Tunable Photonic Crystals with Semiconducting Constituents

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We propose that the photonic band structure (PBS) of semiconductor-based photonic crystals (PCs) can be made tunable if the free-carrier density is sufficiently high. In this case, the dielectric constant of the semiconductor, modeled as $\varepsilon(\omega) = \varepsilon_0(1 - \omega_p^2/\omega^2)$, depends on the temperature T and on the impurity concentration N through the plasma frequency ω_p. Then the PBS is strongly T and N dependent; it is even possible to obliterate a photonic band gap. This is shown by calculating the 2D PBS for PCs that incorporate either intrinsic InSb or extrinsic Ge.

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It is a well-known fact of semiconductor physics that band gaps are temperature dependent. In this Letter we demonstrate that *photonic* band gaps (PBGs) may also depend on temperature. The two phenomena are, however, unrelated.

Photonic crystals (PCs) or PBG materials [1] are periodic structures (in 1D, 2D, or 3D) constructed of two or more (homogeneous) materials, at least one of which is transparent to light. Early investigations involved dielectrics such as glasses. The periodically spaced inclusions and the lattice constant were measured in millimeters. With a judicious choice of the structure, and sufficiently large dielectric contrast between the two constituent materials, a PBG was then found in the microwave region [2]. Applications include high-power mirrors, low-loss waveguides, and antenna substrates [1].

The photonic band structure (PBS) is known to scale with the inverse lattice constant; hence downsizing of PCs soon began in an attempt to attain PBGs in the optical range of the spectrum. In these studies very pure semiconductors—essentially insulators—were used; AlGaAs compounds are favored because they have large dielectric constants (DCs) and relatively wide band gaps that minimize absorption. By now 2D and 3D PCs with lattice constants on the order of hundreds of nanometers are being fabricated by means of microlithographical techniques [3]. The ensuing PBGs are then indeed in the optical region. Such structures are of great interest for thresholdless lasers and, in general, optoelectronics [1–3].

To date, the PBS of any given PC has been immutable. Namely, once the PC has been fabricated, its PBS remains unaltered. Obviously, the possibility to change the PBS externally would invest PCs with considerable flexibility, and could lead to novel applications such as an optical shutter whose performance is controlled in some specified manner. It has already been proposed that PCs constructed with ferroelectric or ferromagnetic materials could be tuned by means of an external electric or magnetic field, respectively [4]. Very recently, it was also suggested that PCs of the inverse opal type could be doped with a liquid crystal; in order to achieve a desired optical response, such a structure could be tuned and even reprogramed by means of a mesh of surrounding wires, each of which can produce a localized electric field [5]. In this Letter we describe a third possibility for tuning PCs—such that incorporate a semiconducting constituent. The idea is based on variations of the concentration of free carriers within the semiconductor by means of changes in the temperature or in the density of dopants.

Of course, even a very pure semiconductor has an intrinsic density of electrons and holes in its conduction and valence bands, respectively. Such concentrations of free carriers can be substantial for narrow-gap semiconductors. Nevertheless, the effect of free carriers on the PBS has not been considered previously. Now, doping by means of current injection provides a mechanism for manipulating the PBS. Further, variations in the temperature of the semiconductor will change the density of free carriers; this could lead to a simple, external control of the PBG. We consider that the physical interest and possibility of applications, involved in these ideas, outweigh the detrimental aspect of free charges, namely, absorption. Below we present an outline of a theory of PBS that incorporates finite densities of electrons and holes [6]. This theory is applied to 2D PCs that include a semiconducting constituent, characterized by a simply modeled dielectric constant $\varepsilon(\omega)$. Specifically, we study the dependence on temperature of the PBS of an array of intrinsic InSb rods in air. We also consider intrinsic Ge that is delta doped in such a way that an array of extrinsic Ge cylinders forms. We show how doping or temperature variation can change, and even close, the PBG.

A convenient measure of the amount of free charge is the screened plasma frequency ω_p. It depends on the densities n_i and effective masses m_i of the free electrons and holes in the relevant conduction and valence bands (labeled i).

As is well known [7],

$$\omega_p^2 = \sum_i 4\pi n_i e^2/m_i\varepsilon_0\,, \tag{1}$$

where ε_0 is the static (background) DC. As a first approximation, we neglect absorption (to be considered later on), which implies a real DC. Then, provided that the frequencies of interest are well below the far infrared resonance region [8], our model DC is

$$\varepsilon(\omega) = \varepsilon_0(1 - \omega_p^2/\omega^2)\,. \tag{2}$$

If, on the other hand, ω is substantially above the phonon resonance, then ε_0 in Eqs. (1) and (2) is replaced by ε_∞, the optical DC.

