Comb-shaped photonic crystal structure for efficient broadband light diffraction and funnelling in solar cells

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A B S T R A C T

We present a comb-shaped photonic-crystal (PhC) rods-lattice structure of broadband light diffraction and funnelling for solar cell applications. It is shown that the photonic band of this PhC structure is very dispersive over a broad bandwidth so that light will be efficiently diffracted in the wavelength region of solar radiation. The PhC structure also creates resonance modes leading to further diffraction and funnelling of light so that the light propagates in many pathways in the whole PhC lattice region, which will greatly facilitate light–matter interaction when light-absorbing elements are embedded in the PhC structure. The proposed structure is also valid for photodetection applications.

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1. Introduction

Light-absorbing devices such as solar cells are normally in the form of thin films. In order to increase the light–matter interaction, reflection from the device surface is to be decreased. The conventional method is to use anti-reflection coating layer [1]. The second major issue is to increase the pathways of the photon traveling inside the active light-absorbing region in order to increase the chances of interaction between the photon and the photon-absorber such as dye molecules and colloidal quantum dots (QDs) [2,3]. It was shown by the geometrical optics approach that a light ray in a textured thin film may be expected to make up to $4n^2$ passes on average before escaping the thin film due to total internal reflection, where $n$ is the refractive index of the sheet [4]. Light diffraction can be achieved by using optical gratings [5,6]. There will be upper limits for the absorption enhancement using normal diffraction gratings [7]. These are the limit in the geometrical optics regime, which can however be surpassed in subwavelength regime [8–10]. Plasmonic excitation using metallic nanoparticles in the solar cells has also been extensively studied to harvest light [11–13]. Wave optics based photonic crystals (PhCs) have shown to be able to further exceed the $4n^2$ limit and improve the light trapping via combined effects of reflection, diffraction, and refraction [14,15]. Micro/nanorods array or PhCs [16–23] were exploited to trap light in solar cells, and PhC back-scatters and forward-scatters were also utilized to retain incident light inside the absorbing medium [24,25]. Solar cell applications of these novel structures are limited because of their narrow bandwidths.

There are two types of PhC-based solar cells, one is to construct the light-absorbing materials into PhC structures, e.g., silicon rods and organic material rods extended along the $z$ direction were positioned periodically on the $xy$ plane, forming two-dimensional (2D) photonic crystals [16,17], while the other type consists of PhC structured electrodes with light-absorbing elements embedded in them, such as silicon or organic light-absorbing layers in patterned electrodes [18–21], QDs embedded in a nanowire array [22] and in a patterned photovoltaic cell [23]. All these demonstrate significantly enhanced light–matter interactions. A 2D PhC structure is superior to a 1D one for solar cells, because a 2D lattice can provide more resonances to trap the light.

In this work, we present a 2D comb-shaped PhC lattice structure as a framework which can effectively diffract and funnel broadband lights from their incident directions (in wave optics regime), thus increase photon pathways and traveling time inside the solar cell. These effects can help to enhance light absorption after light-absorbing elements are embedded in the comb-shaped PhC structure.

2. The comb-shaped PhC lattice structure

The comb-shaped PhC structure is shown in Fig. 1a. It is based on a 2D perfect square PhC (the $y$ direction is extended) with
square dielectric rods characterized by lattice constant $a$ and rod size $b = 0.55a$. We adopt the dielectric refractive index of 2.75 (for TiO$_2$) for the square dielectric rods. Such a value is adopted as we aim at a model solar cell that uses TiO$_2$ rods (see more details in Section 4). The dielectric refractive index in other spatial area is set to be 1.0 (also see the model in Section 4). The photonic band structure of transverse electromagnetic (TE) field in the 2D perfect square PhC lattice is shown in Fig. 1b calculated by the plane wave expansion method. There is no overall stop band in a perfect square PhC lattice is shown in Fig. 1b calculated by the plane wave expansion method [27]. There is no overall stop band within which electromagnetic modes are not able to propagate [28]. The main concept of our work here is to utilize the photonic band states to diffract the broadband light. Light funnelling into the PhC lattice is obtained through the light inlet channels by removing a few rods in the perfect PhC lattice, which eventually turns the PhC into a comb shape, as shown in Fig. 1a.

