Absorption enhancement using photonic crystals for silicon thin film solar cells

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Abstract: We propose a design that increases significantly the absorption of a thin layer of absorbing material such as amorphous silicon. This is achieved by patterning a one-dimensional photonic crystal (1DPC) in this layer. Indeed, by coupling the incident light into slow Bloch modes of the 1DPC, we can control the photon lifetime and then, enhance the absorption integrated over the whole solar spectrum. Optimal parameters of the 1DPC maximize the integrated absorption in the wavelength range of interest, up to 45% in both S and P polarization states instead of 33% for the unpatterned, 100 nm thick amorphous silicon layer. Moreover, the absorption is tolerant with respect to fabrication errors, and remains relatively stable if the angle of incidence is changed.

OCIS codes: (160.5298) Photonic crystal; (310.6845) Thin film devices and applications; (040.5350) Photovoltaic.

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#111893 - $15.00 USD Received 27 May 2009; revised 24 Jun 2009; accepted 24 Jun 2009; published 31 Jul 2009

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1. Introduction

Using advanced optical engineering schemes is a key solution in order to provide new designs and new concepts of photovoltaic (PV) solar cells. The goal of these schemes is twofold: first, they should decrease light reflection at the top surface of the PV device, and second, they are expected to provide a sufficient photon path, or lifetime, within the absorbing material. Combining these objectives, optical engineering in PV solar cells is expected to enhance photon absorption, and finally conversion efficiency. In the particular case of second generation devices, i.e. using thin absorbing layers, both the cost and the quantity of active material may be reduced, but at the expense of the conversion efficiency. More precisely, using a thin layer tends to decrease the photon path within the absorbing material, which tends to decrease light absorption. As an example, in PV cells using amorphous silicon films with a total thickness of absorbing material around 1 µm, even if an anti-reflection (AR) structure is used to collect as much photons as possible, the combination of optical and electrical losses tends to limit the conversion efficiency to about 10% [1]. A deeper insight in the operation of these devices shows that the optical path needed to achieve significant absorption at long wavelengths exceeds the thickness of the silicon layer. Indeed, the absorption length is about 5 µm at 700 nm. At these wavelengths, novel optical engineering schemes are therefore needed to overcome this low absorption. In order to reach this goal, various concepts have been proposed in the recent years. They all exploit patterned structures which dimension is of the order of the wavelength of light. In particular, Bermel et al. [2] proposed to implement a diffraction grating and a reflector at the back side of a 2 µm thick silicon solar cell. Another way to improve light collection and absorption using a collection of gold nanoparticles on the front side of a silicon PV cell was recently proposed by Matheu at al [3]. The authors demonstrated that localised plasmon resonances can be used to enhance light trapping around 600nm. An alternative way consists in the sub-wavelength patterning of the absorbing layer itself, which could then behave as a planar photonic crystal (PC). It was recently proposed to make use of surface addressable slow light mode in order to collect the incident light, and to couple it to waveguided slow light resonances that stand within the absorbing layer [4–8]. Such resonances have successfully been used in order to realize surface addressable photonic devices such as microlasers [9] or wide bandwidth reflectors [10,11]. If carefully designed, such surface addressable resonances may at the same time assist sun light collection, reduce reflection losses, and control light absorption in the patterned absorbing layer.

In this paper, we will show the interest of this concept in the particular case of solar cells based on amorphous silicon (a-Si) layers with thicknesses of the order of 100 nm. The thickness of the absorbing layer is limited not only for economical reasons, but also because of the low diffusion length of the photocarriers in this material. One dimensional PC (1DPC) obtained by a full etching of the a-Si layer can enhance the optical absorption of such layer, and are thus expected to enhance the efficiency of PV cells. The introduced concepts are however more general, and can be applied to other kind of PV cells, as long as the refractive index of the absorbing material is in the same range (around 3).

