THERMAL EXPANSION OF PHOTONIC BAND GAP FOR ONE DIMENSIONAL PHOTONIC CRYSTAL

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Abstract—The effect of temperature on the photonic band gap has been investigated. One dimensional photonic crystal in the form of Si/air multilayer system has been studied in this communication. The refractive index of silicon layers is taken as a function of temperature and wavelength both. Therefore, this study may be considered to be physically more realistic. It may be useful for computing the optical properties for wider range of wavelength as well as temperature. We can use the proposed structure as temperature sensing device, narrow band optical filter and in many optical systems.

1. INTRODUCTION

Photonic crystals (PCs), in particular, photonic band gap (PBG) materials have become area of interest for considerable number of researchers during the last few decades following the pioneering works of Yablonovitch [1] and John [2]. Many studies on photonic crystals suggested various potential applications of photonic crystal based devices [3, 4]. The main attraction of PBG materials is the existence of forbidden band gaps in their transmission spectra. The PBG in a PC is analogous to the electronic band gap in a solid as there is a similarity between the structural periodicity of a PC and the periodic potential energy in a solid. Of the various applications of PCs, some of important

applications are optical filters, optical switches, resonance cavities and waveguides [5–8]. Recently, many studies have been focusing on changing the parameters in a PC to fabricate devices with modulation capability. For example, a slight change of the dielectric constant can be applied to optical switching devices [9].

In addition to the existence of wide band gaps in some properly designed PCs, the feature of a tunable PBG attracts much attention in recent years. The PBG can be tuned by means of some external agents. For instance, it can be changed by the operating temperature and we call it T-tuning. A superconductor/dielectric PC belongs to this type because of the temperature-dependent London perturbation length in the superconducting materials [10–12]. Using a liquid crystal as one of the constituents in a PC, the T-tuning optical response is also obtainable [13]. Recently, PCs containing semiconductor as one of the constituents have also been investigated by many researchers. PCs with intrinsic semiconductor belong to T-tuning devices because the dielectric constant of an intrinsic semiconductor is strongly dependent on temperature [14].

However, earlier reports on the thermally modulated tunable PBGs were mainly based on the linear variation of refractive index with temperature and non-dispersive media [15, 16]. In the present communication, we consider a semiconducting medium as one of the constituents of a one-dimensional photonic crystal, since the dielectric property of semiconductors depends not only on temperature but also on wavelength. Here we consider the Si/air multilayered one-dimensional system. The refractive index of air is independent of temperature and wavelength. But the refractive index of silicon layer is taken as a function of temperature and wavelength both [14]. Therefore, this study may be considered to be more physically realistic.

2. THEORETICAL MODEL

We consider a one-dimensional photonic crystal structure, as shown in Figure 1, that is periodic along z-direction, with lattice constant $d = d_1 + d_2$ being the corresponding spatial periodicity. Here, d_1 and d_2 are the thicknesses of the two slabs of the primary unit supercell corresponding to the materials with refractive indices n_1 and n_2, respectively.

The optical properties of the proposed structure can be calculated using Abeles theory [17]. For TE wave, the characteristic matrix for a
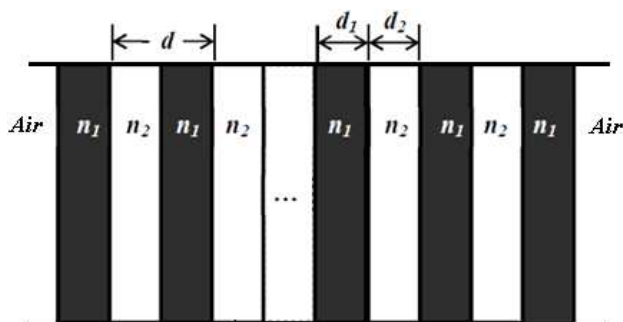
Figure 1. Schematic diagram of 1-D photonic crystal structure.

single period is given by

$$M(d) = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} = \prod_{j=1}^{2} \begin{bmatrix} \cos\delta_j & -\frac{i}{p_j}\sin\delta_j \\ -ip_j\sin\delta_j & \cos\delta_j \end{bmatrix} \quad (1)$$

Here, p_j and δ_j are given by the following relation

$$p_j = n_j \cos\theta_j \quad \text{and} \quad \delta_j = \frac{2\pi d_j}{\lambda} n_j \cos\theta_j \quad (2)$$

where θ_j is the ray angle inside the layer and $j = 1, 2$.

