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Electromagnetic Bloch waves at the surface of a photonic crystal

Robert D. Meade, Karl D. Brommer, Andrew M. Rappe, and J. D. Joannopoulos
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
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We find that electromagnetic modes are localized at the interface between air and a photonic crystal. General arguments that surface modes must always exist for some termination of any surface of a photonic crystal are presented, and the importance of the surface band structure for semiconducting laser systems is discussed.

The recent discovery[1,2] that periodic structures of dielectric materials (photonic crystals) can be made to have an optical band gap in which propagating electromagnetic modes are forbidden has been greeted with enthusiasm. These materials possess many unique physical properties. For instance, defects in photonic crystals have been predicted[3] and observed[4] to localize electromagnetic modes. Moreover, the absence of radiating modes will inhibit the decay of excited states whose energies lie in the band gap, which may lead to unusual electronic[2] and chemical properties of atoms or molecules embedded in the photonic crystal. The absence of zero-point fluctuations in the photonic band gap also has physical consequences, such as an anomalous Lamb shift.[5] In addition, interest in these materials has also been generated by their potential applications. In fact, the prediction that photonic crystals would lead to efficient semiconducting lasers has been a strong motivation for their development.[6]

In previous work, authors have considered properties of bands,[1,2,7–9] defects,[3] and atoms[5] in *infinite* photonic crystals. In this paper, we will determine the effect of terminating the crystal by examining the surface band structure of an interface between air and a photonic crystal. We will show that photonic crystals have electromagnetic surface modes, in which light is exponentially localized to the surface plane. However, unlike the familiar case of metal surfaces,[10] in which the localization of electromagnetic surface waves is a result of a negative dielectric constant in the metal, surface Bloch waves are localized because of interference effects in the photonic crystal. Thus these surface waves are analogous to the electromagnetic Bloch waves occurring on the surface of multilayer films.[11] We will also discuss the impact of these results on the design of semiconducting lasers. Understanding the surface band structure is of particular importance to these devices, because by choosing a proper termination of the photonic crystal one can eliminate the losses associated with radiation into surface modes.

In order to study the surface of a photonic crystal we have performed a series of calculations of interface states. We have found that the surface states can be cataloged as one of four types: extended both in the crystal and the air (EE), decaying in the air but extended in the dielectric (DE), extended in the air and decaying in the dielectric (ED), and decaying in both the dielectric and the air (DD). In the final case, which we will discuss in detail, the light is exponentially localized at the surface. We will find that the surface electromagnetic states are of two general types, having primarily transverse electric (TE) or transverse magnetic (TM) fields. We will also present general arguments that surface modes must always exist for some termination of any surface of a photonic crystal.

It has been noted by several authors[1,9] that there is a similarity between electronic states in a periodic potential and electromagnetic states in a periodic dielectric. We can take advantage of this similarity by applying the methods developed for electronic-structure calculations, such as plane-wave expansions, in order to solve for the eigenstates of an electromagnetic system. These methods, which have been described in detail by a number of authors,[1,7,8] provide a simple and powerful way to solve problems in electrodynamics which takes full account of the vector nature of the electromagnetic radiation.

Although we would like to study the surface of a semi-infinite photonic crystal, computationally it is desirable to choose a system with a finite unit-cell size. Therefore, we employ the supercell method in which slabs of dielectric material alternate with slabs of vacuum. We employ a supercell with six double layers of photonic crystal and six double layers of vacuum. Because the surface states are strongly localized to the uppermost dielectric layer, the error introduced by the finite size of the slab is negligible, less than 0.1% as judged by the splitting between states on opposite surfaces. We expand in plane waves up to a finite frequency, including ~ 130 plane waves per polarization, per primitive unit cell. We found that this was a sufficient plane-wave cutoff to describe the surface states accurately, and increasing the plane-wave cutoff to 250 plane waves per polarization, per primitive unit cell changed the frequencies by less than 0.1%.

