try approach was time consuming, but it helped 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 of nearly 3.5:1. The early predictions had been much more optimistic, anticipating a gap opening up at an index contrast of 1.21:1 in one case¹ and 1.46:1 in the other.² In our experiments all the test structures except one turned out to be "semimetals," and only one particular geometry having an index contrast of 3.5:1 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



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

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

EXPERIMENT

These investigations employed the experimental arrangement that is shown in Fig. 1. A monopole antenna (a 6-mm pin over 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 fcc dielectric structure at the opposite end of the chamber. (Henceforth the fcc dielectric structure will be called the crystal.) Only the plane wave passing directly through the crystal can be seen by the receiving monopole. A microwave oscillator feeds the homodyne detection system with a frequency sweep from 1 to 20 GHz. This homebuilt system resembles an optical Mach-Zehnder interferometer. (Alternatively, a Hewlett-Packard 8510 Network Analyzer was also used to perform the amplitude and phase measurements.) The X-Y recorder plots the interference pattern as a function of microwave frequency.

An example of such a series of interference fringes is shown in Fig. 2 for the transmission of microwaves through a quarter-wavelength stack of nine polystyrene plates (index 1.6, thickness 6 mm) spaced by quarter-wavelength air layers. In such a simple one-dimensional layered structure, a pronounced stop band or one-dimensional band gap occurs around 6.5 GHz. Two curves are present in Fig. 2. The heavy curve is a reference interference fringe pattern showing the antenna transmission function if the stack of plates is removed. Variations in the wave envelope as a function of frequency are simply due to variations in the antenna efficiency. The lighter curve represents the experimental signal, the interference fringe pattern observed if the quarterwavelength stack of plates is inserted into the path of the microwave beam. Over a 2-GHz band, centered on 6.5 GHz, the transmitted beam is severely attenuated. This is the stop band.

Notice also the phase shift with respect to the reference beam in Fig. 2. At 4.5 and at 9 GHz, on either side of the stop band, the signal fringes and the reference fringes are essentially in phase. At the band edges, the behavior is quite different. Owing to group-velocity dispersion, the signal beam is shifted roughly 180 deg compared to the reference beam at the upper-band-edge and lower-band-edge frequencies, 5.5 and 7.5 GHz, respectively. The relative



Fig. 2. Interference pattern produced when a microwave signal being transmitted between antennas interferes with a local oscillator wave. The heavy curve is a reference fringe pattern for the case of transmission through an empty space. The envelope fluctuations are due to variations in antenna efficiency. The lighter curve is for transmission through nine polystyrene plates spaced at one-quarter wavelength. A band gap opens up between 5.5 and 7.5 GHz. Furthermore, on either side of the band gap there is an \sim 180-deg phase shift.



Fig. 3. Three-dimensional periodic structure that had a photonic band gap. This fcc crystal consisted of spherical air atoms that were larger than close packed. The resulting overlap of the air atoms permits us to see visible light transmitted all the way through the structure along the $\langle 111 \rangle$ direction. The interstices between the atoms are filled with dielectric material of a refractive index of 3.5. The overall structure is 86% air and only 14% solid material.



Fig. 4. Three-dimensional fcc crystal consisting of Al_2O_3 spheres of a refractive index of 3.06. These dielectric spheres are supported in place by the blue foam material, of refractive index 1.01. These spherical dielectric atom structures failed to show a photonic band gap at any volume fraction.

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phase shift is linearly proportional to wave vector k. In principle, with an apparatus of this type, it is possible to map out the full dispersion relation, i.e., frequency versus wave vector or ω versus k. Similarly, such commercial equipment as the Hewlett-Packard 8510 Network Analyzer can read out directly in terms of group velocity versus frequency.

