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OPTICAL ABSORPTION ENHANCEMENT IN SOLAR CELLS VIA 3D PHOTONIC CRYSTAL STRUCTURES

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Abstract—Light concentrating structures with three-dimensional photonic crystals (3D PhCs) for solar cell applications are investigated via simulation. The 3D opal PhCs are suggested as an intermediate layer in the concentrator system for solar cells. It is found that the light absorption is significantly enhanced due to the adding of diffractive effects of PhCs to the concentrator. Three types of PhCs are considered in four scenarios to verify the absorption enhancement by such a light concentrating structure. Our calculations show that the face-centered cubic PhC can create an absorbing efficiency superior to the others under a specified lattice orientation pointing to the sun, which results in an enhancement factor of 1.56 in absorption for the 500–1100 nm spectral range.

1. INTRODUCTION

Most solar cells are made from single-crystalline silicon, microcrystalline silicon (μc-Si) or amorphous silicon (a-Si:H) which possesses an indirect band gap [1]. This results in weak absorption of light in the near infrared and increases the absorption length. The critical issue of such Si solar cells is increasing the conversion efficiency. Nevertheless, higher conversion efficiency demands a longer optical path to increase optical absorption, which is especially important for materials with low

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absorption coefficients. In order to concentrate sunlight and reduce escape losses, a light trapping structure is needed to obtain more efficient absorption.

Traditional light trapping schemes used in solar cells are based on geometrical optics via scattering at textured surfaces and reflecting at backside mirrors. Other common elements equipped in solar cells are the antireflective coating (ARC) to minimize light reflection and surface diffraction gratings to increase the optical path [2]. Furthermore, the light trapping approaches based on wave optics can be capable of surpassing geometrical optics approaches in some cases. Wave optics approaches can be aimed at enhancing absorption for a certain range of wavelengths, which can be more advantageous for efficiency [3, 4]. Several light trapping approaches of wave optics were studied such as plasmonics based designs [5], grating couplers [6], fluorescent concentrator systems [7], and photonic crystals (PhCs) [8–10]. A variety of means to refract, diffract, and reflect light are with the aim of increasing the absorption path length of light in the materials.

PhCs are periodic dielectric structures with a spatial scale on the order of the optical wavelength to give a particular dispersion to photons. In general, PhCs can be used in three ways in order to improve light absorbing efficiency. The first approach is the design of reflecting a range of wavelengths with low losses or the inhibition and redistribution of light spectrum via the significant feature of PhCs, the photonic band-gaps (PBGs) [11–13]. This option generally leads to the requirement of a sufficiently large refractive index contrast to open a full PBG. The second approach is the diffraction of light due to the scattering produced by the periodic array, which diffracts the incoming beams into highly oblique angles or guided modes [14–16]. The frequencies above a certain spectral threshold for the onset of diffraction are relative to the period of the fabricated surface lattice, the shape of the scattering object, and the refractive indices and their contrast of the medium and the surrounding. The third approach is the slow Bloch mode which leads to a very strong light-matter interaction for amplifying the absorption [17]. Using extremely strong material dispersion in PhCs, slow light in the vicinity of the photonic band edge is generated to spend more time inside the device. Design and optimization of the PhCs are difficult due to the multi-parameter problem of a nanostructured texture. There are many consequences in connection with the combinations of intermixing materials, lattice symmetry, lattice constant, filling factor, shape of the scattering object, etc. It is not easy to confirm which one gives the most efficient PhC structure in the improvement of light absorbing efficiency in solar cell structures.

In this work, we present a new structure which integrates a three-dimensional (3D) PhC structure on a glass substrate surrounded with a mirror and solar cells. In addition, an impedance match layer as an ARC is placed on top of the optical concentrator. Based on the PhC dispersion properties, the applicability of the concentrator system is evaluated by the finite difference time domain (FDTD) method. The simulation study is also intended to compare the light absorbing efficiencies of the concentrator systems based on different types of 3D opal PhC structures with spherical particles and to estimate the most practical design among these model structures. The relevance between the predictions of the plane wave expansion method (PWEM) [18] and the consequences of the 3D FDTD calculation is demonstrated for the increase of absorbing efficiency coupled to the concentrator structure.

