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A J Ward†, J B Pendry† and W J Stewart‡

† The Blackett Laboratory, Imperial College, London SW7 2BZ, UK
‡ GEC–Marconi Materials Technology Limited, Caswell, Towcester, Northants NN12 8EQ, UK

Abstract. Using the transfer matrix method for calculating the band structure, transmission and reflection coefficients of photonic systems, we present a method for calculating photonic dispersion surfaces. We then show how dispersion surfaces are excellent tools in the search for photonic insulators by applying the method to a simple system. We also explore the potential of metals for incorporation in photonic structures.

1. Introduction

In one dimension, the idea of a photonic band gap has been exploited for some time. In such a material there is a range of frequencies (the photonic band gap or PBG) for which photons cannot propagate. Within the gap, the wave vector is complex and the wave field decays exponentially, and in the limit of a thick sample all the incident energy is reflected. In one dimension, a periodic dielectric multilayer or Bragg stack fulfills this task, being totally reflecting for certain frequencies of radiation normally incident upon it. Unfortunately, this structure only has a band gap in one direction; as we move away from normal incidence the reflectivity falls rapidly beyond a modest angle.

Yablonovitch [1] made the first attempts to improve on this, investigating dielectric structures which were periodic in all three dimensions. These were fabricated on millimetre length scales, and were probed using microwave techniques. He managed to produce a full photonic insulator, that is a structure which, for a range of frequencies, does not permit propagation in any direction. It was hoped that the band structure could be scaled up to optical frequencies by scaling the structure down to micrometre length scales. Unfortunately, this proved too difficult for current fabrication techniques, motivating a search for other structures which are simpler to make but which still exhibit a complete photonic band gap. Such a structure could have applications in producing an almost fully closed lasing cavity for a semiconductor laser, the PBG material being used to make highly reflecting cavity walls with very low losses. This provides control over the spontaneous leakage that limits conventional laser thresholds. Alternatively, if non-linear media were used, a structure with a band gap, and not necessarily a complete one, could be used to make an optical switch, the position of the band gap being controlled by the intensity of the radiation incident upon it [2].

The method which we use to calculate photonic band structures is based on the calculation of a transfer matrix and is explained in some detail elsewhere [4]. Our first task is to take Maxwell's equations and convert them to a form discretized on an orthorhombic real space lattice of points defined by $r = \lambda a + \mu b + \nu c$ (where λ, μ, ν are integers and

a, b, c are the unit lattice vectors). Our resulting formulae are transfer equations. That is to say, if we know the E and H fields at all points within a plane $z = z'$, then we can calculate the fields in the next plane, $z = z' + c$. Repeating this we can find the fields throughout space.

In matrix form this can be written

$$\mathcal{F}(r + c) = \sum_{r'} \hat{T}(r, r')\mathcal{F}(r') \tag{1}$$

where $\mathcal{F}(r) = \begin{pmatrix} E_x(r) \\ E_y(r) \\ H_x(r) \\ H_y(r) \end{pmatrix}$, r and r' lie within a plane.

Let our photonic crystal be periodic on a lattice defined by the orthogonal primitive lattice vectors a', b', c'. (Notice these are not the same as the vectors a, b, c which define the discretization mesh.) Thus $\varepsilon(r) = \varepsilon(r + R)$ and $\mu(r) = \mu(r + R)$ where $R = \alpha a' + \beta b' + \gamma c'$ (α, β, γ are integers). Thus a', b', c' define the unit cell for our crystal.

