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Modeling of light trapping in thin crystalline Si solar cells using surface Mie scatterers

We systematically study with numerical simulations the absorption of light into thin (1-100 µm) crystalline Si solar cells patterned with Si nanocylinder arrays on top of the cell. We then use an analytical model to calculate the solar cell efficiency, based on the simulated absorption spectra. Using realistic values for bulk and surface recombination rates we find that a 20-µm-thick Si solar cell with 21.5% efficiency can be made, by using the Si nanocylinder Mie coating.

7.1 Introduction

Crystalline Si (c-Si) is currently the most widely used semiconductor for photovoltaic applications. Despite continued technological developments that bring down the production costs of c-Si solar cells, the intrinsic Si material costs in these cells still remains high. For this reason, making thinner c-Si solar cells in order to use less of this expensive material continues to be a main driving force for the photovoltaic research community. Recent technological advances have lead to the fabrication of thin-film c-Si solar cells on glass substrates by laser crystallization [133], liquid phase crystallization [134], and layer transfer [135][136]. However, thinner c-Si solar cells do not fully absorb the incoming light, especially in the near-bandgap spectral range where the absorption length of Si exceeds the
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Thickness of the cell. Light trapping is thus needed in order to achieve complete absorption of light in the cell.

Standard c-Si solar cells usually have a thickness of around 180 µm. At the front side they are covered with a pyramidal light trapping texture coated with a 80-nm-thick Si₃N₄ anti-reflection layer [2]. The typical feature size of the texturing is in the range 5-10 µm [115]. Therefore, it is impossible to apply this light trapping texture to thinner cells with thicknesses in the micron range. Recently, metal and dielectric nanostructures have been considered as light-trapping coatings for ultrathin solar cells [40, 51, 53–55, 85, 98]. We have shown that an array of dielectric nanoparticles placed on top of a Si wafer acts as an efficient anti-reflection coating [137]. This is due to the preferential scattering of light towards the high index substrate from leaky Mie resonances that are excited in the nanoparticles [83, 138]. In particular, we have shown that an optimized array of Si nanocylinders (NCs) yields broadband and omnidirectional ultra-low reflectivity, reducing the reflection of a Si wafer to an average value as small as 1.3% [137].

In this Chapter, we investigate the potential of these Mie resonator coatings for light-trapping in thin (1-100 µm) Si solar cells. Using numerical methods, we systematically study light absorption into thin Si slabs patterned with dielectric nanoparticle arrays with different geometries on top of the slab. We use Finite Difference Time Domain (FDTD) simulations (employing periodic boundary conditions) to calculate light absorption of the c-Si slabs and compare it to that of a flat Si slab with a standard Si₃N₄ antireflection coating. An analytical model is then used to calculate, based on the simulated absorption spectra, the photocurrent, open circuit voltage and efficiency of a c-Si solar cell with a Mie scattering surface coating and a metallic backcontact. The model includes Shockley-Read-Hall bulk carrier recombination, surface recombination, as well as radiative and Auger recombination. Using realistic values for the recombination rates and a perfectly reflecting back contact we find that an efficiency as high as 21.5% can be achieved for a 20-µm-thick cell with a Si NC Mie coating. This is a significant improvement compared to the efficiency that we find for a planar c-Si cell with a standard Si₃N₄ anti-reflection coating of the same thickness (17.5%). We also investigate the effect of an absorbing Ag back contact on the efficiency.

7.2 Simulation results

We use FDTD simulations [90] to calculate the absorption of light in thin Si slabs covered with square arrays of Si NC Mie scatterers, for wavelengths in the range 300-1150 nm. The Si NC coating is comprised of 250 nm wide, 150 nm high Si cylinders in an array with 450 nm pitch, conformally coated with a 50-nm-thick Si₃N₄ layer. These parameters are optimized for minimizing the reflection of a bulk Si wafer with a Si NC coating [137]. A perfect reflector is applied at the back of the Si slab and periodic boundary conditions are used. The absorption in both the Si slab and the Si NCs is calculated, as well as the reflection. Figure 7.1 shows the absorption per
7.2 Simulation results

Figure 7.1: Numerically calculated absorption per unit volume (color scale) in a vertical cross section of a 5-µm-thick Si slab coated with the Si NC Mie coating. Each panel represents a different wavelength and shows 3 horizontal unit cells. The absorption of light takes place according to complicated patterns determined by interference of the light scattered by the NCs.