2. ENHANCEMENT APPROACHES OF 3D PHOTONIC CRYSTALS

A schematic view of the new optical concentrator structure of interest is depicted in Figure 1. It is composed of an ARC, a uniform μc-Si or μc-Si-PhC layer (a thin-film solar cell), a glass substrate covered by μc-Si solar cells on the four sides, and a back reflector. In addition, several such concentrator structures can be placed side-by-side to form a two-dimensional array. In order to facilitate the identification of the utility, we simplify the geometry and the assumptions on the

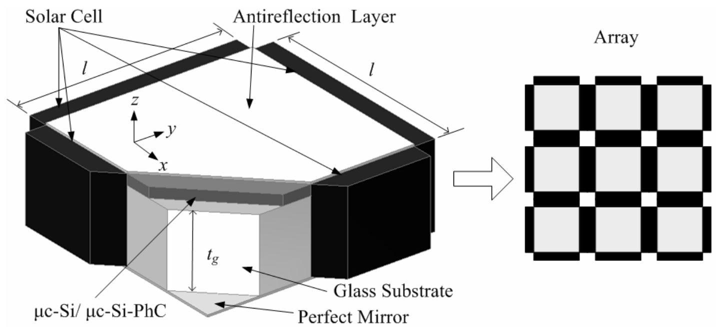

Figure 1. Schematic of the optical concentrator covered by a perfect mirror at the bottom and solar cells on the four sides and the top. In the structure, the μc-Si layer can be replaced by the PhCs to improve light trapping. The model structure can be fabricated into an integrated array (top view).

material properties. The back reflector is assumed to be a perfect mirror. The incident light is normal to the optical concentrator. A quarter wavelength transparent layer of SiO_2 with the refractive index $n = 1.5$ is used as an ARC on μc-Si. Such a coating, which is a common solution based on interference, can perform well in a limited spectral range and for normal incidence. The investigation of surface recombination and carrier collection is an important aspect. With proper passivation to the PhC layer, the surface recombination can be greatly reduced. Besides, the benefits of light trapping are far likely to outweigh the loss of efficiency due to the surface recombination for a thin-film structure. Since we focus on modeling light trapping in a concentrator system, the surface recombination effect is neglected. For the simulation comparison, no shadowing and 100% carrier collection are assumed.

In general, different diffraction phenomena due to the PhC structure can be employed to enhance absorption in solar cells. Firstly, it may reduce Fresnel reflections at the interface between the absorption layer and the surrounding [19]. Secondly, it may excite the guided modes in the substrate [10]. Thirdly, it diffracts light into higher orders to permit for an elongation of the optical path in the absorption layer [9]. Finally, it may produce longitudinal slow-group-velocity effects and the parallel interface refraction associated with transverse slow modes [15]. Upon excitation of these modes, Figure 2

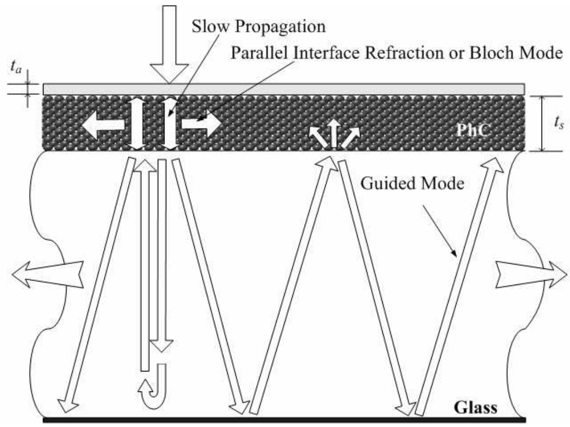

Figure 2. The cross section view of the model structure showing the action of PhCs. The texture increases the effective path length via Bragg diffraction, parallel interface refraction, (slow) Bloch modes, and the light guiding effect relying on total internal reflection.

shows a schematic optical path for our optical concentrator structure that may significantly enhance the absorption.