Our most interesting crystal, exhibited in Fig. 3, is the one that has a photonic band gap. Its structure is most unusual. The spherical atoms consist of air, while the space between the atoms is filled with a dielectric material. This commercial low-loss dielectric material, Emerson and Cumming Stycast-12, has a microwave refractive index of 3.5. The volume fraction occupied by the spherical air atoms is 86%. In fcc close-packed structures, the atomic volume is only 74%. Therefore the atomic spheres in Fig. 3 are actually closer than close packed, i.e., they overlap slightly. Owing to the overlapping atoms, it is possible to see all the way through the crystal along certain directions. The bright spots of light emerging on the top surface of the crystal in Fig. 3 are being channeled from below along the $\langle 111 \rangle$ direction.

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 hemisphere diameter.

The beauty of spherical air-atom crystals is that they are self-supporting. The more obvious fcc structure consisting of dielectric spheres is self-supporting only for the case of close packing. For any smaller volume packing fraction, the dielectric spheres must be supported in position. The dielectric spheres consisted of polycrystalline Al_2O_3 , 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 a refractive index of ~1.01. Precision molds were built of aluminum jig plates having 6mm-diameter steel ball bearings embedded in them. Dielectric foam pads were molded at 95°C, with the molds released at 40°C. The hemispherical depressions in the molded foam were then filled with the Al_2O_3 spheres and the structure built up into many layers. Figure 4 is a photograph of such a crystal consisting of dielectric spheres supported by the blue dielectric foam.

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 interference fringe pattern in Fig. 5 is an example of such a measurement on the 86% spherical air-atom crystal of Fig. 3. These fringes are produced in the homodyne detection system by an electromagnetic wave propagating toward the L-U line of the hexagonal L plane in reciprocal space. This wave was predominantly s-polarized; i.e., it was polarized parallel to the X plane. Two important items emerge from Fig. 5: the lower-gapedge frequency and the upper-gap-edge frequency. The lower edge is defined by the sudden drop in microwave transmission relative to a reference scan with the crystal absent. The upper edge is defined by the frequency at which the transmitted signal recovers.

These two frequencies define band edges, but these band



Fig. 5. Forbidden gap observed on the crystal displayed in Fig. 3 and measured along the L-U line of the L plane. The electromagnetic wave is polarized parallel to the X plane (s polarization).

edges do not necessarily fall at exactly the same point on the surface of the Brillouin zone. The reciprocal space position of these frequency edges is determined by momentum conservation between the external and internal electromagnetic waves. In our experiments, the incoming plane wave was generally incident on the $\langle 100 \rangle$ face of the crystal. (The (100) face is, by definition, perpendicular to the (100) momentum direction.) On transmission through the crystal surface, only the component of wave-vector momentum that is parallel to the surface plane is conserved. This is similar to the principle that leads to Snell's law. In our geometry it means that the component of wave-vector momentum that is perpendicular to the (100) direction, $(0, k_y, k_z)$, is conserved on entering the crystal. The position of the frequency edge in reciprocal space is the point on the Brillouin zone surface having those identical momentum components k_{y} and k_z . In our experiments, the external angle of incidence is held fixed as the frequency is swept. Therefore the uppergap-edge and lower-gap-edge frequencies will have different $k_{\rm v}$ and $k_{\rm z}$ and different Brillouin zone positions.

Owing to the limitations on the external wave vector $\langle 0, k_y, k_z \rangle$ that could be attained in air, some parts of the internal 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, were made of polymethyl methacrylate (microwave refractive index of 1.6) in order to increase 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. Our measurements concentrated on the high-symmetry planes X-U-L and X-W-K, though lower symmetry points were also occasionally investigated. (See Fig. 6 for a description of the Brillouin zone point labels.) Unfortunately, with this method it is not possible to learn much about the higher-frequency bands above the two lowest band edges. At higher frequencies, a superposition of allowed electromagnetic modes can become excited by an incident plane wave. This makes it difficult to disentangle any higher band edges. Accordingly, we determine only the first gap edge where transmission is cut off and the second gap edge where transmission cuts on again. In keeping with the electron-band-structure analogy, the first gap edge may be called the valence band and the second gap edge may be called the conduction band.

