Biomimetic spiral grating for stable and highly efficient absorption in crystalline silicon thin-film solar cells

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Abstract: By emulating the phyllotaxis structure of natural plants, which has an efficient and stable light capture capability, a two-dimensional spiral grating is introduced on the surface of crystalline silicon solar cells to obtain both efficient and stable light absorption. Using the rigorous coupled wave analysis method, the absorption performance on structural parameter variations of spiral gratings is investigated firstly. Owing to diffraction resonance and excellent supericies antireflection, the integrated absorption of the optimal spiral grating cell is raised by about 77 percent compared with the conventional slab cell. Moreover, though a 15 percent deviation of structural parameters from the optimal spiral grating is applied, only a 5 percent decrease of the absorption is observed. This reveals that the performance of the proposed grating would tolerate large structural variations. Furthermore, the angular and polarization dependence on the absorption of the optimized cell is studied. For average polarizations, a small decrease of only 11 percent from the maximum absorption is observed within an incident angle ranging from −70 to 70 degrees. The results show promising application potentials of the biomimetic spiral grating in the solar cell.

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1. Introduction

To pursue renewable and green energy, research efforts have been concentrated on developing economical thin-film crystalline silicon (c-Si) solar cells [1-2]. An obvious dilemma is that the thin film tends to have weak light-absorption efficiency if the film thickness is lower than the absorption length of the material. To overcome this issue, researchers have employed various light-trapping structures to enhance the absorption such as nano-periodic [3–8], random [9–11] and quasi-random [12–16] surface structures, including plasmonic nanoparticles structures [17–19]. Recently, inspired by bionics, biomimetic artificial trapping nanostructures like moth-eye grating and the genetic algorithm-optimized structure are proposed [20,21]. With deliberate designs, the coupling of the incident light into the quasi-guided modes could be improved [22–24], leading to significant absorbance enhancements. However, it is also necessary to check how stable the absorbance of the trapping structures would be with respect to the variations of the structural dimensions. Because in reality, the dimensions of trapping structures could deviate from the nominal geometry due to fabrication errors. As a result, the absorption could be compromised considerably. Therefore, both absorption enhancement and dimension tolerance should be taken into account simultaneously to obtain solar cells with stable and efficient absorption.

In this paper, by emulating the spiral phyllotaxis structure of natural plants which has a superior and stable light capture capability, a two-dimensional (2D) spiral grating is introduced on the surface of c-Si solar cells to obtain both sustainable and efficient light absorption. By using the rigorous coupled wave analysis (RCWA) method [25], the absorption of the spiral grating c-Si thin-film solar cell is calculated within a wavelength range from 300 to 1000 nm. Compared with the conventional slab cell, absorption enhancement of 77 percent in an optimized spiral grating is obtained. Moreover, the proposed spiral grating cell demonstrated a good structure tolerance. Even in the case of 15 percent structural deviation, the maximum integrated absorption only decreases by 5 percent. Furthermore, the proposed cell also manifests excellent angle and polarization tolerance. For average polarizations, only 11 percent decrease of the maximum absorption is observed within an incident angle range from −70 to 70 degrees. Therefore, we could conclude that the proposed grating derived from the spiral phyllotaxis is effective for achieving both stable and highly efficient absorption in the c-Si thin-film solar cells.