Because it is the structure most likely to be employed in the production of a semiconductor laser system, we have chosen to study the (111) surface of the photonic crystal proposed by Yablonovitch, Gmitter, and Leung.[2] This structure is described in detail in Ref. 2. Qualitatively, this structure can be thought of as a set of dielectric columns connecting the sites of a diamond lattice (in the same way that the bonds connect atoms in a silicon crystal). These columns, then, point along the [111], $[\bar{1}\bar{1}1]$, $[\bar{1}1\bar{1}]$, and $[1\bar{1}\bar{1}]$ directions. The three columns along the $[\bar{1}\bar{1}1]$, $[\bar{1}1\bar{1}]$, and $[1\bar{1}\bar{1}]$ directions are identical, but the fourth column in the [111] direction has a larger diameter. A $(1\bar{1}0)$ cross section of this surface is shown in the inset in Fig. 1. The columns along the [111] direction

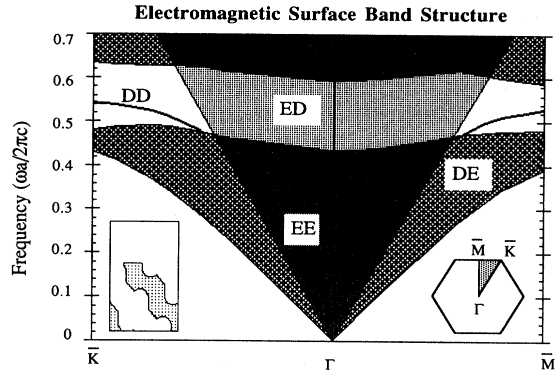

FIG. 1. The band structure of the (111) surface of the Yablonovitch crystal along special directions in the surface Brillouin zone. The shading denotes regions in which light is transmitted (EE), internally reflected (DE), and externally reflected (ED). The lines in the gap correspond to surface bands in which light is exponentially localized to the surface (DD). The surface Brillouin zone is shown in the lower right, with the irreducible BZ shaded. The $\bar{M}$ point is directed along $(1,\bar{2},1)$ a distance of $(\frac{2}{3})^{1/2}(2\pi/a)$ from $\bar{\Gamma}$. The $\bar{K}$ point is directed along $(0,\bar{1},1)$, a distance of $(\sqrt{8}/3)(2\pi/a)$ from $\bar{\Gamma}$. This surface band structure corresponds to a termination of $\tau=0.75$, shown in the inset with air above and photonic crystal below (dielectric regions are shaded, and air regions are unshaded). Frequencies are in units of $(2pc/a)$, where a is the conventional lattice constant.

point vertically in this picture, and the diagonal rib connecting these [111] columns is a $[\overline{1}\overline{1}1]$ column. This surface contains a C_{3v} symmetry, with the rotational axis normal to the surface and passing through the center of the [111] column. Although we have chosen to look at the (111) surface of the Yablonovitch structure, we expect that many of the features of the electromagnetic surface states will be common to all photonic crystals.

Before we consider the band structure of the interface, let us first consider the projected band structure of the air and photonic crystals separately. The union of regions EE and ED shown in Fig. 1 is the projection of the free photon modes into the surface Brillouin zone. For a given $\mathbf{k}=(k_x,k_y)$, there are light modes at all frequencies $\omega \geq ck$. Along the line $\omega=ck$, the light travels parallel to the surface, and increasing ω represents an increasing component of k_z. Similarly, the union of regions EE and DE represents the projected band structure of the photonic crystal. Note that the photonic crystal contains a gap $0.49 < \omega a/(2\pi c) < 0.59$ in which there are no allowed states.

It is now straightforward to understand the four types of surface states, transmitted (EE), internally reflected (DE), externally reflected (ED), and surface modes (DD). In the region of $(\mathbf{k},\omega)$ marked EE, the modes are extended in both the air and in the dielectric and so it is possible to have light transmitted through the crystal. In the DE region, there are modes in the dielectric, but they are beneath the band edge for the air states. Thus the light is extended in the dielectric but exponentially decaying into the vacuum, which constitutes total internal reflection. In the ED region, the situation is reversed; and these states are extended states in the air but they are in the gap of the dielectric. In this case, the modes are extended in the vacuum region but exponentially decaying into the dielectric and so incident light is reflected. Finally, we find there can be states in the region marked DD. In this regime, the states are below the band edge of the light in the air, as well as in the gap of the dielectric material. Thus the light is exponentially decaying in both directions, and so it is localized to the surface plane.

The fields associated with the zone edge $(\bar{M})$ surface mode are shown in Fig. 2(a), which is a (110) cross section through the surface plane. Because the crystal contains a mirror symmetry through this plane, the **D** field lies in the plane, while the **H** field is everywhere normal to the plane, and is displayed in contours. Note that the fields are strongly localized in the plane of the surface, with most of their character in the uppermost dielectric layer. As is the case for the bulk modes and defect states,[3,4] most of the power of the **D** field is concentrated in the dielectric regions. Figure 2(b) displays the fields associated with the $\bar{M}$ surface mode in a (111) plane passing through the top layer of the surface. Although this is not a mirror plane, the **H** field is primarily in the plane, and is shown as vectors, and the **D** field is primarily normal to the plane, and is shown in contours.

