The Traditional Multilayer Film:
A One-Dimensional
Photonic Crystal

We begin our study of photonic crystals with the simplest possible case: a one-dimensional system. To understand the propagation of light through a one-dimensional photonic crystal, we apply the principles of electromagnetism and symmetry that we developed in the previous chapters. Even in this simple system we can see the important features of photonic crystals in general—specifically, photonic band gaps and localized modes at defects. Although the optical properties of dielectric layers may be familiar, by casting the discussion in the language of band structures and band gaps we will prepare for the more complicated two- and three-dimensional systems that lie ahead.

The Multilayer Film

The simplest possible photonic crystal, shown in figure 1, consists of alternating layers of material with different dielectric constants. This arrangement is not a very new idea—the optical properties of such multilayer films have been widely studied. As we will see, this photonic crystal can act as a perfect mirror for light with a frequency within a sharply-defined gap, and can localize light modes if there are any defects in its structure. This arrangement is commonly used in dielectric mirrors and optical filters (see, for example, Hecht and Zajac 1974).

The traditional approach to an understanding of this system is to allow a plane wave to propagate through the material and to consider the multiple reflections that take place at each interface. In this chapter, we will use a different approach—the analysis of band structures
Figure 1 The multilayer film—a one-dimensional photonic crystal. The term “one-dimensional” refers to the fact that the dielectric is only periodic in one direction. (We imagine that the film extends indefinitely in the z-direction.) It consists of alternating layers of materials (blue and green) with different dielectric constants, spaced by a distance $a$.

which is easily generalized to the more complex two- and three-dimensional photonic crystals.

We begin in the spirit of the previous chapter. By applying symmetry arguments, we can describe the electromagnetic modes sustainable by the crystal. The material is periodic in the $z$-direction, and homogeneous in the $xy$-plane. As we saw in the previous chapter, this allows us to index the modes using $k_y$, $k_z$, and $n$: the wave vector in the plane, the wave vector in the $z$-direction, and the band number. The wave vectors tell how the phase of the mode varies with position, and the band number increases with frequency. We can write the modes in the Bloch form:

$$H_{n, k_y k_z} (r) = e^{i k_y y} e^{i k_z z} u_{n, k_y k_z} (z).$$

Here, $u(z)$ is a $z$-periodic function, so that $u(z) = u(z + R)$ whenever $R$ is an integral multiple of $a$, the layer spacing. The crystal has continuous translational symmetry in the $xy$-plane, so the wave vector $k_y$ can assume any value. However, we restrict $k_z$ to a finite interval, the one-dimensional Brillouin zone, because the crystal has discrete translational symmetry in the $z$-direction. Using the prescriptions of the previous chapter, if the primitive lattice vector is $a \hat{z}$, then the primitive reciprocal lattice vector is $(2\pi/a) \hat{z}$ and the Brillouin zone is $\pi/a \leq k_z \leq \pi/a$. 
The Physical Origin of Photonic Band Gaps

For now, consider light that happens to propagate entirely in the $z$-direction, crossing the sheets of dielectric at normal incidence. In this case, $k_y = 0$, so only the wave vector component $k_z$ is important. Without possibility of confusion, we can abbreviate $k_z$ by $k$.

In figure 2, we plot $\omega_n(k)$ for three different multilayer films. In the left plot, all of the strips have the same dielectric constant, so the medium is completely homogeneous. The center plot is for a structure with alternating dielectric constants of 13 and 12, and the right-hand plot is for a structure with a much higher dielectric contrast of 13 to 1.\footnote{We use these particular values because the static dielectric constant of gallium arsenide (GaAs) is about 13, and for gallium aluminum arsenide (GaAlAs) it is about 12, as reported in Sze (1981). These materials are commonly used in devices. Au has a dielectric constant $\varepsilon = 1$.}

