Photonic band-engineering absorption enhancement of amorphous silicon for solar cells

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ABSTRACT

We report on enhancement of thin layer absorption through photonic band-engineering of a photonic crystal structure. We realized amorphous silicon (aSi) photonic crystals, where slow light modes improve absorption efficiency. We show through simulation that an increase of the absorption by a factor of 1.5 is expected for a model film of 100nm of aSi. The proposal is then validated by an experimental demonstration, showing a 50% increase of the absorption of a demonstrator layer of $1\mu m$ thick aSi over a spectral range of $0.32 - 0.76\mu m$. This shows new possibilities of increasing the efficiency of thin film photovoltaic cells. Photonic crystal based architecture are proposed and discussed.

Keywords: Photonic crystals, slow light, thin films, solar cells.

1. INTRODUCTION

The efficiency of photovoltaic solar cells is limited, to a large extent, by optical losses. In the case of classical first generation devices, these losses are overcome using anti-reflection coatings and surface texturation.[1] In the case of more prospective solar cells using advanced concepts, new materials and thin absorbing layers, many possibilities are explored to control light absorption. Using nanophotonics through surface plasmons[2] or photonic crystals (PCs), it is possible to control further photon capture and absorption, and larger conversion efficiencies may be expected. In this sense, nanostructured materials have been extensively used for solar energy conversion along a wide variety of conceptual and technological approaches. In particular, wavelength-scale patterning has been efficiently realised by several groups, with an approach usually based on random or periodic structuration of the top surface[3,4] or patterning of the reflector.[5]

We propose to use photonic crystal (PC) slow light modes in order to improve the absorption efficiency of thin absorbing layers, for subsequent embedding in solar cells. It is possible to control the properties of their photonic bands in order to obtain such a slow light mode; through tuning of the parameters of a one (1D) or two-dimensional (2D) PC, etched into the absorbing layer, in order to optimize light absorption rate. Indeed, when using an absorbing medium for the fabrication of the PC, photons at resonances have higher probabilities to be absorbed thanks to their longer lifetime inside the structure, as was previously shown.[6] The quality factor of the slow light modes may be tuned in order to set the photon lifetime, and their very flat dispersion characteristics should widen the angular aperture of photon collection. Photonic slow Bloch modes may be exploited in various configurations, and allow to produce several kinds of functionalities, such as wide-band reflectors,[7] or high quality factor resonators for laser applications.[8] The concepts we want to demonstrate here is valid in principle for any absorbing material. For demonstration purposes, we will focus in this letter on 1D PCamorphous silicon (aSi). A model structure is shown on Fig. 1.

This approach is complementary with other technological schemes, specially antireflection coatings. Presently, the best antireflection (AR) coating performances reached on thin solar cells[9] allowed to reduce light reflection

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until $\approx 4\%$, on a spectral width of $\approx 150nm$. But the spectral limits imposed by the solar spectrum and the material absorption (usually aSi or crystaline silicon) are wider than that; thus the mode engineering we are proposing here can be done both in order to enhance the absorbing layer performance out of the AR coating spectral limit, and to further reduce the 4% reflection reached through absorption enhancement in the thin absorbing layer.

In order to allow a demonstration of the absorption enhancement principle, we chose to work first with a simple thin layer of amorphous silicon. We will develop the simulation method, and discuss the absorption as a function of the various parameters. We will then show the realization of an experimental demonstrator. In a second part we will discuss, based on these experimental results, the possibility of designing a complete solar cell based on a photonic crystal absorbing layer.

2. AMORPHOUS SILICON ABSORPTION ENHANCEMENT

2.1 Concept and simulations

2.1.1 Methodology

We consider a basic structure as presented in Fig. 1. It consists in an aSi patterned layer on a glass substrate; this constitutes a planar 1D PC structure. The parameters are the lattice constant L, the thickness, the filling factor ff which corresponds to the ratio between the silicon rods width and the period. The rods are supposed to be infinite along the x direction. The incident light is considered at normal incidence.

