Improving Solar Cell Efficiencies With Photonic Crystals

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Abstract: The efficiency of thin-film crystalline or nanocrystalline silicon (c-Si or nc-Si) technology is currently limited by weak optical absorption in the near infrared. In this paper, a photonic crystal-based light-trapping scheme capable of compensating for this problem is proposed and analyzed. The simulations predict that for a 8 μm-thick slab of c-Si or nc-Si, absorption can be enhanced by more than a factor of five for optical wavelengths between 1040 and 1060 nm. Overall power generation is predicted to be enhanced by a relative amount of 13% for three layers of 2D photonic crystal, 14% for a 1D grating, and 20% for a 2D grating. Further improvements should be possible with refinement of the photonic crystal lattice design.

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References and links
1. Introduction

One of the foremost challenges in designing silicon photovoltaic cells is devising an efficient light-trapping scheme. Crystalline silicon (c-Si) and nanocrystalline silicon (nc-Si) have an indirect bandgap, which gives rise to weak absorption of light in the near infrared (near-IR), with an absorption length that increases from over 10 µm for λ = 800 nm to over 1 mm for λ = 1108 nm \[\text{1}\]. However, that range of wavelengths contains 36.2% of solar photons with energies above the bandgap of c-Si \[\text{2}\]. Thus, a c-Si solar cell with a plain wafer geometry less than 1 mm thick will fail to absorb a significant number of photons that could otherwise be used to generate power in the cell. At the same time, the expense of c-Si for a thick wafer with a correspondingly long diffusion length prevents such a design from being used in practical applications. As a result, efficient light trapping schemes that can achieve high levels of absorption for thin films of silicon are needed. In this paper, two distinctive approaches to light-trapping are discussed: geometrical and wave optics. The wave optics approach is implemented using photonic crystals \[\text{3}\].

The vast majority of light-trapping schemes used in solar cells today are based on geometrical optics. This approach is illustrated in Fig. [1] In the first part of the design, the path length is doubled by a back reflector. In the second part of the design, the average path length of the light is increased further via scattering at the front surface. Combining perfect random scattering with a lossless reflector in the back theoretically enhances the effective path length by a factor of \(4n^2\), corresponding to a value of about 50 for Si, and 30 for TiO\(_2\) \[\text{4}\]. There are two related ways to introduce this scattering: a Lambertian surface, or surface texturing. A Lambertian surface is designed to randomly scatter light into a uniform distribution of forward angles, known as a Lambertian distribution. However, no actual scattering surface is perfectly Lambertian in nature – the extent to which it replicates the ideal is typically called the “Lambertian fraction” \(\Lambda\), and is typically 55% or less \[\text{5}\]. An alternative approach is to introduce surface texturing at the front of the solar cell. If one patterns the front surface of c-Si with an inverted pyramid structure, for example by etching (100)-oriented c-Si wafers with KOH to form (111)-oriented pyramids, normally incident light will now be refracted into large angles inside the c-Si. Theoretically, in the best case of a random distribution of pyramids, the performance comes close to the ideal Lambertian scattering case \[\text{6}\]. However, it has been found that the fill factor (a measure of efficiency) is generally decreased by both Lambertian surfaces \[\text{7}\] and textured surfaces \[\text{8}\] – in the latter case, from 75% to 70%. This decrease is 6.7% in relative terms, which corresponds to the loss of a significant fraction of the gains associated with this light trapping technique.

The light-trapping approach illustrated in this paper uses wave optics, which has been shown to be capable, in principle, of outperforming all geometrical optics approaches for a certain range of wavelengths \[\text{9}\]\[\text{10}\]. This is because in contrast to geometric optics approaches that treat all wavelengths of light equally, wave optics approaches can be targeted to enhance ab-
Fig. 1. Illustration of two conventional solar cell designs: (a) a flat front surface with a bottom reflector, and (b) a textured front surface with a bottom reflector. Note that texturing increases the effective path length via refraction into an oblique angle.