The leftmost plot is for a uniform dielectric medium, to which we have artificially assigned a periodicity of $a$. But we already know that in a uniform medium, the speed of light is reduced by the index of refraction. The frequency spectrum is just the light-line given by

$$\omega(k) = \frac{ck}{\sqrt{\varepsilon}}. \tag{2}$$

Because we have insisted that $k$ repeat itself outside the Brillouin zone, the lines fold back into the zone when they reach the edges. The center plot, which is for a nearly-uniform medium, looks like the light-lines with one important difference. There is a gap in frequency between the upper and lower branches of the lines—a frequency gap in which no mode, regardless of $k$, can exist in the crystal. We call such a gap a photonic band gap. As we can see on the right, as the dielectric contrast is increased, the gap widens considerably.

We will devote a considerable amount of attention to photonic band gaps, and with good reason. Most of the promising applications of two- and three-dimensional photonic crystals to date hinge on the location and width of photonic band gaps. For example, a crystal with a band gap might make a very good, narrow-band filter, by rejecting all (and only) frequencies in the gap. A resonant cavity, carved out of a photonic crystal, would have perfectly reflecting walls for frequencies in the gap.

The natural question arises: Why does the photonic band gap appear? We can understand the gap's physical origin by considering the
Figure 2 The photonic band structures for on-axis propagation, shown for three different multilayer films, all of which have layers of width 0.5a. Left: each layer has the same dielectric constant $\varepsilon = 13$. Center: layers alternate between $\varepsilon = 13$ and $\varepsilon = 1$. Right: layers alternate between $\varepsilon = 13$ and $\varepsilon = 1$.

electric field mode profiles for the states immediately above and below the gap. The gap between bands $n = 1$ and $n = 2$ occurs at the edge of the Brillouin zone, at $k = \pi/a$. For now, we focus on the band structure in the center panel of figure 2, corresponding to the configuration that is a small perturbation of the uniform system. For $k = \pi/a$, the modes are standing waves with a wavelength of $2a$, twice the crystal’s lattice constant.

There are two ways to center a standing wave of this type. We can position its nodes in each low-$\varepsilon$ layer, as in figure 3a, or in each high-$\varepsilon$ layer, as in figure 3b. Any other position would violate the symmetry of the unit cell about its center.

But in our study of the electromagnetic variational theorem in chapter 2, we found that the low-frequency modes concentrate their energy in the high-$\varepsilon$ regions, and the high-frequency modes concentrate their energy in the low-$\varepsilon$ regions. With this in mind, it is understandable why there is a frequency difference between the two cases. The mode just under the gap has its power concentrated in the $\varepsilon = 13$ regions as shown in figure 3c, giving it a lower frequency. Meanwhile, the mode just above the gap has most of its power in lower $\varepsilon = 12$ regions as shown in figure 3d, so its frequency is raised a bit.

The bands above and below the gap can be distinguished by where
Figure 3 Schematic illustration of the modes associated with the lowest band gap of the center panel of figure 2. (a) Electric field of band 1; (b) electric field of band 2; (c) local energy of band 1; (d) local energy of band 2. In the pictures of the multilayer film, the blue region is the layer of higher dielectric constant ($\varepsilon = 13$).

Figure 4 The photonic band structure of a multilayer film with lattice constant $a$ and alternating layers of different widths. The width of the $\varepsilon = 13$ layer is $0.2a$, and the width of the $\varepsilon = 1$ layer is $0.8a$. 
the power of their modes lies—in the high-\(\varepsilon\) regions, or in the low-\(\varepsilon\) regions. Often the low-\(\varepsilon\) regions are air regions. For this reason, it is convenient to refer to the band \textit{above} a photonic band gap as the “air band,” and the band \textit{below} a gap as the “dielectric band.” The situation is analogous to the electronic band structure of semiconductors, in which the “conduction band” and the “valence band” surround the fundamental gap.

Our heuristic, based on the variational theorem, can be extended to describe the configuration with a large dielectric contrast. In this case, we find that the fields for both bands are primarily concentrated in the high-\(\varepsilon\) layers, but in different ways—the bottom band being more concentrated than the top. The gap arises from this difference in field energy location. Consequently, we will still refer to the upper band as the air band, and the lower as the dielectric band.