The matrix elements of Equation (1) can be calculated as follows

$$M_{11} = \cos\delta_1 \cos\delta_2 - \frac{p_2}{p_1}\sin\delta_1\sin\delta_2, \quad (3a)$$

$$M_{12} = -\frac{i}{p_1}\sin\delta_1\cos\delta_2 - \frac{i}{p_2}\cos\delta_1\sin\delta_2, \quad (3b)$$

$$M_{21} = -ip_1\sin\delta_1\cos\delta_2 - ip_2\cos\delta_1\sin\delta_2, \quad (3c)$$

$$M_{22} = \cos\delta_1\cos\delta_2 - \frac{p_1}{p_2}\sin\delta_1\sin\delta_2. \quad (3d)$$

The total characteristic matrix of the proposed structure for N unit cells is given by

$$M_T(Nd) = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} = [M(d)]^N = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}^N \quad (4)$$

where the matrix elements of M_T can be written in terms of the elements of the single-period matrix, namely

$$m_{11} = M_{11}U_{N-1}(a) - U_{N-2}(a), \quad (5a)$$

$$m_{12} = M_{12}U_{N-1}(a), \quad (5b)$$

$$m_{21} = M_{21}U_{N-1}(a), \quad (5c)$$

$$m_{22} = M_{22}U_{N-1}(a) - U_{N-2}(a). \quad (5d)$$

where U_N are the Chebyshev polynomials of the second kind given by

$$U_N(a) = \frac{\sin\left[(N+1)\cos^{-1}a\right]}{\left[1-a^2\right]^{1/2}} \tag{6}$$

where

$$a = \frac{1}{2}[M_{11} + M_{22}], \tag{7}$$

The transmission coefficient of the multilayer is given by

$$t = \frac{2p_A}{(m_{11} + m_{12}p_S)p_A + (m_{21} + m_{22}p_S)} \tag{8}$$

where for TE-polarization $p_A = n_A \cos\theta_A$ and $p_S = n_S \cos\theta_S$.

Thus, the transmittance of the proposed structure is given by

$$T = \frac{p_S}{p_A}|t|^2 \tag{9}$$

Since the structure has a linear periodicity, one can assume that the electromagnetic field in the super cell is a Bloch wave, i.e., $F(z + d) = e^{ikd}F(z)$, and hence one can easily derive the dispersion relation of the photonic modes is given by the following equation [18, 19]

$$\cos(K \cdot d) = a \quad \text{or} \quad K = \frac{1}{d}\cos^{-1}a \tag{10}$$

Substituting the values of the matrix elements, we find the following dispersion relation [18]

$$K = \frac{1}{d}\cos^{-1}\left[\cos\delta_1\cos\delta_2 - \frac{1}{2}\left(\frac{p_1}{p_2} + \frac{p_2}{p_1}\right)\sin\delta_1\sin\delta_2\right] \tag{11}$$

It is well known that the refractive index is not constant within wide range of wavelength as well as with respect to the temperature of the material. So, the refractive index of the medium should be the function of wavelength and temperature and may be represented by a refractive index function $n(\lambda, T)$. From phase Equation (2) it is clear that the phase δ is also the function of refractive index so that the phase δ is also the function of wavelength and temperature.

As temperature is considered over a large range, the thickness of medium also changes due to thermal expansion effect. In certain range of temperature, the thermal expansion of any material layer is given by

$$\Delta d(T) = \alpha d(\Delta T) \tag{12}$$

where, α represents the thermal expansion coefficient of the medium, and ΔT indicates the variation of the temperature. Here we consider

linear dependence of thermal expansion on temperature only as the contribution of second and higher order coefficients of thermal expansion are very small.

Air is chosen as another medium of 1-D photonic crystal considered. The thermal expansion in semiconductor medium can be accommodated by shrinkage of the air medium in the photonic crystal so that the lattice constant of the structure does not change with the variation of temperature. So, the thicknesses of higher and lower refractive index materials will be functions of temperature. Thus, the thickness of higher refractive index layer is given by

$$d_1(T) = d_1 + \Delta d_1(T) = d_1 + \alpha d_1 \Delta T \tag{13}$$

As the structure embedded in air, there will be contraction in air corresponding to the expansion in Si layer. The contraction in the layer of air can be written in the following manner;

$$d_2(T) = d_2 - \Delta d_1(T) = d_2 - \alpha d_1 \Delta T \tag{14}$$

Here, d_1 and d_2 are the respective thicknesses of higher and lower refractive index (air) materials at room temperature.