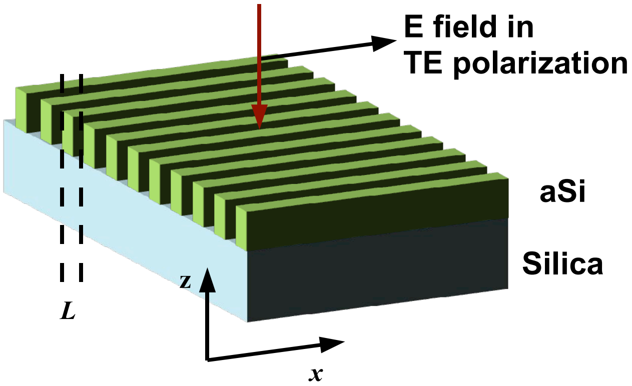

Figure 1. Model structure. General Scheme of the 1D Photonic Crystal structure to increase the absorption.

The Rigorous Coupled Wave Analysis (RCWA) module available in CAMFR* is a well suited method for the electromagnetic study of 1D or 2D periodic grating in multilayer structures. This way of solving the Maxwells 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. Such calculations are done at a given wavelength, 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 to be studied. Due to the modal properties of the 1D PC developed hereafter, most of the calculations will be done at normal incidence. The index of the absorbing material considered is taken from reference[10] and was measured by ellipsometry on amorphous silicon.

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 $0.32\mu m$ to $0.76\mu m$ since the considered material does not absorb any more at larger wavelengths.

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[*] CAMFR is a programming tool developed by the Ghent University, see http://camfr.sourceforge.net/

2.1.2 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.[6,11] 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 $\alpha = \frac{1}{\tau_a \frac{c}{n}}$, 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. The optimization method is further developed in ref.[12]

In the present case, we consider a *100 nm* thick aSi layer deposited on glass as a model system. Indeed the order of magnitude of the usual aSi layers thickness for photovoltaic applications is between tens of nanometers and $1\mu m$, smaller than the carrier diffusion length in order to ensure an efficient carrier collection.

We then calculate the integrated absorption in such a structure on a $0.32\mu m - 0.76\mu m^{\dagger}$ spectral range, with the RCWA based method mentioned in 2.1.1 as a function of the photonic crystal parameters: the period (L) and the aSi filling factor (ff). In order to comment the results we plot a mapping of the absorption, shown on Fig. 2(a).

