Silicon nanodisk array design for effective light trapping in ultrathin c-Si

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Abstract: The use of ultrathin c-Si (crystalline silicon) wafers thinner than 20 μm for solar cells is a very promising approach to realize dramatic reduction in cell cost. However, the ultrathin c-Si requires highly effective light trapping to compensate optical absorption reduction. Conventional texturing in micron scale is hardly applicable to the ultrathin c-Si wafers; thus, nano scale texturing is demanded. In general, nanotexturing is inevitably accompanied by surface area enlargements, which must be minimized in order to suppress surface recombination of minority carriers. In this study, we demonstrate using optical simulations that periodic c-Si nanodisk arrays of short heights less than 200 nm and optimal periods are very useful in terms of light trapping in the ultrathin c-Si wafers while low surface area enlargements are maintained. Double side texturing with the nanodisk arrays leads to over 90% of the Lambertian absorption limit while the surface area enlargement is kept below 1.5.

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References and links

1. Introduction

Crystalline silicon (c-Si) is one of the most popular materials in commercialized solar cells. c-Si has inherently a high reflectance in a wide spectral range and a low absorption coefficient especially near bandgap because it has high refractive index (n ~ 3.5) and its electronic transition is indirect [1]. In this regard, practically suppressing surface reflectance and enhancing light trapping are required for solar cell applications. The surface texturing of c-Si surface with a shape of pyramids in micron scale and antireflection coating with dielectric materials such as SiO₂, Si₃N₄, and ZnS are a general scheme for effective light management. Periodic or random c-Si cones, rods and holes in nano scale have been suggested and demonstrated for ultrathin c-Si wafers; thus, nano scale texturing must be introduced. A variety of shape design for nano scale texturing have been suggested and demonstrated for effective light trapping in c-Si. Periodic or random c-Si cones, rods and holes in nano scale have been suggested and demonstrated numerically and experimentally for ultrathin c-Si wafers [2–6]. The use of ultrathin c-Si wafers is a straightforward method to reduce the cell cost by lowering material consumption [7]. However, the thinner c-Si wafers leads to reductions in optical absorption, which needs to be compensated by effective light trapping [8]. The conventional pyramidal texturing in micron scale, however, is not applicable to the ultrathin c-Si wafers; thus, nano scale texturing must be introduced. A variety of shape design for nano scale texturing have been suggested and demonstrated for effective light trapping in c-Si. Periodic or random c-Si cones, rods and holes in nano scale have been suggested and demonstrated numerically and experimentally for ultrathin c-Si wafers to achieve the 4n² classical absorption limit [9–14]. Quasi-random nanostructures, which are combinations of long range periodicity and short range randomness was reported to be very effective for light trapping in the ultrathin c-Si wafers, and the optimized quasi-random nanostructures were shown to capture 98% of the classical absorption limit in 1 μm c-Si wafers [15]. Recently, the classical absorption limit in c-Si wafers thinner than 35 μm was demonstrated by the use of nanocones at the front side combined with random pyramids at the
back side coated with a dielectric back reflector [16]. High aspect ratios of those nanostructures on c-Si wafers are effective for reducing the reflectance from the c-Si wafers because the effective index from the surrounding medium to c-Si wafers changes gradually [17]. However, the nano texturing in this manner inevitably leads to significant surface area enlargements. Although the enlarged surface of c-Si can be passivated in well-controlled processes with SiO\textsubscript{2}, SiNx, Al\textsubscript{2}O\textsubscript{3} and amorphous Si [18–20], generally surface recombination velocity increases with surface area [21]. For this reason, the surface area enlargement with nano texturing needs to be minimized while strong light trapping is maintained. In this study, we demonstrate using optical simulations that periodic silicon nanodisks of shorter than 200 nm on ultrathin c-Si with periods larger than 600 nm are promising nanostructures for effective light trapping with a very low surface area enlargement less than 1.5. Another benefit from low aspect ratio nanostructures is low material consumption during etching for nanostructure fabrication. We investigate the effects of geometrical parameters of the nanodisk arrays such as disk height, period and filling factor for ultrathin c-Si wafers thinner than 20 μm. We show that single side texturing of the c-Si ultrathin wafers thinner with periodic nanodisk arrays of optimal dimensions lead to around 90% of the Lambertian absorption limit. Also it was found that double side texturing with silicon nanodisks of different periods allows for even higher absorption.

