Enhanced absorption in thin silicon films by 3D photonic band gap back reflectors for photovoltaics

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Since thin-film silicon solar cells have limited optical absorption, we explore the effect of a nanostructured back reflector to recycle the unabsorbed light. As a back reflector we investigate a three-dimensional (3D) photonic band gap crystal made from silicon that is readily integrated with the thin films. We numerically obtain the optical properties by solving the 3D time-harmonic Maxwell equations using the finite-element method, and model silicon with experimentally determined optical constants. The absorption enhancement relevant for photovoltaics is obtained by weighting the absorption spectra with the AM 1.5 standard solar spectrum. We study thin films in two different regimes, much thicker (L_{Si} = 2400 nm) or much thinner (L_{Si} = 80 nm) than the wavelength of light. At L_{Si} = 2400 nm, the 3D photonic band gap crystal enhances the spectrally averaged (λ = 680 nm to 880 nm) silicon absorption by 2.22× (s-pol.) to 2.45× (p-pol.), which exceeds the enhancement of a perfect metal back reflector (1.47 to 1.56×). The absorption is considerably enhanced by the (i) broadband angle and polarization-independent reflectivity in the 3D photonic band gap, and (ii) the excitation of many guided modes in the film by the crystal’s surface diffraction leading to greatly enhanced path lengths. At L_{Si} = 80 nm, the photonic crystal back reflector yields a striking average absorption enhancement of 9.15×, much more than 0.83× for a perfect metal. This enhancement is due to a remarkable guided mode that is confined within the combined thickness of the thin film and the photonic crystal’s Bragg attenuation length. An important feature of the 3D photonic band gap is to have a broad bandwidth, which leads to the back reflector’s Bragg attenuation length being much shorter than the silicon absorption length. Consequently, light is confined inside the thin film and the remarkable absorption enhancements are not due to the additional thickness of the photonic crystal back reflector.

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I. INTRODUCTION

To provide sustainable solar energy for the entire world’s population, including at locations away from industrialized areas, it is an economical step to harness the sun’s energy with solar cells. These cells employ the photovoltaic effect to absorb light and convert the absorbed energy into electricity using semiconductor materials [1, 2]. Being a highly abundant and non-toxic material available in the earth’s crust, silicon is an ideal choice to fabricate the many solar cells needed to provide energy to the whole world [3, 4]. While thick silicon solar cells are widely used, thin silicon solar cells are enjoying a rising popularity since they require less material and hence less resources and costs [5]. Moreover, they are mechanically flexible so they can be deployed on many different platforms, including freely shaped ones.

Since crystalline silicon (c-Si) has an indirect band gap at 1.1 eV, the absorption of light is low in the near infrared range that contains 36% of all solar photons [6]. Conversely, the absorption length is long namely $l_a = 1 \text{ mm}$ just above the gap at $\lambda = 1100 \text{ nm}$ (1.12 eV) and still only $l_a = 10 \text{ µm}$ at $\lambda = 800 \text{ nm}$ (1.55 eV) [7]. Since the thickness of thin silicon film solar cells is much less than the absorption lengths, the absorption of incident solar light is low [8–11], which adversely affects the cost and the flexibility advantages [12–15].

![Design of a solar cell](image)

FIG. 1. Design of a solar cell that consists of a thin silicon film (orange) with a 3D photonic band gap crystal (purple) and a perfect metal (black) as back reflectors. Here, 0 corresponds to the 0th diffraction order that corresponds to specular reflected light by the photonic crystal or the perfect metal. $I_0$ and $R_1$ represent the light incident and reflected at the front surface of the thin film, respectively. $I_1$ represents the light refracted into the thin film medium and incident on the photonic crystal. $-1, 1, 2$ are nonzero diffraction orders. Blue arrows represent the propagation of guided modes in the thin silicon film.

Efficient light trapping enhances the photovoltaic efficiency of silicon solar cells while sustaining the advantages of thin silicon film [8–11]. In traditional light trapping approaches one increases the light paths in a solar cell using random texturing [14, 18], to scatter incident light into long oblique light paths and using a back reflector to reflect unabsorbed light back into the solar cell. In practice, perfect scattering is impossible to achieve, which limits the attainable efficiency [19]. An ideal back reflector reflects light incident from any angle, known as omnidirectional reflectivity [20], and ideally for all wavelengths and all polarizations of light. As illustrated in Fig. 1, a perfect metal with 100% reflectivity at all wavelengths and all polarizations would thus seem to be an ideal back reflector. In practice, no metal has 100% reflectivity at all wavelengths due to Ohmic losses [21]. Moreover, light that is not reflected by a real metal gets absorbed, which produces heat and further limits the photovoltaic efficiency of a solar cell.

Recently, much work has been devoted to light trapping strategies based on wave optics [22–26]. These strategies outperform random scattering optics approaches, typically over broad wavelength ranges, where one takes advantage of enhancements caused by constructive interference. To manipulate the interference, specially designed nano-structures are pursued, including 1D (“Bragg stack”), 2D and 3D photonic crystals [27–37].

In this paper, we explicitly focus on photonic crystal back reflectors with a complete 3D photonic band gap [38, 39], a frequency range for which the propagation of light is rigorously forbidden for all incident angles and all polarizations simultaneously, as recently demonstrated in experiments and calculations [10, 14]. To illustrate the concept, Fig. 1 shows a design of a thin silicon film (orange) with a 3D photonic band gap crystal back reflector (blue). Incident light with intensity $I_0$ is Fresnel diffracted to intensity $I_1$ within the thin film. When the photon flux $I_1$ has a frequency in the photonic band gap, it is reflected by the photonic crystal [38]. The specular reflected beam corresponds to the 0th diffraction order. Figure 1 illustrates non-zeroth order diffraction modes, e.g., $-1, 1,$ and $2,$ that are generated at the
periodic interface between the thin film and the photonic crystal. These diffraction modes couple light into guided modes that are confined inside the thin silicon film via total internal reflection. Consequently, guided photons obtain a long path length inside the film and have thus an enhanced probability for absorption. Hence, different from a perfect metal, a 3D photonic crystal will enhance the absorption of a thin film by (i) profiting from perfect reflectivity inside the band gap for all incident angles and polarizations, and (ii) by generating guided modes [33, 36].