Now, the modified dispersion relation for one-dimensional Si/air multilayered photonic crystal with temperature dependence is given by

$$K(\lambda, T) = \frac{1}{d(T)} \cos^{-1} \left[\cos \delta_1(\lambda, T) \cos \delta_2 - \frac{1}{2} \left(\frac{p_1(\lambda, T)}{p_2} + \frac{p_2}{p_1(\lambda, T)} \right) \right.$$
$$\left. \sin \delta_1(\lambda, T) \sin \delta_2 \right] \tag{15}$$

Also, the group velocity can be calculated by using formula [19]

$$V_g = \left(\frac{dK}{d\omega} \right)^{-1} \tag{16}$$

3. RESULTS AND DISCUSSION

Photonic band structure for one-dimensional Si/air multilayered photonic crystal has been studied considering dependence of refractive indices of constituent materials both on the temperature of the structure and wavelength of incident electromagnetic waves. Here, silicon and air are respectively chosen as higher and lower refractive indices materials. The geometrical parameters are chosen for the thickness of higher refractive index $d_1 = 250\,\text{nm}$ and thickness of lower refractive index $d_2 = 350\,\text{nm}$ at $0\,\text{K}$ temperature. So, the lattice constant of 1D PC is chosen to be equal to $600\,\text{nm}$ and number of the unit cells taken to be equal to 10. The linear thermal expansion

coefficient for silicon is taken to be equal to 2.6×10^{-6}/K [20] and is considered to be constant throughout the range of temperature considered in our computation. The second layer is taken as air whose refractive index is 1, not affected with wavelength and temperature. The refractive index of Silicon (Si) in the range of wavelength of electromagnetic waves from 1.2 to 14 μm and in the temperature range 20–1600 K can be written as a function of wavelength and temperature as [14]

$$n^2(\lambda, T)$$
$$= \varepsilon(T) + \frac{e^{-3\Delta L(T)/L_{293}}}{\lambda^2}\left(0.8948 + 4.3977 \times 10^{-4}T + 7.3835 \times 10^{-8}T^2\right) \quad (17)$$

where

$$\varepsilon(T) = 11.4445 + 2.7739 \times 10^{-4}T + 1.7050 \times 10^{-6}T^2 - 8.1347 \times 10^{-10}T^3$$

and

$$\frac{\Delta L(T)}{L_{293}} = -0.071 + 1.887 \times 10^{-6}T + 1.934 \times 10^{-9}T^2 - 4.554 \times 10^{-13}T^3$$
$$\text{for} \quad 293\,\text{K} \leq T \leq 1600\,\text{K}$$

$$\frac{\Delta L(T)}{L_{293}} = -0.021 - 4.149 \times 10^{-7}T - 4.620 \times 10^{-10}T^2 + 1.482 \times 10^{-11}T^3$$
$$\text{for} \quad 20\,\text{K} \leq T \leq 293\,\text{K}$$

The plot of the refractive index as the function of wavelength and temperature is shown in Figure 2. From Figure 2, it is clear that the refractive index of silicon layers is more dispersive in the range 1.2–5.2 μm. We are also interested in this wavelength region (1.5–4.0 μm) because this wavelength region is also used in optical fiber communication. In our study, the photonic band structure is
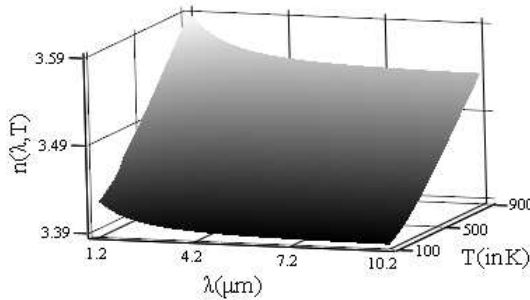

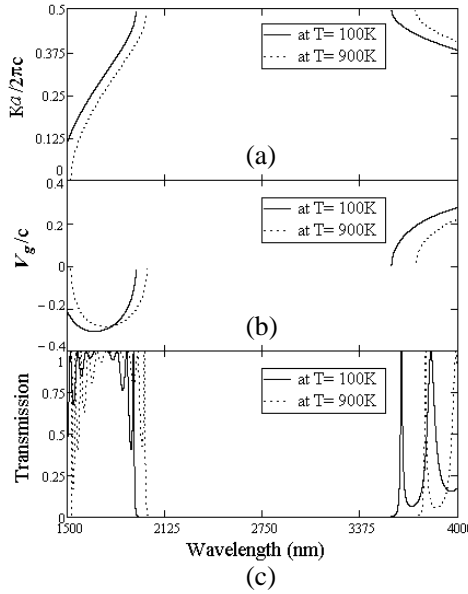**Figure 2.** Variation of refractive index as a function of wavelength and temperature.