2. Nanostructure design and simulation methods

The schematic of the c-Si nanodisk design for the optical simulations in this study is illustrated in Fig. 1. The nanodisk arrays are adjusted to be hexagonal in two dimensions. The hexagonal arrays of nanostructures can be fabricated using cost effective nano lithography such as nanosphere lithography, and laser interference lithography [22, 23]. For the systematic study on the correlations of the geometrical parameters of the nanodisks with the light trapping effects, height and period of nanodisks were varied in submicron from 100 nm to 900 nm while filling factor is kept for 50% unless stated otherwise. Filling factor is defined by the fractional area of nanodisks. The diameter of nanodisks is determined by filling factor. A rigorous coupled wave analysis (RCWA) method was used for the calculations of reflectance and transmittance of nanostructured c-Si wafers depending on the order of diffraction. The commercial software package (Gd-Calc), which runs in MATLAB environment, was used for the RCWA simulations. Incident light was considered to be randomly polarized by averaging transverse magnetic (TM) and transverse electric (TE) polarizations. The number of absorbed photons in ultrathin c-Si wafers with perfect back reflectors was calculated from the simulated reflectances and transmittances, and in turn, converted into photocurrent assuming incident solar radiation is a standard spectrum of AM (air mass) 1.5G at a light intensity of 100 mW/cm\textsuperscript{2}. The perfect electric conductor (PEC) condition was set for a perfect reflector. The base thickness in Fig. 1 was adjusted for the wafers to have the same volume as the planar c-Si wafers without texturing of which thickness is the effective thickness.

![Fig. 1. Schematic of nanodisk arrays on an ultrathin c-Si wafer. c-Si nanodisk arrays are placed on the ultrathin c-Si wafers in two dimensional hexagonal arrays.](image)

3. Calculation results

For the semi-infinite c-Si wafers with texturing of the silicon nanodisks, the reflectances were simulated as a function of wavelengths using the RCWA simulations to investigate
antireflection effects by nano texturing. The reflectances in all the diffraction order were summed up for obtaining the total reflectances. The simulated total reflectances were averaged over the standard solar radiation of AM 1.5G in the wavelength range from 350 nm to 1100 nm [24]. The period and height of the nanodisks were varied from 100 nm to 900 nm. The filling factor of the nanodisks was kept at 50%. The weighted average reflectances are plotted in Fig. 2(a). The average reflectance of planar c-Si wafer is 35%. With introducing the nanodisks, the reflectances decrease compared with the planar c-Si. However, as seen in the figure, the nanodisks higher than 200 nm do not suppress the reflectance below 15%. This result is very contrary to that of the silicon nanocones with high aspect ratios in literature [25]. In the case of the nanocones, the taller nanocones are reported to be more effective to suppress the reflectances. In this study, interestingly, the nanodisks shorter than 200 nm with periods narrower than 500 nm lead to less than 10% of the average reflectance as seen in Fig. 2(a). This antireflection by the short silicon nanostructures can be explained by substrate coupled Mie resonances [26]. The silicon nanostructures lying in proximity to a high refractive index substrate such as c-Si strongly induces forward scattering into the substrate, resulting in greatly suppressed reflections. The forward scattering is weakened as the nanostructures become taller, supporting that the nanodisks taller than 200 nm result in the increased reflectances as shown in Fig. 2(a). The reflectances as a function of wavelengths are shown in Fig. 2(b) for the cases of the nanodisks of 100 nm height and for three different periods of 300 nm, 500 nm and 800 nm. For comparison, the reflectance of planar c-Si with a single layer of antireflection coating (ARC) is shown together. The refractive index of ARC is set to be 1.9 and its thickness 70 nm. The short period nanodisks of 300 nm showed superior antireflection to the single layer ARC in a broad spectral range. As seen in Fig. 2(a), the reflectance showed the minimum at the period of 200 nm, and as the periods increase, the average reflectances increase. The nanodisks of a 800 nm period showed high reflectances over 20% below the wavelength of 700 nm in Fig. 2(b). The nanodisk arrays on the silicon wafers can be considered to act as an interfacial layer of which effective refractive index is intermediate between the incident medium (air) and the silicon substrate when incident wavelengths are greater than the physical dimensions of the nanodisks or the periods. In this case, the optimal height of the nanodisks would provide a destructive interference at a certain wavelength, resulting in vanishing of the reflectances, similar to ARC of a single dielectric layer as seen in Fig. 2(b) for the cases of 300 nm and 500 nm periods. However, when the physical dimensions of the nanostructures are greater compared with incident light wavelengths, the nanostructures do not serve as an effective medium. This is the reason why the nanodisks of long periods show high reflectances in short wavelength regions as seen in the case of the nanodisk arrays of a 800 nm period in Fig. 2(b). The reflectances from the nanodisks of various heights with the period of 500 nm are also plotted as a function of wavelength in Fig. 2(c). As the nanodisks become taller, more oscillations of the reflectances are observed, which is attributed to Fabry-Perot interference. The average reflectances from the nanodisks taller than 200 nm are all in the similar range of 16%~18%.