In the next section of this paper, we introduce our methodology, which consists in the calculation of the reflection, transmission and absorption spectra of the 1DPC, using Rigorous Coupled Wave Analysis (RCWA) [12]. In section 3, we discuss on the influence of the patterning of a thin absorbing layer on the spatial and spectral characteristics of the absorption. In section 4, we will discuss on the maximisation of the integrated absorption of such a solar cell, through a scan of the geometrical parameters of the 1DPC. The optical absorption of each structure is thus integrated over the solar spectrum on the earth, i.e. from 300 nm up to the transparency of a-Si at 750 nm. All the calculations take into account the significant dispersion of both refractive index and extinction coefficient over this spectral range. The influence of the polarization state is studied, and we will address the tolerance with

#111893 - $15.00 USD Received 27 May 2009; revised 24 Jun 2009; accepted 24 Jun 2009; published 31 Jul 2009

regards to technological imperfections. Lastly, section 5 concerns the implementation of such a PC structure in a photovoltaic solar cell device.

2. Methodology

We consider a basic structure as presented in Fig. 1. It consists in a patterned layer, including silicon rods separated by air slits; this constitutes a planar 1D PC structure. The parameters are the lattice constant *a*, the thickness *t*. The filling factor *ff* corresponds to the ratio between the silicon rods width and the period. The rods are supposed to be infinite along the *y* direction. The incident light lies in the plane (*x*, *z*)

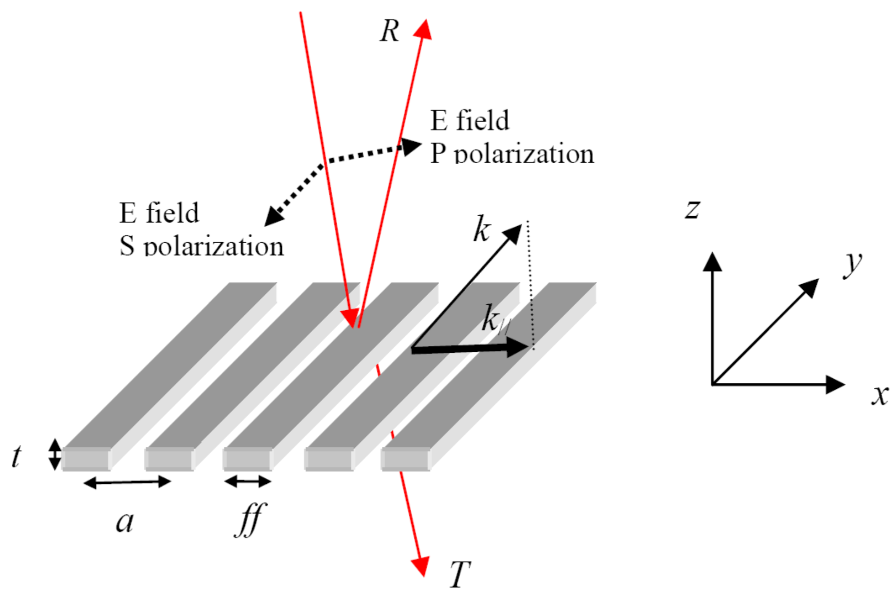

Fig. 1. General Scheme of the 1D Photonic Crystal Structure to increase the absorption

The RCWA module available in CAMFR [13] is a well suited method for the electromagnetic study of 1D or 2D periodic grating in multilayer structures. Indeed, any material dispersion property can be taken into account using this spectral method. This way of solving the Maxwell's equations allows the calculation of the reflectance *R*, the transmittance *T*, and thus of the absorption $A = 1 - R - T$ of a plane wave incident on our structures, as well as the plot of the electromagnetic field distribution in the structure. The absorption is calculated all over the structure, meaning that it takes into account the reduced area of the active layer due to the patterning. Such calculations are done for a given angle of incidence and a given polarization state: the electric field of the S-polarization state is parallel to the direction of the grating. Since the sun light is generally unpolarized, the sensitivity of the proposed structure to the polarization state of the incident light has thus to be studied.

Due to the modal properties of the 1D PC developed hereafter, most of the calculations will be done at normal incidence, but the dependence of the absorption to the angle of incidence will also be developed.