Recently, we reported a numerical study on the enhanced energy density and optical absorption for realistic and finite 3D silicon photonic band gap crystals with an embedded resonant cavity [46, 47]. The absorption was found to be substantially enhanced, but only within the tiny cavity volume, as opposed to the present case where the absorption occurs throughout the whole film volume, which avoids local heating and non-linear or many-body effects that adversely affect the photovoltaic efficiency [2]. While a structure with a 3D photonic band gap is from the outset relevant as an omnidirectional, broadband, and polarization-robust back reflector for solar cells, they have been hardly studied. Therefore, we investigate nanostructured back reflectors with a 3D photonic band gap that is tailored to have a broad photonic band gap in the visible regime. Using numerical finite-element solutions of the 3D time-harmonic Maxwell equations, we calculate the absorption of light in a thin silicon film solar cell with an inverse woodpile photonic crystal as a back reflector. To make our calculations relevant to experimental studies, we employ a dispersive and complex refractive index obtained from experiments [48] and compare the photonic crystal back reflector to a perfect metallic back reflector. We verify that the absorption is not enhanced by the extra material volume. We aim to understand the physics behind large enhancements by identifying the relevant physical mechanisms compared to a standard back reflector.

II. METHODS

A. Structure

The solar cell design in Fig. 1 consists of a thin silicon film as an absorbing layer and a cubic inverse woodpile photonic crystal [49–51] as a back reflector. The 3D inverse woodpile crystal structure consists of two 2D arrays of identical pores with radius \( r \) running in two orthogonal directions X and Z [49]. Each 2D array has a centered-rectangular lattice with lattice parameters \( c \) and \( a \) (see Appendix A). For a ratio \( \frac{a}{c} = \sqrt{2} \), the diamond-like structure has cubic symmetry. Cubic inverse woodpile photonic crystals have a broad maximum band gap width \( \Delta \omega/\omega_c = 25.3\% \) relative to the central band gap frequency \( \omega_c \) for pores with a relative radius \( \frac{r}{a} = 0.245 \) [50, 51]. Our prior results reveal that reflectivity in excess of \( R > 99\% \) - hence transmission \( T < 1\% \) - occurs even for a thin inverse woodpile photonic crystal with a thickness of a few unit cells \( \left( L_{3DPC} \geq 3c \right) \) [39, 43]. Therefore, we choose here a cubic inverse-woodpile crystal with an optimal pore radius \( \frac{r}{a} = 0.245 \) and with a thickness \( L_{3DPC} = 4c = 1200 \text{ nm} \) as a back reflector for the calculation of the absorption of light by the solar cell.

B. Computations

![Diagram of computational cell](image-url)

**Absorbing boundary**

- Thin silicon film with thickness \( L_{Si} = 2400 \text{ nm} \) is the absorbing layer and a 3D inverse woodpile photonic crystal with thickness \( L_{3DPC} = 1200 \text{ nm} \) is the back reflector. The blue color represents the high-index material with a dielectric function similar to silicon.

To calculate optical absorption in a thin silicon film, we employ the commercial COMSOL Multiphysics finite-element (FEM) software to solve the time-harmonic Maxwell equations [52]. Figure 2 illustrates the computational
cell viewed in the $YZ$ plane. The incident fields start from a plane at the left that is separated from the silicon layer by an air layer. Since the plane also absorbs the reflected waves $[33]$, it represents a boundary condition rather than a true current source. The incident plane waves have either $s$-polarization (electric field normal to the plane of incidence) or $p$-polarization (magnetic field normal to the plane of incidence), and have an angle of incidence between $\theta = 0^\circ$ and $80^\circ$. We employ Bloch-Floquet periodic boundaries in the $\pm X$ and the $\pm Y$ directions to describe the infinitely extended thin silicon film $[38]$. To describe a solar cell with finite support, absorbing boundaries are employed in the $-Z$ and $+Z$ directions. We calculate reflectivity and transmission of the thin film at the absorbing boundaries in the $-Z$ and $+Z$ directions, respectively. The light with a given wavelength $\lambda$ incident at an angle $\theta$ with respect to the surface normal is either reflected or transmitted, or absorbed by the thin film $[21]$. To calculate the absorption $A_{Si}(\lambda, \theta)$ we employ the relation

$$A_{Si}(\lambda, \theta) = 1 - R_{Si}(\lambda, \theta) - T_{Si}(\lambda, \theta),$$

(1)

with $R_{Si}(\lambda, \theta)$ the reflectivity and $T_{Si}(\lambda, \theta)$ the transmission spectra that are normalized to the incident light intensity $I_0$.

To gauge the performance of a 3D photonic band gap back reflector, we define the wavelength and angle-dependent absorption enhancement $n_{abs}(\lambda, \theta)$ of the thin film solar cell in Fig. 2 as

$$n_{abs}(\lambda, \theta) \equiv \frac{\int_{\lambda-\Delta \lambda}^{\lambda+\Delta \lambda} P_{AM1.5}(\lambda) A_{(Si+3DPC)}(\lambda, \theta) d\lambda}{\int_{\lambda-\Delta \lambda}^{\lambda+\Delta \lambda} P_{AM1.5}(\lambda) A_{Si}(\lambda, \theta) d\lambda},$$

(2)

with $A_{(Si+3DPC)}$ the absorption in a thin silicon film with a 3D photonic crystal back reflector, and $A_{Si}$ the absorption in a thin silicon film with the same thickness, yet no back reflector. Using Eq. 2 the enhancement is averaged over a bandwidth $(2\Delta \lambda)$ at every discrete wavelength $\lambda$. Furthermore, $\cos(\theta)$ is the ratio of incident light captured at a given angle of incidence $\theta$ compared to the total incident light captured at normal incidence $[54]$. Equation 2 also gives the current generated in the idealized situation that every absorbed photon generates an electron-hole pair, where the absorption is weighted with the solar spectrum using the air mass coefficient $P_{AM1.5}(\lambda)$ $[6]$.

