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Abstract: The absorption of an amorphous silicon thin film with periodic gratings formed by an array of nanowires with varied heights and different profile shapes is studied. Optimized parameters, including period, duty ratio, and the angle of unit cell and the shape of the profile, namely, tented, triangular, and concave type, are used to achieve the optimal results of light absorption and conversion efficiency. The enhancement of conversion efficiency occurs both in TE and TM polarizations. The photovoltaic conversion efficiency of the solar cell with triangular profile can be increased by 58.21%, 42.45%, and 20.38%, compared with those with flat surface, equal-thickness nanowires, and periodic triangular textures, respectively.

Index Terms: Photovoltaic, subwavelength structures, nanostructures, nanowires.

1. Introduction

Photovoltaic (PV) solar cells [1]-[3], which convert sunlight into electrical power, have attracted much attention recently as a competitive candidate for renewable and clean energy. However, the cost of PV solar cells should be reduced and the conversion efficiency should be enhanced in order for them to become a major alternative for electrical power generation. According to these objectives, the increase of conversion efficiency in PV solar cells is expected to enhance photon absorption. Most photovoltaic devices choose silicon as the light absorbing material because of its abundance and good electrical and optical properties. Yet, the crystalline silicon type solar cell consumes more material and is less flexible for some applications. With the use of thin amorphous silicon as absorbing layer [4]–[6] in the range of 1 μ m, both the cost and the amount of active material may be reduced. In addition, the technology of thin amorphous silicon films may facilitate the realization of the promising building integrated photovoltaic devices. However, the optical path within the absorbing material could be too short to fully utilize the shorter wavelengths of light and the longer wavelengths may even pass through the thin absorbing layer. As a result, the conversion efficiency is limited. In order to overcome the low light absorption in such thin structures, various concepts have been proposed in recent years [7]-[9]. Using nanostructures [10]-[12] is one possible solution to provide innovative designs of photovoltaic (PV) solar cells. The goal of these schemes is twofold: first, to reduce the reflection of light from the top surface of the PV device; and second, to enhance the scattering and diffraction of light in the device to provide a sufficient optical path, or photon lifetime, within the absorbing material. Studies of silicon nanostructures [13]-[16] for solar cell may provide promising approaches due to their unique optical and electrical characteristics [17]-[20]. The nanowire structure makes it feasible to decouple the light trapping



Fig. 1. Schematic diagram of the cross section view of the grating structure with periodic nanowires.

from the photon-generated carrier extraction [21]–[23] because the diameter of nanowire structures is smaller than the diffusion length of carriers. In this paper, we demonstrate the interest of this concept in the particular case of solar cells formed by an amorphous silicon (a-Si) absorbing layer with a thickness in the order of 500 nm, using periodic nanowire gratings of different designs with an average thickness of 1000 nm. The thickness of the absorbing layer is limited not only for economical reasons, but also to increase optical absorption because of the low diffusion length in this material. It is shown that adding the periodic nanowire grating to the amorphous silicon thin films can significantly enhance the light absorption.

This work presents a novel grating structure design for a-Si solar cell, in which the a-Si absorption layer decorated with the shaped grating profile enhances performance of the solar cell due to the high light absorption over a broad spectral range. The shaped grating formed by separated nanowires with optimized periodicity and duty ratio can further reduce the reflection of incident light, while enhancing the absorption at some specific wavelengths, so the overall conversion efficiency can be significantly improved.

2. Optical Simulation Model

The optical propagation and scattering of sunlight within the PV solar cells with surface gratings formed by nanowires can be analyzed and the efficiency of the solar cells may be optimized using numerical methods to rigorously solve the Maxwell's equations. In this paper, the finite element method (FEM) simulation tool (COMSOL Multiphysics) was used to investigate the propagation of optical waves in thin film amorphous silicon solar cells decorated with periodic nanowire grating. By doing so, the absorption characteristics of the solar cells with nanowire structures can be investigated. Since the finite element method is appropriate for the analysis of arbitrarily shaped structures, the method described here is also applicable to any nanostructured solar cell design. Our design utilizes both periodic profile and nanowires, and it also incorporates metal films as electrodes. The schematic diagram of the nanotextured surface is shown in Fig. 1.

