PHYSICAL REVIEW B

CONDENSED MATTER AND MATERIALS PHYSICS

THIRD SERIES, VOLUME 59, NUMBER 3 **15 JANUARY 1999-I**

BRIEF REPORTS

Brief Reports are accounts of completed research which, while meeting the usual **Physical Review B** *standards of scientific quality, do not warrant regular articles. A Brief Report may be no longer than four printed pages and must be accompanied by an abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

Interband transitions in photonic crystals

Joshua N. Winn, Shanhui Fan, and John D. Joannopoulos
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

Erich P. Ippen
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
and Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

(Received 6 October 1998)

We present a formalism to describe transitions between photon modes in a photonic crystal with a temporally and spatially varying dielectric constant, in analogy to optical transitions between electronic states in metals and semiconductors. Resonant transitions between different photonic bands are discussed, and predictions of the theory are compared to electromagnetic simulations. We contrast the cases of electronic and photonic transitions, and explore how the photonic band structure allows opportunities for phase matching and stationary-wave generation in nonlinear optical frequency-conversion processes. [S0163-1829(99)11503-0]

The analogy between the physics of an electron in a periodic potential (a crystal) and a photon in a periodic dielectric medium (a photonic crystal) has stimulated many approaches to the problem of controlling light propagation.[1–3] The common thread in these ideas is to employ periodic dielectric materials to alter the dispersion relation for photons in order to produce desirable features, such as photonic band gaps, which have well-known electronic counterparts.

The purpose of this paper is to extend the analogy to the case of photon transitions between bands in a photonic crystal, achieved by perturbing the dielectric constant of the underlying medium with the proper frequency and wave vector. These perturbations can be generated in a number of ways. One particularly simple method is the mechanical vibration of the crystal. Since this vibration must be executed at a frequency comparable to the frequencies of the photon modes of the crystal, this method is only feasible for the microwave regime.

Another method of achieving the perturbation, for microwaves through optical waves, is to exploit the nonlinear properties of one of the materials composing the crystal. In this case, the present work is a generalization of familiar notions from nonlinear optics,[4,5] cast in a different formalism. In a $\chi^{(2)}$ medium, for example, an optical wave may couple with another via the perturbation in the dielectric constant that it induces. The familiar requirements for such coupling to accumulate and generate a new propagating wave are those of frequency and phase (wave vector) matching between initial and final waves. In a photonic crystal, the novelties are that the dispersion relation for photon modes can be altered drastically, and the unperturbed photonic modes can have very different spatial intensity and polarization configurations than plane waves.

The use of a periodicity to assist phase matching has been demonstrated in one dimension with grating dispersion[6] and with a modulated nonlinearity (quasiphase matching)[7] to overcome phase mismatch due to material dispersion, and in a colloidal lattice of spheres, for efficient second-harmonic generation.[8] Resonant enhancement of second-harmonic generation in a one-dimensional grating has also been discussed by various authors.[9–12] The perturbation need not be optically induced. For example, perturbation of a fiber Bragg grating by an acousto-optic modulator has also been demonstrated,[13] and described with a time-independent formalism.[14]

The present work extends these notions to describe the

detailed time-evolution of states in a fully two- or three-dimensional photonic crystal (for which the dispersion relation is highly modified by the high dielectric contrast of the component materials) during an arbitrary temporal and spatial perturbation of the dielectric function. In a photonic crystal, the index contrast is usually large and a perturbative treatment of the effect of index variation is not valid. In this formalism, we begin with the exact eigenmodes of a photonic crystal, with the effects of temporal and spatial perturbations treated in terms of interactions between these eigenmodes. Although it is based on a formalism inspired by the analogy with optically induced electronic transitions in solids, the differences between the electronic and photonic cases are also explicated.

The first step in the analogy is to cast Maxwell's equations in a Schrödinger-like form. This can be done with the appropriate definitions:

$$i\frac{d}{dt}|\mathbf{F}\rangle=[\Theta+V(\mathbf{r},t)]|\mathbf{F}\rangle, \tag{1}$$

$$|\mathbf{F}\rangle\equiv\begin{bmatrix}\mathbf{D}\\ \mathbf{H}\end{bmatrix},\quad \Theta\equiv\begin{bmatrix}0 & i\nabla\times\ldots\\ -i\nabla\times\left(\frac{1}{\varepsilon}\cdots\right) & 0\end{bmatrix},$$

$$V\equiv\begin{bmatrix}0 & 0\\ i\nabla\times\left(\frac{\delta\varepsilon}{\varepsilon^2}\cdots\right) & 0\end{bmatrix}. \tag{2}$$