At normal incidence $(\theta = 0^\circ)$ the absorption enhancement $n'_{abs}(\lambda)$ is reduced from Eq. 2 to

$$n'_{abs}(\lambda) \equiv \frac{\int_{\lambda-\Delta \lambda}^{\lambda+\Delta \lambda} P_{AM1.5}(\lambda) A_{(Si+3DPC)}(\lambda, \theta) d\lambda}{\int_{\lambda-\Delta \lambda}^{\lambda+\Delta \lambda} P_{AM1.5}(\lambda) A_{Si}(\lambda, \theta) d\lambda}.$$  

(3)

To calculate the angle-averaged absorption enhancement $n''_{abs}(\lambda)$, the enhancement $n_{abs}(\lambda, \theta)$ (Eq. 2) is averaged over $n$ incident angles $\theta_i$ to

$$n''_{abs}(\lambda) \equiv \frac{1}{n} \sum_{i=1}^{i=n} n_{abs}(\lambda, \theta_i).$$  

(4)

Figure 2 illustrates the finite element mesh of tetrahedra that are used to subdivide the 3D computational cell into elements $[55]$. Since the computations are intensive due to a finite element mesh of 167000 tetrahedra, we performed the calculations on the powerful “Serendipity” cluster $[56]$ at MACS in the MESA+ Institute (see also Ref. $[46]$).

To enhance the weak absorption of silicon above the electronic band gap at wavelengths in the range 600 nm $< \lambda < 1100$ nm, we tailor the lattice parameters of the inverse woodpile photonic crystal to $a = 425$ nm and $c = 300$ nm such that the band gap is in the visible range. The chosen lattice parameters are 37% smaller than the ones usually taken for photonic band gap physics in the telecom range $[39–44, 57–59]$. The required dimensions are well within the feasible range of nanofabrication parameters $[60–62]$.

To benchmark our proposition of using a 3D inverse woodpile photonic crystal as a back reflector, we compare the absorption spectra to spectra for the same thin silicon layer with a perfect and omnidirectional metallic back reflector. Therefore, in our simulations we replace the photonic crystal and the air layer on the right in Fig. 2 with a homogeneous metallic plane with a large and purely imaginary refractive index $n' = -i \cdot 10^9$.

### III. RESULTS AND DISCUSSION

In the first two subsections, we show the main results, namely the absorption enhancements for silicon films thicker and thinner than the wavelength. In the subsequent subsections, we discuss detailed physical backgrounds, including film thickness, angular acceptance, and absence of photonic crystal backbone contributions to the overall absorption.
A. Supra-wavelength silicon film

Figure 3 shows the normal incidence absorption enhancement spectra $\eta_{abs}(\lambda)$ (Eq. 3) of a supra-wavelength $L_{Si} = 2400$ nm thin silicon film for both the perfect metal and the 3D photonic crystal back reflectors. For the 3D inverse woodpile back reflector, the absorption enhancement varies between $\eta_{abs} = 1 \times$ and $9 \times$ inside the stop bands between $\lambda = 640$ nm and 900 nm. The wavelength-averaged absorption enhancement is about $<\eta_{abs}> = 2.22 \times$ for the $s-$stop band and $<\eta_{abs}> = 2.45$ for the $p-$stop band. In comparison, for a perfect metal back reflector the wavelength-averaged absorption enhancement is about $<\eta_{abs}> = 1.47$ for the $s-$stop band and $<\eta_{abs}> = 1.56$ for the $p-$stop band. Since a perfect metal back reflector has 100% specular reflectivity only in the specular 0th diffraction order, the absorption enhancement $\eta_{abs}$ is always less than two ($<\eta_{abs}> \leq 2$). In contrast, a photonic band gap crystal back reflector also has non-zero order diffraction modes, see Fig. 1, that scatter light into guided modes where light is confined inside the thin silicon film via total internal reflection. Since the effective optical path length travelled by a photon in a guided mode is longer than the path length travelled with only the 0th order diffraction mode, a photonic crystal back reflector yields a greater absorption enhancement $<\eta_{abs}> \geq 2$ for the diffracted wavelengths, as is apparent in Fig. 3. This observation is a first support of the notion that a 3D photonic band gap back reflector enhances the absorption of a thin silicon film by (i) behaving as a perfect reflector with nearly 100% reflectivity for both polarizations, and (ii) exciting guided modes within the thin film.

Since the high-index backbone of the 3D inverse woodpile photonic crystal consists of silicon, one might surmise that the absorption is enhanced by the addition of the photonic crystal’s silicon backbone to the thin silicon film. To test this hypothesis, we calculate the absorption enhancement within the thickness $L_{Si}$ of the thin silicon film.
part (see Fig. 2) using the volume integral of the total power dissipation density from Ref. [52]. Figure 3 shows that the absorption enhancement spectra for the thin film volume agree very well with the spectra of the complete device (both thin film and photonic crystal) in the stop bands between $\lambda = 640$ nm and 900 nm. Therefore, the high-index backbone of the 3D photonic crystal contributes negligibly to the absorption inside the stop bands, even in the visible regime. Apparently, light that travels from the thin film into the photonic crystal is reflected back into the thin film, even before it is absorbed in the photonic crystal. To bolster this conclusion, we start with the notion that the typical length scale for reflection by a photonic crystal is the Bragg attenuation length $\ell_{Br}$ [63] that qualitatively equals the ratio of the central stop band wavelength and the photonic interaction strength $S$ times $\pi$: $\ell_{Br} = \lambda_c/(\pi S)$ [64, 65], where the strength $S$ is gauged by the ratio of the dominant stop band width and the central wavelength ($S = \Delta \lambda/\lambda_c$).

From the stop band between $\lambda = 640$ nm and 900 nm ($S = 260/770 = 0.34$) we arrive at $\ell_{Br} = 770/(\pi 0.34) = 725$ nm, which is much less than the absorption length of silicon: $\ell_{a} < l_{a}$. Thus, the broad bandwidth of the back reflector’s 3D photonic band gap is an important feature to enhance the absorption inside the thin silicon film itself, as the broad bandwidth corresponds to a short Bragg length.

