Surface effects and band measurements in photonic crystals

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An analytic study of Bloch waves near photonic crystal surfaces has been carried out. This is a generalization of Heine's theory of metal/semiconductor interfaces. The main concern of this study is how the surfaces of a finite system affect band determination—which usually involves transmission measurements on small photonic crystals. An analytic expression for transmission is obtained. The results show that the usual band measurements could lead to considerable errors, especially when they involve narrow band gaps. A possible method to improve band measurements has been suggested. The analytic surface analysis has been demonstrated to be fairly accurate, even for a small system. The theory is expected to be applicable to other surface-related problems of photonic systems.

Recently, Yablonovitch and Gmitter (YG) (Ref. 1) demonstrated the existence of photonic band structure in periodic dielectric materials. This system has generated many research efforts.[2–10] Fascinating phenomena such as anomalous Lamb shifts[5] and possible applications in semiconductor lasers[3,9] have been suggested and studied. Electromagnetic (EM) waves in a periodic dielectric, like electrons in a solid, are described by the Bloch theory. In solids, however, the many-body effect due to the Coulomb interaction causes significant modifications to the one-body Bloch states, as is exemplified by the Na conduction band.[11] The interaction among photons is negligible, suggesting that photonic crystals can be an ideal test ground for the decades-old Bloch theory. Accurate band determination is important in regard to photonic crystal applications.

Photonic bands are normally determined[1] with transmission measurements on a finite, usually small, photonic structure. For example, the photonic crystal employed in the YG measurement is made of an Al_2O_3 bulk with 8000 air cavities, which serve as "atoms" and are arranged into the fcc structure. About one-quarter of these atoms are on the surfaces. An interesting question here is how the band structure, which is a property of an infinite system, should be determined from such a small sample. Some insights are necessary before a detailed comparison of measured photonic bands with various theoretic band calculations[4,6,7,10] is possible.

Briefly stated, the purpose of this work is to investigate the surfaces of photonic crystals in general, and their effect on band measurements in particular. A photonic crystal surface is very similar to a metal/semiconductor interface. Near the Fermi level of the latter, there is a band gap on the semiconductor side and there are propagating states on the metallic side—just like a photonic crystal surface in the gap region. Heine[12] investigated the metal/semiconductor interfaces with a one-dimensional (1D) model. Mainly, he established that states inside a band gap have complex crystal momentum, i.e., $k=G/2\pm iq$, where G is a reciprocal wave vector. The imaginary part implies that electrons with energy in the gap can actually tunnel into the semiconductor by a distance $\sim 1/q$ from the interface. Heine's 1D theory has been the basis for understanding metal/semiconductor interfaces. It is generalized here for finite photonic crystals. Analytic results for Bloch states at surfaces and for transmission have been derived.

The transmission spectra of YG's crystal have been evaluated in the $\Gamma\rightarrow X$ and the $\Gamma\rightarrow L$ directions. The results are then compared with YG's measurements. Experimentally, band gaps are put at where the transmission rate drops substantially. This study shows that band gaps can, at best, be qualitatively determined this way. The error may be considerable (e.g., $\sim 60\%$) and it could get even worse if the gap size (E_g) becomes smaller. This is mainly because the imaginary part of the crystal momentum (q) is proportional to E_g; therefore, a large system of sizes $\propto 1/q \propto 1/E_g$ would be necessary for transmission to diminish inside a small gap. Based on the analytic results, we suggest an alternative but accurate way to employ finite-crystal transmission to determine the band dispersions—not just the gap sizes. This will be discussed in connection with Fig. 1.

The surface effect revealed from this 1D theory is expected to hold, probably qualitatively, in 3D photonic crystals. The results could even by quantitatively correct, for example, near the X point where a single lattice scattering component dominates. Experiences with simple metals have illustrated that[11] 1D models are valuable in analyzing important effects in 3D systems. A thorough 3D study of the photonic surface effect should be very interesting, but that would require extensive numerical calculations. An analytic 1D study could be very helpful in our understanding of such numerical results.