The amorphous silicon solar cell structure is made of amorphous silicon (a-Si:H) with a total thickness of 1500 nm which consists of bottom a-Si layer with a thickness of 500 nm. To this are added nanowires with varied heights, and average nanowire thickness of 1000 nm to form a periodic shaped grating, and it is supported by an aluminum back contact of 200-nm-thick aluminum. The same average thickness presents the same amount of absorbing materials, which should have the same capacity for light absorbing. In addition to light properties, this nanowire structure may be made as a radial p-n junction to express its electrical properties, using an ITO coating as the electrode to conduct electrons and holes to allowing the light to penetrate into the absorbing material. In this paper, the duty ratio (r), which is defined as the diameter of nanowire



Fig. 2. (a) Light absorption spectra for various periods. (b) Light reflectance spectra for various periods. (c) Light absorption spectra for various duty ratios. (d) Light reflection spectra for various duty ratios.

divided by nanowire periodicity, and the incline angle (θ), which is defined as the height divided by half period. The number of nanowires in one period has been investigated though calculating the absorption of three, five, seven, and nine nanowires separately. According the results, when the number of nanowires is greater than five, it has little influence on the profile shape and light absorption characteristics, but when the number is three, the absorption is 5% less than others. Therefore, in this study, five nanowires are applied to one period of unit cell to build the profile shape for feasibility of fabrication, consideration of time consumption and accuracy of the simulation result. The period of the unit cell was varied from 50 nm up to 5000 nm and the height was varied from 0 nm up to 800 nm. Alternatively, the triangular structure can be described by the angle of the triangle, which was varied from 0 to 88°. The unit cell was illuminated under normal incidence of the light within 300–1100 nm of the solar spectrum at the Air Mass 1.5.

3. Results and Discussion

The absorption for longer wavelengths of thin film solar cell is limited due to the longer optical path for longer wavelengths compared to thinner material. Most energy with longer wavelengths passes through a thin film without converting into electrons. Changing the average nanowire thickness has a similar effect on flat nanowire arrays, where thicker nanowires can enhance the absorption at longer wavelengths (600–800 nm), while the absorption remains unchanged for shorter wavelengths. Since the absorption length for blue and green light of the spectrum is smaller than the thickness of the solar cell, it will be absorbed within the first few hundred nanometers of the cell so that adding total thickness seems to have no influence on absorption in high energy region of light spectrum.

It illustrates that for smaller period in Fig. 2(a) the reflection decreases and the absorbed light with short wavelength is mainly improved. It is found that absorption is near 95% at shorter wavelengths from 300 nm to 600 nm when period is 100 nm. This is because that the nanowire grating acts as an effective index matching layer if the grating period is smaller than $\lambda/2n$, where λ is the wavelength of the incident light and *n* is the refractive index of the grating [10]. This statement is further evidenced by the reflection spectral in Fig. 2(b) for both samples in the corresponding energy region.

Whereas decreasing the period, the influence of light absorption for longer wavelengths is significantly reduced because the light wavelength in the low energy region is much longer than the period of the triangular profile with short period. Accordingly, incident light waves can easily penetrate through the nanowire profile without interacting with it, and reaching the bottom a-Si layer. Furthermore, the period of 500 nm tends to reach higher light absorption at a range of wavelength of 500 nm to 680 nm since it helps the incident waves to change their direction to neighboring unit cells, and further increases the constructive interference and effective light trapping. According to equation (1), light is diffracted into different diffraction angles to increase efficient optical path, but when the periods of NWs are much larger than λ , the diffraction angles are too small to trap light in unit cells. This can be explained by

$$\sin \theta_t = \sin \theta_i + m \cdot \frac{\lambda}{P} \quad (m = 0, \pm 1, \pm 2, \ldots)$$
(1)

where θ_t is the diffraction angle inside the nanowire, θ_i is the incident angle which is equal to 0°, *P* is the period of the grating, λ is the incident wavelength under refractive index of the propagating media, and *m* specifies the diffraction order.