2. Structure of spiral grating cell and method

In nature, the spiral phyllotaxis is widely found in plants. Because the spiral curve could utilize the least amount of material and the lowest energy consumption to make plants leaves extend to the place where the light is sufficient, it is vital for plants to maximize the utilization efficiency of light in photosynthesis [26–29]. More importantly, even if the size of leaves slowly changes during plant growth, strong light absorption could still be maintained. Based on the facts above, a trapping structure that has the feature of spiral curve should be expected to obtain the merits of both high absorption and good structural tolerance. However, the natural spiral structures are often of complex patterns. As a result, the direct duplication of them is challenging in both theoretical design and fabrication procedure. Thus, the leaf spiral structures ought to be simplified. As shown in Fig. 1, a biomimetic 2D spiral grating is introduced on the surface of the c-Si solar cells to inherit the merits from the Archimedean spiral curve [30] and the sophisticated grating structure. Figure 1(a) shows the three-dimensional (3D) schematic of the spiral grating cell. The cross-sectional view of the spiral grating cell is presented in Fig. 1(b). From top to bottom, the cell consists of an indium tin oxide (ITO) layer, an absorbing layer comprising c-Si, and finally a silver (Ag) layer for back contact. Figure 1(c) shows the top view of a unit lattice of the 2D spiral grating cell. In Fig. 1(c), the period of a unit lattice is denoted as \( a \), and the 2D spiral grating in the solar cell is within a square lattice. In order to simplify the spiral curve and to inherit the merits of
traditional grating, the spiral curve here is transformed to an extended rotational square shape, and the rotating circles in one unit lattice are limited to two rounds for simpler theoretical design and fabrication. Also, to be make the solar cell model more realistic, a popular stack structure for our proposed spiral grating solar cell was adopted, as shown in Fig. 1. In Fig. 1(c), the black cross in the center of the spiral structure denotes the origin point, and the forward rotation direction for extension is clockwise. Because the most inner part of the spiral curve is relatively dense as shown in the inset image of the begonia [31] in Fig. 1(a), the rotation arm of spiral grating is chosen with a starting from the X axis as shown in Fig. 1(c), which means that the most inner half round of spiral curve is omitted. Hence, except the air slot near the starting position being denoted as \( p_1 \) has a width of \( p/2 \), the other air slots are all with the same width of \( p \). The linewidth of spiral arm is denoted as \( d \). Thus, the whole extension length of spiral structure \( l \) is equal to three times of \( p \) and four times of \( d \).

As shown in Fig. 1, there are multiple structural parameters of the spiral grating cell, including \( a, d, p \), the grating height, and also the thicknesses of the three layers (ITO, c-Si, and Ag). Because the purpose of this paper is to study whether the spiral grating could favor stable and efficient absorption, we perform dependence studies on the key surface structural parameters \( (d \) and \( p \)) of spiral grating. The values of other structural parameters cell are chosen consistently with previous literatures. The thickness of the ITO layer is fixed to 80 nm [10], the refractive index and extinction coefficient value for ITO material are set to 1.52 [10] and 0 [9,10,14,32], respectively. The Ag layer is used as a back contact, and the thickness of Ag layer is set to 200 nm [9,10,33]. Because a 2D grating with a periodicity of 300-600 nm has been shown to be effective [6,7]. Thus, here \( a \) is fixed to 600 nm, which is also the same with previous investigations [5,32–34]. The thickness of c-Si layer is set to 1000 nm [5,9,10,32-34]. Moreover to improve the anti-reflection property in the visible and near-infrared region, the c-Si layer is moderate etched with a thickness of 500 nm [5,33,34], which will also enable more realistic conformal passivation and ITO deposition. The optical properties of c-Si and Ag are taken from the literatures [35,36].

To study the light absorption characteristics of the spiral grating cell, the RCWA method is used [25]. In our calculations, to distinguish small changes of structure parameters and also to obtain a reasonable accuracy, the maximum number of in-plane (X and Y) Fourier expansion orders is set to 100. Also, circular truncation of the lattice is chosen, which meant that the Fourier lattice k-vectors are selected to have shortest length by L2 norm [25]. The configuration is chosen through a systematic transmission stability research on a reference square grating solar cell before our investigation on spiral grating solar cell. In the transmission stability research, the Fourier expansion orders are changed from 40 to 160 with a step of 10. And we noticed that when the Fourier expansion orders are above 100, the
change of the transmission results of the spiral grating are minimal. The incidence lights are assumed to be from an infinite air layer, and the direction of incident light is firstly set to be normal to the surface unless otherwise specified. Below the Ag contact layer, an infinite air layer is also used. Then the absorption in the c-Si layer \( A_{cSi}(\lambda) \) can be expressed as:

\[
A_{cSi}(\lambda) = 1 - R(\lambda) - T(\lambda)
\]

Here, \( \lambda \) is within a wavelength range from 300 to 1000 nm. \( R \) is the reflectance from the upper surface of the ITO layer. \( T \) is the transmittance at the c-Si/Ag interface. \( R \) and \( T \) in this study are obtained by the RCWA method. By assuming that each photon absorbed in the c-Si layer generates an electron-hole pair, the short-circuit current of solar cells \( J_{sc} \) can be characterized as [16]:

\[
J_{sc} = \frac{e}{h} \int \lambda A_{cSi}(\lambda) S(\lambda) d\lambda
\]

where \( e \) is the electron charge, \( h \) is the Planck constant, \( c \) is the speed of light in vacuum, and \( S(\lambda) \) is the air mass (AM1.5G) solar spectrum [37].