Sorption only in the range where it can be most beneficial, e.g., the near-IR. The wave optics approach is implemented using a photonic crystal, which is defined as a low-loss periodic dielectric medium [3]. Photonic crystals are the best choice for a wave optics approach, because they offer complete control over the propagation of light. One of the key concepts associated with a photonic crystal is the so-called photonic band gap, a range of wavelengths which are reflected for any incident angle and polarization. Closely associated with the photonic band gap is the phenomenon of slow light. One can understand both phenomena by the following: in a periodic medium, waves must oscillate in a specific form, dictated by Bloch’s theorem. When the energy of the medium oscillates with the same period as the lattice, the waves can concentrate their energy in the low-energy region or in the high-energy region, which gives rise to two different energies for the same spatial period. The energies in between those two limits form the bandgap, a range of energies that cannot propagate in the bulk. As a result, photons with the forbidden energies that enter the photonic material are reflected. The reason why slow light also occurs in these systems is that the photonic bandgap induces an anti-crossing that flattens the photonic bands, giving rise to slow group velocities.

There are three ways in which photonic crystals can improve light-trapping efficiency. First, they can be designed to reflect a range of wavelengths with arbitrarily low losses for all incident angles and polarizations, e.g., an omnidirectional reflector [11]. Second, they can be designed to diffract incoming beams into highly oblique angles. This diffraction takes advantage of the increased density of states associated with a high-index medium. With the proper choice of periodicity, this effect can be targeted to the key near-IR region of the solar spectrum. Third, the photon density of states in the photonic crystal can be selectively enhanced in order to improve absorption efficiency [2]. These modes can be coupled to from outside the photonic crystal via superprism-type effects. Note that these approaches are especially advantageous for thin cells.
40 µm or less in thickness, which are not amendable to coarse texturing approaches that introduce features 5-10 µm in depth. The features discussed in this manuscript can work for even very thin cells of only a few microns. Thin cells offer the advantage of lower materials usage as well as lower bulk recombination losses and potentially higher open-circuit voltages [12].

To date, there has been some initial research considering wave optics approaches to light-trapping. Some groups have used gratings to enhance the effective path length via diffraction [13, 14, 15, 16]. Two groups considered using slow light in an inverse opal structure to enhance absorption for a dye-sensitized photovoltaic cell [20, 21]. More recent work has attempted to combine a distributed Bragg reflector (DBR) with a grating [22]. However, there is still need for further theoretical study which extends the problem to include photonic crystals more generally, and looks at both diffraction and superprism-type effects simultaneously.

2. Design

Two well-known designs, along with the proposed photonic crystal thin-film c-Si structure, are shown in Fig. 2.

Fig. 2. Illustration of solar cell designs involving a distributed Bragg reflector (DBR): (a) simple design, displaying only spectral reflection; (b) periodic grating etched into the DBR, displaying spectral reflection and diffraction; and (c) a photonic crystal consisting of a three-layer deep 2D square lattice of air holes, displaying spectral reflection, diffraction and transmission into the photonic crystal layer. Crystalline silicon is in green, low dielectric in yellow, and air is transparent.

First, consider something very similar to the conventional solar cell design, an anti-reflection coating covering a high index semiconductor layer of thickness $d$ with a distributed Bragg reflector (DBR) at the bottom, as shown in Fig. 2(a). In creating a design that reflects strongly in the near-IR, the materials are chosen to be c-Si ($n \approx 3.5$) and SiO$_2$ ($n = 1.5$) because they represent a low cost and readily available method of making an omnidirectional reflector [23]. Given the target wavelength range and materials, a period $a = 218.5$ nm is chosen. For the specific design used, consisting of five and a half bilayers of c-Si/SiO$_2$, 99% or greater reflection is observed at normal incidence for wavelengths from 767 to 1150 nm.