The electric field, $\mathbf{E}(\mathbf{r})$, of an EM wave in a periodic medium obeys the Maxwell equation

$$-\nabla^2\mathbf{E}(\mathbf{r})-\frac{\omega^2}{c^2}\epsilon'(\mathbf{r})\mathbf{E}(\mathbf{r})=\frac{\omega^2}{c^2}\epsilon_0\mathbf{E}(\mathbf{r}) , \tag{1}$$

where the dielectric function has been separated into two parts: $\epsilon(\mathbf{r})=\epsilon_0+\epsilon'(\mathbf{r})$. ϵ_0 is the averaged dielectric constant and $\epsilon'(\mathbf{r})$ the periodic part. This equation is very similar to the Schrödinger equation for electrons in a

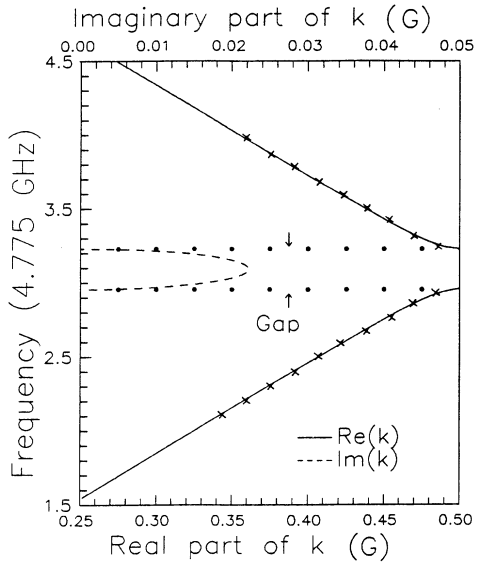

FIG. 1. The calculated band structure near the X point of a fcc photonic crystal. The crystal parameters are taken from YG's measurement, with the atomic size $R_s=0.372b_0$. Inside the band gap, the wave vector is complex: $k=G/2\pm iq$. The nonvanishing q implies a nonvanishing transmission rate in the gap region. The crosses represent bands determined from the calculated transmission spectra of Fig. 2 (see text below).

solid. Following the standard theory of band electrons, we treat $\mathbf{E}(\mathbf{r})$ as scalar waves and expand it into Bloch states

$$E(\mathbf{r})=\sum_{\mathbf{G}}\sum_{\mathbf{k}} C_{\mathbf{k}-\mathbf{G}}e^{i(\mathbf{k}-\mathbf{G})\cdot\mathbf{r}} , \tag{2}$$

where $\sum_{\mathbf{k}}$ is summed over the first Brillouin zone. The periodic $\epsilon'(\mathbf{r})$ can be expanded as

$$\epsilon'(\mathbf{r})=\sum_{\mathbf{G}} U_{\mathbf{G}}e^{i\mathbf{G}\cdot\mathbf{r}} . \tag{3}$$

For a fcc crystal, like the one in YG's measurement,

$$U_{\mathbf{G}}=-\frac{16\pi}{b_0^3 G}(\epsilon_a-\epsilon_b)\left[\frac{1}{G^2}\sin(GR_s)-\frac{R_s}{G}\cos(GR_s)\right] . \tag{4}$$

b_0 is the lattice constant and R_s the radius of the atom. ϵ_a and ϵ_b, respectively, are the dielectric constants of the atom and of the background. $b_0=1.27$ cm, $\epsilon_a=1$, and $\epsilon_b=12.25$ in YG's measurement. They have employed different R_s's (i.e., for different U_G's) and studied the band structures.

Of particular interest here are bands near the X ($k=G_X/2$) and L ($k=G_L/2$) points, where detailed band measurements exist.[1] Near X, the Bloch scattering due to U_{G_X} dominates, since $k=\pm G_X/2$ are degenerate states. With only this dominating potential component retained, the scalar-wave approximation employed in Eq. (2) is reasonable. Equation (1) can thus be rewritten as

$$\begin{aligned}\left[k^2-\epsilon_0\frac{\omega^2}{c^2}\right]C_k&=\frac{\omega^2}{c^2}U_G C_{k-G} ,\\ \left[(k-G)^2-\epsilon_0\frac{\omega^2}{c^2}\right]C_{k-G}&=\frac{\omega^2}{c^2}U_G C_k ,\end{aligned} \tag{5}$$

where $G=G_X$ for bands near X. This two-band mixing formalism should work equally well for bands near L, with $G=G_L$. Effectively, the problem has been reduced in Eq. (5) to a 1D one. This approximation enables us to study the problem analytically.

Nontrivial solutions of Eq. (5) have the general form

$$k=\frac{G}{2}\pm\sqrt{F(\omega)} , \tag{6}$$

where

$$F(\omega)=(G^2/4)+\epsilon_0(\omega^2/c^2)-\sqrt{G^2\epsilon_0(\omega^2/c^2)+U_G^2(\omega^4/c^4)} .$$

$F(\omega)>0$ corresponds to band modes, for which k is real. $F(\omega)<0$ corresponds to gap modes, which have complex $k=G/2\pm iq$, where $q=\sqrt{|F(\omega)|}$. Figure 1 is the calculated band structure near the X point of YG's photonic crystal. Both the real and the imaginary parts of k have been shown in units of G (G_X here). The result illustrates the general band feature in a gap region: q increases from zero at gap edge to a finite value near midgap. These gap modes exist only at surfaces or interfaces since, otherwise, the amplitude of the field would grow exponentially and that is unphysical. The presence of these gap modes is important for transmission in the gap region—especially for a small crystal.