For $\varepsilon_0 = 1$, Eq. (2) describes the DC of a simple metal. The PBS for metallic inclusions thus modeled, surrounded by air, was calculated for periodic systems in 1D, 2D, and 3D [9]. A PBG can arise at low frequencies and just above the plasma frequency; well above ω_p, however, there can be no PBGs. This is because, for $\omega \gtrsim 2\omega_p$, $\varepsilon(\omega) \sim 1$; hence the PBS becomes very similar to that obtained from the empty-lattice model applied to vacuum. The low-frequency behavior (for $\omega \ll \omega_p$) was confirmed experimentally for metallodielectric PCs in the GHz regime [10]. Of course, ω_p for metals is strictly constant, with the consequence that the PBS cannot be altered. On the other hand, the plasma frequency of a semiconductor may depend strongly on the temperature T. In order to exhibit the ideas involved, first we consider InSb, which has the advantages of a small band gap and a high mobility. The narrow gap (0.18 eV at room temperature) gives rise to $\omega_p = 1.6 \times 10^{13}$ s^{-1} in the intrinsic case. As we see in Fig. 1 (dashed line on right side), ω_p increases essentially exponentially with temperature. Hence $\varepsilon(\omega)$ is very sensitive to temperature variations in the far infrared. Thus, for a PC with an InSb constituent, we can expect substantial variations of the PBS with temperature in this important spectral region. Moreover, sufficiently below the phonon resonance ($\omega_T = 3.5 \times 10^{13}$ s^{-1}), damping effects should be moderate [11].

For semiconductors $\varepsilon_0 \gtrsim 10$, and this, as we shall see, causes strong departure from the empty-lattice behavior. For the sake of generality, the DCs of the (infinitely long) cylinders and of the host material are both modeled according to Eq. (2), however with different values of the parameters ε_0 and ω_p. The special case of semiconductor cylinders in air is obtained by substituting $\varepsilon_{0b} = 1$ and $\omega_{pb} = 0$, while the conjugate case is specified by $\varepsilon_{0a} = 1$ and $\omega_{pa} = 0$. Note that ε_0 and ω_p are both doubly periodic functions of the position vector $\boldsymbol{r}$ in the plane of periodicity. The wave equation for the electric field $\boldsymbol{E}(\boldsymbol{r})$ is

$$\nabla \times \nabla \times \boldsymbol{E} = (\omega/c)^2\varepsilon(\omega)\boldsymbol{E} = (\omega/c)^2\varepsilon_0[1 - \omega_p^2(\boldsymbol{r})/\omega^2]\boldsymbol{E}\,. \tag{3}$$

By defining $\eta(\boldsymbol{r}) = 1/\varepsilon_0(\boldsymbol{r})$ and $\Omega(\boldsymbol{r}) = \omega_p^2(\boldsymbol{r})/c^2$, Eq. (3) may be written as

$$\eta(\boldsymbol{r})\nabla \times \nabla \times \boldsymbol{E}(\boldsymbol{r}) + \Omega(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r}) = (\omega/c)^2\boldsymbol{E}(\boldsymbol{r})\,. \tag{4}$$