3. Numerical results and discussion

3.1 Structural engineering and absorption stability analysis

To find out how the key structural parameters of the spiral grating influence the absorption, the \( J_{sc} \) of the spiral grating cell as a function of \( p \) and \( d \) is plotted in Fig. 2. As shown in Fig. 1(c), \( l \) is equivalent to three times of \( p \) and four times of \( d \), and it should not be larger than \( a \). Then \( p \) and \( d \) have to be restricted in a reasonable range. Here, \( p \) is varied with an interval of 5 nm in a range from 20 to 60 nm, and \( d \) is varied with an increment of 15 nm in a range from 30 to 105 nm. From Fig. 2, we can see that as either \( p \) or \( d \) increases, the \( J_{sc} \) firstly rises and then drops. The \( J_{sc} \) gets its maximum value of 26.38 mA/cm\(^2\) when \( p \) and \( d \) are 36 and 78 nm, respectively. This phenomenon can be easily understood. When \( d \) is small (or \( p \) is large), the limited amount of c-Si absorbing material which constitutes of the spiral grating would lead to low absorption. On the contrary, when \( d \) is large (or \( p \) is small), the amount of c-Si absorbing material in the spiral grating will become greater. For silicon has a larger refraction index than ITO, thus the volume averaged index for one period will get larger. Then the
effective index contrast between the upper ITO and the grating interface get larger accordingly. This would result in a considerable index contrast between the layers, thus causing a large reflection from the surface of the absorption layer, which will also make the absorption weak. Therefore, the maximized $J_{sc}$ is obtained with intermediate structural parameters.

Then, the absorption stability is investigated by deviating the structural parameters from the optimums. When $p$ is fixed at 36 nm, the largest variations of $J_{sc}$ is only 7.3 mA/cm² within the whole investigated range of $d$. Similarly, when $d$ is fixed at 75 nm, the largest variation of $J_{sc}$ is only 2.38 mA/cm² within the whole changing range of $p$. In addition, when $p$ and $d$ are simultaneously departed from the optimal geometry by 5 percent, the $J_{sc}$ only reduces by 0.84 percent, as presented in the domain enclosed by the contour line of 26.13 mA/cm² in Fig. 2. In contrast to the previously reported grating cell with stable absorption, in which the $J_{sc}$ decreased by 1 percent when the lattice parameter was 5 percent away from the optimized geometry [8], a smaller deviation of $J_{sc}$ is obtained in our proposed spiral grating cell with the same structural deviation. Moreover, even if $p$ and $d$ are simultaneously deviated from the optimized structure by 15 percent, shown in the area enclosed by the contour line of 25.08 mA/cm², only 5 percent decrease of the maximum $J_{sc}$ happens. Therefore, we conclude that the absorption of the proposed spiral grating cell is stable amid large structural parameter variations. The proposed spiral grating cells could indeed inherit the stability feature of the spiral phyllotaxis.

After optimized the spiral grating with fixed height of 500 nm, we also take consideration of the influence on $J_{sc}$ by using different etching heights from 200 nm to 800 nm, while the whole silicon layer is kept with a fixed value of 1 μm, as shown in Fig. 3(a). The $J_{sc}$ is heavily changed by the grating thickness. It firstly increases and then drops, and it gets its maximum of 26.38 mA/cm² when the etching of thickness is of 500 nm. We then also take consideration of the influence on $J_{sc}$ by using different silicon grating heights from 200 nm to 1100 nm, while the bottom un-etching silicon layer is kept with a fixed thickness of 500 nm, as shown in Fig. 3(b). In this case, the $J_{sc}$ is firstly increased largely while the grating height increasing. When the grating height is above 500 nm, further increasing the height of the grating will make $J_{sc}$ only weakly increased, and fluctuation in a weak amplitude also could be found. These phenomena are similar to previously investigation about the influence of thickness on absorption [33,38,39]. Thus, we choose 500 nm as the etching of thickness.