We set the plane-wave incident direction as the $z$ direction which is perpendicular to the PhC rods in our calculation, the incident TE field is described by $E(x,z,t) = [E_x(x,z,t), 0, E_z(x,z,t)]$.

### 3. Results and discussions

As mentioned before, a large $E_z$ component parallel to the $z$-axis, i.e., the direction of the incident light, indicates a good ability of light diffraction. Fig. 2a and b shows the averaged $\langle E_z^2 \rangle$ in monitor “1”. It is very small in the perfect PhC except for a few individual resonances, while the diffraction in the comb-shaped structure occurs over a much broad wavelength range. For comparison, we also calculated $\langle E_z^2 \rangle$ in the same area of a slab with common rectangular groove grating (substrate refractive index=2.75, depth of rectangular groove=0.15a, period=0.6a, filling factor=1/3) [5] and the results are shown in Fig. 2b showing a much weaker diffraction than the comb-shaped PhC structure. Such results are naturally expected due to the combined effects of reflection, diffraction, and refraction in wave optics based PhC structures [14, 15]. It is reasonable to exceed the $4n^2$ limit in a broad region of wavelengths in the comb-shaped PhC structure.
after reaching steady state. Fig. 4 a and b shows when light absorption by light-absorbing elements embedded in noticed that the reflections from PhC structures consist of largely Therefore, both the perfect PhC and comb-shaped structure do plotted in Fig. 3, which shows a reduced reflection in the comb-shaped PhC structure. It takes about 1 ps (when \( a = 1 \mu m \)) to reach the steady-state power flow in the comb-shaped PhC structure, while it needs only about 0.2 ps to reach the steady state in the perfect PhC.

Reflected powers

\[
\left( \int S_{z}(x,z,t)_{|z=-9a} \right)_{t}
\]
detected at \( z = -9a \) from the PhC structures at steady states are plotted in Fig. 3, which shows a reduced reflection in the comb-shaped PhC structure in some wavelength ranges as compared with the perfect PhC structure. On the other hand, it is easy to estimate by the Fresnel equations that the total reflectance from a substrate slab with a refractive index of 2.75 is around 0.36. Therefore, both the perfect PhC and comb-shaped structure do not significantly reduce the total reflectance. However, it is noticed that the reflections from PhC structures consist of largely the contributions from multiple diffractions by the PhC rods. It is easy to envisage that such reflections will be significantly reduced when light absorption by light-absorbing elements embedded in the PhC structures has been taken into account.

Now we discuss the spatial distribution of the electric field after reaching steady state. Fig. 4 a and b shows \( \langle |E_{z}(x,z,t)| \rangle_{x} \) as functions of the wavelength in both the comb-shaped and the perfect PhC structures. We observe that in the perfect PhC, \( \langle |E_{z}(x,z,t)| \rangle_{x} \) is normally very weak except for a few resonance modes. Resonance modes such as \( \lambda \in (0.9a, 1.1a) \) can create a strong field of \( \langle |E_{z}(x,z,t)| \rangle_{x} \) at the PhC surface, whereas in Fig. 4 b strong and almost continuous \( \langle |E_{z}(x,z,t)| \rangle_{x} \) distribution is observed in the comb-shaped PhC structure over a broadband range.

Fig. 5 shows the spatial distributions of \( \langle |E_{z}(x,z,t)| \rangle_{t} \) at \( z = -2.5a \) and \( z = 3.5a \), i.e., monitors “2” and “3” in Fig. 1 a in the perfect and the comb-shaped PhC structures. We notice again that \( \langle |E_{z}(x,z,t)| \rangle_{t} \) is very strong in comb-shaped PhC structure (with nodes and valleys due to resonance modes), while it is nonzero only at a limited number of wavelengths in the perfect PhC. Quite interestingly, \( \langle |E_{z}(x,z=-2.5a,t)| \rangle_{t} < \langle |E_{z}(x,z=3.5a,t)| \rangle_{t} \) at some wavelengths in the perfect PhC structure even though \( z = -2.5a \) is closer to the light source located at \( z = -8a \). This is due to the resonance modes in the spatial distribution of \( E_{z} \), as shown in Fig. 4 a.

