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Modeling of spectral energy density as thermal radiation characteristic on the basis of porous silicon photonic crystals

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ABSTRACT

The influences of porosity on thermal radiation were studied for enhancement of light absorption in porous silicon (pSi) photonic crystal (PhCs). A 2D concept of unit-cell for square and triangular lattice of circular air holes was formulated and solved using plane wave expansion (PWE) technique and Fourier expansion method. The spectral energy density (SED) of the thermal radiation at different porosity consideration of silicon PhC was investigated for both mentioned lattices including the effect of these lattice structures in the creation of photonic band gaps. It revealed useful to increase the number of frequency band gaps by subjecting the PhC to a square lattice at low porosity. Moreover, a triangular lattice beyond 50% of porosity would be suitable in thermal radiation control where the band gap stabilization applications are required.

1. Introduction

Porous silicon (pSi) is a nanostructured and biodegradable material that has a wide range of properties which has spurred its application in photonics and energy technologies as well as other allied fields [1–11]. On the other hand, thermal radiation from photonic crystal (PhC) which is also referred as complex electromagnetic structures has recently attracted the attention of several researchers [12–17]. Lin et al. indicated that the thermal radiation from metallic PhCs may even exceed that of a blackbody in free space [15]. The effect of thermal oxidation and oxide etching on silicon PhCs of triangular lattice has been studied. Using plane wave expansion (PWE), Thitsa & Albin [18], modeled the latter and proposed advantageous processes for tuning the photonic band gap and defect frequency. There are numerous proposed applications relating to pSi based PhCs. This is largely due to their ability to control light propagation within them [7]. Luo et al. presented a classical simulation of equilibrium thermal emissivity from dispersive lossy PhCs [19]. They indicated the potential usefulness of PhCs in incandescent lighting and thermal photovoltaic applications. Furthermore, a basis for manipulating the thermal emission and absorption of radiation in complex photonic structures and the design of novel solar cell devices has been presented by Florescu et al. [20]. These authors revealed that controlling the thermal emission and absorption of radiation in a PhCs enables the realization of high-efficiency solar cells. Florescu et al. in another study, analyzed the origin of thermal radiation enhancement and suppression inside PhCs as a prerequisite for the understanding the thermal radiation properties of finite PhCs [21]. Moreover, Gesemann et al. presented measurements of the thermal emission properties of 2D and 3D silicon PhCs which depended on substrate heating (resistively and passively) with an aluminum hotplate [22]. A decrease in the averaged energy of 2D PhCs based on bulk and pSi materials was revealed by Szabo et al. who applied finite differential time domain (FDTD) method in calculating wave propagation [23]. Tong et al. indicated that both dispersion characteristic analysis and numerical simulation of field patterns can verify the effective phase indexes of 2D triangular PhCs with dielectric rods in air background [24]. Indeed, the dielectric properties of pSi are mainly governed by the porosity. However, there are several models that relate the porosity of a pSi layer and its refractive index. One of such is the Vegard's law which considers pSi as a homogeneous mixture of silicon and air [7]. Furthermore, Maxwell-Garnett or the Bruggeman models can be used to describe the dielectric constant of a two-component materials system [25,26]. The latter is used in this work and relates porosity and effective refractive index through the following expression:

$$p = 1 - \left[\frac{(1 - n_{pSi}^2)(n_{Si}^2 + 2n_{pSi}^2)}{3n_{pSi}^2(1 - n_{Si}^2)}\right] \quad (1)$$

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Nomenclature

a	lattice constant, m
$\vec{a}_1$; $\vec{a}_2$	primitive basis vectors in real space
A	area, m^2
A_{pol}	potential vector
$\vec{b}_1$; $\vec{b}_2$	reciprocal basis vectors
c^2	phase velocity in vacuum, m/s
c_M^2	phase velocity in dielectric material, m/s
$c(\vec{r})^2$	phase velocity, m/s
$F_{\alpha,\beta}$; $\gamma_{m,n}$	coefficients in Fourier series
$\vec{G}$	reciprocal lattice vector
$\hbar$	reduced Planck's constant, J s
J_1	first kind of Bessel function
$\vec{k}$	wave vector
k_B	Boltzmann constant, J/K
n	refractive index
n^2	dielectric constant
p	porosity, %
pol	polarization
pSi	porous silicon
$\vec{r}$	position, m
R	hole radius, m
Si	silicon
T	temperature, K
$u(\omega, T)$	energy spectral density, J s/radm^2
∇^2	Laplace operator