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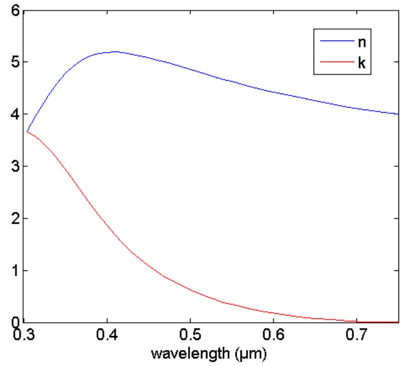

Fig. 2. Refractive index n and extinction coefficient k of the absorbing material in the visible range, measured by ellipsometry on an amorphous silicon layer.

The index of the absorbing material considered is shown in Fig. 2. It corresponds to values measured by ellipsometry on amorphous silicon [14]. For simplicity, the surrounding low index material is supposed to be air, having a refractive index of 1 all over the spectral range.

Finally, the integrated absorption of the structure is defined as the integration of the absorption taking into account the spectral irradiance of the sun (norm AM1.5). Thus, the integration is done from 0.3 µm to 0.75 µm, since the considered material doesn't absorb any more at larger wavelengths. The polarization states will still be distinguished for simpler explanations.

3. Absorption in a planar PC structure

We will consider a simple PC structure patterned in an absorbing layer made of a-Si. Such a structure exhibits surface addressable resonances, corresponding to slow Bloch modes located over the light line and thus to low values of the in-plane component of the wavevector. Compared to an unpatterned layer, the absorption in a PC structure is then expected to be controlled by the quality factor Q_0 of the resonance. Indeed, the absorption may be enhanced if the "impedance matching" between the incident wave and the absorbing medium is achieved, quite similarly to the optical process in resonant photodetectors [15]. Such an impedance matching is achieved provided the photon lifetime, τ_0, related to the optical losses (i.e. related to the quality factor: $Q_0 = \omega\tau_0$, in the transparent PC structure) is equal to the photon lifetime τ_a, related to the absorption losses in the non patterned absorbing medium. Introducing the absorption coefficient $\alpha = \frac{1}{\tau_a \, c/n}$, the matching condition $\tau_0 = \tau_a$ leads to the simple following relation:

$$Q_0 = \frac{2\pi n}{\alpha\lambda} \tag{1}$$

In the case of an amorphous silicon layer, with a refractive index around 4, and an absorption coefficient of a few 1000 cm^{-1}, impedance matching is expected using optical resonance with Q_0 factors in the range between 10 and 100.

First, let's consider a planar 1D PC structure made of a theoretical high index transparent material. To enable easy comparison with the following, this material is supposed to have the same refractive index as the absorbing a-Si. A 500 nm lattice constant is considered, the filling factor is 50%, and the film thickness is 100 nm. The electric field is supposed to be S-polarized.

In Fig. 3(a), the reflectivity is plotted as a function of the normalized frequency (a/λ), and of the in-plane wavevector $k_{//}$. This plot is obtained from reflectivity spectra calculated at

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various angles of incidence. The highly reflective areas (in red) arise from resonant coupling of the incoming plane wave light to modes of the 1D PC that can be addressed from the surface. Therefore, this plot gives an indication of the band structure of this 1D PC in the spectral domain of interest, and over the light line, i.e., for $\omega > ck_{//}$. It can then be noticed that the bands are quite flat, leading to low group velocity modes, especially around the Γ−point ($k_{//} = 0$) of the dispersion characteristics. This leads to a reduced spectral sensitivity of the PC with regards to the incidence angle. This robustness against the angle of incidence is further enhanced for larger bandwidth or lower quality factor optical resonances of the 1D PC.