Since 1987, obvious progress has been made toward the theoretical study and the fabrication of 3D PhCs [20]. Especially as mentioned above, the different light absorbing efficiencies originate from the diffraction phenomena, which could be discussed using the photonic band structures. The photonic band diagrams, which are calculated using the PWEM, are shown in Figure 3 for the three types of opal-based PhCs (simple cubic (SC); body-centered cubic (BCC); face-centered cubic (FCC)) in air background. The complex dielectric constant for the microspheres of μc-Si is obtained from [21]. In the band diagram, relative "flat bands" and more Bloch modes in Γ-X direction for the SC structure (Γ-N for the BCC; Γ-X and Γ-K for the

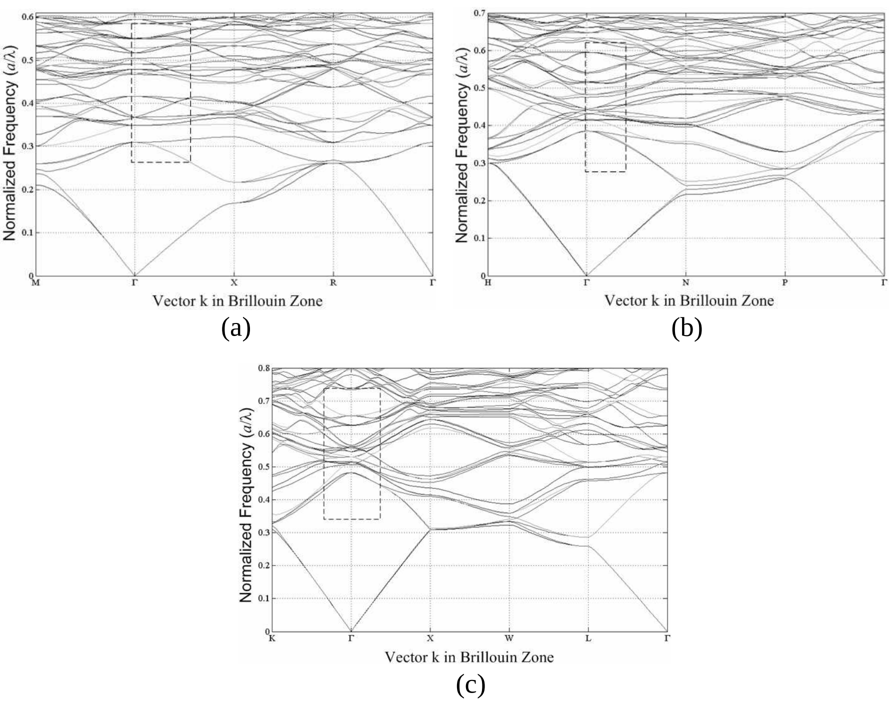

Figure 3. Photonic band structures for the three types of silicon-opal PhCs in air background: (a) SC; (b) BCC; (c) FCC. The black dashed boxes indicate the spectral regions and the corresponding incident directions for simulation. The incident direction relative to the orientation of the SC/BCC/FCC PhC is Γ-X/Γ-N/Γ-X & Γ-K, respectively.

FCC) predict a high absorption at this direction pointing to the sun. A flat dispersion represents the consequence of a large density of modes and a low group velocity. Therefore, a higher concentration of light in the material is expected resulting in enhancement of absorption. Besides, the dispersion curves indicate the permitted energy states for light harvesting from an external source. If the number of reciprocal points near the Γ point grows more, light is diffracted more and guided modes are created further in the substrate.

3. COMPARISON OF VARIOUS NANO-STRUCTURED SOLAR CELL CONCENTRATORS

According to the maximum external quantum efficiency (EQE) of μc-Si solar cells, which appears near the wavelength $\lambda_0 = 700\,\text{nm}$ [4], the quarter-wavelength optical thickness t_a of the ARC and the lattice constant a related to the diameter of the spheres are designed with the operation eigenfrequency $a/\lambda_0 = 0.42$ for the SC structure in Figure 3(a) ($a/\lambda_0 = 0.44$ for the BCC in Figure 3(b); $a/\lambda_0 = 0.53$ for the FCC in Figure 3(c)). The selection is the reason that relatively flat bands around these normalized frequencies exist near the Γ point so that this very high density of states enhances the absorption by efficiently coupling of light into the Bloch modes of the PhCs. The dashed boxes in Figure 3 indicate that the absorption enhancement in the 500–1100 nm range, where the properties of the μc-Si solar cells are characterized by their EQEs [4], is interested in our study.