We conclude this section with the observation that in one dimension, a gap occurs between every set of bands, at either the Brillouin zone’s edge or its center. This is illustrated for the band structure of a multilayer film in figure 4. Finally, we note that band gaps always appear in one-dimensional photonic crystal for any dielectric contrast. The smaller the contrast, the smaller the gaps, but the gaps open up as soon as \(\varepsilon_1/\varepsilon_2 \neq 1\).

\textbf{Evanescent Modes in Photonic Band Gaps}

The key observation of the previous section was that the periodicity of the crystal induced a gap into its band structure. No electromagnetic modes are allowed in the gap. But if this is indeed the case, what happens when we send a light wave (with frequency in the photonic band gap) onto the face of the crystal from outside? No purely real wave vector exists for any mode at that frequency. Instead, the wave vector is complex.

The wave amplitude decays exponentially into the crystal. When we say that there are no states in the photonic band gap, we mean that there are no \textit{extended} states like the mode given by equation (1). Instead, the modes are \textit{evanescent}, decaying exponentially:

\[
\mathbf{H}(r) = e^{ikz}\mathbf{u}(z)e^{-\kappa r}.
\]  

(3)

They are just like the modes we constructed in equation (1), but with a complex wave vector \(k + i\kappa\). The imaginary component of the wave vector causes the decay on a length scale of \(1/\kappa\).
Figure 5  Schematic illustration of the complex band structure of the multilayer film. The upper and lower blue lines correspond to the bottom of band 2 and the top of band 1, respectively. The evanescent states occur on the red line. The maximum decay occurs roughly at the center of the gap.

We would like to understand how these evanescent modes originate, and what determines $\kappa$. This can be accomplished by examining the bands in the immediate vicinity of the gap. Return to the right-hand plot of figure 2. Suppose we try to approximate the second band near the gap by expanding $\omega_2(k)$ in powers of $k$ about the zone edge $k = \pi/a$. Because of time-reversal symmetry, the expansion cannot contain odd powers of $k$, so to lowest order:

$$\Delta \omega = \omega_2(k) - \omega_2\left(\frac{\pi}{a}\right) = \alpha \left(k - \frac{\pi}{a}\right)^2 = \alpha (\Delta k)^2. \quad (4)$$

Now we can see where the complex wave vector originates. For frequencies slightly higher than the top of the gap, $\Delta \omega > 0$. In this case, $\Delta k$ is purely real, and we are within band 2. However, for $\Delta \omega < 0$, when we are within the gap, $\Delta k$ is purely imaginary. The states decay exponentially since $\Delta k = i\kappa$. As we traverse the gap, the decay constant $\kappa$ grows as the frequency reaches the gap's center, then disappears at the lower edge. This behavior is depicted in figure 5.

We should emphasize that although evanescent modes are genuine solutions of the eigenvalue problem, they do not satisfy the translational-symmetry boundary condition of the crystal. There is no way to excite them in a perfect crystal of infinite extent. However, a defect or an edge in an otherwise perfect crystal might sustain such a mode. One or more evanescent (exponentially decaying) modes may be compatible with the structure and symmetry of a given crystal defect. In those cases, we can create a localized, evanescent light mode within the photonic band gap. And, as a general rule of thumb, we can localize states near the middle of the gap much more tightly than states near the gap's edge.
Figure 6  Schematic illustration of possible sites of localized states for a one-dimensional photonic crystal. The states are planar and would be localized near the differently-colored regions, which break the symmetry in the z-direction. We will call a mode at the edge of the crystal (green) a surface state, and a mode within the bulk of the crystal (blue) a defect state.

Of course, one-dimensional photonic crystals can only localize states near a given plane, as shown in figure 6. In the upcoming section, “Localized Modes at Defects,” we will discuss the nature of such states when they lie deep within the bulk of a photonic crystal. In certain circumstances, however, an evanescent mode can exist at the face of the crystal. We will also discuss these states, called surface states, later in this chapter.