![Graphs](image-url)

3.2 Discuss of the optimal spiral grating

To understand the high-absorption capability of the optimal spiral grating cell, the reflection, transmission and absorption spectra are studied as shown in Fig. 4. The reflection spectra of
the optimized spiral grating cell and the slab cell are both presented in Fig. 4(a). In the broad spectrum from 300 to 970 nm, less reflection of the spiral grating cell is observed compared to that of the slab cell. And in the relative narrow bandwidth from 970 to 1000 nm, the reflection spectra of the spiral grating cell and the slab cell possess almost the same amplitude. This appearance demonstrates that the antireflection of spiral grating cell in the short-wavelength range is stronger than that in the long wavelength range. On the other hand, it illustrates that the loss of light from spiral grating cell surface is lower than the conventional slab cell. In the wavelength range from 500 to 1000 nm, the reflection peaks for spiral grating cell are of complex and irregular shapes, while the reflection peaks of the slab cell possess regular shapes. The irregular shapes of reflection peaks are due to the coherent resonant Bloch modes for the spiral grating cell [6,16], while the regular shapes of reflection peaks are a result of Fabry-Perot optical interference for the slab cell [20]. The transmission spectra of spiral grating cell and the slab cell are shown in Fig. 4(b). In the short wavelength region from 300 to 450 nm, the transmission for both spiral grating cell and slab cell is nearly zero. This is because the short wavelength light could not transmit deep in the c-Si absorbing layer due to the grating absorption [39]. At wavelengths above 450 nm, the transmission of the spiral grating cell is found higher than that of the slab, while the magnitude of transmission is still very low.

Subsequently, the absorption spectra of spiral grating cell and the slab are plotted in Fig. 4(c). When the thickness of grating is much greater than the wavelength of light in the ray-optics regime, the maximum absorption for weakly absorbed rays is defined as Yablonvitch limit [24]. Light passing through the material only once, and assumes a perfect antireflection, which is the single-pass absorption. Because both reflection and transmission of the spiral grating cell are very low, the absorption of spiral grating cell is close to the Yablonvitch limit.
In addition, the irregular absorption peaks of spiral grating slightly exceed the Yablonvitch limit in the wavelength range from 600 to 970 nm. This is because when the period of the light trapping structure is comparable to the incident light wavelength, the enhancement ratio of the absorption can be as high as $12n^2$, where $n$ is the refractive index of the absorbing material [40]. As shown in Fig. 4(d), the $J_{sc}$ of the spiral grating cell and the slab cell are calculated. The short circuit current 26.38 mA/cm² of spiral grating is close to the Yablonvitch limit (29.62 mA/cm²), and that also represents an enhancement of 77.28 percent over the conventional slab cells (14.88 mA/cm²). Moreover, a comparison between the optimized spiral grating and square grating solar cells is made. For the conventional square grating cells, all other structure parameters are set to have the same configuration as the spiral grating cells. Therefore, only the square side length of the square grating cell could be engineered to obtain high absorption performance. The optimized square grating cell having a square side length of 330 nm attains $J_{sc}$ of 23.5 mA/cm². Thus, the proposed spiral grating solar cell shows a 12.25 percent enhancement in $J_{sc}$. This result implies the spiral grating carries the highly-absorptive feature of the spiral phyllotaxis.

