Dipole emission rates in one-dimensional photonic band-gap materials

M. Scalora¹, J.P. Dowling¹, M. Tocci¹,², M.J. Bloemer¹, C.M. Bowden¹, J.W. Haus³

¹ Weapons Sciences Directorate, AMSMD-WS-WS-51, U.S. Army Missile Command, Redstone Arsenal, AL 35898-5248, USA
(Fax: 1-205/876-4759, E-mail: JPD2@aip.org)
² Physics Department, University of Alabama, Huntsville, AL 35899, USA
³ Physics Department, Rensselaer Polytechnic Institute Troy, NY 12180-3590, USA

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Abstract. We numerically investigate dipole emission rates in one-dimensional photonic band-gap structures. Both the temporal and spatial dynamics of the electromagnetic field and the atomic polarization are treated by a unique propagation method that allows us to easily and realistically model material boundary conditions for finite structures. We find that for our structure the total power emitted is enhanced near the photonic band edge by more than an order of magnitude, and that this power is drastically reduced by nearly three orders of magnitude when the dipole oscillation frequency is tuned near the center of the forbidden photonic band gap.

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In recent years, much interest and time has been devoted to the study of Photonic Band-Gap (PBG) structures. In one dimension, these materials may consist of dielectric layers, each about a quarter wavelength thick, alternating between a high and a low index of refraction [1, 2]. This one-dimensional, periodic arrangement gives rise to a band-gap structure for photons, in full analogy to semiconductor devices that exhibit band gaps for electrons. In both cases, a range of frequencies or energies is not allowed to propagate through the crystal (Fig. 1). Interest in three-dimensional PBG structures has steadily been growing because these materials possess the potential to revolutionize photonics in the same way that semiconductor devices have already revolutionized electronics [2].

For three-dimensional PBG structures, a topologically complicated dielectric function is needed in order for a full three-dimensional gap to exist [2]. However, even in one dimension, where constructing a gap is trivial, there is much to be learned. For example, the dynamics of ultrafast pulses in such one-dimensional PBG structures has been explored only recently by our group when the principles of a photonic band-edge laser [3], a nonlinear ultrafast optical limiter and switch [4], and a nonlinear optical diode [5], were all demonstrated to be possible in these structures. Therefore, in what follows we adopt the simple one-dimensional model of John and Wang [1b, c]; they assume a material such that, regardless of polarization or direction of propagation, a photon would always encounter precisely the same periodic index variation. Although such materials in reality do not exist, the approximation allows us to treat three-dimensional structures as being effectively one-dimensional in nature, while retaining the three-dimensional flavor of the interaction.

There are several reasons to study real-time pulse propagation in PBG materials. Any realistic device is finite in length, and hence an incoming pulse whose carrier frequency is well within the forbidden band gap, and whose linewidth is finite, cannot detect a gap unless it probes several dielectric layers. From a dynamical standpoint, then, a photonic band gap does not exist unless the radiation can probe the structure first. We have found that the implications of this conclusion can be far reaching. An example is provided by our theoretical development of the nonlinear, ultrafast, photonic band edge optical limiter and the optical diode [4, 5]. In these devices, the idea of a local band gap is exploited to induce changes in the width of the gap that can lead to left–right symmetry breaking and dynamical shifts of the photonic stop band. Further development of these ideas can therefore lead to efficient devices for all-optical switching and logic.

In order to highlight the importance of the dynamics of the radiation inside a layered one-dimensional structure, in this short note we study the dynamics of a dipole radiating inside a one-dimensional PBG material. The temporal evolution of the atom–field system in finite, one-dimensional, quasi-periodic structures – to our knowledge – has not been investigated before from this point of view. The study of spontaneous emission rates in layered structures is important because it addresses the question

It is a pleasure for us to dedicate this work to H. Walther on the occasion of his 60th birthday.
of emission rates for one-dimensional laser cavities, in particular, zero-threshold, semiconductor vertical-cavity surface-emitting lasers that utilize quarter-wave Bragg reflectors for mirrors.

Purcell was the first to predict that the emission rate of an excited atom could be altered by positioning physical boundaries in the neighborhood of the atom [6]. The reason for the change in the emission rate can be understood if we recall that, according to Fermi's golden rule, the rate of decay is proportional to the density of final photon states \( \rho(\omega) \), that is;

\[
\gamma = \frac{2\pi}{\hbar} \rho(\omega) | < f | \mu \cdot E | i > |^2,
\]

where \( |i > \) and \( |f > \) are the initial and final atom-field states, respectively, of the radiating system; \( \mu \) is the dipole moment; and \( E \) is the electric field. For example, in a parallel mirror cavity, the spontaneous emission process can be almost completely stopped if the atomic transition frequency is smaller than the cavity cutoff frequency. Several theoretical [7] and experimental studies have shown this effect in microcavities [8], including a particularly elegant experiment using the micromaser by Walther and his co-workers in Garching [9].