Consider a semi-infinite photonic crystal first which, by assumption, occupies the $x>-a/2$ half-space, where a is the layer separation. The allowed modes inside the crystal thus have the form

$$\psi_k(x)=\begin{cases}e^{ikx}+\eta e^{i(k-G)x} & \text{for band modes} ,\\ e^{-qx}\cos\left[\dfrac{G}{2}x+\delta\right] & \text{for gap modes} .\end{cases} \tag{7}$$

The factors η and δ are determined from Eq. (5): $\eta=[k^2-\epsilon_0(\omega^2/c^2)]/[U_G(\omega^2/c^2)]$ and $\sin2\delta=qG/[U_G(\omega^2/c^2)]$. In deriving these results we have assumed a small gap size (i.e., $U_G\ll\epsilon_0$), which is normally satisfied [see Eq. (4)]. We have also assumed that the first layer atoms are located at $x=0$; that is one-half the layer separation from the crystal surface. Take the [100] surface in the fcc structure, for example, which corresponds to transmission in the $\Gamma\rightarrow X$ direction; the crystal surface is put at $x=-a/2=-b_0/4$. Such a surface condition, on which the following calculations are based, is how a surface is normally defined in a solid.[13] We do not have to put the surface this way, but different surface conditions would give different factors η and δ, which, in turn, would result in different transmission spectra (see below).

We remark that the gap states at surfaces we study here correspond to the ED surface states of Meade *et al.*,[8] and the band states to their EE states. The first

letter E stands for extended waves in vacuum and the second letter D (E) for decaying (extended) waves in the crystal. These are the only surface modes that are relevant to transmission measurements. Other surface modes, denoted as DD and DE states,[8] also exist on surfaces. They are not discussed here; their analytic properties can be studied in a similar fashion.

The EM wave transmission through a finite crystal is analogous to quantum tunneling across a potential barrier. Consider a $2N$-layer crystal located at $-a/2 < x < (2N-\frac{1}{2})a$ and an incident wave traveling in the $+x$ direction, which, for example, could represent a finite crystal with N layers of fcc cells. The wave is described by

$$E(x)=\begin{cases} e^{ik_0x}+re^{-ik_0x}, & x<-\dfrac{a}{2}, \\ C_k\psi_k(x)+C_{-k}\psi_k(-x), & \\ & -\dfrac{a}{2}<x<(2N-\frac{1}{2})a, \\ te^{ik_0x}, & x>(2N-\frac{1}{2})a. \end{cases} \quad (8)$$

$k_0=\sqrt{\epsilon_0}k$ is the wave vector in vacuum. The component $\psi_k(-x)$ comes from the surface reflection at $x=(2N-\frac{1}{2})a$. It is clear from Eqs. (7) and (8) that the transmission in the band (gap) region is like quantum tunneling across a potential well (barrier). The coefficients r, t, C_k, and C_{-k} are determined by the continuity of $E(x)$ and $dE(x)/dx$ at the surfaces. The transition rate so obtained can be expressed analytically:

$$T=t^*t=\begin{cases} \dfrac{1}{1+\left[\dfrac{B^2}{A^2}-1\right]\sin^2[2kNa]} & \text{in band regions}, \\ \dfrac{1}{1+\left[\dfrac{B'^2}{A'^2}+1\right]\sinh^2[2qNa]} & \text{in gap regions}, \end{cases} \quad (9)$$

$$A=2k_0[\eta^2G-k(1+\eta^2)],$$

$$B=(k_0^2+k^2)(1+\eta^2)+\eta^2G^2-2\eta^2Gk,$$

$$A'=2k_0[q\cos2\delta-(G/2)\sin2\delta],$$

and

$$B'=[k_0^2+(G^2/4)-q^2]\cos2\delta+qG\sin2\delta.$$

Within a band, T exhibits an oscillatory pattern as a function of ω, and is enveloped between 1 and $A^2/B^2<1$. There is a finite transmission rate inside a gap. The rate could be considerably large near band edges where q goes to 0 (see Fig. 1). For a sufficiently large crystal, however, $T\sim e^{-4Naq}$, which vanishes as $N\to\infty$. Figure 1 shows that $q\approx0.02G$ at the gap center where q reaches its maximum. Thus, it takes $N\gg10$ for T to diminish even at the midgap; N is only about 10 in YG's measurement. It is interesting to examine how, in a finite crystal, the transmission rate drops as ω crosses from a band region into a gap. Such studies are obviously important in determining the gap size from transmission measurements.