We can write down Bloch's law for the electromagnetic fields in our unit cell:

$$\mathcal{F}(r + a') = \exp(ik_x a')\mathcal{F}(r) \tag{2}$$
$$\mathcal{F}(r + b') = \exp(ik_y b')\mathcal{F}(r) \tag{3}$$
$$\mathcal{F}(r + c') = \exp(ik_z c')\mathcal{F}(r) \tag{4}$$

If we specify k_x and k_y, then equations (2) and (3) set the boundary conditions on the fields in the x and y directions. By iterating our transfer equations through the unit cell we can also write

$$\mathcal{F}(r + c') = \hat{T}\mathcal{F}(r) \tag{5}$$

where $\hat{T}$ has the form of a product of N transfer matrices, N being the number of layers of discretization cells in one crystal unit cell. Comparing (4) and (5) we see that $\hat{T}$ has eigenvalues of the form $\exp(ik_z c')$. So this is our method: we calculate $\hat{T}$ for a given frequency, ω. We then find the eigenvalues of $\hat{T}$ which give us all the k_z values for that ω. Repeating this for different frequencies gives us the band structure, $k_z(\omega)$.

Notice that we calculate all the values of k for a given ω. This is in contrast to most other methods [5, 6, 7] used for calculating photonic band structures which expand the wave field as a series of plane waves and as a result find the ω values for a given k. However, this method makes working at a fixed energy somewhat difficult. We shall see that by fixing the energy and searching for all the allowed k values, we can develop useful techniques to help in the search for a photonic insulator.

Incidentally, we can also use the transfer matrix to calculate the reflection and transmission coefficients of our system by integrating the fields through the unit cell and using multiple scattering formulae to add cells together. This is also explained in detail elsewhere [3, 4].

2. The strategy

By working at a fixed energy (fixed ω) we can find all the allowed (real) k_z values for a given k_x, k_y. If this is repeated for different k_x, k_y we can map out all the allowed k vectors for a given energy for either photon polarization. The tips of these vectors describe

a constant energy surface in k space. This is called a dispersion surface. The Fermi surface is a familiar example.

The dispersion surfaces for photons in a homogeneous, isotropic dielectric ('free' photons) are two coincident spheres, one for each polarization, the radii of which are proportional to ω ($k = \omega\sqrt{\varepsilon}/c$). If we turn on the effect of a periodic dielectric function we find that the free photon spheres are distorted as they approach a Brillouin zone boundary, and in general the degeneracy between polarizations is lost. Figure 1 shows a schematic diagram of what we have in mind. The first Brillouin zone for a system with cubic symmetry is a cube. The dispersion surface for a single polarization for an energy with a band gap in some direction will be a distorted sphere, but with necks forming where the surface comes close to touching the edge of the Brillouin zone to leave forbidden regions where there are no allowed k vectors.
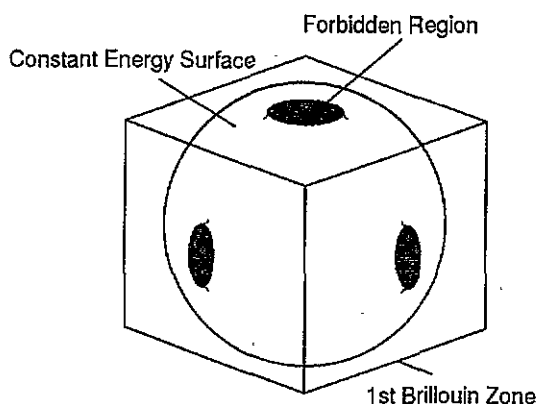

Figure 1. A sketch of a dispersion surface. Forbidden regions appear when the surface touches the edge of the Brillouin zone.

The rules controlling distortion of a photonic dispersion surface are the same as those which control the effect of a periodic potential on a Fermi surface. That is, the surface is distorted towards the Brillouin zone edge, the degree of distortion being controlled by the strength of the dielectric modulation. If the dispersion surface touches the Brillouin zone boundary then they must intersect at right angles.

Figure 2 shows the effect of a periodic potential on a series of free-photon spheres of increasing radius. Contour 1 is for an energy just below a photonic gap. Contour 2 is at an energy within the gap; notice that there are no states at the centres of the faces of the Brillouin zone. It is not a complete gap, however, as there are still some allowed states in the corners of the zone. Contour 3 is at an energy just above the gap. Notice that pockets of allowed states in the second Brillouin zone have now appeared.