![Fig. 2. (a) Reflectance contour map from c-Si bulk wafers with the nanodisk arrays of various periods and heights. The dashed line denotes a contour line of 10% reflectance. (b) Reflectance as a function of wavelength from c-Si bulk wafers with the nanodisk arrays of 100 nm height and three different periods (300 nm, 500 nm, 800 nm). For the sake of comparison, the weighted average reflectances of planar c-Si wafer and a single layer of antireflection coating (ARC) are plotted. (c) Reflectance as a function of wavelength from c-Si bulk wafers with the nanodisk arrays of 100 nm, 300 nm, and 500 nm periods. For the sake of comparison, the weighted average reflectances of planar c-Si wafer and a single layer of antireflection coating (ARC) are plotted.](image)
reflectance from planar c-Si with ARC was also plotted together. (c) Reflectance as a function of wavelength from c-Si bulk wafers with the nanodisk arrays of 500 nm period and four different heights (100 nm, 300 nm, 500 nm, 900 nm).

The reflectances from the nanodisks can be further suppressed by introducing ARC. A dielectric layer of a 70 nm thickness ($n = 1.9$) was added onto the top of the nanodisks, and the reflectances were calculated as shown in Fig. 3(a), 3(b) and 3(c). As shown in Fig. 3(a), the reflectances from the nanodisks with ARC are greatly suppressed down to below 6% for all the cases, and similarly to the previous results, the nanodisks shorter than 200 nm and below the period of 600 nm lead to even lower reflectances (below 4%). As seen in Fig. 3(b), the nanodisks with ARC for a long period of 800 nm show a very low reflectance even in long wavelength regions above 700 nm. When the height of the nanodisks becomes taller than 100 nm, similar oscillations arising from the Fabry-Perot interference are observed but the oscillation amplitudes are distinctly reduced as shown in Fig. 3(c).

Another benefit we expect from the nanotexturing is light trapping in long wavelength regions above the wavelength of 700 nm, where the absorption coefficient of c-Si is poorer compared with that in the shorter wavelength regions. Fractional high order diffracted transmittances in the wavelength range from 600 nm to 1100 nm by varying the periods were simulated and plotted in Fig. 4(a) for the cases with the nanodisks of a 100 nm height. A fractional high order transmittance is a fraction of a total transmittance excluding a zero order diffracted transmittance. The high order diffracted light would take lengthened light path lengths and lead to enhanced photocurrent. As the period increases, the high order diffracted transmittances increase in the long wavelength regions. This can be understood by the following basic diffraction equation. For simplicity, one dimension diffraction equation is considered here and the incidence angle of light is assumed to be normal to the interface between air and c-Si. Two dimension equation can be found in literature [27].

$$\sin \theta_m = m \left( \frac{\lambda}{n_{si}} \right)$$  \hspace{1cm} (1)

In the above equation, $m$, $\theta_m$, $p$, $n_{si}$ are the diffraction order, diffraction angle in the $m$-th order, nanodisk array period and refractive index of c-Si, respectively. $\lambda$ is the wavelength of incident light. From the above equation, we can see that the period of nanodisk arrays must be greater than the wavelength of incident light divided by refractive index of c-Si for existence of 1st order transmitted diffraction. For higher order diffraction, the denominator or period must be greater than $\lambda / n_{si}$ multiplied by $m$. This clearly support that greater periods are needed for higher order diffraction in the longer wavelength region. Assuming incident light
is a standard solar spectrum of AM 1.5G at a light intensity of 100 mW/cm² and all the transmitted photons are converted into electricity, the maximum photocurrents by the high order transmittances were calculated and plotted in Fig. 4(b). The photocurrents substantially increase with increasing the period from 100 nm to 300 nm, followed by a plateau above 300 nm.