Figure 7.1 shows the combined absorption in Si slab and Si NCs as a function of wavelength for the patterned slab (red), compared to that for a flat Si slab with a standard 80 nm Si₃N₄ coating (blue). Data are shown for 5-µm-thick (a) and 20-µm-thick (b) Si slabs. The graphs show that absorption is enhanced over the entire...
300-1100 nm spectral range by the presence of the Mie nano-scatterers on the front surface. This can be explained by two main mechanisms. First, the Mie scatterers provide an antireflection effect, due to the preferential forward scattering towards the Si slab, as we demonstrated earlier for thick Si wafers [137]. This effect improves the absorption over a broad spectral range from the ultraviolet to the near-infrared. Second, the array of Mie scatterers couples the incoming light to waveguide modes in the thin Si slab. This effect is responsible for the absorption enhancement in the near-infrared spectral range. The main sharp peaks at 910, 960 and 1100 nm for the 5-µm-thick slab with the Mie coating (red, see also absorption profiles in Fig. 7.1) are ascribed to coupling to Fabry-Perot and waveguide modes by the Mie resonances in the Si NC [139]. These main peaks are not observed for the flat reference. The smaller oscillations in the absorption spectrum of both the Mie-coated sample and the flat slab (blue) are due to Fabry-Perot interferences in the Si/Si₃N₄ layer stack. For the 20-µm-thick slab a broad enhancement is observed above λ=900 nm, on top of the Fabry-Perot resonances, which we ascribe to coupling to a broad continuum of waveguide modes; for this large thickness individual waveguide-coupling peaks cannot be spectrally separated due to the high density of modes in the waveguide.

![Absorption spectra](image)

**Figure 7.2:** Simulated absorption spectra for a 5-µm-thick (a) and a 20-µm-thick (b) Si slab with (red) and without (blue) a surface coating of Si nanocylinders. Absorption in the particles and in the Si slab are both taken into account. The flat and patterned geometries are coated with 80 nm and 50 nm thick Si₃N₄ coatings, respectively. The absorption of the slab with the Mie coating is larger than that of a standard coating over the entire spectral range. This is due to an improved antireflection effect and to light coupling to waveguide modes of the thin slab.

### 7.3 Solar cell modeling

The absorption data shown in Fig. 7.2 can be used to calculate the total photocurrent generated in the thin Si cell. First, a uniform photocarrier generation rate is assumed throughout the thickness of the Si slab. In practice, this means that the absorption profiles shown in Fig. 7.1 are averaged out over the volume of the slab.
This is a valid assumption for crystalline Si, for which the carrier diffusion length is larger than the thickness of the solar cell considered in this work. The generation rate $G$ per unit volume can be calculated by:

$$G = \frac{1}{t} \int_{\lambda_1}^{\lambda_2} \frac{\lambda}{hc} I(\lambda) A(\lambda) d\lambda$$  \hspace{1cm} (7.1)

where $t$ is the Si slab thickness, $I(\lambda)$ is the AM1.5 solar power spectrum, $A(\lambda)$ is the simulated absorption spectrum, $h$ is Planck’s constant and $c$ the speed of light. Assuming the slab is made of n-type Si, the generation rate $G$ is then used in the diffusion equation for holes in the quasi-neutral region \[2\]:

$$D_h \frac{d^2 \Delta p}{dx^2} = \frac{\Delta p}{\tau_b} - G$$  \hspace{1cm} (7.2)

where $D_h$ is the minority carrier diffusion constant, $\Delta p$ is the excess hole concentration, $\tau_b$ is the bulk lifetime for holes and $x$ the position across the thickness of the cell. Equation 7.2 can be solved assuming the boundary conditions:

$$\Delta p |_{x=0} = \frac{n_i^2}{N_D} \left( e^{qV/kT} - 1 \right)$$  \hspace{1cm} (7.3)