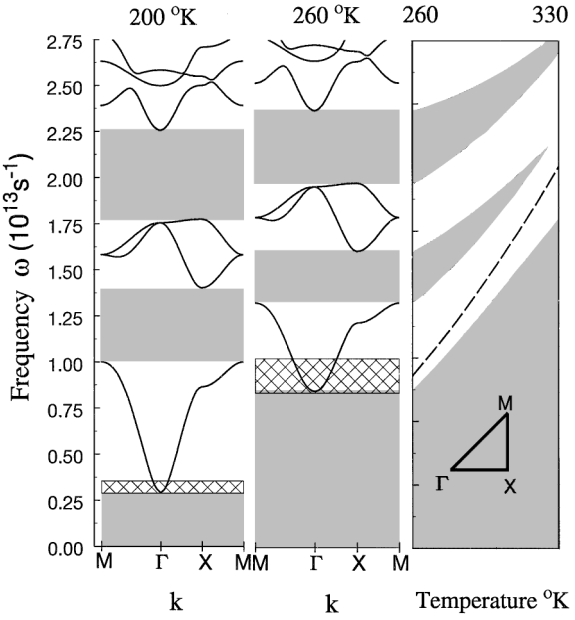

FIG. 1. PBS for two temperatures of circular semiconducting InSb cylinders that form a square lattice. The light is polarized parallel to the cylinders. The DC of the intrinsic InSb cylinders is modeled according to Eq. (2), with $\varepsilon_0 = 17.7$, $m_e/m = 0.015$ [7], and $n_e = 5.76 \times 10^{14} T^{3/2} \exp(-0.13/k_B T)$ (T in K, $k_B T$ in eV, and n_e in cm^{-3}); the lattice constant is $a = 40\ \mu$m and $f = 0.25$. The cross-hatched bands extend from $\omega_p - 1/\tau_e$ to $\omega_p + 1/\tau_e$, making regions of exclusion where absorption is strong. The first three PBGs (shaded) and the passbands (blank) in between are displayed on the right side as functions of temperature. Note that the second gap closes at $T = 325$ K. The dashed line is $\omega_p(T)$, with strong absorption in its vicinity. The inset is the irreducible part of the Brillouin zone.

Of course, $\eta(\boldsymbol{r})$ and $\Omega(\boldsymbol{r})$ are also periodic functions of their argument, and hence can be expanded in 2D Fourier series.

We consider only waves that propagate parallel to the plane of periodicity. Then 2D PCs support two independent modes, with either the electric or the magnetic field being parallel to the cylinders [13]. Here we shall study only the former, so-called E mode. It is a transverse wave, hence the double rotational in Eq. (4) reduces to $-\nabla^2 E(\boldsymbol{r})$. By applying the Bloch theorem to $E(\boldsymbol{r})$, Eq. (4) becomes

$$\sum_{\boldsymbol{G}'}[\eta(\boldsymbol{G} - \boldsymbol{G}')|\boldsymbol{k} + \boldsymbol{G}'|^2 + \Omega(\boldsymbol{G} - \boldsymbol{G}')]E_{\boldsymbol{k}}(\boldsymbol{G}') = (\omega/c)^2 E_{\boldsymbol{k}}(\boldsymbol{G})\,. \tag{5}$$

Here $\boldsymbol{G}$ is the reciprocal lattice vector, $\eta(\boldsymbol{G})$ and $\Omega(\boldsymbol{G})$ are the Fourier transforms of $\eta(\boldsymbol{r})$ and $\Omega(\boldsymbol{r})$, and $E_{\boldsymbol{k}}(\boldsymbol{G})$ is the amplitude of the Bloch wave of wave vector $\boldsymbol{k} + \boldsymbol{G}$.

Equation (5) constitutes the eigenvalue problem for $\omega = \omega(\boldsymbol{k})$ and thus determines the PBS for our 2D semiconductor system. It is notable that the matrix operator on the left side does not depend on the eigenvalue, which is to say that the eigenvalue problem has been cast in the standard form—much easier to solve numerically [14]. Of course,

such a simplification is not feasible for an arbitrary model of $\varepsilon(\omega)$. The function $\Omega(\boldsymbol{G})$ is

$$\Omega(\boldsymbol{G}) = \frac{1}{A_c}\int_{A_c} d\boldsymbol{r}\,\Omega(\boldsymbol{r})e^{-\boldsymbol{G}\cdot\boldsymbol{r}} = \begin{cases} \overline{\Omega}, & \boldsymbol{G} = 0, \\ F(\boldsymbol{G})\delta\Omega, & \boldsymbol{G} \neq 0, \end{cases} \tag{6}$$

where A_c is the area of the unit cell, $\overline{\Omega}$ is the average of $\Omega(\boldsymbol{r})$, $\delta\Omega$ is the "contrast" $\Omega_a - \Omega_b = (\omega_{pa}^2 - \omega_{pb}^2)/c^2$, and $F(\boldsymbol{G}) = A_c^{-1}\int_a d\boldsymbol{r}\, e^{-i\boldsymbol{G}\cdot\boldsymbol{r}}$ is the structure factor; the integral is taken over the cross-sectional area of one cylinder. In the special case of circular cylinders, $F(\boldsymbol{G}) = 2fJ_1(GR)/GR$, where R is the cylinder radius, J_1 is a Bessel function, and $f = \pi R^2/A_c$ is the filling fraction. The formulas for $\eta(\boldsymbol{G})$ are completely analogous to Eq. (6).