The result of these measurements on our 86% spherical air-atom fcc dielectric structure (Fig. 3) is plotted in Fig. 6. For electromagnetic waves, two band structures must be shown, thus allowing for the two different polarization states of electromagnetic waves. The forbidden band gap in Fig. 6 is filled in by slanted lines. The lines that are slanted up to the right fill in the band gap for linear polarization that is parallel to the X plane (mostly s polarized). The lines slanted up to the left 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 electromagnetic 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



Fig. 6. Experimentally observed photonic band structure in reciprocal space of the fcc spherical air atoms surrounded by dielectric configuration of Fig. 3. The lines sloping up to the right represent predominantly s polarization relative to the Brillouin zone, while the lines sloping up to the left represent predominantly p polarization. The cross-hatched region for which both polarizations are forbidden in all directions in k space is the photonic band gap.

given on Fig. 6, 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.

The band structure in Fig. 6 plots frequency versus real wave vector. At frequencies within the forbidden gap, the wave vector is pure imaginary, and it measures the attenuation length within the crystal. Attenuation was generally 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 narrow, however, particularly for *p*-polarized waves at the point *U*, the attenuation length was much longer, approximately 10–20 unit cells.

All the 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. An example of such a band structure is shown in Fig. 7 for the case of 50% volume fraction spherical air atoms embedded in polystyrene of a refractive index of 1.6. In our experiments we found that it was essential to start out with large forbidden gaps at the points X and L at centers of the square and hexagonal facets of the Brillouin zone. Invariably if band gaps at the X and the L points were inadequate, band overlap would become established at peripheral points between facets, such as U, W, or K. In our experimental survey, a semimetallic band structure occurred in all cases but one.

Let us now analyze more of the band structure properties as a function of volume fraction and structure type. Figure



Fig. 7. Example of a photonic band structure similar to that of a semimetal. The fcc structure was 50% volume fraction air atoms but was made of polystyrene, with a refractive index of only 1.6. The conduction band at the L point overlaps the valence band at the U and W points. In order to get a band gap, both the volume fraction of atoms must be increased and the index contrast must be increased.



Fig. 8. Effective long-wavelength refractive index $c/a\nu_X$ measured on two basic crystal structures of various volume fractions, where cis the speed of light in vacuum, a is the length of the unit cube, and ν_X is the center frequency of the X gap. Fcc close packing occurs at 74% volume fraction. Spherical dielectric atoms and spherical air atoms are the two basic types. Of all these structures, only the one marked photonic band gap had a forbidden frequency band at all directions in reciprocal space.

8 gives the refractive index of the different crystal structures as a function of volume filling fraction. The effective refractive index is defined as $c/a\nu_X$, in terms of the center frequency, ν_X , of the X-point gap. We found that the X-point center frequency was a good extrapolation of the low-frequency dispersion out to the X point. Therefore $c/a\nu_X$ is a good surrogate representation of the long-wavelength refractive index of the composite structure represented by these fcc crystals. For both the spherical air atoms and the dielectric sphere atoms, a simple linear interpolation of refractive index with volume fraction seems to describe the experimental indices in Fig. 8. Neither of the effective medium theories, not Maxwell-Garnett nor Bruggeman were any more accurate in modeling Fig. 8. Only the one structure marked photonic band gap on Fig. 8 had a forbidden gap all the way around the Brillouin zone. All the others were semimetals as mentioned earlier.

In view of the importance of having large gap widths at the L point and at the X point, we present those results in Fig. 9. The measured gap width normalized to ν_X is plotted against spherical air-atom volume fraction. All the results in Fig. 9 were taken on Emerson and Cumming Stycast-12, a material with an index contrast of 3.5:1 relative to air. It is clear from Fig. 9 why the 86% volume fraction spherical air-atom structure has an overall photonic band gap. Its gap widths are far larger than any of the others.