and

$$\frac{d \Delta p}{dx} |_{x=t} = - \frac{S}{D_h} \Delta p(t)$$  \hspace{1cm} (7.4)

where $N_D$ is the doping level, $V$ the voltage across the cell, $n_i$ is the intrinsic carrier concentration, and $S$ the back surface recombination rate. An infinitely thin p-n junction is assumed at the front surface ($x=0$). Realistic devices that come close to this approximation are, e.g., heterojunction a-Si/c-Si solar cells, where the a-Si emitter is only a few nanometers thick \[140\]. Solving equation 7.2 for $\Delta p$ and calculating the current density as $J = -qD_h \frac{d\Delta p}{dx}$ yields the solution for $J(V)$ below:

$$J = j_0 \left( e^{qV/kT} - 1 \right) - qLG \left( \frac{L}{L_{j0}} - \frac{LS}{F} \right)$$  \hspace{1cm} (7.5)

with:

$$L = \sqrt{\tau_b D_h}$$

$$L_{j0} = L \frac{D_h \cosh(x) + SL \sinh(x)}{SL \cosh(x) + D_h \sinh(x)}$$

$$j_0 = \frac{qD_h n_i^2}{L_{j0} N_D}$$

$$F = D_h \cosh(x) + SL \sinh(x)$$

which is in agreement with Ref. \[141\], for the case of uniform carrier generation rate. Equation 7.5 represents the J-V characteristic of the solar cell based on the
assumptions above. The short-circuit current density $J_{SC}$, the open-circuit voltage $V_{OC}$, the fill factor and efficiency $\eta$ are easily calculated from this relation. The free parameters in the model are the bulk lifetime $\tau_b$, the surface recombination velocity $S$ and doping level $N_D$. The bulk lifetime $\tau_b$ can be written as:

$$\frac{1}{\tau_b} = \frac{1}{\tau_{SRH}} + \frac{1}{\tau_{Auger}} + \frac{1}{\tau_{rad}}$$  \hspace{1cm} (7.6)

where $\tau_{SRH}$ lifetime representing Shockley-Read-Hall bulk recombination, $\tau_{Auger}$ is the lifetime representing Auger recombination and $\tau_{rad}$ is the radiative recombination lifetime. For n-type Si, a semi-empirical expression for equation 7.6 is [142]:

$$\frac{1}{\tau_b} = \frac{1}{\tau_{SRH}} + \left( N_D + \Delta n \right) \left( 1.8 \times 10^{-24} N_D + 3 \times 10^{-27} \Delta n + 9.5 \times 10^{-15} \right)$$  \hspace{1cm} (7.7)

where $N_D$ is expressed in units of cm$^{-3}$, and $\Delta n$ is the injected carrier concentration in units of cm$^{-3}$, which is directly related to the open circuit voltage $V_{OC}$, as shown in Ref. [143]. The set of equations 7.5-7.7 can be solved recursively. In the following, we assume a fixed $N_D = 10^{16}$ cm$^{-3}$, and $\tau_{SRH}$ and $S$ are varied.

Figure 7.3 shows calculations of $J_{SC}$ (panels a, d, g), $V_{OC}$ (b, e, h) and efficiency (c, f, i) as a function of Si slab thickness. The top row assumes $\tau_{SRH} = 1$ ms and $S = 10$ cm/s (good bulk material quality and surface passivation), the middle row $\tau_{SRH} = 1$ ms and $S = 100$ cm/s (good material quality and poor surface passivation) and the bottom row $\tau_{SRH} = 0.1$ ms and $S = 10$ cm/s (poor material quality and good surface passivation). Each panel shows data for a Si slab with a standard 80 nm Si$_3$N$_4$ coating (blue) and for a Si slab with a Mie coating (red, same Si NC geometry as in Fig. 7.2). The latter is calculated considering absorption spectra that include both the absorption in the Si slab and absorption in the Si NCs at the surface. For reference, Fig. 7.3 also shows data for a Si slab with perfect anti-reflection coating and a perfect Lambertian light trapping surface where the (geometrical) path length enhancement at long wavelengths equals $4n^2$, with $n$ the refractive index of Si (black dashed lines) [42, 116].