Equations (5) and (6) have been applied to a PC made up of intrinsic InSb cylinders in air. The PBSs are displayed in Fig. 1 for the temperatures 200 and 260 K. There is a low-frequency PBG that extends up to a frequency slightly below $\omega_p(T)$, and the first passband is parabolic. Such a behavior is characteristic of the E mode, if the DC of the cylinders is sufficiently negative [9,10]. There are also two higher-lying PBGs in the exhibited frequency region. This situation differs from the metallic case [with $\varepsilon_0 = 1$ in Eq. (2)], where no gaps were found above the second band [9]. The most dramatic aspect of Fig. 1 is the rapid increase with T of low-frequency PBG. This can be attributed directly to the increase in $\omega_p(T)$ (dashed line in Fig. 1), namely, to more and more electrons being excited from the valence band of InSb to its conduction band. On the other hand, all the subsequent PBGs *decrease* with T. The explanation for this is that, for a given ω, $\varepsilon(\omega)$ becomes smaller as the temperature is raised, giving rise to a diminished dielectric contrast in comparison to the air cylinders. We also note that the midgap frequencies and, indeed, the entire PBS keep rising with T. However, because our neglect of the lattice contribution in Eq. (2), the upper part of Fig. 1 has only semiquantitative validity (although absorption there remains small).

On the right side of Fig. 1, the first three PBGs (shaded) and the passbands (blank) between them are shown as a function of T beyond 260 K. It is seen that the second PBG is actually obliterated at $T = 325$ K; in this sense the PC is "completely tunable." Clearly, the equifrequency surfaces $\omega(k) = \text{const}$ are expected to undergo dramatic changes, similar to those described in Ref. [4]. The dashed line is $\omega_p(T)$; in its vicinity absorption is important because $\text{Im}\varepsilon \gg \text{Re}\varepsilon$ for the semiconductor. Similar results were obtained for air cylinders in an InSb host.

The other PC that we consider is made entirely of Ge. We assume that an intrinsic sample of Ge is delta doped by donor impurities, in such a way that a 2D, periodic array of strongly *extrinsic, n*-type Ge cylinders is formed. By Eq. (1), in this regime ω_p is proportional to the square root of the impurity density N. Then, using an experimental value of ω_p for $N = 10^{19}$ cm^{-3} [15], we may write $\omega_p(N) = 1.45 \times 10^{14}[N(\text{cm}^{-3}) \times 10^{-19}]^{1/2}$ s^{-1}. As we see on the right side of Fig. 2, for $N = 3 \times 10^{19}$ cm^{-3}, the dielectric contrast between extrinsic and intrinsic Ge is sufficiently great for the formation of two PBGs. As N decreases, these gaps also decrease. The first gap disappears when the cylinders become intrinsic themselves, while the second gap is obliterated at $N = 0.4 \times 10^{19}$ cm^{-3}.

Figures 1 and 2 demonstrate that the PBS can be very sensitive to changes in the temperature or the impurity concentration. This is to say that the PBS can be externally controlled or tuned by means of suitable variations of temperature or current injection. There are important implications for the optical response of PCs with a substantial density of free carriers. For example, consider the PC constituted by the intrinsic InSb cylinders. Suppose illuminating this PC by light incident in a direction perpendicular to the cylinder axes, and that is polarized parallel to the axes, giving rise to the E modes considered here. For $\omega = 1.75 \times 10^{13}$ s^{-1}, the light will be reflected in part and transmitted in part (see Fig. 1) if $T < 281$ K. If, now, the temperature is raised slightly, no propagation is possible in the PC, and the light will be totally reflected. With an additional increase of the temperature, to $T > 297$ K, transmission will occur again. Clearly, these ideas could serve as the basis for a temperature-controlled optical shutter. Further, at fixed T, the PC has passbands defined by certain lower and upper bounds. By changing T, these bounds shift. Simply stated, the passband is tunable. The same considerations remain valid if temperature control is replaced by current injection control, as is clear from Fig. 2.