Figure 2 illustrates the calculated $T(\omega)$ (solid curves) for four different finite crystals. $N=4$, 8, 16, and 32 indicate the numbers of lattice layers of the crystals. The parameters chosen here simulate YG's measurements near the X point. The atomic size $R_s=0.372b_0$ gives a gap size of $E_g=1.312$ GHz, the location of which is shown by the two vertical curves in the figure. There is a steady decrease in T as ω enters the gap from the band region. This result suggests no obvious criterion as to how the band edge should be determined from the spectra. The rate does not drop abruptly at the edge as might have been expected,[1] at least not for $N<30$. If we had employed a smaller E_g, the outcome would have been even worse. To see this, we note that at the gap center [i.e., where $\epsilon_0(\omega^2/c^2)=G^2/4$] Eq. (6) can be expanded for a small E_g and gives $q\simeq GU_G/4\epsilon_0\propto E_g$ in the lowest-order approximation. Small q, then, would need a large N for T to drop down appreciably. There is thus a systematic error involving the gap measurement and it gets worse rapidly as E_g reduces in size.

In deriving Eq. (9) we have made several assumptions. A very important one is that the waves in a finite crystal are describable by Bloch waves [Eq. (8)]. Its validity needs to be checked, especially for small N's. Recall from Eq. (5) that the problem is essentially one dimensional. The band near $k=G_X/2$ can thus be studied in an alternative way by, for example, employing a periodic multislab structure in which the band parameters a, U_G, and ϵ_0 are kept unchanged. This can easily be achieved with a construct which contains two uniform slabs in the unit cell, each with a different dielectric constant. The transmission rate of such a multislab system can easily be calculated by means of the so-called transfer-matrix

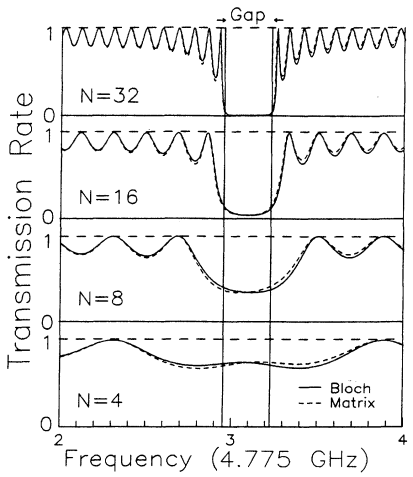

FIG. 2. The calculated transmission spectra in the [100] direction for finite photonic crystals with $2N$ layers; $N=4$, 8, 16, and 32. The same crystal parameters as those in Fig. 1 have been employed. The two vertical curves indicate where the ideal band gap is located (i.e., when $N\to\infty$). The finite transmission rate inside the gap is important for small systems and can cause errors in the band-gap measurements.

method,[14] in which EM waves in neighboring slabs are related by a 2×2 matrix. The method is equivalent to solving the Maxwell equation numerically for the finite multislab system. Dashed curves in Fig. 2 are such exact results, in which the same band parameters as those used for the solid curves have been used. Very close agreement between the two calculations is obtained. It suggests the validity of the analytic expressions, Eqs. (7) and (9), for photonic crystals with $N>4$. The close agreement at such small N's is surprising—the band nature is already eminent in an $N=4$ crystal. The close agreement found in Fig. 2 also indicates that similar Bloch state analysis may be applied to other surface-related problems; for example, the localized, interfacial states between two photonic crystals. Localized impurity states have been suggested[2,9] to have important applications in semiconductor lasers.