Off-Axis Propagation

So far we have considered the modes of a one-dimensional photonic crystal which happen to have $k_y = 0$; that is, modes that propagate only in the z-direction. In this section we will discuss off-axis modes. Figure 7 shows the band structure for modes with $k = k_x \hat{y}$ for the one-dimensional photonic crystal described in the caption of figure 4.

The most important difference between on-axis and off-axis propagation is that there are no band gaps for off-axis propagation when all
possible \( k \), are considered. This is always the case for a multilayer film, because the off-axis direction contains no periodic dielectric regions to coherently scatter the light and split open a gap.

Another difference involves the degeneracy of the bands. For on-axis propagation, the electric field is oriented in the \( xy \)-plane. We might choose the two basic polarizations as the \( x \)- and \( y \)-directions. Since those two modes differ only by a rotational symmetry which the crystal possesses, they must be degenerate. (How could the crystal distinguish the two?)

However, for a mode propagating in some off-axis \( k \)-direction, this symmetry is broken. The degeneracy is lifted. There are other symmetries; for example, notice that the system is invariant under reflection through the \( yz \)-plane. For the special case of propagation down the dielectric sheets, in the \( y \)-direction, we know from the symmetry discussion of chapter 3 that the possible polarizations are in the \( x \)-direction or in the \( yz \)-plane. But there is no rotational symmetry relationship between these two bands, so they will generally have different frequencies. All of this information is displayed in figure 7.

![Figure 7](image-url)

**Figure 7** The band structure of a multilayer film. The on-axis bands \((0, 0, k_z)\) are shown on the left side, and an off-axis band structure \((0, k_y, 0)\) is displayed on the right. On-axis, the bands overlap—they are degenerate. Along \( k_y \), the bands split into two distinct polarizations. Red indicates modes polarized so that the electric field points in the \( x \)-direction, and blue indicates modes polarized in the \( yz \)-plane. The layered material is the same as the one described in the caption of figure 4.
Although \( \omega(\mathbf{k}) \) for these two different polarizations have different slopes, both are approximately linear at long wavelengths (\( \mathbf{k} \to 0, \ \omega \to 0 \)). This long-wavelength behavior is characteristic of all photonic crystals, regardless of geometry or dimensionality:

\[
\omega_\nu(\mathbf{k}) = c_\nu (\hat{\mathbf{k}}) k. \tag{5}
\]

Here \( \nu \) indexes the two possible polarizations, or equivalently, the first two bands. In general, \( c_\nu \) will depend on both the direction of \( \mathbf{k} \) and the band index.

Why is the dispersion always linear at long wavelengths? At long wavelengths, the electromagnetic wave doesn’t probe the fine structure of the crystal lattice. Instead, the light effectively sees a homogeneous dielectric medium; the microscopic bumps of varying \( \varepsilon \) in the crystal are smoothed out on the light’s length scale.

The medium may be anisotropic, having a different average dielectric constant for each direction—these are the effective dielectric constants that we would measure by applying a static field in a capacitance measurement, for example. Typically, we measure three dielectric constants, one for each principal axis of the effective medium. Even if an analytic expression for the effective dielectric constants of a general photonic crystal is not known, they can be calculated numerically.\(^2\)

Returning to the multilayer film, we would like to understand why modes polarized in the \( x \)-direction (band 1 in fig. 7) have a lower frequency than modes polarized in the \( yz \)-plane (band 2). Once again we use our heuristic: the lower modes concentrate their electrical energy in the high-\( \varepsilon \) regions. In this case, we focus on the long-wavelength limit of each mode.

The fields for both bands are shown schematically in figure 8. For the \( x \)-polarized wave, the displacement fields lie in the high-\( \varepsilon \) regions. But at long wavelengths, the polarization of band 2 is almost entirely along the \( z \)-direction, crossing both the low-\( \varepsilon \) and the high-\( \varepsilon \) regions. Continuity forces the field to penetrate the low-\( \varepsilon \) region, leading to a higher frequency.