**B. Sub-wavelength silicon film**

![Graph showing absorption enhancement spectra](image)

**FIG. 4.** Absorption enhancement spectra for a sub-wavelength thin silicon layer ($L_{Si} = 80$ nm), taken as ratio of absorption $A$ with a back reflector and absorption $A_{Si}$ without back reflector, all at normal incidence computed using Eq. 3. Top panel: $s$-polarized, bottom panel: $p$-polarized light, with $s$- and $p$-stop bands shown as yellow highlighted regions. Red circles pertain to the thin film with a 3D photonic crystal back reflector and the black diamonds are for the silicon part only. The blue dashed curves pertain to a thin film with a perfect metal back reflector and the green line are the reference level of the thin film without reflector.

Figure 4 shows the normal incidence absorption enhancement $\eta_{abs}'(\lambda)$ (Eq. 3) of a $L_{Si} = 80$ nm thin silicon film, whose thickness is much less than the wavelength in the material ($L_{Si} << \lambda/n$), hence no guided modes are sustained in the film itself. Since the thickness is also much less than the silicon absorption length $L_{Si} << l_{a} = 1000$ nm between $\lambda = 600$ nm and 900 nm [48], the absorption $A$ of the thin film itself is low, namely about 4.5% at the blue edge of the photonic stop bands) and 0.2% at the red edge of the stop band, see Fig. 5. These results agree with
a Fabry-Pérot-analysis of the thin film, which reveals a broad first order resonance near 570 nm that explains the increased absorption towards the short wavelengths.

For the perfect metal back reflector in Fig. 4 the absorption is reduced ($\eta'_{\text{abs}}(\lambda) < 1$) at wavelengths $\lambda < 730$ nm, and enhanced ($\eta'_{\text{abs}}(\lambda) > 1$) at longer wavelengths. This result is understood from the Fabry-Pérot behavior of the thin film in presence of the perfect metal, that induces an additional $\pi$ phase shift (due to the exit surface reflectivity) to the roundtrip phase. Consequently, a first order resonance appears near $\lambda = 1140$ nm, and the next anti-resonance near 600 nm. Therefore, the absorption is enhanced towards $\lambda = 1140$ nm and reduced towards 600 nm, in agreement with the results in Fig. 4. The corresponding wavelength-averaged absorption enhancements are $< \eta_{\text{abs}}' > = 0.8$ for $s$-polarized and $< \eta_{\text{abs}}' > = 0.85$ for the $p$-polarized stop band. In other words, a perfect metal back reflector hardly enhances the absorption for thin films with the thickness corresponding to a Fabry-Pérot minimum for the desired wavelengths of absorption enhancement.

In presence of a photonic band gap back reflector, the wavelength-averaged absorption enhancement is surprisingly larger, see Fig. 4. The strong increase is clearly illustrated by the use of a logarithmic scale. We see several peaks between $\lambda = 600$ nm and 900 nm in Fig. 4 four absorption resonances (S1, S2, S3, and S4) inside the $s$-polarized stop band and two absorption resonances (P1 and P2) inside the $p$-polarized stop band with enhancements as high as $\eta_{\text{abs}}' = 100$ for both polarizations. The wavelength average enhancement is $< \eta_{\text{abs}}' > = 13.5$ for the $s$-polarized stop band and $< \eta_{\text{abs}}' > = 11.4$ for the $p$-polarized stop band. Since the thickness of the silicon $L_{\text{Si}} = 80$ nm does not sustain guided modes at the wavelengths within these stop bands, the enhanced absorption peaks must be induced by the presence of the photonic crystal back reflector, which has an effective refractive index smaller than that of silicon (see Appendix A), and hence leads to no phase shift like the metallic back reflector.

Considering that this Si layer is much thinner than the one in Sec. III A, there is a likelihood that the absorption is
enhanced by the extra silicon volume from the photonic crystal’s backbone, whose thickness is much greater thickness than of the film, namely $L_{3DPC} = 1200 \text{ nm}$ versus $L_{Si} = 80 \text{ nm}$. To test this hypothesis, we calculated the absorption within the volume of the thin silicon film part only ($L_{Si} = 80 \text{ nm}$), using the power per unit volume formulae of Ref. [52], as shown in Fig. 5 (from which Fig. 4 is deduced) with various back reflectors for $s-$ and $p-$polarizations. The enhanced absorption at all six resonances S1-S4, and P1-P2 occur in the thin film volume only. The wavelength-averaged absorption enhancement within the thin film part is $\eta_{abs} = 10.46$ averaged over the $s-$polarized stop band and $\eta_{abs} = 7.84$ for the $p-$polarized stop band, which are nearly the same as in the full device. Therefore, we conclude that the absorption in the photonic crystal contributes only a little to the enhanced absorption and does not induce the presence of the absorption peaks. Fig. 4 reveals that the absorption within the thin film part and the one within the complete device (both thin film and photonic crystal) match very well near the center of the $s-$ and $p-$ stop bands and differ at the edges. The reason is that the Bragg attenuation length $l_B$ is smallest near the center of the stop band, while it increases toward the band edges, where it leads to more absorption in the crystal before the light is reflected within a Bragg length.

To investigate the physics behind these intriguing peaks, we discuss the electric field distributions for the exemplary resonances S3 and P1. The incident light with wavevector in the Z-direction has either $s$-polarization ($E$-field in the X-direction) and or $p$-polarization ($E$-field in the Y-direction). To filter the scattered electric fields that are guided in the plane of the thin layer from possibly overwhelming incident fields, we plot in Fig. 6 the field components that are absent in the incident light. Thus, we plot the $E_z$ and $E_y$ field components of the S3 resonance that is excited by $s-$polarized light ($E_{in}, X$), and the $E_z$ and $E_x$ components of the P1 resonance that is excited by $p-$polarized light ($E_{in}, Y$).

