Design of photonic crystal enhanced light-trapping structures for photovoltaic cells

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Abstract

A new concept of the optical collector including a three-dimensional photonic crystal (3D PhC) is proposed in the study for microcrystalline silicon photovoltaic cells. The goal is to couple the normally incident light into various modes diffracted and guided in the collector structure. To achieve a higher absorption, a 3D periodic structure is patterned within the presented collector as an intermediate layer providing the absorption enhancement mechanism. By select proper PhC or photonic sponge architectures, the spectral positions of the induced modes can be controlled so as to improve the light harvesting.

Keywords: Photonic crystals, photovoltaic cells, light trapping, optical collector

1. Introduction

Silicon-based photovoltaic cells, such as single-crystalline silicon, microcrystalline silicon (μc-Si) or amorphous silicon (a-Si:H), are guaranteed to be an alternative energy source. However, such materials possess an indirect band gap [1]. This results in weak absorption of light and increases the absorption length. The critical problem in the Si-based photovoltaic cells is increasing the conversion efficiency. To overcome the difficulty, higher conversion efficiency demands a longer optical path to increase optical absorption. Thus, a light trapping structure is needed to obtain more efficient absorption.

To increase the light-harvesting efficiency, classical strategies combine the integration of an anti-reflection film (ARF), a textured top surface, and a reflector on the back side. Traditional light trapping schemes used in photovoltaic cells are based on geometrical optics. 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 [2, 3]. Various schemes have been explored to overcome the intrinsic limitation and to harvest more photons from solar radiation, such as plasmonics based designs [4], grating couplers [5], fluorescent collector systems [6], and photonic crystals (PhCs) [7-9]. PhCs that have such an ordered structure with a modulation of refractive index or dielectric constant have attracted considerable attention from both fundamental and practical points of views. Generally speaking, PhCs can be used in three ways in order to improve light absorbing efficiency. The first method is the design of reflecting a range of wavelengths with low losses or the inhibition and redistribution of light spectrum via the photonic band-gaps (PBGs) [10]. The second method is the diffraction of light due to the scattering from the periodic objects, which redirect the incoming beams into highly oblique angles or guided modes [11-13]. The third method is the slow light which results in a very strong light-matter interaction for amplifying the absorption [14]. Design and optimization of the PhCs are difficult due to the multi-parameter
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problem of a multidimensional structure. There are many influences 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 determine which one gives the most efficient PhC structure in the improvement of light absorbing efficiency in photovoltaic cell structures.

In this study, a model which integrates a three-dimensional (3D) PhC structure on a glass substrate surrounded with a mirror and photovoltaics is presented as a new concept for optical collectors. In addition, an impedance match film as an ARF is placed on top of the optical collector. According to the PhC dispersion properties, the applicability of the collector 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 collector systems based on different types of PhC structures with spherical particles. The most practical design can be estimated between these model structures. The relevance between the predictions of the plane wave expansion method (PWEM) [15] and the results of the 3D FDTD calculation is demonstrated for the increase of absorbing efficiency.

2. Model Structure and Band Diagrams of 3D PhCs

Figure 1 shows the schematic view of the new optical collector structure. It is composed of an ARF, a uniform μc-Si or μc-Si-PhC layer (a thin-film photovoltaic cell), a glass substrate covered by μc-Si photovoltaic cells at the four rims, and a back reflector. In order to facilitate the understanding of the utility, the geometry and the assumptions on the material properties are simplified. The back reflector is assumed to be a perfect mirror. For the simulation comparison, no shadowing and 100% carrier collection are assumed. The incident light is normal to the optical collector. A quarter wavelength transparent layer of SiO₂ with the refractive index n=1.5 is used as an ARF on μc-Si. The investigation of surface recombination is an important issue. With proper passivation to the PhC structure, the surface recombination can be greatly reduced. In addition, 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 collector system, the surface recombination effect is neglected.

Figure 1. Schematic of the optical collector.
A 3D PhC has the potential to combine all mentioned effects in a photonic device. The enhancement of absorption in photovoltaic cells can be achieved via the PhC structure. Firstly, it may reduce Fresnel reflections at the interface between the absorption layer and the surrounding [16]. Secondly, it may excite the guided modes in the substrate [9]. Thirdly, it diffracts light into higher orders to permit for an elongation of the optical pathway in the absorption layer [8]. Finally, it may produce longitudinal slow-group-velocity effects and the parallel interface refraction associated with transverse slow modes [12]. Based on these mechanisms, Fig. 2 shows a schematic optical pathway for the presented collector structure that may significantly enhance the absorption.