One interesting feature of the fields shown in Fig. 2(b) is that the magnetic field is primarily in the transverse direction, perpendicular to the surface and to the **k** vector. For this reason, we describe the mode as TM-like. However, the surface modes of a photonic crystal are not rigorously TE or TM. To understand why this is so, let us consider the simpler case of the surface of a multilayer

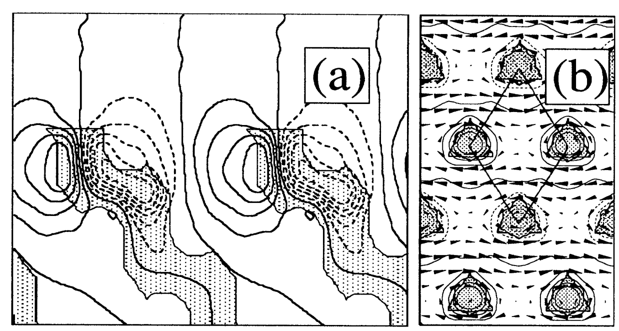

FIG. 2. The fields associated with the zone-edge $(\bar{M})$ surface mode for a surface termination of $\tau=0.75$. The regions of dielectric are shown shaded, while the regions of air are left unshaded. (a) The fields shown in the (110) plane. The contours indicate lines of constant **H**. (Dashed lines indicate contours of negative value.) Because **D** is the curl of **H**, **D** is always parallel to the equipotential lines of **H**, and is large only where the gradient of **H** is large (where the equipotential lines are closely spaced). In this cross section, **k** lies in the plane of the figure. (b) The fields associated with the $\bar{M}$ surface mode, in a plane passing through the top layer of the surface. The **H** field is primarily in the plane, and is shown as vectors, and the **D** field is primarily normal to the plane, and is shown as contours. The surface unit cell is circumscribed by the parallelogram, and the fields change sign in alternate unit cells, consistent with a zone-edge state. In this figure, **k** is directed vertically.

film. In this case the distinction between modes which are TE and TM is exact. This can be seen from symmetry arguments. The surface of a multilayer film has a continuous translational symmetry parallel to the surface plane, so we can label the states by in-plane **k** vector. Consider the mirror plane defined by the **k** vector and the surface normal. Fields must be either even or odd with respect to this mirror plane. Fields which are odd are normal to the plane, while fields that are even lie in the mirror plane. If the **H**(**D**) field is normal to the plane, then the mode is TM(TE). However, at the surface photonic crystal, the symmetry is lower and so there is no rigorous distinction between TE and TM modes. Even though the rigorous distinction between TE and TM breaks down at the surface of a photonic crystal, the fields displayed in Fig. 2(b) lead us to describe the mode qualitatively as TM-like.

Until this point, we have considered the band structure of the one particular termination of the (111) surface, shown in the inset in Fig. 1. However, the surface can be terminated at many levels [see the inset in Figs. 3(a) and 3(b)]. By specifying the Miller indices of a surface we determine the surface normal, and for periodic arrays of atoms this uniquely describes the physical system whose surface properties we wish to investigate. However, a photonic crystal has a lattice constant of macroscopic dimensions, and so we need a nomenclature to determine not just the surface normal, but also the termination of the surface inside a unit cell. To do so, let us introduce a termination parameter τ $(0 \leq \tau < 1)$, which describes the termination of any surface. Let $\tau = 0$ when the surface is terminated through the bond center, as shown in the inset in Fig. 3(b), and increase linearly as the height of the surface is raised, normalized so that the surface terminates at

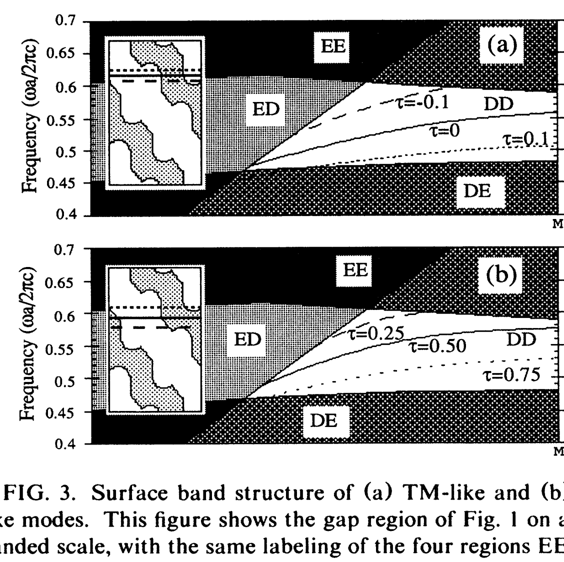

FIG. 3. Surface band structure of (a) TM-like and (b) TE-like modes. This figure shows the gap region of Fig. 1 on an expanded scale, with the same labeling of the four regions EE, ED, DE, and DD. The insets indicate the surface terminations corresponding to the three values of τ for which the surface bands have been plotted (see Fig. 1, inset). Larger values of τ correspond to vertically higher terminations on the inset, which contain more dielectric on the surface. Note that higher τ yields lower values of surface band frequency.