\(^2\)One useful analytic constraint for the effective dielectric constant of a general photonic crystal is provided by the Weiner bounds, as in Aspnes (1982). Specifically, for a two-material composite, each effective dielectric constant \( \varepsilon_{\text{eff}} \) is bounded by

\[
(1/f_1 + 1/f_2)^{-1}, \quad \varepsilon_{\text{eff}} \leq f_1 \varepsilon_1 + f_2 \varepsilon_2,
\]

where \( f_1 \) and \( f_2 \) are the volume fractions of the materials with dielectric constants \( \varepsilon_1 \) and \( \varepsilon_2 \).
Figure 8 A sketch of the displacement field lines for a long wavelength mode traveling in the $y$-direction (out of the page). In the left figure, the fields are oriented along $x$. In the right figure, the fields are oriented primarily along $z$. The blue regions are the high-$\varepsilon$ regions.

Figure 9 Two superimposed band structures of a multilayer film, showing how the bandwidths vary with $k_y$. The blue lines refer to bands along $(0, k_y, 0)$, while the green lines are the bands along $(0, k_y, \pi/a)$. Only modes with electric field oriented along the $x$-direction are shown. The red line is the light-line, $\omega = ck_y$. The layered material is the same as the one described in the caption of figure 4.
We can also understand the asymptotic (short-wavelength, large-$k$) behavior of the modes with a simple argument. In figure 7, note that the range of frequencies spanned by each band (the bandwidths) is determined by the difference between frequencies at the zone center ($k = 0$) and zone edge ($k = \pi/a$). At large $k$, the bandwidths decay to zero. This is illustrated in figure 9, which shows the superposition of two band structures. The blue lines represent states along $\mathbf{k} = (0, k, 0)$ and the green lines represent states along $\mathbf{k} = (0, k, k_z = \pi/a)$.

As we saw for the case of a plane of glass, once the frequency goes below the light line $\omega = ck_y$ the modes decay exponentially into the vacuum region. Therefore, the overlap between modes in neighboring layers of high-$\varepsilon$ material goes exponentially to zero. When the coupling between neighboring planes is small, each guides its own mode independent of its neighbors. In this case, the dependence on the on-axis wave vector vanishes, and every mode in the band becomes the frequency of a guided mode, trapped by the high-$\varepsilon$ layers.

**Localized Modes at Defects**

Now that we understand the features of a perfectly periodic system, we can examine systems in which the translational symmetry is broken by a defect. Suppose that the defect consists of a single layer of the one-dimensional photonic crystal that has a different width than the rest. Such a system is shown in figure 10. We no longer have a perfectly periodic lattice, but if we move many wavelengths away from the defect, the modes should behave as before.

For now, we restrict our attention to on-axis propagation and consider a mode with frequency $\omega$ in the photonic band gap. There are no extended modes with frequency $\omega$ inside the periodic lattice, and introducing the defect will not change that fact. The destruction of periodicity prevents us from describing the modes of the system with wave vector $k$, but we can still employ our knowledge of the band structure to determine whether a certain frequency will support extended states inside the rest of the crystal. In this way, we can divide up frequency space into regions in which the states are extended and regions in which they are evanescent, as in figure 11.

\footnote{In solid state physics, the analogous system is the tight binding model, in the limit of small hopping. See, for example, Harrison (1980).}
Figure 10  A defect in a multilayer film, formed by enlarging one of the layers of dielectric. Note that this can be considered to be an interface between two perfect multilayer films. Also sketched is the displacement field strength associated with a defect state.