![Figure 2. Schematic optical paths inside the collector.](image)

Different light absorbing efficiencies originate from the diffraction phenomena, which could be analyzed using the photonic band structures. The photonic band diagrams, which are calculated using the PWEM, are shown in Fig. 3 for the two kinds of inverse-opal PhCs (inverse-opal simple cubic, iSC; inverse-opal body-centered cubic, iBCC). The complex dielectric constant for the \( \mu \)-Si background is obtained from [17]. In the band structure, relative flat bands and more Bloch modes in \( \Gamma X \) direction for the iSC structure (\( \Gamma N \) for the iBCC) predict a high absorption at this direction pointing to the sun. A flat dispersion represents the result of a large density of modes and a low group velocity. Hence, a higher concentration of light in the material is expected resulting in enhancement of absorption. In addition, the dispersion curves indicate the permitted energy states for light harvesting from an external source. If the number of reciprocal points near the \( \Gamma \) point becomes more, light is diffracted more and guided modes are created further in the substrate.

### 3. Results and Discussion

Based on the maximum external quantum efficiency (EQE) of \( \mu \)-Si photovoltaic cells appearing near the wavelength \( \lambda_0=700 \) nm [3], the quarter-wavelength optical thickness \( t_a \) of the ARF and the lattice constant \( a \) related to the diameter of the air holes are designed with the operation eigenfrequency \( a/\lambda_0=0.42 \) for the iSC structure in Fig. 3(a) and \( a/\lambda_0=0.44 \) for the iBCC in Fig. 3(b), respectively. The choice is the reason that relatively flat bands around these eigenfrequencies exist near the \( \Gamma \) point so that this very high density of states enhances the
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absorption by efficiently coupling of light into the Bloch modes of the PhCs.

Figure 3. Band diagram for the 3D silicon PhCs of inverse opal: (a) iSC; (b) iBCC.

To confirm the improvement of the absorption enhancement, the 3D FDTD through the Optiwave OptiFDTD software is exerted for the numerical analysis of the photovoltaic 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×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=5λ_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 \( \Delta x, \Delta y, \Delta z \leq \lambda/(2n) \), where \( n \) is the refractive index and \( \lambda \) is the vacuum wavelength.

The absorbance of different 3D PhC-based collector systems and the effects of the enhancement on the absorption of interest are shown in Fig. 4. 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 \( \lambda/2 \) apart from the top of the collector structure. The calculated absorption is weighted by the Air Mass (AM) 1.5 direct normal and circumsolar spectrum [18]. Figure 4 shows the absorption as a function of wavelength for the collector systems with a PhC-based μc-Si slab and for those with a μc-Si slab of equivalent volume. The impact of the discussed optical properties is apparent from the results. The average absorptions for the two cases (a) and (b) with the equivalent
volume solid slabs in Fig. 4 are 16.1% and 20.9%, respectively. The average absorptions for the cases with the PhC-based slabs are 31.9% (iSC, incident in ΓX direction) and 27.6% (iBCC, incident in ΓN direction), respectively. The enhancements in optical absorption for the collectors with a PhC-based slab over those with a solid slab of equivalent volume are also shown in Fig. 4. The enhancement factor (Ef) is defined as the ratio of the average absorption of a modified collector system with a PhC-based slab to the average absorption of a collector system with a solid slab of equivalent volume. For a given spectrum range near the band edge (1100nm), the evaluation of the Ef is calculated using the formula [19]

\[
Ef = \frac{\int_{\lambda}^{1000} A_{PhC}(\lambda)I(\lambda)d\lambda}{\int_{\lambda}^{1000} A_{0}(\lambda)I(\lambda)d\lambda},
\]

where \(A_{PhC}(\lambda)\) represents the absorption features of an enhanced collector system with a PhC-based intermediate layer. \(A_{0}(\lambda)\) represents the absorption of a collector 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 collector system design augments the reflective and diffractive properties of the 3D PhC, which improve the optical absorption. In the 500 – 1100 nm range where the properties of the μc-Si photovoltaic cells are characterized by their EQEs [3], the Ef s for the two cases in Fig. 4 are 1.98 (iSC, ΓX) and 1.32 (iBCC, ΓN), respectively. From the average absorptions and the Ef s, the collector design with an iSC PhC intermediate structure has higher absorbing efficiency. The PhC intermediate structure is designed with a specified eigenmode at \(\lambda_0 = 700\) nm. Referring to the dispersion curves in Fig. 3, the curves near the specified eigenmode in the case of Fig. 3(a) with respect to the ΓX direction reveal the characteristics of flatter bands and more Bloch modes than those in the other case. Therefore, such a design allows a more light-harvesting near the eigen-wavelength as shown in Fig. 4(a).
4. Conclusion

A theoretical analysis for the potential and impact of a 3D PhC intermediate layer in the design of optical collectors is presented for the improvement of the absorption efficiency in the μc-Si photovoltaic cells. The diffractive effects via the PhCs lead to the desired spectrally selective absorbance spectrum with a limited but sufficiently large spectral width. The device performance is evaluated based on the absorption characteristics of two PhC modified collector structures to those non-modified (with equivalent volume) structures. The highest performance is achieved by the iSC PhC intermediate structure. This structure reaches an Ef of 1.98 for a specified lattice orientation pointing to the sun. The 3D PhCs are an effective approach to light trapping in the photovoltaic cell system with such a collector. Theoretical investigations for the optimization of PhC-based collector systems should further follow to address basic principles for photon management in photovoltaic applications.

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