First, we discuss the S3 $E_y$ and P1 $E_x$ field components that are transverse to the incident direction, and perpendicular to the incident polarization. Both components are maximal inside the thin silicon film, as expected for guided waves. The field distributions show periodic variations in the plane of the thin film that are also characteristic of guided modes [26, 66]. The periods match with the crystal’s lattice parameter, which suggests that the fields are part of a Bloch mode. The fields extend into the photonic crystal by about one unit cell, in agreement with a Bragg attenuation length of about $L_B = 0.6c = 180 \text{ nm}$ at the $p-$stop band center that was computed in Ref. [39].

For the other two field components S3 $E_z$ and P1 $E_z$, the maximum fields are located at the air-silicon and at the
silicon-photonic crystal interfaces, and the amplitudes decay away from the interfaces. The components show less conventional guiding behavior: the S3 $E_z$ component is maximal just inside the photonic crystal (by about a quarter unit cell), and has a nodal plane parallel to the thin film. The P1 $E_z$ component has maxima on either side of the thin Si film, somewhat like the field pattern of a long-range surface plasmon polariton (LRSPP) on a thin metal film \[67\]. This field extends about $\Delta Z = 1$ unit cell into the crystal. These field distributions are the plausible signature of the confinement of a surface mode \[38, 68\]. Hence, the device can be viewed as a thin absorbing dielectric film on top of a photonic crystal, which thus acts as a surface defect on the crystal and sustains a guided surface state. Consequently, the remarkable peaks observed in Fig. 4 correspond to guided modes confined in a thin layer consisting of two separate contributions: (i) a non-zero thickness layer due to the Bragg attenuation length of the crystal’s band gap, and (ii) a deeply sub-wavelength thin Si film.

C. Wavelength-resolved transmission and absorption

To analyze the physics behind the results in Sections III A and III B, we break the problem down into several steps. Firstly, we briefly recapitulate the known situation of a thin silicon film only. Secondly, we study the thin film with a photonic crystal back reflector, where we only consider dispersion, but no absorption. This fictitious situation allows a comparison to the dispersion-free results that pertain to frequencies below the silicon band gap, see Ref. \[39\]. Thirdly, we study the complete device structure with the full silicon dispersion and absorption taken from Ref. \[48\].

\[1\] There is an important difference with a LRSPP, namely that here the field is maximal at the center of the thin film, whereas LRSPP fields are minimal at the center of a thin metal film.

FIG. 7. Transmission spectra calculated for a thin silicon film solar cell ($L_{Si} = 2400 $ nm) at normal incidence. Top panel: $s$–polarization, bottom panel: $p$–polarization. Black dashed curves are the transmission spectra for a thin film. Green solid curves are results for the thin film with a 3D inverse woodpile photonic crystal back reflector, with dispersion but no silicon absorption ($\text{Im}(n_{Si}) = 0$). Red dashed-dotted curves are results for the thin film with a 3D inverse woodpile photonic crystal back reflector, including silicon absorption ($\text{Im}(n_{Si}) \neq 0$). The vertical dashed lines are the edges of the $s$– and $p$–stop bands that are shown as yellow bars.
Figure 7 reveals oscillations between λ = 600 nm and λ = 1100 nm for both polarizations in the transmission spectra for the thin silicon film (L_{Si} = 2400 nm). These oscillations are Fabry-Péot fringes resulting from multiple reflections of the waves inside the film at the front and back surfaces of the thin silicon film.

In Fig. 7 we observe nearly 0% transmission between λ = 600 nm and λ = 900 nm for a thin film with a photonic crystal back reflector, both with and without silicon absorption. These deep transmission troughs are photonic stop bands between λ = 647 nm to 874 nm for p-polarization and λ = 634 nm to 892 nm for s-polarization. These gaps were previously identified to be the dominant stop gaps in the Γ − X and Γ − Z high-symmetry directions (see Appendix B) that encompass the 3D photonic band gap. From the good agreement of the stop bands, both with and without silicon absorption, we deduce that an inverse woodpile photonic crystal behaves as a perfect reflector in the visible range, even in presence of substantial absorption. This result further supports the observation above that the absorption length of silicon is much longer than the Bragg attenuation length of the 3D inverse woodpile photonic crystal. Hence, waves incident on the photonic crystal are reflected before being absorbed by the high-index backbone of the photonic crystal. Thus, the Fabry-Péot fringes in transmission between λ = 600 nm and λ = 860 nm are completely suppressed by strong and broadband reflection of the 3D photonic crystal back reflector [39].

FIG. 8. Absorption by a thin silicon film (L_{Si} = 2400 nm) in the stop band of a 3D inverse woodpile photonic crystal. Top panel: s-polarized, bottom panel: p-polarized light. Green solid curves are absorption spectra for a thin silicon film. Red dashed-dotted curves are absorption spectra for a thin silicon film with a 3D inverse woodpile photonic crystal. The vertical dashed lines are the edges of the s- and p-stop bands. The stop bandwidths are shown as the yellow bar.

Furthermore, oscillations below λ = 600 nm are present in the transmission spectra for the thin silicon film with a photonic crystal back reflector without absorption, but not in the system with absorption. Since the transmission spectra with realistic absorption show nearly 0% transmission below λ = 600 nm, where silicon is strongly absorbing, all light is absorbed and the Fabry-Péot fringes are suppressed.

Figure 8 shows the absorption spectra for a thin silicon film without and with a 3D photonic crystal back reflector. We consider the dispersive and complex refractive index for the silicon and the high-index backbone of the photonic crystal. Fabry-Péot fringes appear below λ = 900 nm, corresponding to standing waves in the thin silicon film. Since the imaginary part of the silicon refractive index increases with decreasing wavelength (see Fig. 15), the absorption in silicon also increases with decreasing wavelength.