Figure 11  The division of frequency space into extended and evanescent states. In this sketch the density of states (the number of allowed modes per unit frequency) is zero in the band gaps of the crystal (yellow). Modes are allowed to exist in these regions only if they are evanescent, and only if the translational symmetry is broken by a defect. Such a mode is shown in red.
Defects may permit localized modes to exist, with frequencies inside photonic band gaps. If a mode has a frequency in the gap, then it must exponentially decay once it enters the crystal. The multilayer films on both sides of the defect behave like frequency-specific mirrors. If two such films are oriented parallel to one another, any \( z \)-propagating light trapped between them will just bounce back and forth between these two mirrors. And because the distance between the mirrors is of the order the light’s wavelength, the modes are quantized. The situation bears strong resemblance to the quantum-mechanical problem of a particle in a box (as in Liboff 1992), or the electromagnetic problem of microwaves in a metallic cavity (as in Jackson 1962).

Consider the family of localized states generated by continuously increasing the thickness of the defect layer. The bound mode associated with each member of this family will have a different frequency. As the thickness of the high-\( \varepsilon \) layer is increased, the frequency will decrease, because the field will be concentrated more and more in a high-\( \varepsilon \) region. Moreover, the rate of decay will be largest when the frequency is near the center of the gap, as shown in figure 5. States with frequencies in the center of the gap will be most strongly attached to the defect.

The density of states of a system is the number of allowed states per unit increase in \( \omega \). If a single state is introduced into the photonic band gap, then the density of states of the system in figure 11 is zero in the photonic band gap, except for a single peak associated with the defect. This property is exploited in the band-pass filter known as the dielectric Fabry-Perot filter. It is particularly useful at visible-light frequencies, because of the relatively low losses of dielectric materials.

This treatment can be extended to the interface between two multilayer films with different spacings. Localized states can exist as long as the band gaps of the two materials overlap. We can also obtain states that are localized in the \( z \)-direction, but propagate along the interface \( (k_z = i\kappa, \ k_\parallel \neq 0) \).

**Surface States**

We have seen under what conditions we can localize electromagnetic modes at defects in a multilayer film. In a similar fashion, we can also localize modes at its surface. In the previous section, the mode was bound because its frequency was within the photonic band gap of the
Figure 12  The electric field strength associated with a localized mode at the surface of a multilayer film.

Figure 13  The band structure at the surface of a multilayer film. The shaded regions describe states which are extended in the air region (blue), in the layered material (red), or in both (purple). The green line represents a band of surface states confined at the interface. The layered material is the same as the one described in figure 4. The surface is terminated with a layer of high dielectric with a width $0.1a$. 
films on both sides. But at the surface, there is only a band gap on one side of the interface—the outside air does not present a band gap.

In this case, light is bound to the surface if its frequency is below the light line. We can think of such a wave as being totally internally reflected (see fig. 12). At a surface we must consider whether the modes are extended or decaying in both the air and the layered material, and we must consider all possibilities for \( \mathbf{k}_\parallel \). The appropriate band structure is shown in figure 13. We divide the phase space of modes into four regions, classified by how they behave in the air and crystal regions. For example, the label “DE” means that modes in that region decay in the air region, and are extended in the crystal region.

The EE modes extend on both sides of the surface, the DE modes decay in the air region and extend into the crystal, and the ED modes extend in the air region, but decay inside the crystal. Only if the modes are evanescent on both sides of the surface can we have a surface wave. The region where this is possible is labeled DD. In fact, every layered material has surface modes for some termination, a phenomenon we shall discuss again in chapter 6.

Further Reading

Many of the theorems we have developed and the properties we have observed for photonic crystals have analogs in quantum mechanics and solid-state physics. For readers familiar with those fields, appendix A provides a comprehensive listing of these analogs.

The conventional treatment of the multilayer film, including the calculation of absorption and reflection coefficients, can be found in Hecht and Zajac (1974). The use of the multilayer films in optoelectronic devices is widespread in current literature. For example, Fowles (1975) outlines their use in Fabry-Perot filters, and Yeh (1988, p. 337) explains how they are incorporated into distributed feedback lasers.

The details of the computational scheme used to compute band structures can be found in Meade et al. (1993a). Other methods for computing band structures are outlined in Ho et al. (1990) and Sözüer et al. (1992).