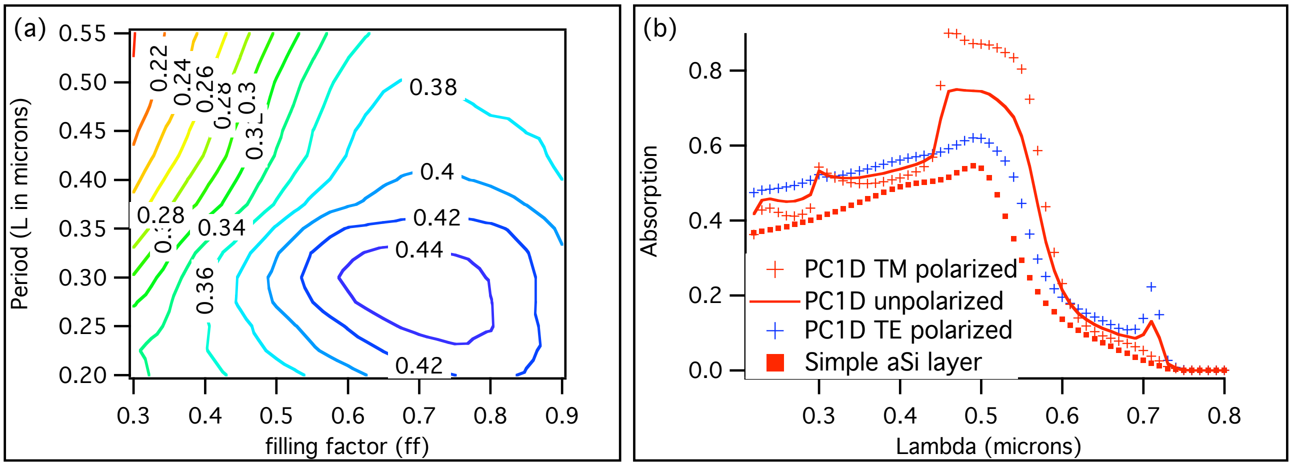

Figure 2. (color online) (a)Contour plot of the integrated absorption as a function of the 1DPC parameters : the period L and aSi filling factor ff. The incident light is considered with the solar spectrum norm AM1.5, at normal incidence the absorption is averaged on both TE and TM polarizations. (b) Absorption spectrum of a simple aSi layer with a period L= 300nm and a filling factor of 70% for TE, TM polarization and an unpolarized light taken as half the sum of the latter. For sake of comparison, a simple aSi layer absorption is plotted.

Fig. 2(a) clearly indicates that the optimal absorption is obtained for a period of $L \approx 300nm$ and an aSi filling factor $ff \approx 70\%$. This mapping shows that there is a good tolerance to variations of the PC parameters, as only 2% in absorption are lost for a variation ≈ 15% in the period or filling factor.

Taking an optimal parameter set (L= 300nm and $ff = 70\%$) it is possible to simulate the absorption spectrum (simply by plotting $A = 1 - R - T$ given by RCWA simulations). It is shown for TE polarization (electrical field

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[†] Taking into account the AM1.5 solar spectrum norm.

parallel to the slits) TM polarizations and for an average on Fig. 2(b). The absorption of a 100nm thickness planar aSi layer, without any PC structure, is also shown for comparison. The absorption peak yielded by the PC is observable around $\lambda = 500nm$. Around this wavelength the patterning allows for a nearly twofold increase of the absorption (from 50 to 90%) in TM polarization and an increase of $1/5^{th}$ in TE polarization. Globally, the integrated absorption for both polarization and for a $0.32 - 0.76\mu m$ spectrum, increases by one half thanks to the PC, from 29% to $\approx 45\%$.

2.2 Demonstrator

In order to allow a first experimental demonstration, we chose to perform experiments on a $1\mu m$ thick layer of amorphous silicon. Indeed, such a thickness should favor a multimode behavior. On the other hand in order to limit the possible non-radiative recombination that may occur on the etched interface, we first designed a thin PC depth, with respect to the layer thickness. Finally we chose to focus on one polarization.

Given these choices we scanned the various PC parameters (period between 0.3 and $0.5\mu m$, $30\% < ff < 70\%$, and etching depth below $0.3\mu m$) to find the optimal PC parameters for absorption enhancement. These simulations lead to a maximum absorption for a photonic crystal period of 400nm, an air filling factor of 75% and an etching depth of $200nm$. The expected total solar light absorption between $\lambda = 0.32\mu m$ and $0.76\mu m$ is then $\approx 64\%$, to be compared with $\approx 43\%$ without patterning.

Therefore, a $1\mu m$-thick amorphous silicon film on glass was fabricated. Patterning was achieved using holographic lithography, and the resist mask was transferred into a hard mask of SiO_2. Amorphous silicon was then partially etched using Reactive Ion Etching, with a gas plasma based on a mixture of SF_6 and Ar.[13]

Before measuring the spectral response of this optimal sample, we simulated its absorption spectrum, shown on Fig. 3(a). Fig. 3(b) shows the corresponding total reflectance (including specular reflection and diffraction), indeed the latter is the accessible experimental data. Simulated spectra are shown for both TE and TM polarizations, and for the arithmetic mean-value of TE and TM data (taken for non-polarized light). Given the considered thickness of amorphous silicon no light is transmitted for wavelengths $\lambda \lesssim 650nm$, therefore reflectivity for these wavelengths is a direct information on the absorption. As for wavelengths $\lambda > 650nm$, the aSi layer becomes transparent, yielding then an interference pattern.

We deduce from Fig. 3(a) an integrated solar absorption of $\approx 65\%$ of the incident TE light for the patterned layer, and $\approx 63\%$ for TM polarization, so 64% on average. This should be compared to 43% for the non-patterned aSi layer.