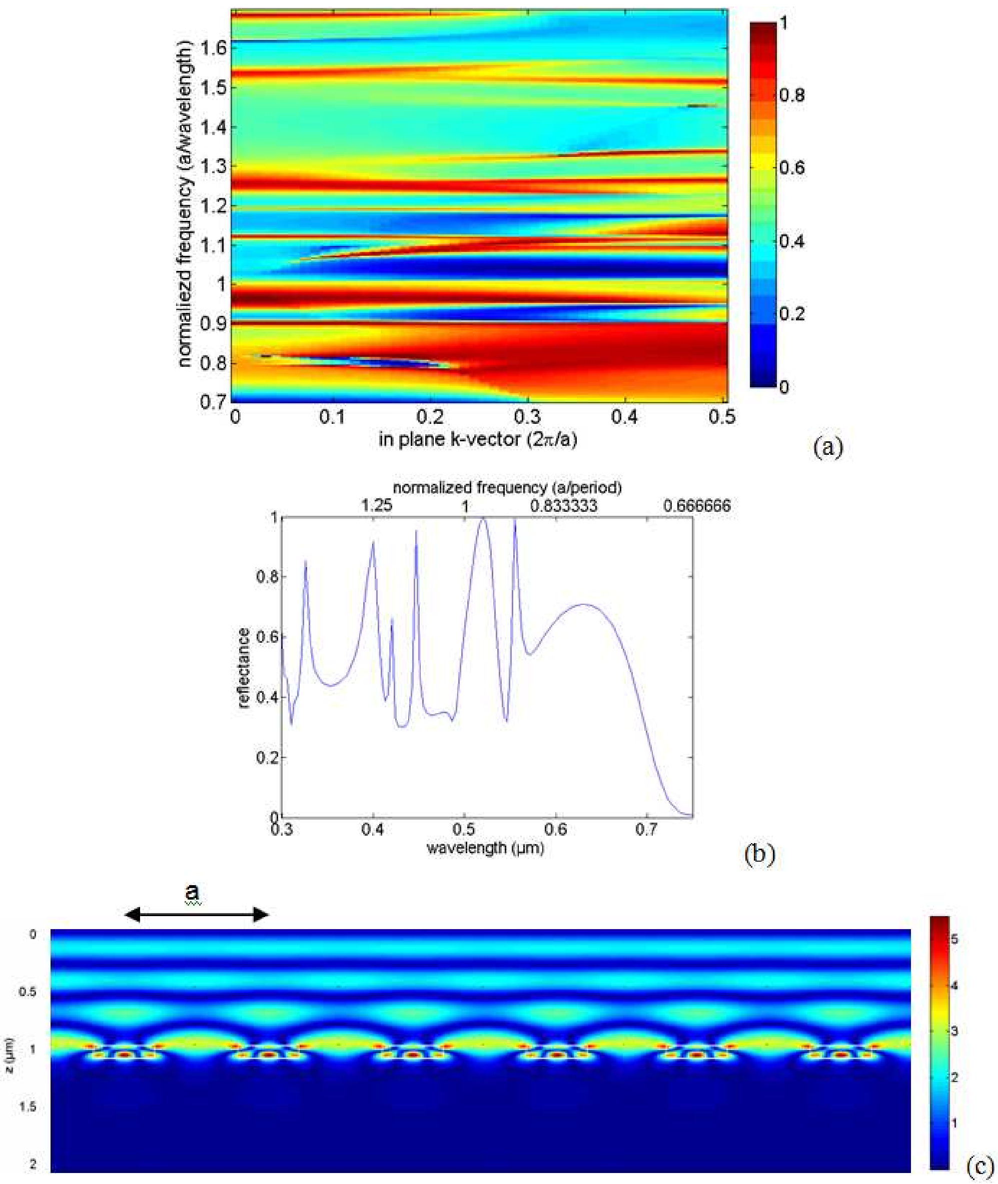

Fig. 3. 1D PC made of high index non absorbing material: reflectance plotted as a function of $k_{//}$ and a/λ (a), reflectance at normal incidence (b) and electric field intensity map of a 6 PC unit cells, at the wavelength 555 nm; the a-Si rods section corresponds to the white border rectangles (c).