$\tau = 1$ when the same physical surface as $\tau = 0$ is achieved.

In fact, we find that the surface band structure varies in an interesting manner as the termination of the surface is changed, as is shown in Figs. 3(a) and 3(b). As the termination of the surface is increased, more dielectric is added, and the frequency of the surface mode is lowered. This can be understood in an intuitive way, recalling that the dielectric is analogous to a region of low potential. As more dielectric is added to the surface, the potential that the surface state experiences decreases, and so its frequency decreases. Thus, as τ is increased, bands sweep down from the conduction band to the valence band. These states may be either TM-like, as shown in Fig. 2(a), or TE-like with the **D** field primarily in the transverse direction. Let us consider the band structure as τ is increased from $\tau = 0$ to $\tau = 1$. The surface bands in the final termination are identical to the surface bands in the initial termination, since the two correspond to equivalent surfaces. As the termination is increased, exactly two states are swept from the conduction band to the valence band, one of which is TM-like and the other is TE-like. Thus, by increasing the termination of the surface from $\tau = 0$ to $\tau = 1$ we have added one bulk unit cell (per surface unit cell), and increased the total number of states in the valence band by two (at each **k** point).

This suggests a general argument, that any $\{nlm\}$ surface (with n,l,m integers) of any photonic crystal with a gap will always have surface states for some termination. If the surface has integer indices, then it has a finite unit-cell size, and a finite surface Brillouin zone. Since the crystal as a whole has a gap, the surface Brillouin zone must also have a gap. Suppose that as the surface termination is varied between any τ and $\tau + 1$, there are b bulk unit cells introduced per surface unit cell. There must then be $2b$ states transferred from the conduction band to valence band. As the frequencies of these states are lowered from the bottom of the conduction band to the top of the valence band, they must sweep through the gap and become surface bands. This argument for the existence of surface states also applies to the case of multilayer films which lack a gap in their full three-dimensional Brillouin zone, but have a gap in the direction normal to the surface.

Finally, we discuss the importance of these results on the design of semiconducting lasers. The possibility of employing photonic crystals to produce efficient semiconducting lasers has been suggested by Yablonovitch.[2] His proposal has several elements, which we will review briefly. As a first ingredient, one uses microfabrication techniques to produce a photonic band-gap structure from a semiconducting material. By choosing the proper structure, one insures that the electronic band-gap energy E_{gap} falls within the photonic band gap. The next ingredient is to create a lasing mode at ω_d in the electromagnetic band gap. This can be done by introducing a defect into the photonic crystal which creates a localized electromagnetic mode. If the defect size is chosen so that $h\omega_d = E_{gap}$, then the system can radiate into the local mode, which acts as a laser cavity. Because there is only a single mode in the gap, there is no possibility for spontaneous emission into other frequencies, which enhances the efficiency of this laser system.

The final step is to extract the light from the local mode. Even if the defect is located several lattice constants below the surface, there will be some overlap between the exponential tail of the surface states, penetrating into the crystal, and the exponential tail of the defect state embedded within the crystal. Because of this overlap, the light confined in the defect mode can escape by tunneling. But, depending on the surface, there are two channels into which the light can escape, into the air states (ED) or into the surface states (DD). Only the radiation which escapes into air is useful. The radiation which is confined to the surface cannot be collected, and so this is a mechanism for loss. Fortunately, by choosing a proper termination for the photonic crystal, one can insure that there are no surface states at the lasing frequency. For instance, at a termination of $\tau = 0.75$ (see Fig. 1), there are no surface states in the region $0.54 < \omega a/(2\pi c) < 0.59$, and so this range would be the optimal choice for the lasing frequency.

In conclusion, electromagnetic states can be localized at the surface of a photonic crystal. We have found that these modes are of two general types, TE-like and TM-like, and have presented general arguments that surface modes must always exist for some termination of any surface of a photonic crystal.

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