In Eq. (2), $\mathbf{D}$ is the displacement field, $\mathbf{H}$ is the magnetic field, $\varepsilon(\mathbf{r})$ is the background dielectric function, and $\delta\varepsilon(\mathbf{r},t)$ is the perturbation in the dielectric function. In an unperturbed photonic crystal, ε is triply periodic and $\delta\varepsilon=0$. The eigenvectors of Θ are the photonic Bloch states of the crystal, and the eigenvalues are their frequencies. With a suitably defined inner product

$$\langle\mathbf{F}_1|\mathbf{F}_2\rangle\equiv\frac{1}{(2\pi)^3}\int d^3\mathbf{r}\left(\frac{1}{\varepsilon}\mathbf{D}_1^*\cdot\mathbf{D}_2\right)+(\mathbf{H}_1^*\cdot\mathbf{H}_2), \tag{3}$$

the operator Θ is Hermitian. Note that V is not a Hermitian operator, which implies that the transitions it induces are not norm conserving. Nevertheless, we may proceed as in quantum mechanics to develop a time-dependent perturbation theory. Supposing that $|\mathbf{F}_n\rangle$ are the Bloch states of the unperturbed crystal, we may derive the following exact equation for the amplitudes $a_m(t)=\langle\mathbf{F}_m|\mathbf{F}(\mathbf{r},t)\rangle e^{i\omega_m t}$:

$$i\frac{d}{dt}a_m(t)=\sum_n V_{mn}a_n(t)\exp[i(\omega_m-\omega_n)t]. \tag{4}$$

In this equation, the perturbation matrix elements V_{mn} are given by

$$V_{mn}=\frac{-\omega_m}{(2\pi)^3}\int d^3\mathbf{r}\,\frac{\delta\varepsilon(\mathbf{r},t)}{\varepsilon^2}\,\mathbf{D}_m^*\cdot\mathbf{D}_n. \tag{5}$$

For coupling to occur, this matrix element must be nonvanishing. The unperturbed states can be written in Bloch form $\mathbf{D}_n(\mathbf{r})=\hat{\mathbf{D}}_n(\mathbf{r})\exp(i\mathbf{k}_n\cdot\mathbf{r})$, where $\hat{\mathbf{D}}_n(\mathbf{r})$ is periodic on the crystal lattice. If the perturbation $\delta\varepsilon$ is itself a Bloch wave $\hat{\delta\varepsilon}(\mathbf{r})\exp[i(\mathbf{k}\cdot\mathbf{r}-\omega t)]$, as would be the case for a perturbation caused by the nonlinear interaction with another optical wave, then for a nonvanishing matrix element it must be the case that $\mathbf{k}_m+\mathbf{k}_n-\mathbf{k}=\mathbf{G}$, where $\mathbf{G}$ is any reciprocal lattice vector of the crystal. This is to be contrasted with the usual phase-matching condition $\mathbf{k}_m+\mathbf{k}_n-\mathbf{k}=0$ in a homogeneous medium. However, phase-matching alone is not a sufficient criterion for coupling between Bloch states. The symmetries of the Bloch states must also be compatible with that of the perturbation $\delta\varepsilon$, in the sense that the integral which remains in Eq. (5) should be nonzero even after the phase-matched factors $\exp(i\mathbf{k}\cdot\mathbf{r})$ cancel out.

One major difference between this case and the case of electrons in a solid is that in a solid, the bands are all occupied with electronic states up to the Fermi level. In a photonic crystal the bands are generally unoccupied. A single Bloch wave can be established as the initial condition for Eqs. (4) by illuminating the crystal with an optical wave of the proper frequency along the desired direction.

In that case, all other modes of the problem may be ignored except for ones which are coupled to the initial condition by way of the perturbation. The simplest case is one in which the perturbation is tuned to the frequency difference between the initial Bloch state and only one other, possibly in a different band. If the phase-matching condition is satisfied, resonant transitions between the states (say, 1 and 2) take place under the influence of the perturbation. In analogy with the corresponding two-state problem in quantum theory, the approximate solutions to Eqs. (4) are

$$a_1(t)=\cos\left(t\sqrt{\frac{V_{12}V_{21}}{2}}\right),$$

$$a_2(t)=\sqrt{\frac{\omega_2}{\omega_1}}\sin\left(t\sqrt{\frac{V_{12}V_{21}}{2}}\right). \tag{6}$$