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The corresponding spectral reflectance calculated at normal incidence is displayed in Fig. 3(b). Let us consider the reflection peak at 555 nm; which signature is typical of a slow Bloch mode which can be coupled from the surface [16]. Its quality factor $Q_0 = \lambda/\delta\lambda \approx 40$ enables efficient coupling of the incident light and confinement in the high index layer, as can be shown on the electromagnetic field intensity profile in Fig. 3(c). Moreover, for this value of Q_0, the PC resonance is expected to enable a reasonable impedance matching between the incident light and the absorbing medium.

Now, let us consider the same structure, but including the extinction coefficient of the high index material.

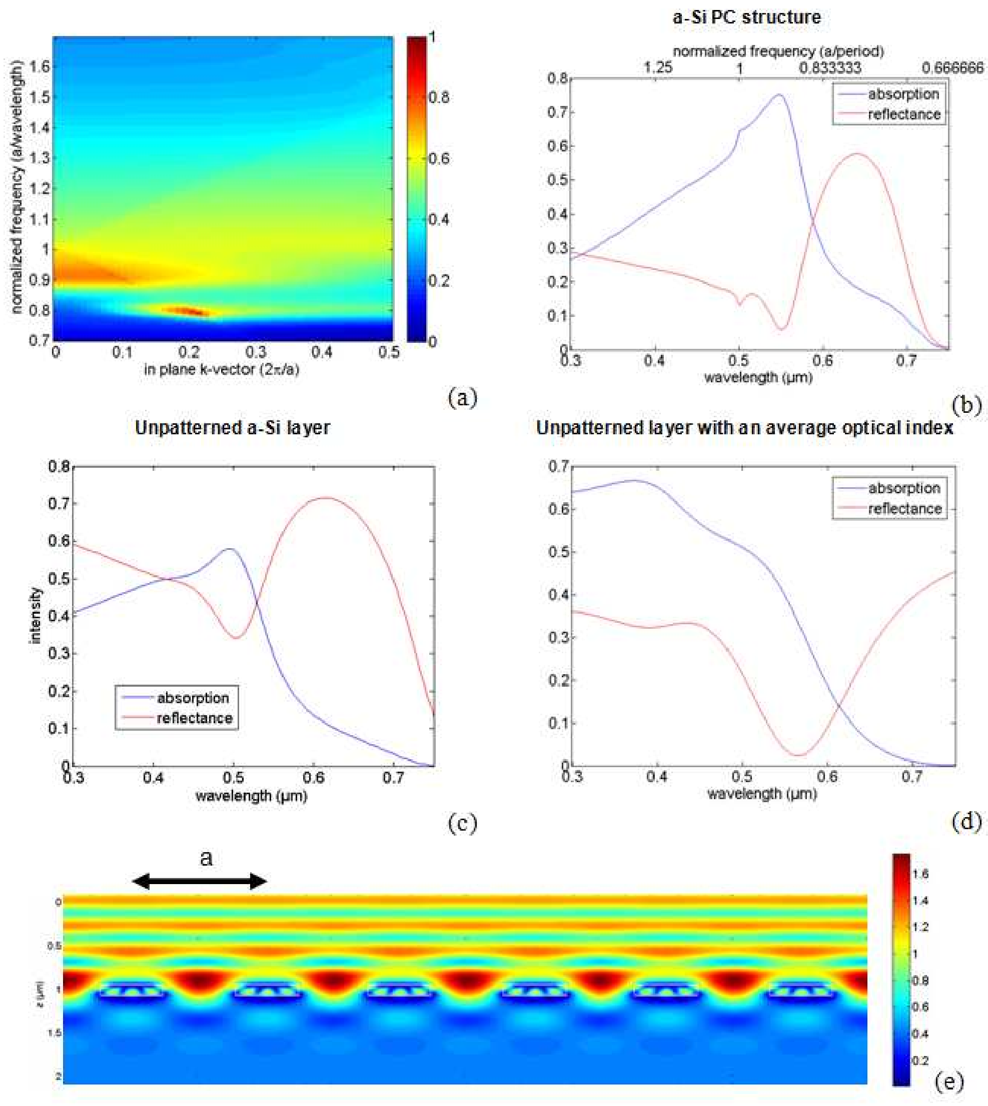

Fig. 4. 1D PC made of high index absorbing material: absorption plotted as a function of $k_{//}$ and a/λ (a), absorption and reflection at normal incidence for the PC structure (b), the unpatterned layer (c) and a layer where the optical indices are mean values between a-Si and air (d). The electric field intensity map of a 6 PC unit cells, at the wavelength 547 nm, is also plotted (e); the section the unit a-Si rod corresponds to the white border rectangle.