We can use plots of photonic dispersion surfaces to look for systems with interesting band structures. These surfaces can tell us many things—whether a given gap is complete or whether there remain allowed states, the size of these allowed regions and their location in k space.

By changing our periodic structure and observing the effect this has on the size and position of the allowed regions in k space, it is possible to search more efficiently for photonic insulators.
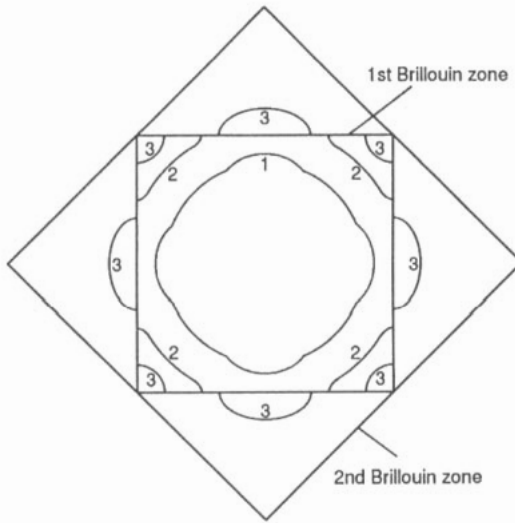
Figure 2. Three dispersion surfaces for a system with a cubic lattice. Contour 1 is for an energy just below the gap, contour 2 is within the gap and contour 3 is just above the gap.
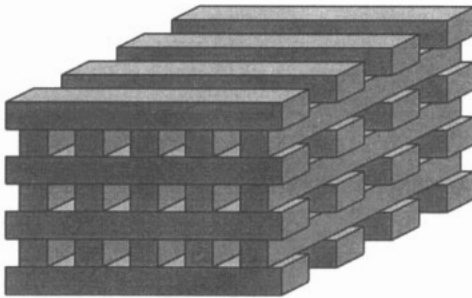

Figure 3. Diagram of the log pile structure.

3. A specific example

We now present the results of calculations of dispersion surfaces for a particularly simple cubic 3D periodic structure—the simple cubic version of the log pile structure. The FCC version of this structure was proved to have a band gap for certain refractive indices by Ho *et al* [9] using ω versus k plots. We use this system to demonstrate the power of the dispersion surface approach. This structure consists of layers of parallel dielectric rods, separated by a distance a, alternate layers being rotated by 90° (see figure 3). These calculations were made using the code PHOTON [8] which is available from the Computer Physics Communications library at Queen's University, Belfast.

We chose rods with a rectangular cross section and a filling fraction of 35%. That is, the height of each rod is $0.5a$ and the rod width $0.35a$. The length a was 0.317 microns but this is arbitrary and only affects the overall energy scale.