Figure 7.3(a) shows that the photocurrent is strongly enhanced for all thicknesses due to the surface Mie scatterers. The photocurrent enhancement is more significant for thicknesses below 20 $\mu$m where the Mie scatterers provide both an antireflection effect and strong light trapping due to coupling to waveguide modes in the thin Si slab. For a 1-$\mu$m-thick cell the photocurrent is enhanced by as much as 75% due to the Si Mie coating, for a large part due to light trapping. For a 20-$\mu$m-thick cell, a photocurrent enhancement of 20% is observed. For thicknesses above 20 $\mu$m, the photocurrent enhancement converges to the same value for all cell thickness, as the light trapping effect becomes less relevant with respect to the anti-reflection effect. The dash-dotted lines in Fig. 7.3(a) represent the photocurrents achieved in the case of an infinitely long carrier diffusion length (i.e., when all the photogenerated carriers are extracted from the cell). As can be noticed, these photocurrents diverge from the actual photocurrents (solid lines) only for cell thicknesses above 50 $\mu$m, i.e. for thicknesses comparable with the minority
carrier diffusion length. The graph of Fig. 7.3(a) also shows that the photocurrents achieved with a Mie coating are roughly halfway between those achieved with a standard flat coating, and those achieved in the $4n^2$ light trapping limit. Similar results are observed in case of high surface recombination velocity $S$ (Fig. 7.3(d)) and short bulk lifetime (Fig. 7.3(g)). In both these cases, the photocurrent for cells thicker than 20 $\mu$m is reduced compared to the case in Fig. 7.3(a), due to reduced carrier collection for large cell thickness. Figures 7.3(b,e,h) show that for cells with Mie coating $V_{OC}$ is always higher than for a flat cell with a standard Si$_3$N$_4$ coating. This is a direct consequence of the higher photocurrent for the Mie-coated cell, as seen in Figs. 7.3(a,d,g). For the Mie-coated cell with low surface and bulk recombination rates (Fig. 7.3(b)) $V_{OC}$ increases for decreasing cell thickness. This is due to the reduced effect of bulk recombination as the cell thickness. For larger surface recombination velocities (Fig. 7.3(e)), $V_{OC}$ decreases with decreasing thickness, as surface recombination then dominates over bulk recombination. In this case an optimum $V_{OC}$ is found for a thickness of 10 $\mu$m for the cell with Mie coating, and 20 $\mu$m for the cell with standard Si$_3$N$_4$ coating. For cells with strong bulk recombination (Fig. 7.3(h)), a lower $V_{OC}$ is observed for all thicknesses. However, in this case the effect is stronger for thicker cells, where the bulk material quality plays a more
important role due to the larger bulk volume.

Finally, Figs. 7.3(c,f,i) show a strong efficiency enhancement for Mie-coated cells. This is a direct consequence of the photocurrent enhancement due to the antireflection and light trapping effects provided by the Mie scatterers and the enhanced voltage. In particular, for a 20-µm-thick cell with low bulk and surface recombination rates an efficiency as high as 21.5% can be achieved, compared to an efficiency of 17.5% for a flat cell. For reference, a cell operating in the 4n^2 light trapping limit would yield an efficiency of 25.3%. The importance of the result for the Mie light-trapping coating relies in the fact that standard random textures commonly used for wafer-based c-Si solar cells cannot be applied to 20-µm-thick cells, as the feature size is comparable to the thickness of the cell. Interestingly, the graph shows that a 5-µm-thick cell with Mie scatterers yields the same efficiency as a flat 100-µm-thick cell with standard Si_3N_4 coating. The Mie scatterers thus allow reducing the cell thickness by a factor of 20, maintaining the same power conversion efficiency. Similar results are observed for high surface recombination velocities S (Fig. 7.3(f)) and bulk lifetimes (Fig. 7.3(i)). In both cases, lower efficiencies are observed than for the cells with lower recombination rates, due to the lower photocurrents and voltages.