Between λ = 600 nm and λ = 900 nm in the top and bottom panels of Fig. 8 there are more Fabry-Péot fringes.
The fringes have a greater amplitude for a thin silicon film with photonic crystal back reflector, compared to a standalone thin silicon film. To interpret the increased number of fringes, we consider diffraction from the photonic crystal surface. In the solar cell design in Fig. 1, light first travels through silicon before reaching the photonic crystal surface. Therefore, the incident wavelength reduces to $\lambda/n_{Si}$ inside the silicon layer. In the entire stop bands (both $s$ and $p$) the wavelength $\lambda/n_{Si}(\lambda)$ between $\lambda = 600$ nm and $\lambda = 900$ nm is smaller than the lattice parameter $c = 300$ nm of the 3D inverse woodpile photonic crystal (along the $\Gamma Z$ direction). In addition, a 3D inverse woodpile photonic crystal introduces a periodic refractive index contrast at the interface with a thin silicon film. Hence, nonzero diffraction modes [26, 58] are generated at the photonic crystal-thin silicon film interface at specific wavelengths inside the stop bands, resulting in additional reflected waves that are then absorbed in the film.

Between $\lambda = 600$ nm and 900 nm, the silicon thickness $L_{Si} = 2400$ nm is larger than half the wavelength $\lambda/n_{Si}$ in the absorbing layer. This is the condition for a photonic crystal-thin silicon film interface to couple the reflected waves into the guided modes [21, 53] that propagate inside the silicon. Hence, the physical mechanism responsible for the additional number of fringes is the occurrence of non-zero diffraction modes coupled into guided modes due to the photonic crystal back reflector. The absorption in guided modes can sometimes approach 100% [33], e.g., at $\lambda = 700$ nm and 720 nm in Fig. 8 (bottom). As a result, the perfect reflectivity of a 3D inverse woodpile photonic crystal extends over the entire stop bands, whereas nonzero order diffraction modes and guided modes are limited to specific wavelengths. This is in contrast to Section III.B where we studied a reduced thickness such that no guided modes are allowed.

D. Absence of absorption inside the photonic crystal backbone

Since we propose the back reflector to be a photonic crystal that is also made of silicon, one might rightfully hypothesize that the mere presence of extra material in the photonic crystal simply increases the total length of silicon, which thus sneakily enhances the absorption. To evaluate this hypothesis, we compute and compare the absorption for three different devices. We first study a thin silicon film of thickness $L_{Si} = 2400$ nm without back reflector, neither perfect metal nor photonic band gap (device #1). Secondly, we consider a silicon film ($L_{Si} = 2400$ nm) with a photonic crystal back reflector with a thickness $L_{Si} = 1200$ nm; this device #2 has a total thickness of 3600 nm. Thirdly, we study a structure with the same total thickness as the second one, namely a silicon layer with a thickness $L_{Si} = 3600$ nm, but without back reflector (device #3).

To investigate the effect of the band gap on the absorption in the thin film, we zoom in on the absorption spectra inside the stop bands in Fig. 9. We observe that the absorption spectra are closely the same for both thin films (devices #1 and #3), including the Fabry-Pérot fringes. Since film #3 is considerably thicker than #1, the similarity strongly suggests that the silicon absorption within the stop band wavelength range is saturated for the thinner layer.

In contrast, device #2 with a photonic crystal back reflector reveals significantly higher absorption, including a larger amplitude of the Fabry-Pérot fringes than the films #1 and #3. Since the total thickness of device #2 is the same as for film #3, we conclude that the enhanced absorption of the film with the photonic band gap back reflector is not caused by the additional thickness of the backreflector itself, hence the ‘sneaky’ effect does not exist. The conclusion that the backreflector does not contribute to the absorption is also reasonable, since we have seen above that the absorption of the light mostly occurs within the films themselves. Using Eq. 2, we find that the wavelength-averaged absorption enhancement due to a photonic crystal back reflector is nearly $\eta_{abs} = 1.8 \times$ for the $s$-stop band and nearly $\eta_{abs} = 1.9 \times$ for the $p$-stop band compared to a thin film with thickness $L_{Si} = 3600$ nm.

IV. PRACTICAL CONSIDERATIONS FOR DEVICES

A. Angular acceptance

In order to optimize the absorption of a thin silicon film for photovoltaic device applications, we first investigate the impact of a 3D photonic crystal back reflector on the angular acceptance. Figures 10(a, b) show transmission maps versus angle of incidence and wavelength. The angle of incidence is varied up to $\theta = 80^\circ$ off the normal. For both polarizations simultaneously we observe a broad angle-independent stop band that is characterized by near 0% transmission. The broad stop band extends all the way from $\lambda = 680$ nm to $\lambda = 880$ nm. This shows that the Bragg attenuation length for the 3D inverse woodpile photonic crystal is smaller than the absorption length of silicon for all incident angles for the omnidirectional stop band. Thus, a 3D photonic band gap crystal acts as a perfect reflector in the omnidirectional stop band for all incident angles and for all polarizations, even with full absorption in the refractive index - in other words, an omnidirectional stop band.
FIG. 9. Verification of the absence of absorption inside the photonic crystal backbone. Top panel: s-polarized, bottom panel: p-polarized light, with s− and p− stop bands shown as yellow highlighted regions. Red dashed-dotted curves pertain to a thin silicon film (thickness $L_{Si} = 2400$ nm) with a photonic crystal back reflector (thickness $L_{3DPC} = 1200$ nm). Blue dotted curves pertain to a thin film with the same overall thickness $L_{Si} = 3600$ nm, and the green solid curves pertain to a thin film only with the same silicon thickness $L_{Si} = 2400$ nm.

Figure 11 shows the absorption enhancement versus incident angle for five representative wavelengths throughout the band gap of a 3D inverse woodpile back reflector. For all incident angles up to $80^\circ$, we observe that the absorption enhancement stays above 1, which corresponds to a standalone thin film. Furthermore, at certain incident angles, the absorption enhancement is as high as 7 or 9. For both polarizations, Fig. 11 also reveals oscillatory absorption enhancement with increasing incident angles, which are signature of the Fabry-Pérot fringes [69]. Hence, a 3D inverse woodpile crystal widens the angular acceptance of a thin silicon film solar cell by creating an omnidirectional absorption enhancement regime.