Dispersion surfaces were plotted for different values of the refractive index n. We plotted the wave vector in units such that the first Brillouin zone runs from $-1 \leqslant k_x \leqslant +1$, $-1 \leqslant k_y \leqslant +1$, $-1 \leqslant k_z \leqslant +1$. For each plot we chose an energy within the first band gap. The dispersion surfaces are projected down onto the k_x, k_y plane. As we were looking for a true photonic insulator, no attempt was made to distinguish between the polarizations and our diagrams in fact show the projections of both surfaces superimposed. Figure 4(a)
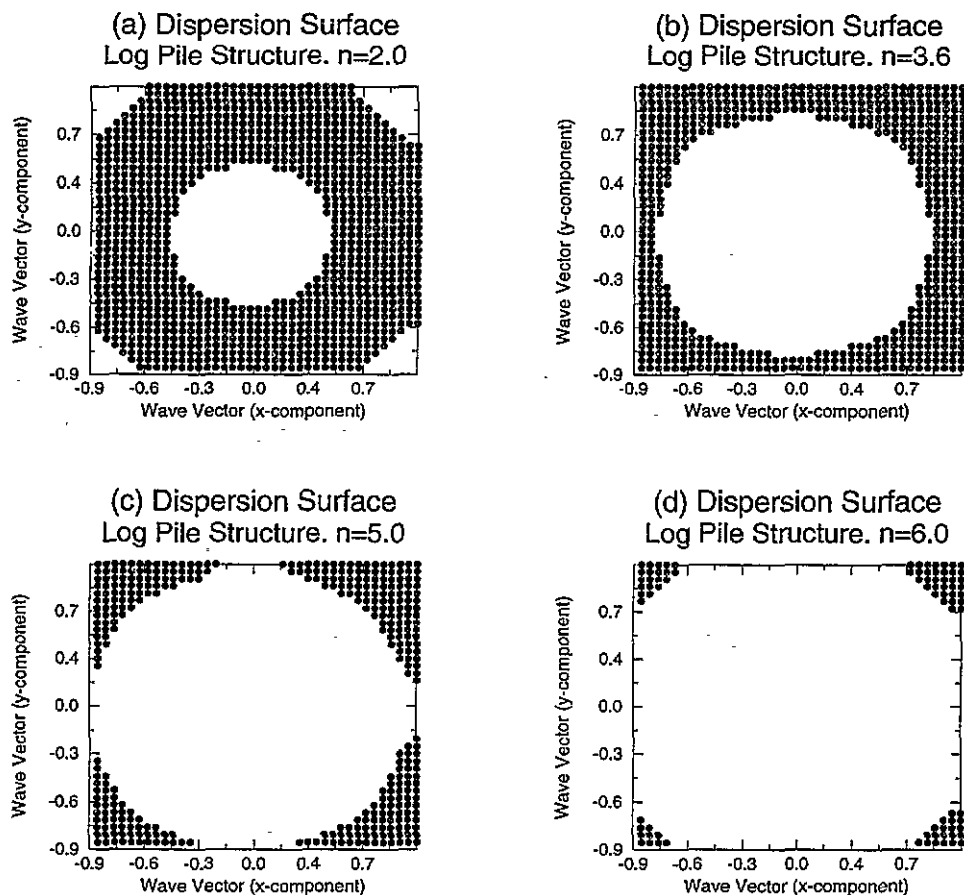
(a) Dispersion Surface
Log Pile Structure. n=2.0

(b) Dispersion Surface
Log Pile Structure. n=3.6

(c) Dispersion Surface
Log Pile Structure. n=5.0

(d) Dispersion Surface
Log Pile Structure. n=6.0

Figure 4. Projections of dispersion surfaces for the log pile structure for different values of the refractive index of the rods: (a) $n = 2.0$, (b) $n = 3.6$, (c) $n = 5.0$, (d) $n = 6.0$.

shows the dispersion surface for refractive index $n = 2$. It is basically spherical (a circle in projection). At the centre of the k_x, k_y plane the surfaces touch the $k_z \pm 1$ Brillouin zone boundary leaving a large forbidden region (the empty circle in the centre of the figure). Similarly at $k_x = \pm 1$ and $k_y = \pm 1$ the surface forms necks to touch the boundary normally leaving forbidden regions in the centres of the k_x, k_z and k_y, k_z planes. Notice that the forbidden regions at $k_x = \pm 1$, $k_y = \pm 1$ are a little larger than at $k_z = \pm 1$.

Figure 4(b) gives the dispersion surfaces for $n = 3.6$ (typical of a semiconductor). The central forbidden region is now much larger, allowed states being forced into the corners of the k_x, k_y plane. By the time n has increased to 5 (figure 4(c)), the forbidden circle has expanded to the edges of the Brillouin zone. The allowed regions are much smaller and have now become disconnected. When $n = 6$ (figure 4(d)) the allowed regions have shrunk further and now only occupy the corners of the plane. By the time $n = 6.33$ the allowed regions have vanished altogether and the gap is complete.

Obviously the dispersion surface gives at a glance a picture of the whole of k space at a single frequency and is therefore invaluable in the search for a photonic insulator. In particular, it enables attention to be focussed on the parts of k space where some dispersion

surface remains, thus suggesting what further steps may be needed to push the structure into the insulating phase.