Fig. 9. Forbidden gap width normalized to v_X and 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 dielectric material between air atoms had a refractive index of 3.5. We have elected to plot the 86% X-point gap width as a negative number since the (200) Fourier component has the opposite sign on either side of the null point at 68% volume fraction.

Notice the unusual behavior of the X gap as a function of spherical air-atom volume fraction. At approximately 68% volume fraction the X-gap width becomes undetectable, while at the higher-volume fraction of 86% it rises again to a large value. While our measurements can assign only an absolute magnitude to the gap width, we have elected to plot this last data point as a negative quantity. As is shown in Ref. 2, the gap width on any plane in reciprocal space is proportional to the corresponding Fourier component of the dielectric constant. We believe that the zero gap at 68% volume fraction is a node at which the Fourier component of dielectric modulation changes sign.

It is not entirely surprising for the X-plane Fourier component of the dielectric constant to change sign at a volume fraction near close packing. Figure 10 is a perspective view of the fcc close-packed structure. Remember that the spheres are air and the spaces between the spheres are filled with dielectric material. At the lower edge of the band gap. the Bloch electric-wave function tends to be concentrated in the high-dielectric-constant layers, while the upper-edge electric-field function tends to concentrate in the low-dielectric-constant layers. For the sake of definiteness let us concentrate on lower-edge or valence-band electric-field function near the X plane. The electric field will seek out those layers that are parallel to the cube faces in Fig. 10 that have the highest dielectric constant. If the spherical air atoms are much smaller than close packed, the electric field will weave between the layers of atoms and avoid the atomic layers themselves. For spherical air atoms larger than close packed, as can be seen in Figs. 3 and 10, there is little dielectric material left between the atomic layers and most of the remaining material is in the cusp-shaped volumes in the planes of atoms. In that case the electric field tends to concentrate in the atomic layers themselves.

The plane containing the most dielectric material shifts



Fig. 10. Close-packed fcc structure. If the atoms are air filled and smaller than close packed, the electric field lines of the valence band edge X-gap mode will tend to weave between atomic layers. If the air atoms are larger than close packed or if they are filled with dielectric material, the electric field lines of the valence band edge X-gap mode will tend to concentrate within the planes of atoms.



Fig. 11. Forbidden gap width normalized to ν_X and observed at the L point and at the X point for a series of fcc crystals made of Al₂O₃ spherical dielectric atoms (refractive index of 3.06). The atomic volume fraction was varied by changing the size of the unit cube. Overall, the L-point gap width was too feeble for the existence of a photonic band gap.

from the interatomic layers to the atomic layers as the spherical air-atom volume fraction increases. As a consequence, the amplitude of the Fourier component of the dielectric constant goes through zero and changes sign. This explains the peculiar behavior of the X-gap width in Fig. 9 and justifies plotting the 86% data point as a negative quantity. In that case the valence-band Bloch electric-wave function tends to concentrate in the planes of atoms along the cube faces.

By inspection of Figs. 3 and 10, it is clear that there is no tendency for the L-plane dielectric Fourier component to change sign. The electric field tends to concentrate between the layers of atoms, and there is no indication of a node in the data. Therefore the L gaps were all plotted as positive quantities.

The gap widths for spherical dielectric Al_3O_2 atoms are displayed in Fig. 11. The gap widths are all rather feeble. which explains why no overall photonic band gap was observed for dielectric spheres. The L-plane gap was particularly weak. It exhibited a polarization dependence even at the center of the hexagonal L plane, where s and p polarization are degenerate. The X-plane gap was stronger. There were some indications that the 74% volume fraction X-gap data point should have been plotted as a negative quantity as above. That data point was unusually sensitive to tiny changes in packing geometry, possibly indicating that it was near a node. It the absence of any additional information, we simply left the 74% X-gap width as a positive number in Fig. 11. The index contrast in this case was 3.03:1, somewhat less than the spherical air-atom case. But that is not the reason for the absence of a photonic band gap for the Al_3O_2 dielectric spheres. Instead the absence must be attributed to the smallness of the L-plane gap at all tested volume fractions.