In Fig. 4(a), the absorption is plotted as a function of the normalized frequency, and of the in-plane wavevector. As in the case of the transparent layer, this plot gives an indication of the

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dispersion characteristics of this new structure, in far as a-Si absorbs light (below 700nm). The absorption spectrum at normal incidence is displayed in Fig. 4(b); only one main band is remaining, displaying a peak at 547 nm, with 75% maximum of absorption, and a remaining reflectance of 6%. The electric field intensity map shown in Fig. 4(e) clearly shows that this is the same mode as shown previously in the non absorbing material: despite of the absorption, the interferences leading to the increase of the photon lifetime in the PC structure still control the shape of the electric field, even if, this time, it appears to be more intense in the air than in the material.

Comparing Fig. 4(b) with Fig. 4(c), which displays the spectra for the unpatterned slab, one can notice that the absorption remains significantly higher for the PC layer in the 500-750 nm range. Moreover, the maximum value of 58% obtained for the unpatterned layer is significantly lower than the maximum value of 75% achieved with the PC structure. The interest of using a slow Bloch mode is further demonstrated by comparing these data with Fig. 4(d), which shows the spectra in the case of a layer which both refractive and extinction indices are mean values between a-Si and air. Around 550 nm, the absorption of this last structure is even lower than in the case of the unpatterned a-Si layer, and the reflection is similar to the value calculated for the PC structure. Therefore, in the case of the PC structure, the absorption enhancement may not be explained by a sole anti-reflection effect due to a lower mean index, or by a vertical Fabry-Perot resonance, but by the specific properties of the slow light mode.

4. Maximization of the PC structure absorption

In section 3, we demonstrated that using a slow Bloch mode resonance may significantly enhance light absorption around the resonant wavelength. In the case of a real PV cell, it is necessary to improve the absorption not only around a certain wavelength, but also over the full spectral range between 0.3 and 0.75 µm. Moreover, the structure has to be as insensitive as possible to the polarization state of the incident light.

In order to reach these goals, the parameters of the 1D PC should be optimized. RCWA simulations were performed on the structure, scanning the lattice parameter and the filling factor with steps of respectively 0.025 µm and 2.5%, for a 100 nm thick a-Si layer. A maximum of the absorption integrated over the whole spectral range of interest has been found for a = 0.45 µm and ff = 67.5%: the integrated absorption reaches 44% of the solar spectrum in the S polarization state and 45% in the P polarization state, whereas it is only of 33.1% for the unpatterned slab.

The corresponding spectral properties are plotted in Fig. 5. Using this new set of parameters, the absorption is higher for most wavelengths in the 1D PC than in the unpatterned slab. The global absorption enhancement may be attributed to a combination of the effect of the slow light modes, with a global reduction of the reflectance, probably due to a lower mean index in the case of the 1D PC structure.

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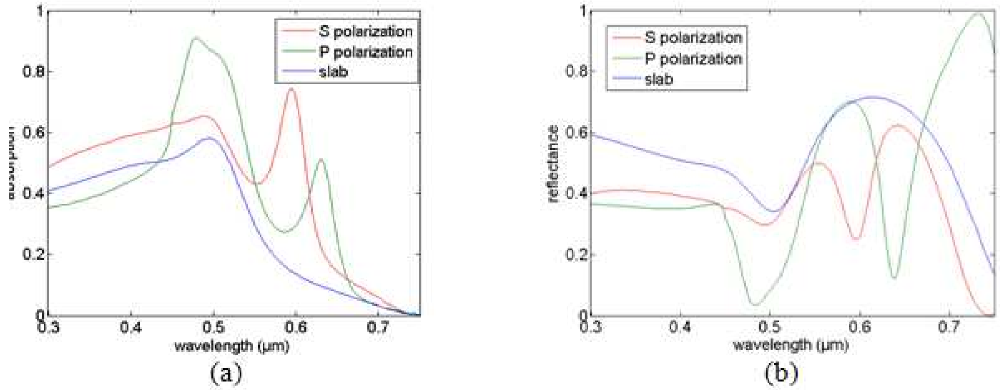