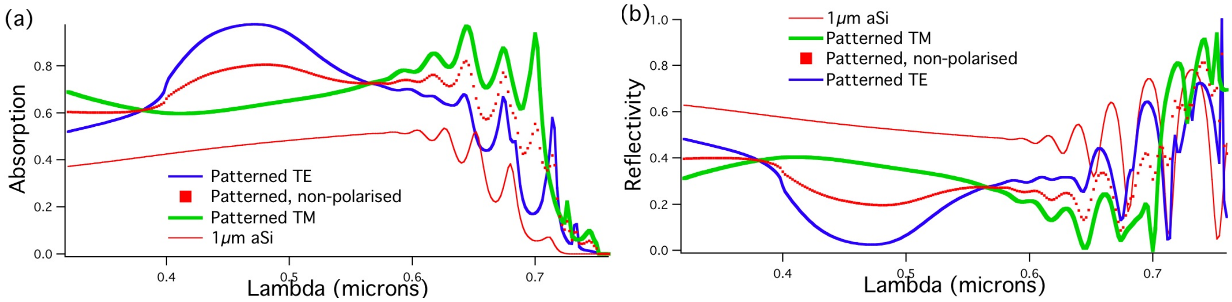

Figure 3. Simulated (a) absorption and (b) resulting reflection of the realised sample for a TE incident light.

2.3 Characterization

In order to characterize the optical properties of this structure, we performed reflectivity experiments integrated over the whole half space around the sample front surface, with an integrating sphere. As mentioned above, given that no light is transmitted below $\approx 650nm$, reflectance $R = 1 - A$ where A is the absorption in this spectral range. For higher wavelengths, we compare simulated and measured reflectance spectra tendencies.

The reflectivity measurement showed that the patterned film reflectivity is drastically reduced with regards to the non-patterned film reflectivity over the whole considered spectrum, as can be seen on Fig 4. This demonstrates, below $630nm$, an equivalent absorption increase.

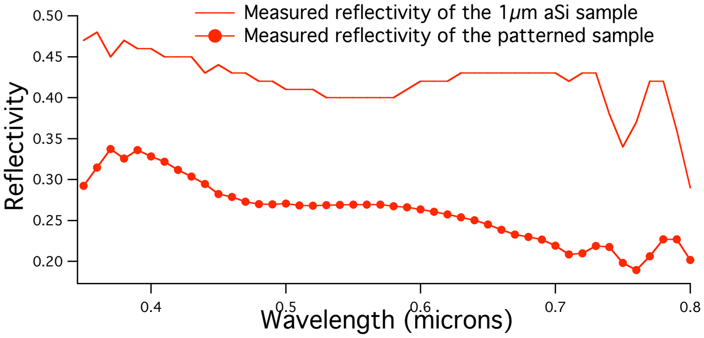

Figure 4. Experimental reflectivity of the patterned sample (round markers) and of the simple $1\mu m$ thick aSi layer (thin line) on glass.

These reflectivity measurements exhibit similar tendencies as those observed on the simulations shown on Fig. 3 (b). As the white light source used in the experiment is non-polarized, the patterned sample reflectivity measurement should be compared to the corresponding simulation. A broad peak can be seen for TE light on the simulated curves around 470nm. This peak is attributed to a mode of the PC structure, as it will be discussed below. In the experimental curve, a significant decrease of the reflectivity is observed just below 500nm ; we attribute this to a smoothed signature of this mode, observed on the patterned simulated reflectivity curve. At high wavelengths, oscillations appear, similarly to what is observed on the simulations but smoothed again, and starting at higher wavelength.

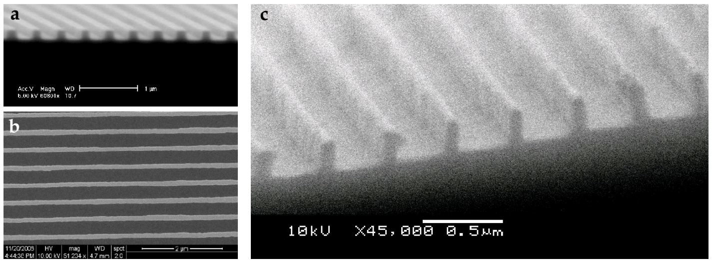

Figure 5. Scanning electron microscope views of patterned aSi: a. Test sample with a metallic film deposited above. b. aSi etched surface seen from above. c. Profile view, the aSi has been etched on $\approx 200 \pm 15nm$.