Now, the key to improving the absorption efficiency in a semiconductor layer lies in increasing the path length of light traversing it. Thus, two modifications of the baseline structure in Fig. 2(a) are also studied: a grating, and a photonic crystal. In Fig. 2(b), a grating similar to
the one studied in Ref. [22] is created by etching the top low-index SiO$_2$ layer of the DBR. It should be noted that the introduction of the grating into the omnidirectional reflector can, in principle, cause coupling into propagating modes in the reflector, thus eliminating perfect omnidirectional reflectivity. This issue is addressed through the numerical results, and found not to be a major problem overall. Following previous work (e.g., Refs. [14, 15, 16]), the periodicity of the grating is chosen such that first order diffraction will occur in the near-IR. The exact value is chosen to be 1.375$a = 300.4$ nm so that the first order diffraction threshold will occur at the wavelength $\lambda = 1068$ nm, just below the indirect c-Si electronic bandgap wavelength, $\lambda_{BG} = 1107$ nm. Alternatively, second order diffraction can be used [17]. In either case, the exact optimal periodicity will depend slightly on the thickness of the active region, and will be shifted to longer wavelengths for thicker cells (since they will already be absorbing shorter wavelengths well). Furthermore, there are a variety of other parameters to be considered, such as profile shape, incident angle and polarization, profile, duty cycle, and etch depth [24]. The rectangular (square-wave) profile is chosen because it is a simple structure that has been shown to perform better than a triangular pattern [18]. The incident angle is chosen to be either normal or oblique incidence, modeled by $k_\parallel = 0$ and $k_\parallel = 0.4(2\pi/a)$, respectively. The incident polarization is assumed to be transverse electric (TE) for simplicity, but the same approach can also be applied to transverse magnetic fields. The etching profile is chosen to be a symmetric square wave, for simplicity. The duty cycle $f$, i.e., the fraction of dielectric that is raised over each period, is chosen to be exactly one-half for the reason that the largest Fourier components (responsible for coupling to diffraction) will occur at that value. Finally, the etch depth is chosen to be 0.46$a = 100.5$ nm, by optimizing over all etching depths less than one period. Spectrally reflected modes are denoted by $r_0$ whereas diffracted modes are denoted by $r_1$, $r_2$, etc. In Fig. 2(c), a design utilizing photonic crystal is depicted, consisting of a three-layer-deep 2D square lattice of air holes, with an air-hole radius of $r = 0.55a$ and periodicity the same as in the grating. Aside from the diffracted modes, which are labeled in the same fashion as those in the grating, additional modes refracted into the photonic crystal are denoted by $t$. Experimentalists should note that results similar to those obtained for air holes in c-Si could also be obtained using silica or other materials for the holes.

In order to determine the light-trapping properties of these structures, a transfer matrix method known as the S-matrix method is utilized [25] (unless noted otherwise). The structure is broken up into slices with uniform symmetry in the z-direction, boundary conditions are imposed at one end, and fields are propagated throughout the structure. Light trapping is calculated by modeling the c-Si regions with a complex dielectric constant that depends on wavelength, as in Ref. [1]. The c-Si region is treated as if it were only intrinsic, i.e., the p— and n—doped regions are assumed to be optically transparent, which is a good approximation for the near-IR wavelengths of interest. Alternatively, one can consider the doping to have a negligible impact on the optical properties of the device. Aside from that issue, in principle, this calculation of the optical properties is exact apart from experimental errors and discretization errors, of which the latter can be reduced systematically by increasing the resolution of the structure. Verification was performed for several simulations using the finite-difference time domain method [26] with perfectly-matched boundary layers [27]. In general, the results were in good agreement, but the FDTD method was much slower for the same resolution, so it was not used for most calculations.

3. Results and Discussion

Now consider the role of diffraction induced by the periodicity of the photonic crystal inside the solar cell. The light-trapping as a function of frequency observed for a 9.15$a$-thick slab of c-Si backed by several different DBRs is shown in Fig. 3. One back-reflector is a plain DBR, one
with 1D etching with period $a_x = 1.375a$, and two with the 2D etchings $a_y = a_x$ and $a_y = 0.95a_x$
(predicted to be close to optimal: see Fig. 5).

Fig. 3. Absorption vs. frequency of a 9.15a-thick layer of c-Si, with several different DBRs on bottom: one which is plain, one with 1D etching with period $a_x = 1.375a$, and two with the 2D etchings $a_y = a_x$ and $a_y = 0.95a_x$. The last case is predicted to be close to optimal for enhancing light-trapping (see Fig. 5).
One can construct a simple analytical model to explain the diffractive light-trapping mechanism. If a bulk region of thickness $d$ is considered, then all resonances should pick up a round-trip phase change which is a multiple of $2\pi$, which gives us the condition $k_\perp = \pi m / d$, where $m$ is an integer, and the frequency of the diffracted mode is given by $\omega = (c/n)[G^2 + (\pi m / d)^2]^{1/2}$. If the only source of loss is the material, then the quality factor is given by $Q = n/2k$. Comparison between this simple analytical model for the mode spacings and quality factors with the results in Fig. 3 shows excellent agreement. Note that one could alternatively have used a second order diffraction grating instead, as in Ref. [17]. However, it was found that the performance of the second order gratings is similar to first order gratings for our choice of periodicity. This may be because for the parameters used, the material absorption was sufficient to cause most of the diffracted beams to be absorbed before being diffracted back into the zeroth order.