We model the emission of radiation from a collection of point dipoles that are located inside a finite one-dimensional PBG structure, or distributed Bragg reflector. We then calculate the energy radiated from the structure in the absence of any defect modes, although these defects can trivially be included. (A defect mode consists of a break in the periodicity of the PBG crystal, as would be the case if a \( \lambda \) or \( \lambda/2 \) phase slip were introduced by removing one of the dielectric layers, or by adding one.) Our previous theoretical studies have shown that, in the absence of defect modes, gain can be enhanced if the optical frequency of laser operation is near the photonic band edge [3], a frequency regime where the group velocity is low and hence the density of modes is high. In addition, due to the finite length of the structure, edge and surface effects that are normally neglected in the usual PBG \( k \)-space calculations can become important. We therefore study dipole emission rates at photonic band-edge frequencies with an eye towards utilizing these effects in order to maximize laser gain and power output.

We model the interaction of a PBG structure with the electromagnetic field that is generated when dipoles located inside the material radiate. For this work, we assume that the active medium is composed of a collection of classical dipole oscillators excited with an initial potential energy. However, these classical dipoles can readily be replaced with a more realistic collection of excited two-level atoms. This can be accomplished by replacing the oscillator equations with the coupled Bloch equations that describe medium inversion and polarization. The qualitative aspects of field dynamics remain the same, so we will address the specifics of this two-level atom model in a later publication.

We therefore begin by assuming that at time \( t = 0 \) the total field \( \Sigma \) is zero, and that the initial volume polarization \( \Pi \) is given by:

\[
\Pi = \frac{1}{2} \left[ P(x, t) e^{-i\omega t} + c.c. \right].
\]

This gives rise to a macroscopic Maxwell field of the type:

\[
\Sigma = \frac{1}{2} \left[ E(x, t) e^{-i\omega t} + c.c. \right].
\]

Here, \( P \) and \( E \) are general envelope functions, and upon direct substitution in Maxwell's equation for the propagation, we may write:

\[
\frac{\partial^2 E}{\partial z^2} - \frac{1}{c^2} \frac{\partial^2 E}{\partial t^2} + \frac{2i\omega}{c^2} \frac{\partial E}{\partial t} + \frac{\omega^2}{c^2} E = \frac{n(z)^2 - 1}{c^2} \left( \frac{\partial^2 E}{\partial z^2} - 2i\omega \frac{\partial E}{\partial t} - \omega^2 E \right) + \frac{4\pi}{c^2} \left( \frac{\partial^2 P}{\partial t^2} - 2i\omega \frac{\partial P}{\partial t} - \omega^2 P \right).
\]

We have assumed that the dielectric medium response can be separated into a linear, non-resonant response that gives rise to the periodic background refractive index \( n(z) \), and a resonant response that can be modeled by a collection of noninteracting classical oscillators. Assuming that the volume polarization is given by \( \Pi = Nex \), where \( N \) is the dipole density, \( e \) is the electric charge, and \( x \) is the charge displacement from equilibrium. The resulting medium polarization obeys a harmonic-oscillator equation of motion of the type:

\[
\frac{d^2 \Pi}{dt^2} + \omega_0^2 \Pi = \frac{Ne^2}{m} \Sigma,
\]

where \( \omega_0 \) is the natural frequency of the oscillator, and \( m \) is the mass of the electron. We now assume that the field and polarization envelopes are slowly varying functions of time, i.e., variations of the envelope functions are small over one optical period. However, these variations are allowed to be arbitrarily rapid in space, since the index of refraction at a dielectric interface can vary sharply within
one optical wavelength. Therefore, retaining all lowest-order terms on either side of (4), we may write:
\[
\frac{\partial^2 E}{\partial z^2} + \frac{2i \omega}{c^2} \frac{\partial E}{\partial t} = -n^2(z) \frac{\omega^2}{c^2} E - \frac{4\pi^2 \omega^2}{c^2} P.
\]  
(6)