Attempts have been made to follow YG's procedure in determining the band gaps at X and L—with our calculated transmission spectra. The results are then compared with YG's measurements (Fig. 3). As we have explained, there is no obvious criterion in locating the gaps, and it is not clearly described how gaps are determined experimentally.[1] We therefore choose an arbitrary cutoff T_c, and put gaps at where $T<T_c$. Results shown are for $T_c=0.1$ (long-dashed curves) and for $T_c=0.01$ (short-dashed curves). The region between these two sets of data has been shaded. The horizontal axis here represents the packing fraction f, which is a measure of R_s and is defined as the volume fraction that is occupied by the air cavities. The actual gap sizes (the solid curves), in general, lie inside the shaded area. However, a serious problem here is that a reasonable T_c cannot be determined prior to the band analysis. Take the gap at the X point, for example. If $T_c=0.01$ is employed, the measured gap would be within 5% of error at $f=0.20$, but the error would be as high as 60% at $f=0.55$—even though the actual gap sizes at these two f's are about the same. It is clear that such band measurements are, at best, qualitatively accurate. The measured results (the circles) at $f>0.2$ generally lie within the shaded region. That they are narrower than the actual gap sizes is probably due to the finite tunneling inside the gaps. The measured E_g at $f<0.2$ is larger than all theoretical values. This result cannot be understood based on our present analysis. We note that the gap must vanish as $f\to0$ (i.e., when the air cavities shrink to zero sizes); measured results do not reflect this trend. A smaller E_g, as we argued earlier, implies a smaller q, which in turn means higher transmission rates inside a gap. Therefore, a larger sample may be necessary to determine the band in the small-f regime.

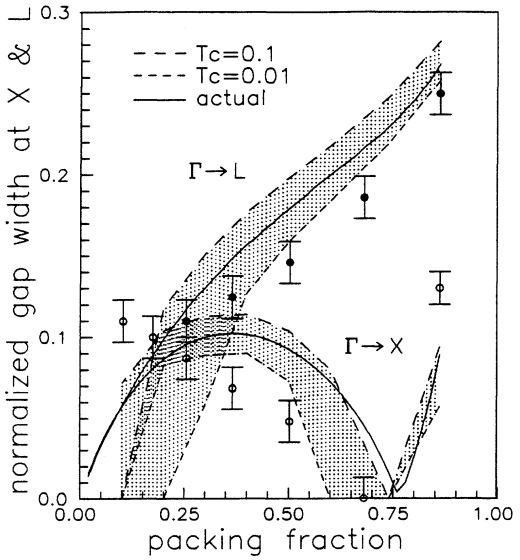

FIG. 3. The gap widths at different packing fractions (i.e., different R_s). The gap sizes have been normalized by the band energy at the center of the gap at X. The long- (short-) dashed curves are from this calculation with the cutoff $T_c=0.1$ (0.01). The solid curves represent the ideal gap sizes for infinite systems and the circles (● and ○) are taken from YG's measurements.

This study suggests no particular T_c to use for an accurate band measurement. However, an analytic relation [i.e., Eq. (9)] between the transmission spectra and the band parameters (e.g., $U_G,\epsilon_0,\ldots$) has been established. This relation has been checked to be valid even for a small system. With the interaction among photons negligible, this result is essentially exact for a photonic system. It is thus possible to gain useful band information by analyzing $T(\omega)$ in accordance with Eq. (9). One possible method is described in the following. It is reasonable to expect that large transmission is associated with Bloch states of the crystal. Equation (9) shows that the maxima of $T(\omega)$ are at the crystal momentum $k=m\pi/2Na$, with m an integer. It is convenient to express k within the reduced-zone scheme. Then the frequencies at which the transmission maxima are located can be associated with $k=(\frac{1}{2}-m'/2N)G$, where $1\le m'\le N$. In regard to the spectra of Fig. 2, $m'=1$ should be associated with the first peaks on either side of the gap, $m'=2$ with the second peaks, etc. The band dispersion determined from the calculated $N=32$ spectrum is shown in Fig. 1 by the crosses—which actually trace out the bands faithfully. The same band structure would have been obtained if the $N=8$ or 16, or even the 4 spectra were employed for analysis. That this is true can easily be seen by matching the peak positions of the various spectra of Fig. 2. This method appears to be useful for determining the whole band structure, not just the gap sizes. It should be very interesting to compare bands measured in this fashion with those of the various band calculations.[4,6,7,10]

In summary, we have included surfaces in a modified Bloch theory for photonic crystals, and the results are expressed analytically. Comparison with exact, numerical calculations indicates that the analytic expressions remain valid for systems as small as only four layers. Transmission rates of finite photonic crystals have been calculated and employed in band studies. It was pointed out that the existing band analysis could lead to large errors, especially when E_g is small. The analytic results of this study have been shown to be helpful for an improved band measurement. Our main results, Eqs. (7) and (9), may also be useful in studies of other surface-related problems too. They have been employed to examine the

localized EM mode at interfaces between photonic crystals.[15] The "one-body" Bloch theory for photonic systems is essentially exact within the 1D model. The result is expected to hold in 3D—possibly quantitatively, in gap regions around certain high-symmetric points in k space.

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