![Fractional high order diffracted transmittance as a function of wavelength by varying the periods of the nanodisk arrays.](image1)

Fig. 4. (a) Fractional high order diffracted transmittance as a function of wavelength by varying the periods of the nanodisk arrays. (b) Photocurrents generated from the high order diffracted transmission in the wavelength range of 700 nm ~1100 nm as a function of the periods of the nanodisk arrays.

The maximum photocurrents in 2 μm effective thickness c-Si wafers with nanodisks of various heights and periods were simulated and shown in Fig. 5(a). The nanodisks were coated with ARC. The perfect reflector was placed at the back surface. The photocurrents sensitively depend on the period rather than the disk height. The maximum photocurrents were calculated in two wavelength regions. One wavelength range is from 350 nm to 700 nm, where the optical absorption is strong and another one from 700 nm to 1100 nm, where the optical absorption is poor relatively. The photocurrents generated in both of the wavelength regions are plot in Fig. 5(b) as a function of period. The photocurrents ($J_{ph1}$) generated in the short wavelength range do not vary much, but distinct increases of the photocurrents ($J_{ph2}$) in the long wavelength range are observed with increasing the period. The enhanced optical absorption in the long wavelength range is clearly observed for the 2 μm thickness c-Si wafer with increasing the period from 300 nm to 800 nm as shown in Fig. 5(c). For the nanodisks of a 100 nm height, the simulated maximum photocurrent is found at the period of 800 nm as seen in Fig. 5(a).

![The maximum photocurrent generated in 2 micron thickness c-Si wafers as a function of nanodisk height and period.](image2)

Fig. 5. (a) The maximum photocurrent generated in 2 micron thickness c-Si wafers as a function of nanodisk height and period. (b) Photocurrents generated from solar radiation in the short wavelength region (350 nm ~700 nm) and the long wavelength region (700 nm ~1100 nm). Total photocurrent ($J_{ph,total}$), which is the sum of $J_{ph1}$ and $J_{ph2}$, is also shown. (c) Absorption spectra of 2 micron thickness c-Si wafers with nanodisk texturing as a function of wavelength for various periods (dotted lines). The solid lines are smoothened data by adjacent averaging, which are displayed only for the eye guide.

In order to investigate the effect of filling factor on light trapping, we simulated the photocurrents in 2 μm thickness c-Si wafers while keeping the period at 800 nm. The disk

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height was also varied from 80 nm to 180 nm in efforts to find the optimal dimension of the nanodisks. Except the cases with a short height (below 100 nm) and a low filling factor (below 20%), the nanodisk texturing leads to high photocurrents exceeding 28 mA/cm². Specifically, the heights between 120 nm and 160 nm and the filling factor between 20% and 70% are optimal choices for effective light trapping.

As stated above, it is desirable that the surface area enlargement with nanotexturing is minimized for suppressing minority carrier recombination at the surface. The surface area enlargement with texturing of the nanodisk with filling factor of 50% was calculated by varying height and period and plotted in Fig. 6. As the height increases and the period decreases, the surface area enlargements increase significantly. Longer periods and shorter heights are desirable in terms of the surface area enlargement. If both of the height and period are too short and long, light trapping becomes poor. To keep the surface area enlargement below 1.5, the period must be greater than 600 nm, and the height be shorter than 160 nm see Fig. 7.