Near resonance, we may assume that \( \omega \approx \omega_0 \), so that \( \omega^2 - \omega_0^2 \approx 2\omega_0 \delta \), where \( \delta = \omega - \omega_0 \) is then a small frequency detuning. Substitution of (2) into (5) then yields
\[
\frac{\partial P}{\partial t} = i\delta P + i \frac{\omega_0^2}{8\pi n_0} E,
\]  
(7)

where \( \omega_0^2 = 4\pi N e^2/m \) is the plasma frequency. It is now convenient to scale to a dimensionless coordinate system in order to maintain generality and to avoid explicit reference to a particular system or a particular range of parameters. For example, the longitudinal coordinate can be scaled by the vacuum wavelength \( \lambda \), and the time can then be scaled with respect to the corresponding optical period \( \lambda/c \). However, scaling is a matter of convenience, and the scaling factor can also be chosen to be the wavelength at the center of the gap, \( \lambda_{cg} \), with the corresponding optical period \( \lambda_{cg}/c \) scaling the time. We also scale the polarization and field envelopes as \( \hat{P} = P/P_0 \) and \( \hat{E} = (\omega_0^2/4\pi \omega^2) E/P_0 \), respectively, where \( P_0 \) is an arbitrary scaling factor that can be chosen according to the initial conditions for the oscillators. For instance, \( \hat{P}_{\tau=0} = 1 \) implies \( P_{\tau=0} = P_0 = N\omega_0 x_0 \), where \( x_0 \) is the initial oscillator amplitude. Then, taking our scaled, unitless space and time parameters as \( \xi = z/\lambda_{cg} \) and \( \tau = c\xi/\lambda_{cg} \), respectively, (6) and (7) reduce to
\[
\frac{\partial \hat{E}}{\partial \tau} = \frac{i}{4\pi \omega} \frac{\partial^2 \hat{E}}{\partial \xi^2} + i\hat{\omega} n^2(\xi) \hat{E} + i \frac{2\pi^2 \omega_0^2}{\omega_{cg}} \hat{P},
\]  
(8)

and
\[
\frac{\partial \hat{P}}{\partial \tau} = -i\hat{\Delta} \hat{P} + i \frac{1}{2} \hat{E},
\]  
(9)

where \( \hat{\omega} = \omega/\omega_{cg} \) and \( \hat{\Delta} = 2\pi \delta/\omega_{cg} \) is now the center-gap scaled frequency detuning. Equations (8) and (9) are not explicitly supplemented by the boundary conditions appropriate for a one-dimensional structure. The boundary conditions are not explicitly introduced, as is usually done in typical PBG calculations, because they are accounted for through the specification of the spatially dependent index of refraction \( n(\xi) \). The polarization initial condition consisting of initially excited oscillators will force the dipoles to radiate into the structure. The nature of the dielectric layers (i.e., their refractive index and width) determines the transmission properties of the lattice, and perhaps most importantly in this case, the emission properties of the dipoles. Our numerical model allows the dipoles to be located at any arbitrary location \( \xi \) inside the structure, and can easily be extended to include all three dimensions. In that case, however, the vector nature of the electromagnetic field must be preserved, but the elegance and simplicity of the method of solution remain intact. More on the method of solution in one-dimensional structures can be found in [3–5, 10].

In order to properly account for all the energy radiated by the dipoles, we calculate the total, spatially integrated energy \( W_\omega(\tau) \) in the field as a function of time, and at a given frequency \( \omega \) of oscillation. This total energy is given by:
\[
W_\omega(\tau) = \frac{1}{8\pi} \int_{-\infty}^{\infty} n^2(\xi) \left| \hat{E}(\xi, \tau) \right|^2 d\xi.
\]  
(10)

We point out that, after a short time, most of the energy that is radiated can be found outside the structure. The instantaneous power radiated by the dipoles at time \( \tau \) is then given by the slope of this function, namely:
\[
P_\omega(\tau) = \frac{dW_\omega(\tau)}{d\tau},
\]  
(11)

which typically approaches a steady-state value for sufficiently large \( \tau \).

We choose a structure that consists of a total of 22 periods, or 44 dielectric layers whose index of refraction alternates between a low and a high value of \( n_1 = 1 \) and \( n_2 = 1.4142 \), respectively. We take the widths of the alternating layers as \( a = \lambda/(4n_1) \) and \( b = \lambda/(4n_2) \), the quarter-wave condition required for a distributed Bragg reflector. Then we locate a thin emitting dipole layer (about 1/7 of the dielectric layer in width) near the center of the structure, roughly in the center of a high index region. This ensures that if the dipole frequency \( \omega_0 \) is tuned to a frequency on the low frequency side of the photonic band gap, then the electric field is localized in the high index layers. In contrast, if the thin emitting layer were to be located inside a low index layer, and \( \omega_0 \) were chosen on the high energy side of the band gap, then the electric field would be localized inside the low index layers. We note that in general the emission rate is a sensitive function of the exact location of the emitting layer. We take the ratio of the squares of the plasma frequency to the center gap frequency to be \( \omega_0^2/\omega_{cg}^2 \approx 10^{-4} \), which is appropriate for optically active dielectric semiconductor materials such as InSb, GaAs, or AlGaAs [11]. However, we note that field dynamics inside the structure are relatively insensitive to the precise value of this ratio, because it only determines the strength of the field–matter coupling, which is already assumed to be weak. This ratio does not affect the spatial dynamics, which is dominated by interference effects arising from the derivatives of the field and the spatial discontinuity of the refractive index, i.e., the first two terms on the right-hand side of (8). Without loss of generality, we may then normalize the initial condition for the polarization by choosing \( \hat{P}_{\tau=0} = 1 \). We also choose a detuning from resonance equal to zero. Here too, the precise value of \( \delta \) cannot affect the qualitative aspects of the dynamics inside the structure, and any small deviation from resonance will not significantly affect the dynamics.