4. Photonic mirrors—better mirrors?

Finally we turned our attention to another simple system, but this time one which includes a metal. We attempted to answer the question: which is a better reflector (at optical frequencies)—a bulk metal surface, or a series of thin metal planes?

The idea is that we can perhaps incorporate metals into photonic structures to give enhanced dielectric contrast. The problem is that metals absorb light and therefore we want to explore whether there is any way of reducing this absorption and making the metallic structures more efficient.

To model the metal we used a frequency-dependent dielectric constant of the form $\varepsilon(\omega) = 1 - [\omega_p^2/\omega(\omega + i\gamma)]$ and chose parameters $\omega = 15.1$ eV, $\gamma = 0.27$ eV (typical for a metal such as aluminium). Figure 5(a) shows the calculated reflection coefficient for the bulk metal. Below the plasma frequency the reflectivity is high but less than unity because of losses due to the finite electrical conductivity.

Figures 5(b) and 5(c) show the band structure and reflection coefficient for a stack of 256 metal planes, the filler between the planes having a refractive index of 1.5. The plane thickness was chosen to be 2.5 nm, to be comparable to the skin depth, and the plane spacing, which simply controls the overall energy scale, was 0.35 microns. Note the peak in the reflectivity corresponds with the position of the photonic band gap. Figure 5(e) compares the bulk reflectivity and the reflectivity of the layered system in the region of the peak. The reflectivity for the layered system is higher over a fairly narrow range of frequencies, having a maximum at around 98% compared with 95% for the bulk at that point.

The asymmetry of the reflectivity peak is due to the redistribution of the electromagnetic field at the top and the bottom of the gap. In each case the photon wave function is a standing wave. The metal acts like a repulsive potential so at the bottom of the gap (the lowest energy state), the nodes of the wave function lie on top of the metal planes ($|\psi(z)|^2 \sim \sin^2(\pi z/a)$ where a is the plane spacing). This means that the overlap between the metal and the electromagnetic field is minimized and the absorption is small. The reflectivity is correspondingly high. At the top of the gap the reverse is true. The nodes of the wave function lie between the planes ($|\psi(z)|^2 \sim \cos^2(\pi z/a)$) and the overlap between the metal and the field is maximized. Therefore the absorption is greater and the reflectivity is correspondingly lower.

To what extent is the gap for this system complete? Figure 5(d) shows the dispersion surface for the metal layers. Since the system is only periodic in the z direction (the stacking direction) there are only Brillouin zone boundaries in the k_z direction. So no forbidden regions open along the k_x, k_y directions. Figure 5(d) shows a small forbidden region but the gap is by no means complete.

In answer to our question then, yes, a stack of layers can have a larger reflectivity than the bulk but only for a limited range in frequency and k space.

5. Conclusions

We have presented the dispersion surface as a useful tool in searching for a photonic insulator. We then applied our transfer matrix method to two systems and confirmed that