Referring to the previous results as seen in Fig. 6, we chose 140 nm of the height and 50% of the filling factor as optimal dimensions of the nanodisks with the 800 nm period for the front surface texturing. Also we introduced the nanodisk arrays on the back surface for light trapping in a broader spectral range [12]. The height of the nanodisk on the back surface is set at 100 nm, and filling factor at 50%. In efforts to find the optimal period of the nanodisk arrays on the back surface, the period at the back surface was varied from 800 nm to 1600 nm and 2400 nm with the 800 nm period of the front surface. In Fig. 8(a), the photocurrents were
simulated using the RCWA method and shown for 2 μm effective thickness c-Si wafers with the above double side texturing, and compared with those of the cases with single side texturing and ARC coated planar wafer. The perfect reflector was placed at the back surface for all the cases. For the cases with double texturing, the nanodisk arrays at the back surface were embedded with a dielectric layer of SiO₂ (n = 1.45). When the period of the nanodisk arrays at the back surface was a double of that at the front surface (1600 nm), the highest photocurrent of 33.2 mA/cm², which is 93% of the Lambertian absorption limit, was provided. Thus, the period of the nanodisks on the back surface was set to be a double of that of the nanodisks on the front surface for the case of the double side texturing. Figure 8(b) shows the absorption spectra for four cases of a 2 μm effective thickness c-Si wafers: (1) planar c-Si with ARC, (2) single side texturing, (3) double side texturing, (4) Lambertian absorption limit. The Lambertian absorption limit is the theoretical maximum, where the front surface is assumed to scatter incident light randomly and the back surface has a perfect reflector. As expected, single side texturing provides enhanced absorbance over planar c-Si with ARC above the wavelength of 700 nm, and the double side texturing leads to even enhanced absorption. We also varied effective c-Si wafer thicknesses from 1 μm to 50 μm for four cases. Similarly, as increasing the c-Si thickness, for all the given thicknesses, the double side texturing with the nanodisks provides much enhanced photocurrents as seen in Fig. 8(c). Note that with the double side texturing, the photocurrents higher than 90% of the Lambertian limit can be generated for all the thicknesses. In this case, the surface area enlargement was less than 1.5 and the disk height is much less than 200 nm. The nanodisk design we proposed in this study would be very promising for effective light trapping in ultrathin c-Si solar cells. The low aspect ratio nanostructures with the low surface area enlargements are highly desirable to realize high efficiency and cost effective solar cells because of low materials loss by etching and little surface recombination. When the surface recombination is minimized in c-Si wafers, the use of the thinner wafers can lead to enhanced open circuit voltage resulting from reduced bulk recombination. Thus, once light harvesting is well preserved in thinner wafers with minimal surface recombination, the ultrathin c-Si solar cells even have higher efficiencies than the bulk c-Si solar cells [28]. In this regard, the nanodisk arrays would be one of very promising nanostructures for the ultrathin c-Si solar cells owing to effective light trapping and low surface area enlargements. If metallic nanostructures for the surface plasmon resonance effect are combined with the nanodisk arrays, even higher absorption enhancements would be expected, and this research work is underway [29, 30].

![Fig. 8.](image)
maintained at 800 nm. The red dashed line indicates the maximum photocurrent in the Lambertian absorption limit. (b) Absorption spectra of 2 μm thickness c-Si wafers with single side or double side texturing of the nanodisk arrays. The absorption spectrum of planar c-Si with ARC is also shown for comparison. The blue and red solid lines are smoothened data for the eye guide. (c) Photocurrent density of c-Si wafers with texturing or without texturing and ARC for various c-Si wafer thickness. The Lambertian absorption limit is shown together. The cross-sectional images of c-Si wafers with single side or double side texturing are illustrated in the top figure. The nanodisk arrays are coated with orange-colored ARC. The yellow colored layer is an optical spacer of SiO₂. The gray layers denote the ideal reflector (PEC).

4. Conclusions

We performed systematic study on light trapping in ultrathin c-Si wafers with the nanodisk array texturing by the RCWA simulations. We numerically demonstrated that the short nanodisk arrays of less than 200 nm with coating of ARC lead to great suppressed reflectances in the wide spectral range and also absorption enhancements by coherent light trapping. The nanodisk texturing is very beneficial to cell cost reductions and efficiency improvements because etching loss of the material during texturing and surface enlargements are low due to the low aspect ratio of the nanodisks. We showed that the double side texturing of the nanodisk arrays can exceed 90% of the Lambertian limit in ultrathin c-Si wafers. We believe that the nanodisk array texturing we demonstrated in this study is practically very promising for the solar cells based on the ultrathin c-Si wafers.

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