We now discuss our results. In Fig. 2, we plot the transmittance \( T(\hat{\omega}) \) and the density of modes \( \rho(\hat{\omega}) \equiv d\kappa/d\hat{\omega} \) for the structure that we have described above, as a function of the center-gap-normalized frequency \( \hat{\omega} = \omega/\omega_{cg} \). The density of modes shown in the figure can be derived analytically from first principles [12] for the simple one-dimensional model by using the matrix transfer method. Here, we simply plot the result (not to scale) for our structure for illustrative purposes. In the present work it is not necessary to explicitly calculate the
density of modes. It is clear from the figure that some frequencies near the center of the gap are not allowed to propagate through the crystal, while near the edges transmission varies. For simplicity, from now on we will concern ourselves with the low-frequency band edge, and simply state that if the emitting layer were located inside a low index layer, the same qualitative behavior would be expected for frequencies at the high-frequency photonic band edge.

In Fig. 3, we plot the temporal evolution of the total, spatially integrated energy radiated by the dipoles $W_d(t)$, eq. (10), for several frequencies near the photonic band edge. The time $t$ is expressed in units of the optical period that corresponds to the frequency at center gap. The rate at which energy is transferred from the dipoles to the field is the power output $P_d(t)$, eq. (11), and it is simply the slope of the $W$ function. From the figure, we can readily establish that steady-state dynamics is quickly achieved, and that for some frequencies near the band edge the steady-state ($t \to \infty$) power output or rate of energy flow $P_d(\infty)$ can be quite large. As expected, $P_d(\infty)$ is very small for frequencies near midgap. We summarize the dynamics in Fig. 4, where we plot the power radiated by the dipoles as a function of frequency, as expressed by (11), in the larger $\tau$ limit. We also calculate the power radiated as if the dipoles were embedded in a host background medium of uniform index of refraction of order unity, i.e., the vacuum. In order to compare the emission rates in the structure with those of the vacuum, we have normalized the total power output of Fig. 4 with respect to the vacuum emission rate: $P_d(\infty) = P_{d,\text{vac}}(\infty) / P_{d,\text{vac}}(\infty)$. Therefore, a normalized power output of $P_d(\infty)$ equal to one in Fig. 4 corresponds to the vacuum radiation rate. One should note that the results in Fig. 4 – which indicate high emission rates near the band edge and emission suppression inside the photonic band gap – come as a direct consequence of placing periodically spaced dielectric boundaries near the dipole emitting layer, and then allowing the layer to radiate. The figure thus suggests that near the band edge, where the density of modes is large (Fig. 2), the power radiated from the lattice can be nearly 15 times greater than the power that is radiated by the dipole layer in free space. In addition, near the center-gap frequency ($\tilde{\omega} \approx 1$), where the density of modes is lowest, the power radiated by the dipoles is reduced to about $10^{-3}$ of the power radiated in vacuum. The total energy radiated from the structure can never be reduced to zero at any frequency within the forbidden gap because we are considering a finite structure, which therefore has an incomplete gap. Hence, left- and right-propagating modes will always tunnel through the crystal, allowing some energy to always escape.

In Fig. 5, we show the spatial distribution of the electric field intensity ($I = |E|^2$) that is emitted inside the PBG crystal. The frequency was chosen to correspond to the maximum power emission of Figs. 3 and 4, i.e., at the band edge where $\tilde{\omega} \approx 0.885$ (recall that at center gap $\tilde{\omega} = 1$). On the other hand, in Fig. 6, we depict the electric field for a frequency further away from the edge such that we are tuned well into the pass band at $\omega/\omega_{eg} \approx 0.86$. The quantitative and qualitative differences in the fields lead to the large differences in the power radiated at those
three orders of magnitude with respect to free space. More efficient suppression could be obtained by exploiting several other structural factors, such as cavity geometry, defects, and a combination of refractive-index profile, and perhaps field-atom coupling coefficients as well as detuning. Finally, we have demonstrated that the power enhancement is strongly peaked near the band edge.

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