Figure 3. The dispersion relation, group velocity and transmission for 1D photonic crystal at $T = 100\,\text{K}$ and $T = 900\,\text{K}$.

plotted from 1500 to 4000 nm (1.5–4.0 μm) on wavelength scale. We are interested to study the effect of temperature on photonic band gap in this region. For normal incidence of light, the photonic band structure has been plotted using the Equation (15) at different temperature 100 K and 900 K, which is shown in Figure 3(a). The values of refractive index of Si are computed by using Equation (17) at various temperature and wavelength, while the refractive index of air is 1. From Figure 3(a), it is found that the photonic band gaps (PBGs) have been shifted towards the higher wavelength regions due to variation in the refractive index values of silicon with temperature. The PBG is also broadened with the rise of temperature. The broadening is due to the increasing in refractive index contrast with temperature. The shifting behavior can be explained by the phase Equation (2). For the Si layers the thickness as well as refractive index is the function of temperature. So, the phase equation given in Equation (2) in terms of wavelength and temperature can be written as

$$\delta_1(\lambda, T) = \frac{2\pi d_1(T)}{\lambda} n(\lambda, T) \cos \theta_1$$

According to this phase equation, as $d_1(T)$ and $n(\lambda, T)$ increases with temperature, the wavelength must increase accordingly to keep the phase $\delta_1(\lambda, T)$ unchanged.

The group velocity and transmittance have been plotted using the Equations (16) and (9) respectively at different temperature 100 K and 900 K are shown in Figures 3(b) and 3(c). The shifting of these curves is according to the shifting of the forbidden bands as in Figure 3(a). From Figure 3(b) it is found that the group velocity shows the anomalous (negative group velocity) behavior corresponding to the first allowed band.

The variation of band gap width with temperature is shown in Table 1 and the variation of band edges and band gap width with temperature is shown in Figure 4. From this table, it is clear that the lower edge of the band gap shifts by 8.76 nm/100 K towards the higher wavelength region, whereas the upper band edge shifts 19.14 nm/100 K. Therefore, the band gap increases 10.38 nm/100 K. From Figure 4, it is clear that the expansion in the band gap is 10.38 nm/100 K.

The plots of the characteristic wavelength of a PBG, i.e., the ratio of the wavelength corresponding to the middle of band gap to the width of band gap and the PBG with temperature are shown in Figure 5. From Figures 4 and 5, it is found that both PBG and mid gap increase with the temperature whereas mid gap to band gap ratio decreases with temperature. So, it is found that the PBG increases with greater value than the midgap with the temperature. Therefore, the characteristic wavelength of the PBG of our interest decreases with the rise of temperature, indicating that the broadening of band gap is more pronounced than the shifting of the entire band gap as the temperature of the structure increases.

Table 1. Band gap width at different temperatures.

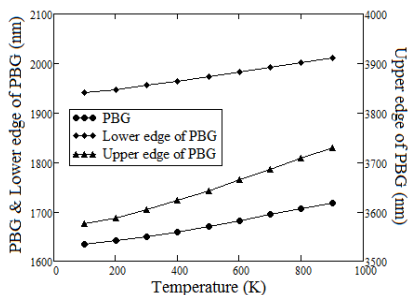| Temperature (in K)	Upper Edge of PBG (in nm)	Lower Edge of PBG (in nm)	Width of PBG (in nm)
100	3576.0	1941.0	1635.0
200	3588.6	1947.3	1641.3
300	3604.7	1955.9	1648.8
400	3622.8	1963.9	1658.9
500	3642.8	1972.9	1669.9
600	3664.2	1982.3	1681.9
700	3686.2	1992.0	1694.2
800	3708.0	2001.7	1706.3
900	3729.1	2011.1	1718.0

Figure 4. The variation of photonic band edges and PBG with temperature.
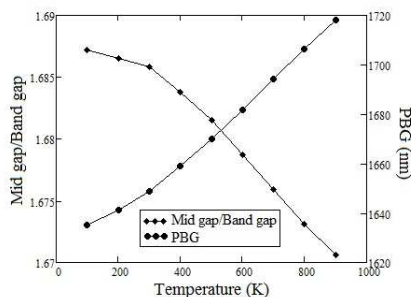

Figure 5. The variation of midgap to bandgap ratio with temperature.

4. CONCLUSIONS

The effect of temperature on photonic band gap has been investigated. The refractive index of silicon layers is taken as a function of both temperature and wavelength. Therefore, this study may be considered to be more physically realistic than other previous works. Also, it may be useful for computing the optical properties for wider range of wavelength as well as temperature. We can use the proposed structure as temperature sensing device, narrow band optical filter and in many optical systems.

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