Seeking for light absorbing efficiency, it is necessary to investigate the effects of these 3D microstructures on the light diffraction properties of the concentrator structure in detail. To confirm the improvement of the absorption enhancement, the 3D FDTD through the Optiwave OptiFDTD$^{\text{TM}}$ simulation software is exerted for the numerical analysis of the solar cell device. This method can be used to describe optical properties for considering the complexity of the model. For the limitation of computer memory capacity, the lateral domain size ($l \times l$) of the FDTD computation is restricted to a 20×20 PhC-lattice array, the thickness for the glass substrate with a refractive index of $n = 1.8$ is $t_g = 5\lambda_0$, and the model structure is surrounded by perfectly matched layers. The thickness of the 3D opal PhC structure is $t_s = 6a$. The corresponding space resolution is based on a mesh limit with $\Delta x, \Delta y, \Delta z \leq \lambda/(20n)$, where n is the refractive index and λ is the vacuum wavelength.

In order to quantify the absorbance of different 3D PhC-based concentrator systems, the effects of the enhancement on the absorption of interest for the μc-Si solar cells are shown in Figure 4. The

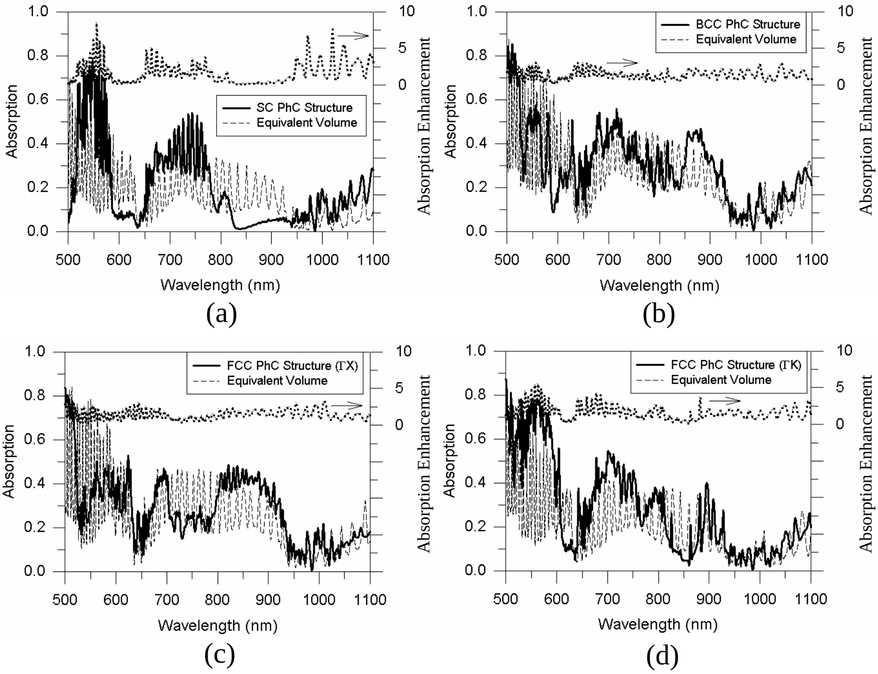

Figure 4. Absorption and absorption enhancement vs. wavelength in the model structure with different types of PhC configurations: (a) SC; (b) BCC; (c) and (d) FCC. The normal incident directions are depicted in the caption of Figure 3.

calculation is done for normal incidence. The absorbance is given by $A = 1 - R - T$, where the reflectance is R and the transmittance is $T = 0$. The detection surface for R is located at the upper position $\lambda_0/2$ apart from the top of the concentrator structure. The calculated absorption is weighted by the air mass (AM) 1.5 solar spectrum [22]. Figure 4 shows the absorption as a function of wavelength for the concentrator systems with a PhC-based μc-Si slab and for those with a μc-Si slab of equivalent volume. Here, the impact of the discussed optical properties is apparent. The average absorptions for the four cases (a)–(d) with the equivalent volume solid slabs in Figure 4 are 18.7%, 28.7%, 27.4%, and 22.9%, respectively. The average absorptions for the cases with the PhC-based slabs are 23.8% (SC, incident in Γ-X direction), 34.4% (BCC, incident in Γ-N direction), 32.1% (FCC, incident in Γ-X direction), and 35.8% (FCC, incident in Γ-K direction), respectively. The enhancements in optical absorption for the concentrator systems with a PhC-based slab over those with a solid slab of equivalent volume are also shown in Figure 4. A quantity for band edge enhancement, the enhancement factor (Ef), is defined as the ratio of the average absorption of a modified concentrator system with a PhC-based slab to the average absorption of a concentrator system with a solid slab of equivalent volume. For a given spectrum range near the band edge (1100 nm), the evaluation of the enhancement factor is calculated using the formula [23]