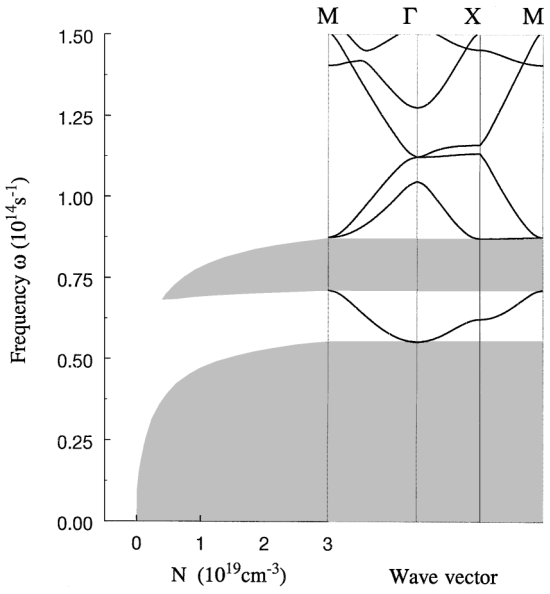

FIG. 2. PBS of a square array of circular cylinders generated by delta doping of an intrinsic Ge host. The right side of the figure corresponds to $N = 3 \times 10^{19}$ donor atoms per cm^3. The left side shows the variation of the two PBGs with N. The low-frequency gap disappears when the cylinders become intrinsic, and the second gap is obliterated for $N = 0.4 \times 10^{19}$ cm^{-3}. Here $\varepsilon_0 = 15.8$ [7], $a = 5$ μm, and $f = 0.25$.

In the figures ω is limited to the far ir, which is the operative regime of mesoscopic PCs at the present. The band gap of InSb is in the far ir itself, hence it is *not* possible to reach the *near* ir. On the other hand, semiconductors with larger gaps would require extremely high levels of doping for ω_p to lie in the far ir; this would likely cause prohibitive absorption. However, it is important to note that such semiconductors are promising for tuning in the microwave and short wave regimes where absorption is negligible. For instance, between 280 and 320 K, intrinsic Ge gives rise to substantial variations of ω_p ($\sim$10 GHz).

In conclusion, we have shown that, in PCs with semiconducting constituents, it is possible to alter and even close the PBGs by means of external control: doping or changing the temperature. Similar calculations for the H mode (magnetic field parallel to the cylinders) and for 3D PCs are of obvious interest. The corresponding PBSs can be readily calculated for Eq. (4) which, conveniently, leads to the standard eigenvalue problem, for any dimensionality of the periodicity. There is a downside, of course, namely, absorption. It can be minimized, however, by careful choices of the materials, the geometric parameters, and the spectral range. Transmission studies, both experimental and theoretic, would be desirable. Preliminary calculations of the reflectivity of semiconductor-based superlattices, incorporating phonon dispersion and damping, are encouraging.

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Note added.—In two recent experiments, PCs were infiltrated with liquid crystals, whose indexes of refraction are temperature dependent. Tuning was achieved by changing the temperature of the samples [16].

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[11] The losses can be attributed to the finite lifetimes of the electrons τ_e, the holes τ_h, and the phonons τ_{ph}. For $\omega^2 \ll \omega_T^2$, their respective contributions to $\mathrm{Im}\varepsilon(\omega)$ can be shown to be, approximately, $\varepsilon_0\omega_{pe}^2/\omega^3\tau_e$, $\varepsilon_0\omega_{ph}^2/\omega^3\tau_h$, and $(\varepsilon_0 - \varepsilon_\infty)\omega/\omega_T^2\tau_{ph}$, where ω_{pe} and ω_{ph} are the electron and hole plasma frequencies. It can be easily verified that, for intrinsic InSb, the electron collisions predominate. Then, by Eq. (2), $\mathrm{Im}\varepsilon(\omega)/|\mathrm{Re}\varepsilon(\omega)| \sim \omega_{pe}^2/|\omega^2 - \omega_{pe}^2|\omega\tau_e$. For $\omega = 2\omega_{pe}$, the value of this ratio is $1/6\omega_{pe}\tau_e \simeq 0.016$ for a mobility $\mu_e = e\tau_e/m_e = 77\,000\ \mathrm{cm}^2/\mathrm{V}$ [7]. Considering that the semiconductor occupies only one-quarter of the volume of the PC, we expect the absorption to be reasonably small. However, as ω approaches ω_p [and $\mathrm{Re}\varepsilon(\omega) \simeq 0$], the losses would obviously become prohibitive. Absorptive effects in the metallic case were investigated in Ref. [12].

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