It can be observed by Figs. 2, 4, and 5 that in the comb-shaped PhC lattice, \( E_{z}(x,z,t) \) is very strong when \( \lambda = 1.8a \), while it is weak at \( \lambda = 1.0a \). To understand the two cases, we now study the spatial distributions of \( \langle |E_{z}(x,z,t)| \rangle_{t} \) in both the perfect PhC and the comb-shaped structure at the two different wavelengths, which are shown in Fig. 6. A strong diffracted field \( E_{z} \) is observed at the surface of the perfect PhC when \( \lambda = 1.0a \) due to the matching of the wavelength with the lattice constant \( a \) (similar matchings are observed when \( \lambda = 0.5a \) and \( 0.25a \) in Fig. 4 a), while the light can be effectively funnelled into the comb-shaped structure due to the broken surface at \( z = -6a \) as shown in Fig. 1 a. The field dwelling at the surface of the perfect PhC also occurs at the backside surface \( (z=4a) \) of the comb-shaped structure, see the large field distribution when \( z > 4a \) in Fig. 6 c. When \( \lambda = 1.8a \), the incident \( E_{z} \) field can hardly penetrate into the perfect PhC, resulting in the weak diffracted \( E_{z} \) concentrated on the surface of the perfect PhC. Note that the width of the light inlet channels in the comb-shaped structure is \( \leq 2a \) so that the incident \( E_{z} \) will be strongly diffracted in the inlet channels, resulting in a strong \( E_{z} \) distribution at \( \lambda = 1.8a \), as shown in Fig. 6 d.

Fig. 2c shows the optical power flows

\[
\frac{1}{A} \int_{1}^{z} E_{z}^{2}(x,z,t) \, dx \, dz
\]
along the \( x \) direction in one period of comb-shaped PhC structure and the same area of the perfect PhC when \( \lambda = 1.8a \). \( A \) is the area of monitor “1”. Note that the initial incident light propagates along the \( z \)-axis so that \( E_{z}(x,z,t) \) is zero at \( t=0 \). We observe here that due to dispersion of the photonic bands, the incident light is diffracted, which is greatly enhanced through the inlet channels in the comb-shaped PhC structure. It takes about 1 ps (when \( a = 1 \mu m \)) to reach the steady-state power flow in the comb-shaped PhC structure, while it needs only about 0.2 ps to reach the steady state in the perfect PhC.

\[
\left( \int S_{z}(x,z,t)_{|z=-9a} \right)_{t}
\]
4. Model solar cell structure

Based on the enormous nanofabrication progress of stacked PhC structures [18,32], we propose a model solar cell based on the comb-shaped PhC structure presented in the previous sections. The PhC structure is to be formed by a stack of dielectric rods fabricated as an alternant sequence of low-index material layers such as indium tin oxide (ITO, dielectric refractive index = 1.17 [33]) films and high-index TiO₂ films with light-absorbing QDs [34,35] embedded inside deposited and patterned by lithographic techniques. These dielectric rods form a square 1D PhC lattice stacked in the z direction as shown in Fig. 7. Light absorbed by the QDs will excite electrons from the valence band to the conduction band in the QD, which are then injected into the TiO₂ rods [36]. They will further diffuse to the nearest ITO layers which are connected to a back contact ITO film to form the photocurrent. Disulfide/thiolate redox couple [37] that has negligible absorption in the visible spectral range is to be used as transparent organic solvent-based, noncorrosive electrolytes to achieve high power conversion efficiencies. Light can be injected into the solar cell structure along either the +z or the −z direction.

5. Conclusions

In conclusion, we present a comb-shaped PhC structure in a thin film format which can efficiently diffract incident radiation from its initial incident direction into the thin film plane over a broadband of wavelengths. The comb-shaped PhC structure efficiently generates a nonzero electric field component along the incident direction of the light. By embedding light-absorbing elements such as organic dyes and QDs in such a PhC lattice, we will obtain not only a much enhanced light–matter interaction in the light-absorbing elements but also a much increased pathways of the photon in the device resulting in a much improved opportunity for the photon to be absorbed. The proposed structure can also be applied in photodetection devices.

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