$$Ef = \frac{\int_{\lambda}^{1100} A_{\mathrm{PhC}}(\lambda) I(\lambda) d\lambda}{\int_{\lambda}^{1100} A_0(\lambda) I(\lambda) d\lambda}, \tag{1}$$

where the value $A_{\mathrm{PhC}}(\lambda)$ represents the absorption features of an enhanced concentrator system with a PhC-based intermediate layer and $A_0(\lambda)$ represents the absorption of a concentrator system with a solid intermediate layer of equivalent volume. The AM 1.5 direct normal and circumsolar spectrum is used for the solar intensity $I(\lambda)$. This new concentrator system design augments the reflective and diffractive properties of the 3D PhC, which improve the optical absorption. In the 500–1100 nm range for μc-Si solar cells, the enhancement factors for the four cases in Figure 4 are 1.27 (SC, Γ-X), 1.2 (BCC, Γ-N), 1.17 (FCC, Γ-X), and 1.56 (FCC, Γ-K), respectively. From the average absorptions and the enhancement factors of the four cases, the concentrator design with a FCC PhC intermediate structure has higher absorbing efficiency when the light beam is incident in the z axis in connection with the Γ-K direction of the reciprocal space path in the PhC. The PhC intermediate structure is designed with a specified eigenmode at $\lambda_0 = 700$ nm. Referring to the dispersion curves in Figure 3, the curves near the specified eigenmode in the case of Figure 3(c) with respect to the Γ-K direction reveal the characteristics of flatter bands and more Bloch modes than those in the other cases so as to allow a more light-harvesting near the eigen-wavelength as shown in Figure 4(d).

For the case of a concentrator system with a solid intermediate layer of equivalent volume, strong Fabry-Pèrot (FP) oscillations due to the plane wave interference between the reflections from the multilayer structure would naturally increase the absorption enhancement as shown in Figure 4. However, the spectral range of enhanced absorption is limited by the linewidth of the oscillations, and the solar cells on the four sides of the concentrator cannot function effectively. From experiments, the interference fringes would also turn out much lower due to roughness and imperfections in the structure. In addition, the spectral positions of possible reflection peaks relative to the absorption edge would reduce the absorbing efficiency so that the overall absorbance would not be actually obvious. For the case of an enhanced concentrator system with a PhC-based intermediate layer, the diffractive effects due to the periodic structure could cause a prolongation of the optical path and permit to excite guided modes which enhance absorption tremendously over a narrow spectral domain. The less ideal absorption in the long wavelength regime near 1100 nm could be amended to overcome the small extinction coefficient of μc-Si. Besides, the periodic interface could suppress some destructive FP resonances so as to improve the overall absorbance as shown in Figure 4, especially for the spectral characteristics near the wavelength 700 nm with respect to the maximum EQE of μc-Si solar cells.

4. CONCLUSION

We have presented a theoretical analysis for the potential and impact of a 3D PhC intermediate layer in the proposed concentrator system. Our calculation shows that the incorporation of a 3D PhC structure is suited to improve the absorbance of the μc-Si solar cells in the concentrator application. The desired diffractive effects via the PhCs give rise to the desired spectrally selective absorbance spectrum with a limited but sufficiently large spectral width. We have compared the device performance in terms of the enhancement factors that compares the absorption characteristics of three PhC modified concentrator structures to those non-modified (with equivalent volume) structures. The highest performance is achieved by the FCC PhC intermediate structure. This structure achieves an enhancement factor of 1.56 for a specified lattice orientation pointing to the sun. The 3D PhCs are an effective approach to light trapping in the solar cell system with such a concentrator. Moreover, the concentrator structure can be set side-by-side to form a two-dimensional array for more efficient application implementations. Further theoretical investigations should follow to address basic strategies for the optimization of 3D PhC-based concentrator systems for photon management in solar cells.

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