(a) Reflection Coefficient
For Bulk Metal

(b) Band Structure
For a series of Metal Planes

(c) Reflection Coefficient
For a series of Metal Planes

(d) Dispersion Surface
For a series of Metal Planes
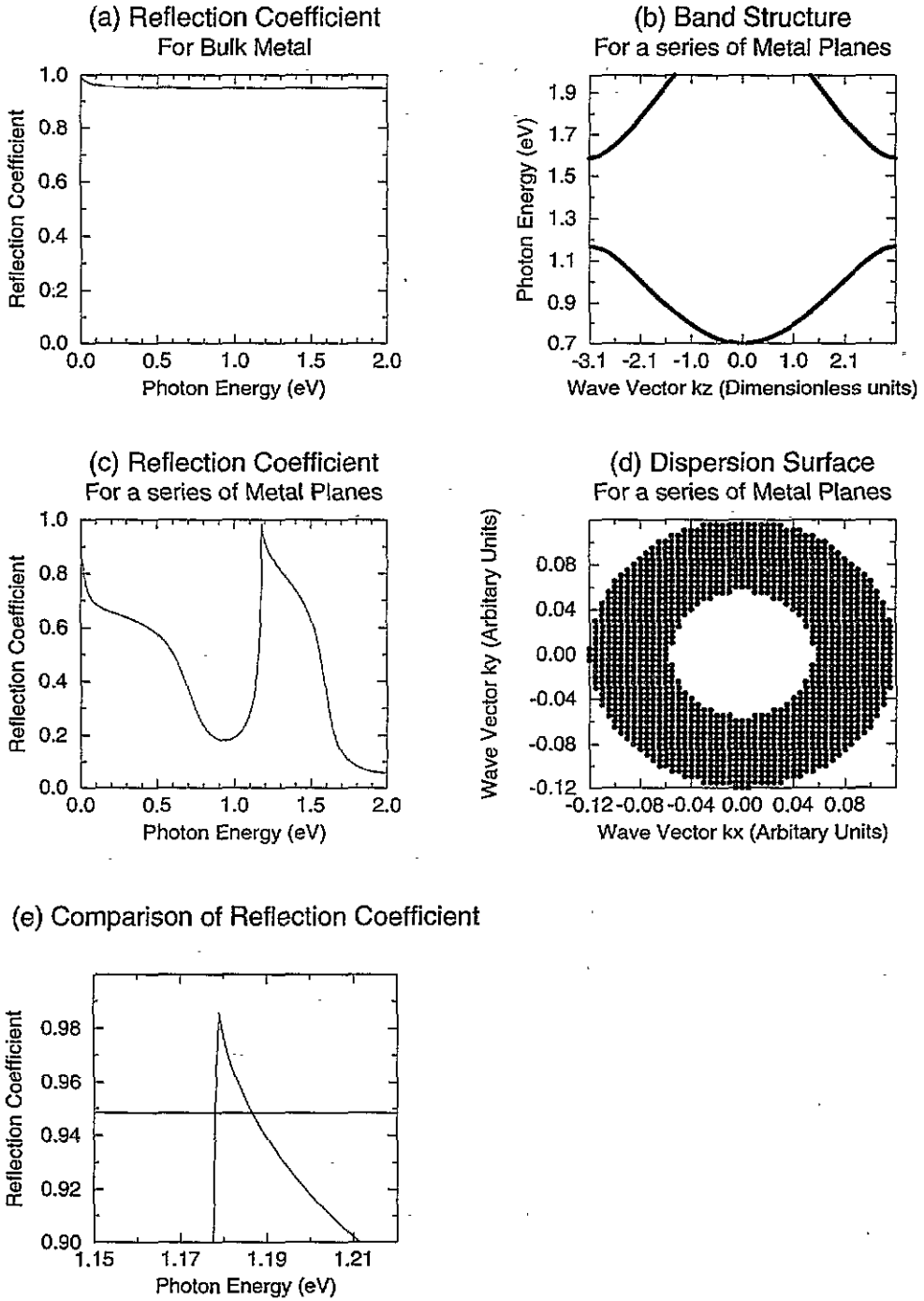

(e) Comparison of Reflection Coefficient

Figure 5. (a) Reflectance of bulk metal, (b) band structure, (c) reflection coefficient and (d) dispersion surface for a stack of planes planes. (e) Comparison of the reflectance of the bulk metal and the layered system.

the simple cubic log pile structure does indeed have a complete gap (albeit for a refractive index $n > 6.33$ which is somewhat artificial). We are limited, however, by the geometry which can be studied. An FCC log pile structure would have a complete gap for a much lower refractive index contrast but our present methods can only handle systems with cubic primitive unit cells. In the future we hope to extend our method to include systems with non-orthogonal unit cells.

We also showed that a series of metal planes can have a higher reflectivity than bulk metal if only for a limited range of frequencies and angles of incidence. We have shown that the inherent absorption of the metal need not necessarily present a problem because of the redistribution of the photon wavefunction at the band edges. In the future it should be possible to include metals in the design of fully three-dimensional photonic systems to obtain an effective enhancement in the refractive index contrast.

Acknowledgment

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