To further investigate the crucial role of the Shockley-Read-Hall lifetime \( \tau_{SRH} \) and of the surface recombination velocities S, Fig. 7.4 shows the calculated solar cell efficiency (color lines) as a function of \( \tau_{SRH} \) (vertical axis) and S (horizontal axis), for a 5-µm-thick cell (a) and a 20-µm-thick cell (b) with a Si NC Mie coating. For a 5-µm-thick cell (a), efficiencies range from 19.5% for \( \tau_{SRH} = 1 \) ms and S = 1 cm/s, down to 15% for \( \tau_{SRH} = 1 \mu s \) and S = 1000 cm/s. Similarly, for a 20-µm-thick cell (a), efficiencies range from 21.5% to 14%. A comparison of the two graphs shows that a 20-µm-thick cell is more sensitive to variations of \( \tau_{SRH} \) than a 5-µm-thick cell, due to the larger volume. Similarly, a 5-µm-thick cell is more sensitive to

![Figure 7.4: Efficiency (colors) as a function of the Shockley-Read-Hall lifetime \( \tau_{SRH} \) (vertical axis) and the surface recombination velocity S, for a 5-µm-thick cell (a) and a 20-µm-thick cell (b) with Mie coating. The efficiency of a 5-µm-thick cell is more sensitive to variations in S, whereas the 20-µm-thick cell is more sensitive to variations in \( \tau_{SRH} \). For thin cells, efficiencies range from 19.5% to 15%; for the thick cell from 21.5% to 14%.](image-url)
7.4 Light trapping with TiO$_2$ Mie scatterers

variations of $S$ than a 20-$\mu$m-thick cell, due to the larger surface-to-volume ratio.

In the analysis conducted so far, a perfect back reflector was considered. Simulations were also used for Si slabs with a back reflector with 97% reflectivity. Figure 7.5 shows the calculated efficiency as a function of thickness, for a Si slab with perfect back reflector (solid), and with a back reflector with 97% reflectivity (dashed). Data are shown for a Si slab with flat Si$_3$N$_4$ coating (blue lines) and for a Si slab with Mie coating (red). Similarly to Fig. 7.3(c), we assume $\tau_{SRH} = 1$ ms and $S = 10$ cm/s. The graph shows a drop in efficiency of about 0.5% (absolute) for a 20-$\mu$m-thick cell with Mie coating, when a realistic back contact is used instead of an ideal back reflector; the efficiency of the 20-$\mu$m-thick Mie-coated cell then drops to 21%. Similar losses are observed for cells with a standard Si$_3$N$_4$ coating.

20-$\mu$m-thick cell with Mie coating, when a realistic back contact is used instead of an ideal back reflector; the efficiency of the 20-$\mu$m-thick Mie-coated cell then drops to 21%. Similar losses are observed for cells with a standard Si$_3$N$_4$ coating.

**7.4 Light trapping with TiO$_2$ Mie scatterers**

The analysis conducted so far shows that Si NC Mie scatterers serve as excellent light trapping coatings for thin c-Si solar cells. From an optical point of view, Si is the best material for the Mie coating, as its refractive index is large ($n \sim 3.5$) and matched to that of the Si substrate. Furthermore, Si Mie coatings can be easily integrated on top of a c-Si wafer by reactive ion etching, as shown in Chapters 2 and 6. However, a Si Mie coating increases the surface area of the cell and may be difficult to passivate, causing enhanced recombination of electrical carriers. As will be shown in Chapter 9, an interesting alternative to the Si-based Mie coating is a TiO$_2$-based Mie coating [45]. In fact, TiO$_2$ has a relatively high index ($n \sim 2.2$-$2.5$) and low absorption. The antireflection and surface passivation properties of the TiO$_2$ Mie coating are studied in detail in Chapter 9. Here, we present the same
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analysis done in the present Chapter for a Si NC array, for an array of TiO$_2$ Mie scatterers. As before, we assume $\tau_{SRH} = 1$ ms and $S = 10$ cm/s.

Figure 7.6: Efficiency of a Si slab with a standard 80 nm Si$_3$N$_4$ coating (blue), with a Si Mie coating (red) and with a TiO$_2$ Mie coating (green), as a function of the slab thickness.