To understand the lower reflection in the short wavelength than that in the long wavelength range, the electric field distributions of one unit lattice for different wavelengths are calculated as shown in Fig. 5. Figures 5(a, d), 5(b, e) and 5(c, f) are obtained in the X-Z plane, with incident light wavelengths of 450, 700 and 940 nm, respectively. Figures 5(d)-5(e) demonstrate that the electric-field intensity is enhanced inside the c-Si absorption grating zone. While in Fig. 5(f), the electric-field intensity enhancement occurs at the surface of spiral grating. This is due to the diffraction resonance of the spiral grating at the short wavelengths, which then could be easily coupled into the absorption material c-Si. That phenomenon verifies the results in Fig. 4(a), where the reflection of spiral grating in the short wavelength region is lower than that in long wavelength region. Compared with the slab cell in Figs. 5(a-c), higher electric fields in Figs. 5(d-f) also evidence that huge absorption enhancements could be achieved by the spiral grating. Also, from the $|E|^2$ maps in Fig. 5, both light absorption in the Ag layer and also reflection above from the Ag surface could be observed. For the thickness direction, Figs. 5(g)-5(i) show that the electric-field intensity enhancement occurs at the absorption material, which manifest that the coupling from air to absorption material c-Si is happening. While for the longer wavelength of 940 nm in Fig. 5(i), the magnitude of electric-field intensity enhancement is lower than Figs. 5(g) and 5(h). One may also easily found that, the $|E|^2$ cross sections shown in Figs. 5(g) and 5(h) roughly look like concentric subwavelength patterns within a unit cell, and this phenomena is known to facilitate the impedance matching. Thus, small reflection from the surface could be observed at these two wavelength as shown in Fig. 4(a). Those differences phenomenon could explain the result shown in Fig. 4(a), in which the irregular shape of reflection peaks only emerge in the long wavelength region.
3.3 Angular and polarization characteristics of the optimal spiral grating

Due to the sun movement, the incident angle and polarization dependence of absorption is critical. The $J_{sc}$ of optimized spiral grating cell as a function of different incident angles for P, S and average polarizations are depicted in Fig. 6. The P polarization follows the X axis, and the S polarization follows the Y axis. The average polarizations $J_{sc}$ firstly increases with incidence angle, and $J_{sc}$ is notably higher at angles around 10 - 20 degrees than at normal incidence. For each polarizations, the maximum $J_{sc}$ is obtained at 10 degrees for S polarization and at 15 degrees for P polarization. Moreover, there is only 11 percent decrease of the maximum $J_{sc}$ within an incident angle range from $-70$ to $70$ degrees for average polarizations. Compared with the previously claimed grating cell with angular stability, in which the integrated absorption is decreased by 25 percent between 0 degree and 70 degree for average polarizations [8]. And the maximum $J_{sc}$ dropped by 11 percent between 0 degree and 60 degree for average polarizations [41]. Furthermore, as a comparison, the maximum $J_{sc}$ of the optimized square grating decreased by 18 percent within an incident angle ranging from $-70$ to $70$ degrees for the average polarizations. Thus, the angular stability of the proposed spiral grating cell is better than the optimized square grating. Then, we could conclude that the proposed spiral grating cell is insensitive to the angle of incident, and the spiral grating cell imitating the spiral phyllotaxis of plants does have an ability of achieving both stable and highly efficient light absorption.

Fig. 5. Electric field intensity profiles at (a, d, g) 450nm, (b, e, h) 700nm, and (c, f, i) 940 nm for slab cell (a-c) and spiral grating (d-i), respectively. The profiles (a-f) and (g-i) are obtained in the X-Z plane and in the X-Y plane, respectively. The black lines present the interfaces between the grating and the ITO material. The magnitudes of electric-field intensity enhancement are indicated by the color scales.
Fig. 6. The short circuit current densities as a function of the incident angle for the optimized spiral grating, under P (follow the X axis), S (follow the Y axis) and average polarized illuminations. The zero-degree angle refers to the normal incidence to the solar cell surface.

4. Conclusion

In summary, based on the merit characteristics of both spiral phyllotaxis and grating structure, a 2D spiral grating is proposed to achieve both highly-efficient absorption with good structural tolerance. The absorption of spiral grating is close to the Yablonvitch limit. About 77 percent enhanced absorption is yielded by the optimal spiral grating cells, as compared with the conventional slab cells. The enhancement originates from diffraction resonance and excellent superficies antireflection across the wavelength from 300 to 1000 nm. Moreover, the absorption performance on structural parameter variations of spiral grating is investigated. The results reveal that the proposed cell demonstrates stable absorption with respect to the structural variation. Finally, the angular and polarization dependence of absorption of the optimized cell is also studied. The proposed grating exhibits good stability with respect to the angle of incidence and polarization. Consequently, the 2D spiral grating derived from the spiral phyllotaxis is effective and feasible for achieving both stable and highly efficient absorption. Considering that the spiral phyllotaxis of plants in nature generally possess 3D structures, we can expect that a 3D spiral grating which inherits the spiral characteristics in the vertical direction could bring further improvement to the solar cell absorption.

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