Greek letters

α; β	arbitrary coefficients for reciprocal lattice vector
ε	permittivity, F/m
μ_0	permeability, H/m
ζ	arbitrary coefficient in the eigenvalue problem
ω	frequency, rad/s

Abbreviation

BZ	Brillouin zone
DOS	density of states
SED	spectral energy density
PhC	photonic crystal
PWE	plane wave expansion

where porosity (p) is the percentage of air in a layer cross section, n_{Si} is the refractive index of silicon, and n_{pSi} is the effective refractive index associated with that porosity. Table 1 depicts the refractive index and dielectric constant versus porosity in Bruggeman model and Fig. 1 shows an example of scanning electron microscope images of monolayer of pSi found in [27].

Currently, applications of thermal light sources through PhCs are being explored, mainly in the field of thermo-photovoltaic power conversion. However, the demands of high-operating temperatures inevitably leads to Nano and microscopic material degradation, presenting a formidable challenge [28–32].

This work is to investigate at high temperature, the spectral energy density (SED) characteristics of silicon material based on square and triangular lattice PhCs in different porosities. This is aimed at exploring new concepts on porosity effect that could be integrated in solar cells improvement. It is to also study the effect of lattice structure on the SED spectrum though pSi PhC in order to retain the reliable design for optimum absorption in solar cells efficiency. These objectives have been achieved by using a PWE algorithm from wave equation based on Fourier expansion method to the first kind of Bessel function. This method was implemented for both dispersion relation and density of states (DOS) where the SED has been deduced. Based on that highlighted methodology, the results have been compared with existing published works in statistical physics.

Table 1
Refractive index and dielectric constant versus porosity in Bruggeman model [25,26].

Porosity (%)	Refractive index (n_{Si})	Dielectric constant (n_{Si}^2)
0	3.47	12.04
10	3.23	10.43
20	2.98	8.88
30	2.72	7.40
40	2.44	5.95
50	2.14	4.58
60	1.84	3.39
70	1.56	2.43
80	1.32	1.74
90	1.12	1.25
100	1	1

2. Numerical methods

2.1. PWE processing

In the electromagnetic theory, Maxwell's equations in free space described the propagation of electromagnetic waves and the solutions of these equations can be approximated by conjugating PWE and Fourier expansion methods [33–37]. Thus, the governing equation for the electric and magnetic component of the light wave is given by Eq. (2):

$$\nabla^2 A_{pol} - \mu_0 \varepsilon(\vec{r}) \frac{\partial^2 A_{pol}}{\partial t^2} = 0 \tag{2}$$

$$\mu_0 \varepsilon(\vec{r}) = \frac{1}{c(\vec{r})^2} \tag{3}$$

where ∇^2 designed the Laplace operator; $\vec{r}$ is the position; A_{pol} the vector potential; pol stands for the polarization; μ_0 is the permeability; $\varepsilon(\vec{r})$ is the permittivity and $c(\vec{r})^2$ is the phase velocity. In the PWE method the phase velocity can be expanded as Fourier series, using the reciprocal lattice vector $\vec{G} = m\vec{b}_1 + n\vec{b}_2$ with $m, n \in \mathbb{Z}$ to ensure invariance of the function to displacement:

$$c(\vec{r})^2 = \sum_{\vec{G}} \gamma_{\vec{G}} e^{i(\vec{G}\cdot\vec{r})} = \sum_{m,n} \gamma_{m,n} e^{i(m\vec{b}_1 + n\vec{b}_2)\cdot\vec{r}} \tag{4}$$

Fig. 2 illustrates the real and the reciprocal space in square and triangular lattice with the primitive basis vectors for both spaces. The vector potential in the wave equation can also be written as a Fourier series:

$$A_{pol} = \sum_{\vec{k}} A_{\vec{k}} e^{i(\vec{k}\cdot\vec{r} - \omega t)}$$

$$A_{pol} = \sum_{o,p} A_{o,p} e^{i\left[(o\vec{b}_1 + p\vec{b}_2 + \vec{k})\vec{r} - \omega t\right]}$$

Introducing Eqs. (4) and (5) into the Eq. (2) and comparing the coefficients, the central equation can be represented as:

$$\sum_m \sum_n \gamma_{m,n} \zeta A_{o-m,p-n} = \omega^2 A_{o,p} \tag{6}$$