To calculate the angle-averaged and wavelength-averaged absorption enhancement $\eta_{abs}$ in the omnidirectional stop band, we employ Eq. 2. Consequently, the angle- and wavelength-averaged absorption enhancement for s−polarization is $\eta_{abs} = 2.11$ and for p−polarization is $\eta_{abs} = 2.68$, which exceeds the maximum absorption enhancement feasible for a perfect reflector. These enhancements are possible only if a photonic crystal back reflector generates non-zeroth order diffraction modes at certain discrete wavelengths for all incident angles. Once these non-zero diffraction modes couple into guided modes and are confined inside the thin film via total internal reflection, the effective optical path length travelled is longer than the one travelled by a zero order diffraction mode. Therefore, a 3D inverse woodpile crystal enhances the absorption of a thin silicon film for all incident angles and polarizations by (i) revealing perfect reflectivity inside the omnidirectional stop band and (ii) generating guided modes for specific wavelengths.

B. Optimal thickness of the absorbing thin film

To investigate the effect of the thickness $L_{Si}$ of the thin silicon film on its absorption, we plot in Fig. 12 the absorption for light at normal incidence for film thicknesses between $L_{Si} = 300$ nm and $2400$ nm in presence of a 3D inverse woodpile photonic crystal back reflector with a constant thickness $L_{3DPC} = 1200$ nm. While the absorption
FIG. 10. Angle- and wavelength-resolved transmission spectra calculated for a thin silicon film \( (L_{Si} = 2400 \text{ nm}) \) with a 3D inverse woodpile photonic crystal back reflector for (a) \( s \)-polarization and (b) \( p \)-polarization. The dark blue color represents nearly 0% transmission that occurs in the stop band at all incident angles. The white dashed box indicates an angle- and polarization-independent range with nearly 0% transmission.

FIG. 11. Absorption enhancement versus incidence angle \( \theta \) off the surface normal to characterize the angular acceptance of a thin silicon film \( (L_{Si} = 2400 \text{ nm}) \) with a 3D inverse woodpile back reflector, for 5 wavelengths throughout the band gap (850 nm, 820 nm, 790 nm, 760 nm, and 730 nm) with connected symbols and colors as shown in the legend. The top panel is for \( s \)-polarized light, and the bottom panel for \( p \)-polarized light.

for a thin film shows a monotonic increase with increasing silicon thickness for both polarizations, Fig. 12 reveals that the absorption for a thin film with a photonic crystal back reflector is always higher than the corresponding standalone thin film. Furthermore, absorption spectra of a thin film with a photonic crystal back reflector reveals oscillations with increasing film thicknesses for both polarizations, showing saturation towards higher wavelength. We surmise that in order to maximize absorption enhancement for a given wavelength, the thickness of a thin silicon film had better be chosen to the maxima of the oscillations in Fig. 12. Therefore based on this normal incidence analysis,
FIG. 12. Absorption versus thickness $L_{Si}$ of a thin silicon film in presence (connected red circles) of a 3D photonic crystal back reflector, and without back reflector (green squares). The data pertain to a wavelength $\lambda = 760$ nm, the gap 3D photonic band gap center of the backreflector. Top panel: $s$–polarized, bottom panel: $p$–polarized light.

when designing a device the thickness of the silicon film had better be tweaked from $L_{Si} = 2400$ nm to one of the fringe maxima in Fig. 12 such as $L_{Si} = 1200$ nm or the range $1800 – 2100$ nm.

C. Various other experimental considerations

To enhance the absorption of light over an even broader wavelength range than reported here, it is relevant to consider different orientations of the 3D photonic crystal back reflector. In case of both direct and inverse woodpile structures, it is interesting to consider light incident in the $\Gamma Y$ direction, since the $\Gamma Y$ stop gap with a relative bandwidth 39.1 % (see Fig. 2 of Ref. [39]) is about 1.3× broader than the $\Gamma Z$ or $\Gamma X$ stop gaps whose relative bandwidth is 30.4 % [39, 50, 51, 57].

To improve the likelihood that photonic band gap back reflectors gain real traction, it is obviously relevant to consider strategies whereby such a back reflector can be realized over as large as possible (X,Y) areas. In the current nanofabrication of silicon inverse woodpiles, an important limitation is the depth of the nanopores that are fabricated by deep reactive-ion etching [41, 61], which limits the X or Z-extent of the nanostructures, whereas the Y-extent has no fundamental limit. Therefore, with the design shown in Fig. 2 the back reflector would have sufficient Z-extent (thickness) and a large Y-extent, but limited X-extent, and thus limited area. A remedy consists of etching the nanopores at 45° to the back surface, as demonstrated by Takahashi et al. [70]. Then, the areal (X,Y)-extent of the photonic crystal equals the areal extent of the pore array, which can be defined by standard optical lithography or by self-assembly. In such a design, light at normal incidence to the thin silicon film arrives at 45° with respect to the inverse woodpile structure, parallel to the $\Gamma U$ high-symmetry direction. The stop gap for this high-symmetry direction has properties that are fairly similar to the $\Gamma Z$ or $\Gamma X$ stop gaps considered here [39, 50, 51, 57]. Therefore the present analysis also pertains to this design.
Having a 3D silicon photonic crystal as a back reflector provides an all-silicon integration with the absorbing thin silicon film. Moreover, this approach makes the solar cell lighter, since the 3D inverse woodpile photonic crystal structure is highly porous, consisting of nearly 80% volume fraction air (see Appendix A). Simultaneously, our design remarkably enhances the overall absorption in comparison to a standalone thin silicon with the same overall thickness, as illustrated by our results.

If one wishes to shift the absorption enhancements discussed here to shorter wavelengths, it is relevant to consider replacing silicon by wider band gap semiconductors such as GaAs, GaP, or GaN. In such a case, an important practical consideration is whether to realize the photonic band gap back reflector from the same semiconductor for convenient integration, or whether to perform heterogeneous integration of silicon photonic band gap crystals, since the latter are readily realizable, see Refs. [41, 60–62].

Since GaAs has a similar real refractive index as silicon, many of the results presented here can be exploited to make predictions for GaAs absorption in presence of a photonic band gap back reflector. For the other semiconductors, this calls for additional detailed calculations, since most semiconductors have different (complex) refractive indices than silicon, with different dispersion. Nevertheless, the computational concepts and strategy presented in this study remain relevant to address the pertinent questions.