After the perturbation acts for time $\pi\sqrt{2/V_{12}V_{21}}$ (or, equivalently, $\omega_1/\sqrt{2V_{12}V_{21}}$ optical cycles of the initial mode), the initial mode has been converted into the target mode. As an example, for a $\chi^{(2)}$ material such as GaAs ($n=3.5$), the modulation strength $\delta\varepsilon/\varepsilon$ can be expected to reach 5×10^{-5} if the intensity of the perturbing electric field reaches 10^{10} W/m^2, as it would if a one-watt laser pulse were focused onto a 10 μm$\times$10 μm region of a photonic crystal.[15] For photonic modes with $\lambda\approx1$ μm and $\omega_2\approx2\omega_1$, an order-of-magnitude estimate with Eq. (5) predicts a transition time of order 100 ps.

Note that the amplitudes of the coefficients in Eq. (6) are not equal—a reflection of the fact that V is not Hermitian and the transitions are not norm conserving. This is to be contrasted with the norm-conserving unitary evolution of quantum mechanics. Another point of contrast to electronic transitions is that the photonic transition may be indirect; that is, between states that propagate in different directions. For this the wave vector of the perturbation must be matched to the difference in wave vectors of the states. In the case of electron bands, momentum conservation demands that optically-induced transitions be very nearly direct ($\Delta\mathbf{k}=0$).

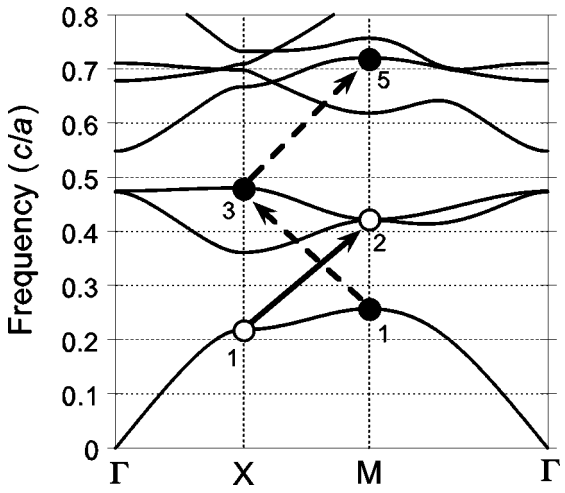

FIG. 1. Photonic bands for the TM-polarized modes of a square lattice of dielectric ($\varepsilon = 11.36$) rods in air. The transitions $X_1 \leftrightarrow M_2$ and $M_1 \leftrightarrow X_3 \leftrightarrow M_5$ are marked.

Interband transitions in photonic crystals also add possibilities for well-known nonlinear frequency-conversion processes. The basic difference is that, in a photonic crystal, the unperturbed modes may be quite different from ordinary plane waves, and the underlying dispersion relation (band structure) governing the allowed transitions may be manipulated by thoughtful design of the crystal geometry.

As a concrete demonstration we have simulated the electromagnetic fields in a typical two-dimensional photonic crystal, a square lattice of columns with dielectric constant $\varepsilon = 11.36$ embedded in a medium with $\varepsilon = 1$. The photonic band structure (computed by a conjugate-gradient scheme[16]) is shown in Fig. 1, for waves polarized with the electric field along the columns. The initial state was chosen to be X_1, and the target state M_2, as indicated by the solid arrow. For phase matching, a perturbation with $\mathbf{k} = (\pi/a)\hat{\mathbf{y}}$ is necessary. A finite-difference time-domain (FDTD) computation of

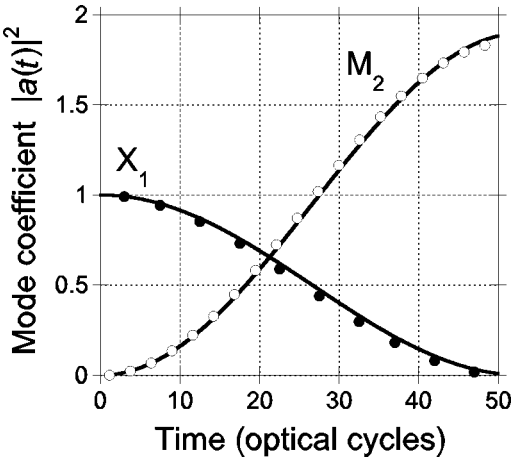

FIG. 2. The time-dependent composition of the electromagnetic field during a resonant $X_1 \leftrightarrow M_2$ transition, caused by a 4.4% nonlinearity. A point was plotted every five optical cycles for each mode, as computed by a FDTD simulation. The time axis is measured in elapsed optical cycles of the initial mode, X_1. The solid lines are the predictions of the two-state coupled-mode model, Eq. (6).