Fig. 5. Spectral absorption (a) and reflectance (b) of the 1DPC maximizing the integrated absorption and minimizing the sensitivity of the integrated absorption to the polarization state of the incident light.

An additional key figure of merit of a PV solar cell is the independence of the conversion efficiency over the incidence angle of the incoming light. Figure 6 represents the angle dependence of absorption spectrum in several solar cell structures. The red line shows absorption graphs in both polarization states in the above optimized structure, and the blue one corresponds to the absorption in the slab. It is noticeable that the 1DPC structure is less sensitive to the angle of incidence, since there is a 25% decrease of the absorption between 0° and 70° for the PC structure, whereas the decrease is as high as 55% for the unpatterned PC slab. As pointed out above, the absorption is controlled using Bloch modes corresponding to rather flat photonic bands. Therefore the variation of their characteristics with regards to the incidence angle is weak, and this may explain the lower decrease of the global absorption in the case of the PC structure. Moreover, as mentioned above, the slow light mode exhibits a low quality factor; its spatial extension is therefore limited [12], and the angular acceptance is further increased.

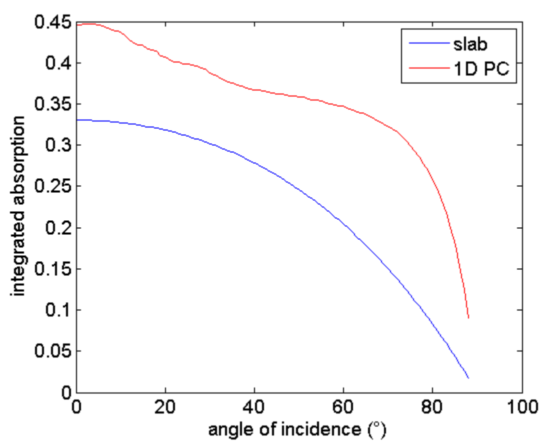

Fig. 6. Angle dependence of integrated absorption in 1D PC and slab

As far as the fabrication of such PC assisted solar cells is concerned, it is necessary to check how tolerant the integrated absorption is with regards to a variation of the topographical parameters. Indeed, we will exploit processing technologies like interference lithography or nano-imprint to generate such sub-wavelength patterns on a large surface, and the final parameters is expected to be slightly different from the nominal geometry.

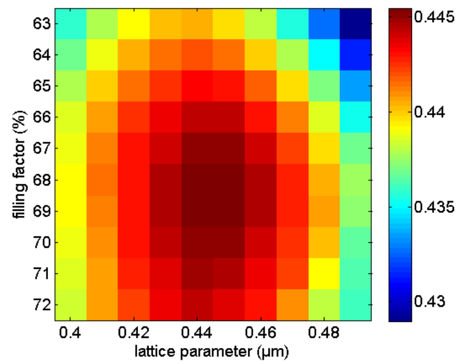

Fig. 7. Contour map of integrated absorption in x-axis of lattice constant (L) and y-axis of material filling factor (ff)

Figure 7 shows the two dimensional colored contours of integrated absorption at each condition point, obtained by changing the lattice constants and material filling factor of 1DPC around the optimal set of parameters. This map shows that the integrated absorption is only decreased by 1% if the lattice parameter and the filling factors are 5% away from the nominal geometry. Therefore, this structure exhibits good tolerance with regards to a variation of the topography of the 1D PC.

Similar results can be obtained using slightly different thicknesses of a-Si layers. The integrated absorption increases as the thickness increases, reaching 48% for a 150 nm thick a-Si layer, whereas it is of 38% for the unpatterned layer: as far as the thickness increases, the gain obtained by the patterning slightly decreases, since the light is more absorbed in the a-Si.