One reason for the experiment/simulation disagreements may be in the amorphous silicon optical index difference between the real and simulated samples. Moreover we also attribute these differences to technological uncertainties. The topographical profile of the sample is shown on Fig.5(a). The actual aSi sample is shown on Fig.5(b) and (c). One can see on Fig.5(c) that, for the etching depth chosen, the sidewalls are quite vertical, but the patterns section is not perfectly rectangular. The lines seen on both Fig.5(b) and (c) are not perfectly smooth, yielding an unavoidable disorder (due both to holographic lithography, and to etching of an amorphous material) this may smoothen the measured electromagnetic spectra.

In order to confirm and to understand better the role of the PC structure, we performed a mapping of the simulated electromagnetic field in the studied structure, for a TE polarized field at a wavelength of 480nm, where the absorption mode is centered. One can see on Fig. 6 that maxima of electromagnetic field intensity distribution are confined into the mesas lines, therefore showing that the PC is yielding most of the absorption.

3. TOWARDS A PHOTONIC CRYSTAL SOLAR CELL DESIGN AND FABRICATION

We demonstrated above both theoretically and experimentally a method to drastically improve the absorption of thin amorphous silicon layers for photovoltaic applications. This method is in principle applicable to any absorbing material, provided the PC parameters are adapted to the complex refraction index of the material. So

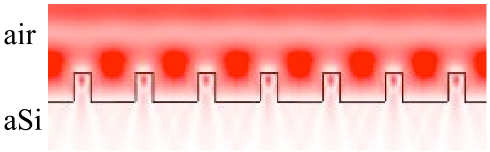

Figure 6. (color online) Mapping of the electromagnetic field intensity in the patterned structure at a wavelength $\lambda = 480nm$.

let us discuss the simulation and design of entire solar cells based on this method, and the potential absorption increase in a complete photovoltaic structure.

As a modeling demonstrator, we will consider a simple design,[14] enumerated hereafter from back to front, and shown on Fig.7(a):

1. A back aluminium reflector of thickness 50nm deposited on a glass substrate.
2. A transparent and conductive oxide (TCO) as an optical spacer, in order to allow for an enhancement of the vertical resonance in the photonic crystal.
3. The amorphous silicon absorbing layer, with a thickness in the range mentioned above.
4. A front TCO layer in order to serve both as an anti-reflection coating and for carrier collection.

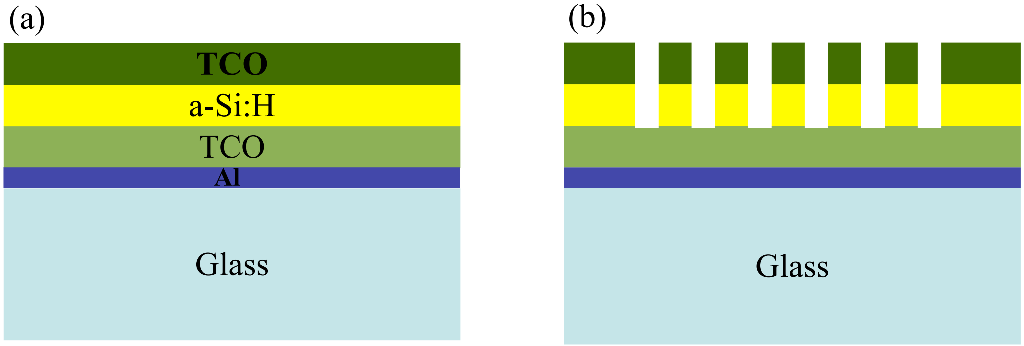

Figure 7. The simple thin film photovoltaic structure considered without (a) and with (b) the PC structure.