![Fig. 4. Illustration of the average enhancement created by a 1D grating with period 1.375a and etch depth 0.46a.](image)

The results for a c-Si wafer with thickness varying from 4 $\mu$m to 32 $\mu$m backed by a 1D grating with period 1.375a and etch depth 0.46a are shown in Fig. 4 (after smoothing over individual closely-spaced peaks as depicted in Fig. 3). In analyzing these results, it is observed that light trapping ability goes up with thickness, as expected, due to the greater number of modes supported by the bulk semiconductor region. However, the relative enhancement of light trapping is greater for thinner films, because they have lower baseline absorption. For a 4 $\mu$m-thick c-Si region, the greatest absorption enhancement of about a factor of 7 occurs over the range 1040 to 1060 nm. This result is consistent with the observation that the density of peaks is greatest near the diffraction limit, as illustrated in Fig. 3.

One can envision improving upon the 1D gratings above by incorporating a second, orthogonal periodicity that is also parallel to the surface of the solar cell, i.e., a 2D grating. However, an interesting but non-trivial question is how to choose the second period. Although one might naively set the second period equal to the first, this approach creates two strongly overlapping sets of diffraction modes, which means that if the light-trapping is already high in one direction,
the other direction may not contribute much. On the other hand, a second period which is too short will only improve light-trapping in a region which already has good light-trapping (e.g., green light). For silicon, therefore, the shorter period should at least roughly 73% of the longer period. The range of light-absorption considered is between $\omega = 0.2\left(\frac{2\pi c}{a}\right)$ and $0.25\left(\frac{2\pi c}{a}\right)$ (for $a = 218.5$ nm, this corresponds to a wavelength range $\lambda = 874$ nm to 1093 nm). This calculation was performed in Fig. 5. Although there is quite a bit of fluctuation, probably due to Fabry-Perot oscillations, a simple quadratic fit (the lowest-order polynomial satisfying the relevant constraints, discussed above) suggests that the optimum absorption for both thicknesses occurs when $a_y \approx 0.94a_x$ (where $a_x$ is assumed to be the longer period without loss of generality).

Now consider the enhancement of light-trapping for a photonic crystal. Clearly, the photonic crystal should be capable of diffraction, as observed for the previous case of a grating etched into the DBR. If the period and index contrast are similar, the same diffraction modes are predicted (and observed in simulations). Furthermore, note that the photonic crystal introduces two possibilities: either it can serve as a reflector, thereby replacing the DBR used earlier, or it can serve as a medium for enhancing the absorption of light. The mechanism is enhancing the density of states in the photonic crystal region for a specific set of target frequencies. In order to study this phenomenon, the eigenmodes of Maxwell’s equations with periodic boundary conditions, also known as a photonic bandstructure, were computed by preconditioned conjugate-gradient minimization of the block Rayleigh quotient in a planewave basis, using a freely available software package [28]. The bandstructure of the TE modes of the photonic crystal used in this problem is shown in Fig. 6. A flat band is observed around $\omega = 0.225$, which should translate into a higher density of states and therefore improved light-trapping in this region.

An absorption spectrum is calculated for three geometries: a source inside the c-Si with no
Fig. 6. Bandstructure for tranverse electric (TE) modes in a photonic crystal consisting of an infinite 2D square lattice of air holes in c-Si with period 1.375a and radius $r = 0.55a$.

photonic crystal, a source inside the c-Si with a photonic crystal consisting of a 2D lattice of air holes, and a source outside the c-Si with the same photonic crystal. Fig. 7 is for normal incidence, and Fig. 8 is for TE modes at oblique incidence. Note that a large enhancement is observed at the diffraction limit $\omega = 0.288(2\pi c/a)$, as would be expected for the results obtained with the grating geometry. Furthermore, some narrow peaks in the absorption are observed, which correspond to resonant photonic crystal modes (superprism-type effects) – for example, at normal incidence, one peak is observed around $\omega = 0.225(2\pi c/a)$ in Fig. 7, as predicted by the bandstructure in Fig. 6. More peaks are observed at oblique incidence around $\omega = 0.18(2\pi c/a)$, 0.245(2\pi c/a), and 0.255(2\pi c/a) in Fig. 8, which correspond to frequencies at which coupling takes place to photonic crystal modes, as can be seen from Fig. 6. The greater number of peaks observed at oblique incidence can be explained by the fact that coupling to certain modes is forbidden in directions of high symmetry, such as normal incidence.