THEORY

A starting point for the behavior of light waves in threedimensional periodic dielectric structures is derived from Maxwell's equations: .

$$-\nabla^{2}\mathbf{E} + \nabla(\nabla \cdot \mathbf{E}) = \epsilon(\mathbf{x}) \frac{\omega^{2}}{c^{2}} \mathbf{E}, \qquad (1)$$

where **E** is the optical electric field, *c* the speed of light, ω is the optical frequency (which plays the role of an eigenvalue), and the geometry of the dielectric structure is contained in the spatial dependence of dielectric constant $\epsilon(\mathbf{x})$. The dielectric constant is related to the refractive index by $\epsilon \equiv n^2$. Equation (1) resembles Schrödinger's equation if $\epsilon(\mathbf{x})\omega^2/c^2$ is identified with the kinetic energy term $2m[E - V(\mathbf{x})]/\hbar^2$, where *m* is the electron mass, \hbar is Planck's constant divided by 2π , *E* is the total energy eigenvalue, and $V(\mathbf{x})$ is the potential energy.

In optics we generally restrict ourselves to positive dielectric constant materials. Metals, which have negative dielectric constants, invariably have significant dissipation as well, i.e., an imaginary component to $\epsilon(\mathbf{x})$. Among the high-quality optical materials, particularly semiconductors, a high positive dielectric constant in the transparent region is accompanied by almost no dissipation. This means that the kinetic energy term $\epsilon(\mathbf{x})\omega^2/c^2$ must always be positive in nondissipative dielectric structures. If potential barriers are permitted, in which the kinetic energy is negative, it would be much easier to confine the wave functions, to produce localization, and to produce forbidden band gaps. In optics with positive dielectric constants, it is challenging to create a photonic band gap. For electrons, in a tight binding model for example, a forbidden band gap occurs right from the outset. The positive kinetic energy for waves in dielectrics is the main reason why only one dielectric crystal, out of the many that we tested, had a photonic band gap.

As is shown in Ref. 2, the vector character of Eq. (1) also contributes to the difficulties of creating a photonic band gap. Waves that are p polarized relative to the local Brillouin zone surface interact more weakly. Vector wave equations are extremely difficult to solve.⁵ This is a pity, since for solid-state-band theorists, our dielectric structures represent the classic muffin-tin potential. In the scalar wave case, this famous potential would be solvable. The various methods for solving wave equations in three-dimensionally periodic media are reviewed in Chaps. 9-11 of Ashcroft and Mermin.⁶ In view of the relatively small gap widths that we have found experimentally and the difficulty of adapting some of the more sophisticated band theory methods to vector waves, we will analyze our data in terms of the socalled nearly free photon model. Our analysis is analogous to the well-known nearly free electron model and is appropriate as long as the wave functions are weakly perturbed plane waves. The widest relative gap width, which measures the strength of perturbation, occurred at the L point in the 86% spherical air-atom crystal and was only $\sim 1/4$. All other gap widths in all the crystals were at least a factor of 2 smaller, which lends reasonable credence to the nearly free photon model.

The nearly free photon model predicts a splitting of bands at the Brillouin zone surfaces:

$$\omega_{\pm} = \omega_0 \left(1 \pm \frac{n_G}{n_0} \right), \tag{2}$$

where ω_{\pm} are the angular frequencies of the upper and lower band edges and ω_0 is the center frequency at that point on the Brillouin zone surface, n_G is the Fourier component of the refractive index corresponding to the reciprocal lattice vector **G** defining that face of the Brillouin zone, and n_0 is the mean refractive index. For the case of a layered structure with refractive-index contrast Δn between layers, the corresponding $n_G = \Delta n/\pi$. In three-dimensional structures, the refractive-index contrast is not organized into simple layers, and the plane-wave Fourier components n_G tend to be much weaker than $1/\pi$ times the index contrast Δn .