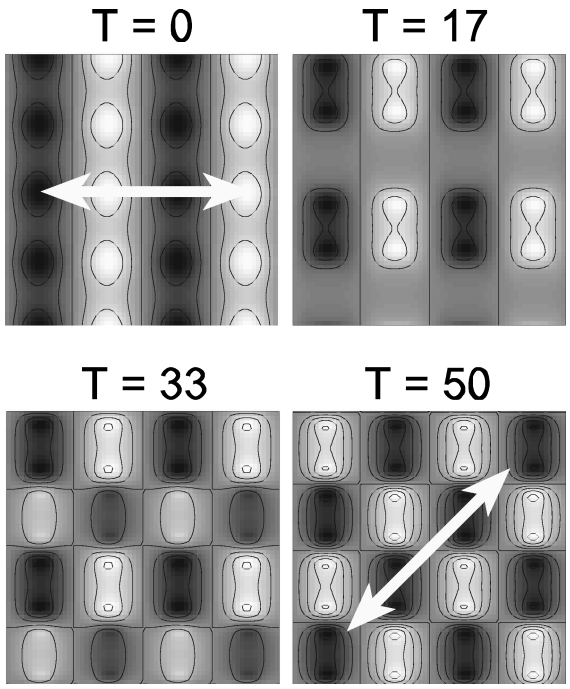

FIG. 3. Representative electric field patterns during the $X_1 \leftrightarrow M_2$ transition. White (black) represents a field pointing out of (into) the page. Contours of field strength are also shown. The arrows show the direction of propagation at the beginning and end of the transition. The time T is the number of optical cycles of the initial mode, as in Fig. 2.

Maxwell's equations on a 32×32 spatial grid containing four unit cells, with a 4.4% dielectric perturbation of the columns, allowed the detailed time evolution of the fields to be observed. The use of an unnaturally large index modulation in the simulation is purely for the purposes of shortening the transition time and thereby making the computation tractable. The physics is independent of the magnitude of the index modulation. Also, for a weaker perturbation the approximations leading to Eq. (6) are even more appropriate as

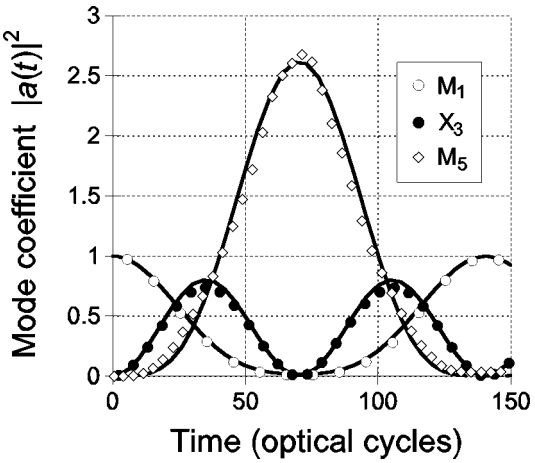

FIG. 4. The time-dependent composition of the electromagnetic field that begins in the M_1 state and is resonantly excited to X_3. A point was plotted every ten optical cycles for each mode, as computed by a FDTD simulation. The predictions of a three-state model derived from Eqs. (4) are plotted as solid lines. The time axis is measured in elapsed optical cycles of the initial mode, M_1.

the transition time becomes correspondingly lengthened.

This time evolution is shown in Figs. 2 and 3. In Fig. 2 the coefficients $|a_n(t)|^2$ are plotted and compared to the predictions of the two-state model. This model agrees with the FDTD simulation almost exactly—the transition time, which scales inversely with the magnitude of the perturbation, agrees with the prediction of Eqs. (6). In Fig. 3, representative field configurations during the transition have been plotted, as the field switches from propagating along the X direction to the M direction. This is a demonstration of an indirect, interband transition, one of the possibilities afforded by the periodicity of the photonic crystal.

The result of this transition is the generation of a standing wave, since M_2 lies on the band edge and has zero group velocity. It is evidently possible to generate stationary modes in a photonic crystal without using counter-propagating waves ($\mathbf{k}$ and $-\mathbf{k}$), as would be the case in a homogeneous material. This is an example of the possibilities introduced by the drastically altered photonic band structure, in this case the flattening of photonic bands near the edge of the Brillouin zone.