Now consider the absorption as a function of wavelength observed for several different solar cell designs, all with an 8 µm-thick region of c-Si. The material parameters for silicon [1] are used to calculate realistic absorption values for the system as a function of wavelength, as shown in Fig. 9. It is clear that substantial absorption enhancement for the latter two designs takes place at near-IR wavelengths (800 - 1100 nm). Furthermore, an abrupt cutoff at $\lambda \approx 1050$ nm occurs at the diffraction limit of both designs, as expected. Taken together, these results suggest that both designs work mostly in the same fashion. Finally, in order to calculate power generation efficiency from our model, we assume that each absorbed photon with energy greater than the bandgap energy generates an electron-hole pair, and both carriers reach the electrical contacts. This corresponds to the statement that the diffusion length $L_D$ is much greater than the distance traveled by each carrier (i.e., $L_D \gg d$). Power generation efficiency is given by $\eta = J[V(\text{max})]/P_{\text{inc}} = (J_{\text{sc}}V_{\text{oc}})/P_{\text{inc}} \times FF$, where $P_{\text{inc}}$ is the solar irradiance, $V(\text{max})$ and $J[V(\text{max})]$ are the voltage and current density at the maximum power point, respectively,
the product of which equals the open-circuit voltage $V_{oc}$ times the short-circuit current density $J_{sc}$ times the fill factor $FF$. Following Refs. [29, 30], the above quantities can be calculated as follows: first, the current density $J$ as a function of the voltage $V$ is given by the sum of the photon-induced current minus the intrinsic current generated by radiative recombination, i.e.

$$J(V) = \int_0^\infty d\lambda \left[ \frac{e\lambda}{hc} \frac{dI}{d\lambda} A(\lambda) \right] - \frac{e(n^2 + 1)E_g^2kT}{4\pi^2\hbar^2c^2} \exp \left( \frac{eV - E_g}{kT} \right),$$

(1)

where $\frac{dI}{d\lambda}$ represents the light intensity experienced by the solar cell per unit wavelength (given by the ASTM AM1.5 solar spectrum [2]), $A(\lambda)$ is the absorption calculated from above, $E_g$ is the bandgap energy, $kT$ is the thermal energy at the operating temperature $T$, and $n$ is the average refractive index of the semiconductor. Next, the open circuit voltage is calculated by setting $J = 0$. Finally, the fill factor is found by setting the derivative $d(JV)/dV = 0$ and solving for $V(\text{max})$ and $J[V(\text{max})]$. This method for calculating $\eta$ can be applied to the absorption spectra of Fig. 9 and yields a relative increase in power generation efficiency of 13% for three layers of 2D photonic crystal, 14% for a 1D grating, and 20% for a 2D grating.

4. Conclusions

In conclusion, two light-trapping schemes in silicon have been studied: geometrical and wave optics. It is found that in principle, wave optics can vastly outperform geometrical optics for a certain range of wavelengths. Fortunately, only a relatively small range of wavelengths, from 800 nm - 1100 nm, requires enhancement in thin films of c-Si. The contribution of diffraction and the DBR have been fully characterized, but more work is needed on coupling to guided modes of the photonic crystal. Also, it may be possible to combine the photonic-crystal based light-trapping approach with geometrical optics-based approaches in order to achieve even higher efficiencies. These may be appropriate subjects for future work.
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Fig. 9. Illustration of the absorption at normal incidence of an 8µm-thick Si cell with a flat distributed Bragg reflector, plus etching in one direction (1D), and a three-bilayer photonic crystal of air holes with a metal reflector. Note that the absorption has been averaged over a range of approximately 10 nm, which suppresses narrow peaks of the type seen in Fig. 3.