Equation (2), as written, applies only to s-polarized electromagnetic waves with respect to the Bragg reflection planes on the Brillouin zone surface. For p-polarized waves, the scattering efficiency is diminished by the projection of the polarization vector onto the new scattered direction. Accordingly, n_G is diminished by $\cos(2\theta) = 2 \cos^2 \theta - 1$, where θ is the angle of incidence onto the Bragg plane forming the Brillouin zone surface. The largest scattering angle on a single facet of the fcc Brillouin zone is $\theta = 39^{\circ}$, subtended by the points L and W. In Yeh⁷ the forbidden gap width is increased by a further angle-dependent factor $1/\cos^2 \theta$. The reason for this additional factor is that they are considering the stop band for a fixed angle of incidence. As explained earlier in the experimental section of this paper, the component of photon momentum that is parallel to the entry plane is conserved. Therefore the upper-band-edge and lower-band-edge frequencies observed experimentally appear at different points along the Brillouin zone surface. The apparent gap width becomes larger by $1/\cos^2 \theta$. By contrast, Eq. (2) gives the band-edge frequencies and gap width at a single point on the Brillouin zone surface.

The quantity n_G/n_0 plays the role of a dimensionless pseudopotential in the nearly free photon model, and we will give it the label V_G . For example, the pseudopotential corresponding to $\mathbf{G} = \langle 111 \rangle$ on the hexagonal L plane of the Brillouin zone can be defined by $V_1 \equiv n_{\langle 111 \rangle}/n_0$. The dimensionless pseudopotential corresponding to $\mathbf{G} = \langle 200 \rangle$ on the square X plane of the Brillouin zone can be defined $V_2 = n_{\langle 200 \rangle}/n_0$. In general these pseudopotentials can also be expected to depend on polarization angles as explained above.

The nearly free photon model becomes particularly interesting at points of degeneracy on the Brillouin zone surface. For example, at the point W, four different plane waves are degenerate and they mix to produce eigenmodes that break the degeneracy. Similarly at the point U, three different plane waves mix to produce a superposition of plane waves. As is shown in Ashcroft and Mermin, the solution requires the diagonalization of the following matrix:

$$\begin{bmatrix} -\Delta\omega/\omega_{W} & V_{1} & V_{1} & V_{2} \\ V_{1} & -\Delta\omega/\omega_{W} & V_{2} & V_{1} \\ V_{1} & V_{2} & -\Delta\omega/\omega_{W} & V_{1} \\ V_{2} & V_{1} & V_{1} & -\Delta\omega/\omega_{W} \end{bmatrix} = 0, \quad (3)$$

where ω_W is the center frequency at point W in the Brillouin zone and $\Delta \omega \equiv (\omega - \omega_W)$, where ω are the new eigenfrequencies. The solutions to Eq. (3) are as follows:

$$\Delta \omega / \omega_W = -V_2 \qquad \text{(twice)}, \tag{4a}$$

$$\Delta \omega / \omega_W = V_2 \pm 2V_1. \tag{4b}$$

Of these four solutions, the two in Eq. (4a) are degenerate. This degeneracy is no accident, nor is it specific to the nearly free photon model. It is quite general and arises directly from the group-theoretical properties of the W point in the fcc structure. In the character tables given by Callaway,⁸ the W₃ representation is doubly degenerate. If Eq. (4a) were to be the lowest-lying frequency at the point W, then a photonic band gap would be impossible, since valence and conduction bands would touch. This can be prevented in two ways: (i) V_1 can be larger than V_2 ; (ii) V_2 can be negative, as is shown in Fig. 9. Either case will ensure that at least one of the two solutions of Eq. (4b) is less than the solutions of Eq. (4a).