For the case of an optically induced perturbation, there must be a Bloch state with just the right frequency (to satisfy the resonance condition) and wave vector (for proper phase matching). This can be achieved by altering the geometry of the crystal until the band structure admits such a mode (for example, in the present case, the state at Y_1 is very close to resonance between X_1 and M_2). Or, the perturbation might be induced in a two-dimensional crystal by utilizing the third dimension—by illuminating the crystal from below the symmetry plane at the proper angle. In that case the allowed states form a continuum: the frequency can be tuned to resonance, and the angle of approach can be chosen to permit phase matching.

As a second illustration, it is possible (for this particular band structure) to couple together three different modes. Figure 4 shows the time evolution of the fields which start in state M_1 and are acted upon by a perturbation (again in the y direction) in resonance with X_3. The field energy oscillates between those two modes and also a third, M_5, which happens to be very nearly frequency- and phase-matched to the states in the lower bands, owing to the band structure of this particular crystal. The FDTD simulations agree with the predictions of a simple three-state coupled-mode model, derived from Eqs. (4) and solved by Runge-Kutta integration.

A simulation of very long duration shows that eventually the fields transfer some power to even higher modes; it is likely that there will exist such modes near resonance since the density of photonic bands increases with frequency. The fields will climb the band structure in sequential jumps given by the frequency and wave vector of the perturbation, and with a temporal sequence determined by the matrix elements V_{mn} between states and the proximity to resonance. This band-climbing behavior is another point of contrast to the case of electronic transitions, where numerous mechanisms exist for de-exciting the electron back to its ground state. Such mechanisms are less important for photon modes in a photonic crystal, since the nonlinear interactions between light and dielectric media are very weak. Proceeding to sequentially higher modes is of course possible through nonlinear conversion processes in homogeneous materials (no photonic crystal) but is generally suppressed by the lack of phase matching.

The hallmark of photonic crystals—a drastically altered dispersion relation for light—may provide opportunities in principle for resonant transitions and frequency conversion in a time-dependent medium. Since band structures and matrix elements are easily computed, the dispersion relation can be designed to permit coupling between desired modes, and the spatial distribution of intensity and polarization of the photon modes may be modified to concentrate wave energy in certain desired locations. Photonic crystals may allow unusual, controllable temporal sequences of electromagnetic fields to be realized.

The authors would like to acknowledge helpful conversations with Mehran Kardar and Eli Burstein. This work was supported in part by the MRSEC program of the NSF under Award No. DMR-9400334. J.N.W. acknowledges the support of the Fannie and John Hertz foundation.

[1] E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).
[2] J. D. Joannopoulos, P. R. Villeneuve, and S. Fan, Nature (London) **386**, 143 (1997).
[3] J. D. Joannopoulos, R. D. Meade, and J. N. Winn, *Photonic Crystals* (Princeton University Press, Princeton, NJ, 1995).
[4] N. Bloemberger, *Nonlinear Optics* (Benjamin, Reading, MA, 1965).
[5] Y. R. Shen, *The Principles of Nonlinear Optics* (Wiley, New York, 1984).
[6] A. Yariv and P. Yeh, J. Opt. Soc. Am. **67**, 438 (1977).
[7] E. J. Lim, M. M. Fejer, and R. L. Byer, Electron. Lett. **25**, 174 (1989).
[8] J. Martorell, R. Vilaseca, and R. Corbalán, Appl. Phys. Lett. **70**, 702 (1997).
[9] J. Trull, R. Vilaseca, J. Martorell, and R. Corbalan, Opt. Lett. **20**, 1746 (1995).
[10] M. J. Steel and C. Martijn de Sterke, Appl. Opt. **35**, 3211 (1996).
[11] M. Scalora, M. J. Bloemer, A. S. Manka, J. P. Dowling, C. M. Bowden, R. Viswanathan, and J. W. Haus, Phys. Rev. A **56**, 3166 (1997).
[12] J. W. Haus, R. Viswanathan, M. Scalora, A. G. Kalocsai, J. D. Cole, and J. Theimer, Phys. Rev. A **57**, 2120 (1998).
[13] W. F. Liu, P. St. J. Russell, and L. Dong, Opt. Lett. **29**, 1515 (1997).
[14] P. St. J. Russell, Phys. Rev. Lett. **56**, 596 (1986).
[15] A. Yariv, *Optical Electronics in Modern Communications*, 5th ed. (Oxford University Press, Oxford, 1997).
[16] R. D. Meade, A. M. Rappe, K. D. Brommer, and J. D. Joannopoulos, Phys. Rev. B **48**, 8434 (1993).