Figure 7.6 shows the calculated efficiency as a function of thickness for a Si slab with a standard 80 nm Si$_3$N$_4$ coating (blue), with a Si Mie coating (red) and with a TiO$_2$ Mie coating (green). The efficiency of the Si slab with the Si Mie coating was calculated considering absorption spectra that include both the absorption in the Si slab and absorption in the Si NCs at the surface. The efficiency of the Si slab with the TiO$_2$ Mie coating was calculated taking into account absorption in the Si slab. As can be seen, the TiO$_2$ Mie coating yields a higher efficiency than the flat Si$_3$N$_4$ coating, but lower than the Si Mie coating. This is due to two main reasons: parasitic absorption in the TiO$_2$ NCs (see Chapter [9]) and less efficient scattering through Mie resonances due to the lower index of TiO$_2$ with respect to Si. The TiO$_2$ Mie coating allows designing 20-µm-thick Si solar cells with 19.8% efficiency, compared with 21.5% for a Si Mie coating. Despite the lower performance, a TiO$_2$ Mie coating has the advantage that it can be easily integrated with a thin passivation layer, yielding very low surface recombination velocity, as will be shown in Chapter [9].

7.5 Light trapping with random and periodic arrays of Mie scatterers

Finally, we compare the light trapping properties of random and periodic arrays of Si Mie scatterers. In Chapter 6 we have shown that random and periodic Si NC arrays on a thick Si wafer yield similar antireflection properties. This is due to the fact that for a thick substrate, the individual scattering of single Si NCs dominates over the collective scattering of the grating. For thinner cells however, the scattering...
from grating orders of the NC array is important for coupling to waveguide modes of the thin slab [65][139][144]. Usually, only a limited number of modes in the slab can be populated by scattering from grating orders, i.e. those modes whose parallel momentum matches the spatial frequencies of the grating [145]. By randomizing the NC array, we broaden the spectral spatial frequencies of the array, and thus we can couple to a larger number of modes in the slab.

Figure 7.7 shows the simulated absorption spectra for a 5-µm-thick Si slab coated with a flat Si$_3$N$_4$ coating (black), with a periodic array of Si Mie scatterers (blue) and with a random array of Si Mie scatterers (red). Both periodic and random configurations yield larger absorption for the entire spectral range 300-1050 nm than for a flat cell. The curves for the periodic and random arrays overlap for wavelengths shorter than 700 nm. In this spectral range, the absorption is enhanced mostly due to an antireflection effect (see Chapter 6). However, in the near-infrared spectral range, the periodic and random arrays show different behavior. The periodic array shows sharp peaks, which are ascribed to coupling to waveguide modes in the thin slab, as discussed above. The random array shows a broadband enhancement over the entire near-infrared spectrum. We attribute this to the fact that the random array couples light to a larger number of modes in the slab, due to its broader spectrum of spatial frequencies. Further studies are needed to obtain deeper understanding of the coupling of resonant Mie modes to waveguide modes. Overall, the AM1.5-weighed average absorption of the random array is 77% compared to 72% of the periodic array. In both cases, a significant absorption enhancement is observed with respect to the case of a flat Si$_3$N$_4$ coating (66%).


7.6 Conclusion

Using numerical simulations, we have shown that strongly reduced reflection and enhanced light trapping can be achieved in thin (1-100 µm) c-Si solar cells covered at the front surface with an array of Mie scattering Si nanocylinders, and coated with a Si$_3$N$_4$ anti-reflection layer. For thin Si slabs near-infrared light trapping due to preferential scattering of light by the Mie scatterers into guided modes of the Si slab is directly observed from spectral peaks in the photocurrent. A strong increase in photocurrent is observed due to the Mie scatterers for all thicknesses in the range 1-100 µm. For thin cells, a strong increase in open circuit voltage is observed. For cells with low bulk and surface recombination ($\tau_{SRH} = 1$ ms and $S = 10$ cm/s) a cell efficiency of 21.5% can be achieved for a 20-µm-thick Mie coated cell, compared to 17.5% for a flat cell. Silicon Mie scatterers are thus good candidates to substitute standard light trapping techniques, such as pyramidal textures, that cannot be applied on thin solar cells. Our study opens new perspectives for designing high-efficiency thin-film c-Si solar cells.