Given this architecture, the most direct way to fabricate a photonic crystal consists in patterning both the top TCO and aSi layers. A passivation layer (as SiN_x) should deposited afterwards. The subsequent generic structure including the PC is shown on Fig.7(b).

Based on these elements, we simulated the optical absorption of such a structure, with and without the PC. In order to isolate the aSi contribution to optical absorption, we considered a completely transparent TCO with a refractive index $n_{TCO} = 2$. Fig. 8 shows the compared simulated absorption spectra of this structure with or without photonic crystal patterning.

An improvement of the optical absorption is obtained for a PC period of $L = 310nm$ and ff= $69 - 74\%$. Two resonance peaks can be seen, clearly due to the patterning. They are spectrally located at the edges of the absorption spectrum, where the usual absorption techniques are the least efficient.[9,14] They yield an increase of the integrated absorption from 52% to 63% of the incident light. The latter is slightly less important than for the bare aSi case, as the non-patterned complete solar cell structure is already optimized, thanks to the back metallic reflector and the front antireflection coating.

These simulations have to be taken as first steps towards a rigorous understanding of absorption in the photonic crystal structure. Indeed here TCO has been taken as a non-absorbant medium, in order to isolate the absorption in the medium of interest (aSi). This approximation of a transparent TCO is valid for wavelengths

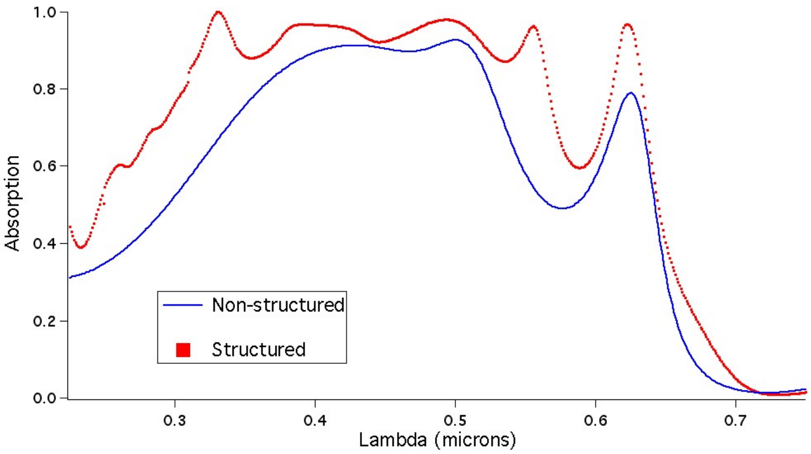

Figure 8. Simulations of the structures absorption for a TM polarised incident light. Continuous blue line: non-patterned structure. Red squares: photonic crystal patterned structure.

below 660nm, above this value, TCO absorbs more than aSi. Further theoretical work should be done in order to take into account the absorbency of TCO and then distinguish between each layer's contribution. PC band engineering may then contribute to enhance the aSi layer contribution. It is also needed to evaluate the photoelectrical losses which may be induced by the etching process. Current simulations performed in our group show that the latter are more than compensated for by the improved absorption yield.[6]

4. CONCLUSION AND POTENTIALITIES

The contribution of a PC structure using light modes coupled in the normal direction was demonstrated both theoretically and experimentally for a simple aSi layer, and proposals were made for a complete solar cell structure, in combination with usual techniques. We showed that despite the high efficiency of existing techniques, a PC patterning may enhance thin layer absorption. This is allowed by the fact that the absorption enhancement can me made higher at the edges of the absorption spectrum. This complementarity should be further studied with more elaborated techniques such as back reflector texturation.

This method is applicable to any absorbing material, such as crystalline silicon or III-V semiconductors, provided the PC parameters are adapted to the complex refraction index of the material. Given the controllability of the spectral properties of the absorption enhancement, we believe this method could also be used to improve the sensitivity of detectors on given spectral bands.[15]

This opens the way to various solar cell architectures, with a wide spectrum of potentialities for efficiency improvement for various types of materials.

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