The difference between the wave functions for the solutions to Eqs. (4a) and (4b) can be visualized from Fig. 10. The mixing of the plane waves along the cubic X axis results in standing waves that peak either within the plane of atoms on the cubic face or between the planes of atoms. Depending on whether the atoms are made up of air or dielectric spheres, one of these standing waves will be bonding (lower in frequency) and the other will be antibonding (higher in frequency). The $\langle 200 \rangle$ standing wave peaking on the cubic face will, at the W point, interact strongly with other standing waves in the $\langle 111 \rangle$ directions, leading to the solution of Eq. (4b). For the other $\langle 200 \rangle$ standing wave, having nodes on the fcc faces, the interaction with $\langle 111 \rangle$ plane waves cancels out, leading to Eq. (4a).

Similarly, the matrix equation for the point U is

$$\begin{bmatrix} -\Delta\omega/\omega_U & V_1 & V_2 \\ V_1 & -\Delta\omega/\omega_U & V_1 \\ V_2 & V_1 & -\Delta\omega/\omega_U \end{bmatrix} = 0,$$
(5)

where ω_U is the center frequency at point U in the Brillouin zone and $\Delta \omega \equiv (\omega - \omega_U)$. The solutions to Eq. (5) are as follows:

$$\Delta\omega/\omega_{II} = -V_2/2,\tag{6a}$$

$$\Delta \omega / \omega_{II} = V_2 / 2 \pm [(V_2 / 2)^2 + 2(V_1)^2]^{1/2}.$$
 (6b)

For the solution of Eq. (6a), as in Eq. (4a), the effect of the $\langle 111 \rangle$ pseudopotential cancels out.

We are now in a position to test Eqs. (4) and (6) against the observed band structure at the points W and U in Fig. 6. It is necessary to take polarization into account. Fortunately, as discussed earlier, in the high-symmetry planes X-U-Land X-W-K, there exist two orthogonal linear polarizations that are not expected to mix. At the U point these divide neatly into s polarizations that are parallel to the X plane and p polarizations that are parallel to the X-U-L plane. At the W point the two polarizations are not purely s or p, but they are orthogonal nevertheless. One polarization is parallel to the X-W-K plane and the other is parallel to the X plane. Each orthogonal polarization leads to its own matrix equation [Eq. (3) or (5)] with its own values of V_1 and V_2 that must be adjusted by polarization-angle-dependent factors. For p polarization at the U point, V_2 is multiplied by $\cos(2\theta) = 7/9$ and V_1 is multiplied by $\cos(2\theta) = 1/3$. Substituting into Eq. (6), we find that the calculations are in

reasonable agreement with experiment for both polarization components of the measured band structure at the point U in Fig. 6.

A similar calculation (requiring more trigonometry) at the W point leads to gap widths that are significantly larger than observed in Fig. 6. We do not know the reason. Evidently, we may possibly have reached the limits of the nearly free photon model at the W point.

CONCLUSIONS

We have found that the idea of a photonic band gap can be experimentally realized in three-dimensionally modulated dielectric structures. It required a refractive-index contrast approaching 3.5:1, and the optimal structure consisted of 86% spherical air-atoms and only 14% dielectric material. All the other structures that we tested were semimetals with the conduction band minimum at the L point overlapping with the valence band maximum at the W or U point. In particular, this included all the tested structures consisting of spherical dielectric atoms.

The mean reason for the difficulty in producing a photonic band gap was that the Fourier components of the index modulation in a three-dimensional structure tend to be much weaker than in a simple one-dimensional layered structure. In the spherical dielectric atom case the $\langle 111 \rangle$ Fourier components tended to be particularly weak.

It should be possible to scale the optimal structure from microwave wavelengths down to near-infrared wavelengths by microfabrication in semiconductors like silicon and GaAs that do possess the required refractive index.

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