5. Towards complete photovoltaic solar cell structure

A possible complete solar cell including the PC structure is presented in Fig. 8.

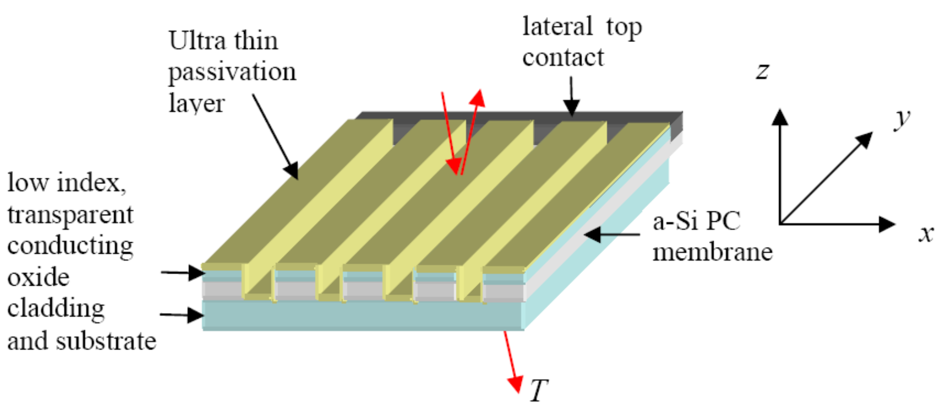

Fig. 8. Targeted configuration of a PV solar cell structure, including an a-Si PC, as well as contact and passivation layers.

It is noticeable that the concept presented in the previous sections, where a-Si is surrounded by air, is still valid provided a-Si is surrounded by transparent materials having a significantly lower refractive index than a-Si. Only the numerical values of the PC parameters and the resulting absorption may be slightly affected by a substrate and a cladding, but the absorption increase remains in the case of the PC structure, compared to the unpatterned stack.

In such a PV solar cell, the cladding and the substrate have to collect the photogenerated carriers. Thus, transparent conductive oxides (TCO) such as ITO or ZnO can be considered, which refractive index is close to 2. Then, a lateral metallic top contact can be placed beside the incoming light absorption area.

Since the proposed design is quite tolerant with regards to fabrication imperfections, the realization of future demonstrators is feasible using nanopatterning technologies such as holographic lithography or nanoimprint. For simplicity, the TCO cladding could be etched in the same time as the a-Si layer. An ultra thin passivation layer like SiN_x, could also be used to reduce the surface recombination, while the impact of the volume recombinations remains low, thanks to the reduced thickness of the a-Si layer (100 nm).

6. Conclusion

We have demonstrated the interest of patterning an absorbing layer as a planar PC, in order to optimize light absorption. Coupling the incident light into slow Bloch modes may significantly increase the absorption of an a-Si layer, using a simple 1D PC pattern. We showed that, using an optimization scheme, the absorption of an 100 nm thick a-Si layer may significantly be increased by 35% over the whole 300-750 nm range, these performances being relatively independent on the incident light polarization. Moreover, due to the unique properties of slow light modes, the integrated absorption exhibits a good stability with respect to the angle of incidence. Finally, the proposed design is quite tolerant with regards to fabrication imperfections, which make feasible a realization of future demonstrators using low cost nanopatterning technologies such as holographic lithography or nanoimprint. The cost of this additional technological step should be overcome by the advantages of using a thinner active layer, with optimized sunlight absorption.

Acknowledgements

Dr Park would like to acknowledge the French Embassy in Korea for a post-doctoral grant which was attributed in the frame of the French-Korean International Associated Laboratory “Centre for Photonics and Nanostructures”. Peter Bienstman is acknowledged for his advice on CAMFR. We would like to acknowledge financial support from the French National Research Agency (ANR) through the Solar Photovoltaic program (SPARCS project).

#111893 - $15.00 USD Received 27 May 2009; revised 24 Jun 2009; accepted 24 Jun 2009; published 31 Jul 2009