V. CONCLUSION

We investigated a thin 3D photonic band gap crystal as a back reflector in the visible regime, which reflects light within the band gap for all directions and for all polarizations. The absorption of a thin silicon film solar cell with a 3D inverse woodpile photonic crystal back reflector were calculated using finite-element computations of the 3D time-harmonic Maxwell equations. We tailored the finite-sized inverse woodpile crystal design to have a broad photonic band gap in the visible range and have used the refractive index of real silicon, including dispersion and absorption, in order to make our calculations relevant to experiments. From the comparison of the photonic crystal back reflector to a perfect metallic back reflector, we infer that a photonic crystal back reflector increases the number of Fabry-Pérot fringes for a thin silicon film, without changing the effective refractive index of silicon. Therefore, we observe that a 3D inverse woodpile photonic crystal enhances the absorption of a thin silicon film by (i) behaving as a perfect reflector, exhibiting nearly 100% reflectivity in the stop bands, as well as (ii) generating guided modes at many discrete wavelengths. Our absorption results show nearly 2.39× enhanced wavelength-, angle-, polarization-averaged absorption between $\lambda = 680$ nm and $\lambda = 880$ nm compared to a 2400 nm thin silicon film. We find that the absorption enhancement is enhanced by positioning an inverse woodpile back reflector at the back end of a thin silicon film, which will keep the length of the solar cell unchanged as well as make the thin silicon film solar cell lighter. In order to maximize the efficiency for a given wavelength, we show that the thickness of a thin film had better be chosen to the maxima of the Fabry-Pérot fringes. For a sub-wavelength thin 80 nm absorbing layer with a photonic crystal back reflector, we identify and demonstrate two physical mechanisms causing the giant average absorption enhancement of 9.15 times: (i) a guided modes due to the Bragg attenuation length and (ii) confinement due to a surface-defect.

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VIII. DISCLOSURES

The authors declare no conflicts of interest.

Appendix A: Primitive unit cell of the 3D inverse woodpile photonic crystal structure

For a cubic inverse woodpile with lattice parameters $c$ and $a$, Fig. 13 (i) shows the tetragonal primitive unit cell for reduced nanopore radii $\frac{r_1}{a} = 0.245$. This unit cell is periodic in all three directions $X, Y, Z$. If the air volume fraction is further increased by increasing the nanopore radii, Fig. 13 (ii) reveals remarkable crescent-like shapes appearing at the front and the back interfaces in the XY view of the unit cell, here for reduced pore radii $\frac{r_2}{a} = 0.275$. Once the pore radii exceed $\frac{r_2}{a} \geq 0.245$, the adjacent pores intersect with each other and hence these crescent-like shapes occur as they preserve the periodicity of the unit cell.
Figure 13 (bottom) shows the calculated volume fraction of air and silicon in the inverse woodpile crystal structure versus the reduced nanopore radius $\frac{r}{s}$ by employing a volume integration routine of the finite element method [52]. To preserve periodicity of the numerically approximated unit cell, we consider the primitive unit cell in (i) for a pore radius between $\frac{r}{s} = 0$ and $\frac{r}{s} = 0.245$ and the modified unit cell in (ii) for a pore radius between $\frac{r}{s} = 0.245$ and $\frac{r}{s} = 0.30$. Our numerical calculation agrees to great precision (within about $10^{-6}$%) with the analytical results for all pore radii. Since an inverse woodpile crystal consists of nearly 80% air by volume fraction at the optimal pore radius $\frac{r}{s} = 0.245$, it is a very lightweight component for photovoltaic applications, in comparison to bulk silicon with the same thickness.

Appendix B: Brillouin zone of the 3D inverse woodpile photonic crystal structure

Figure 14 shows the first Brillouin zone of the inverse-woodpile crystal structure in the representation with a tetragonal unit cell, with real space lattice parameters $(a, c, a)$, and reciprocal space lattice parameters $(2\pi/a, 2\pi/c, 2\pi/a)$. Eight high symmetry points are shown, where $\Gamma$ corresponds to coordinates $(0,0,0)$, $X$ to $(1/2,0,0)$, $Y$ to $(0,1/2,0)$, and $Z$ to $(0,0,1/2)$. The $X$ and $Z$ directions correspond to the directions parallel to the two sets of nanopores in the crystal structure, that turn out to be symmetry equivalent, see Refs. [39, 57].

Appendix C: Complex and dispersive refractive index of silicon

To make our study relevant to practical devices, we employ the dispersive and complex refractive index obtained from experiments to model silicon in all thin films and in the photonic crystal backbone. Figure 15 shows the wavelength dependency of the real and imaginary parts of the refractive index of silicon in the visible regime from several sources [48, 71, 72]. Vuye et al. report the dielectric function of a commercially available silicon wafer using in situ spectroscopic ellipsometry [71]. Jellison measured the dielectric function of crystalline silicon using two-channel polarization modulation ellipsometry [72], and Green gives a tabulation of the optical properties of intrinsic silicon based on many different sources, aiming at solar cell calculations [48]. Figure 15 shows that for the real part of the refractive indices of Refs. [71, 72, and 48] are in very good mutual agreement, and are thus used in our simulations. For the imaginary part of the refractive index, we note that the results of Ref. [72] and [48] agree well with each other between $\lambda = 500$ nm and $750$ nm and differ from the ones from Ref. [71] for reasons unknown to us. All data sets agree well beyond $\lambda = 750$ nm. Since Ref. [48] is based on many different sources of data, we have chosen to adopt it as the imaginary refractive index of silicon in our study.

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FIG. 15. Wavelength dependence of the real and imaginary parts of the refractive index of crystalline silicon (c-Si) in the visible and near infrared spectral ranges. Red circles, black triangles, and green squares are the data obtained from Ref. [48], Ref. [71], and Ref. [72], respectively. The top ordinate shows the frequency in wave numbers (cm$^{-1}$).

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