With changes in the duty ratio, which is defined as the ratio of nanowires in one period, the enhancement of absorption is shown in Fig. 2(c). This makes the periodic profile as a refractive index matching layer because a lower duty ratio means the effective refractive index is closer to the refractive index of air, which indicates a good property of anti-reflection. Furthermore, in Fig. 2(d) the reflectance of NWs with duty ratio equal to 0.2 is close to 1% in the range from 300 nm to 600 nm. Therefore, the shorter wavelength light nearly entirely transmits into the absorbing layer, so the absorptance of the NWs with the lower duty ratio can be improved. The NWs with small period can help more light entering the absorbing layer, and the NWs with small period and small duty ratio can further improve the light absorption. In the long wavelength region, the enhancement of absorptance at some particular wavelengths is observed. The electromagnetic wave inside the nanowire would be reflected many times by the interface between Si and the air, and some electromagnetic waves are guided in the three-layer Air-Si-Al structure, which can be seen as a waveguide structure. For longer wavelengths, the light may not be totally absorbed by the a-Si and the remaining light will be reflected by the lower electrode and then absorbed by the a-Si again, eventually forming a resonant mode inside each single nanowire. In short, these resonant modes allow for good coupling of the incident plane waves, high energy concentrations within the nanowires, and strong Fabry-Pérot resonances between the top and bottom interfaces [24].

Above all, this shows a distinct enhancement by larger periods of grating profile because the optical path length is increased, and a carefully chosen period can couple more light absorption for the red part of the optical spectrum. In addition, reducing the duty ratio can help absorption for the blue and green part of the optical spectrum. Thus a well-designed nanowire grating profile can significantly increase light absorption for visible light. In one careful design, triangular profile formed by nanowires, with a period of 500 nm, the duty ratio is 0.2 and the angle is 75°, enhancing the conversion efficiency by 55.53% compared to flat nanowires and 12.45% compared to the periodic grating thick PV solar cell.

In the next step, the conversion efficiency was determined to determine the influence of parameters of the structure as well. The conversion efficiency is defined as the ratio of the power absorbed in the silicon layer with respect to the total incident power. The conversion efficiency was calculated using

$$\eta = \frac{\int_{0}^{\lambda_{g}} \frac{\lambda}{\lambda_{g}} \cdot I(\lambda) \cdot A(\lambda) d\lambda}{\int_{0}^{\infty} I(\lambda) d\lambda}$$
(2)

where λ_g is the band gap corresponding wavelength for the concerned material ~800 nm for a-Si, λ is the wavelength of the incident photon, $I(\lambda)$ is the solar energy density spectrum corresponding to



Fig. 3. Conversion efficiency versus varied periods for different angles. (a) Wavelengths from 300 nm to 600 nm. (b) Wavelengths from 600 nm to 1100 nm. Conversion efficiency versus varied duty ratios for different angles. (c) Wavelengths from 300 nm to 600 nm. (d) Wavelengths from 600 nm to 1100 nm.

the above solar spectrum, and $A(\lambda)$ is the absorption spectrum. It should be noted that equation (2) is defined as the optical-to-electrical conversion efficiency provided that each incident wavelength shorter than the λ_g , which can be trapped by the solar devices, would be converted into one electron-hole pair with the energy corresponding λ_g . In addition, the collection efficiency taking the electronic properties of the material into account is assumed to be 100%. In other words, the internal quantum efficiency is assumed to be 100%.

The duty ratio was chosen as 0.2 based on the discussion of reflectance mention above, then we adjust the angle and the period of the triangular profiles to find out the best design of NWs. In Fig. 3(a), the conversion efficiency was calculated for a spectral range at shorter wavelengths from 300 nm to 600 nm. The dashed line represents the conversion efficiency of a solar cell on a flat substrate. It can be observed that the efficiency is enhanced after adding nanowires, even without grating profile. The incident light at shorter wavelengths would be absorbed quickly by the top region of a-Si, so light trapping is negligible. The improved light trapping is the reason why nanostructures with smaller periods are investigated for enhancement of the conversion efficiency. Moreover, large angle of small periods tends to be a better refractive index matching layer to have higher efficiency than that of larger period. Furthermore, the incident light at longer wavelength from 600 nm to 1100 nm, is shown in Fig. 3(b), showing that flat nanowires have only slight influence on efficiency compared to without nanowires. As shown by the above discussion, the influence of nanowires on absorption is significant mainly for shorter wavelengths. On the other hand, the guantum efficiency of the nanostructure with the larger incline angle and smaller period with larger wavelengths is not enhanced as much as that at shorter wavelengths. When the period of nanowire profiles is larger than 500 nm, influence of the angle becomes more obvious. In contrast to smaller periods, some particular periods, 700 nm for example, act as gratings on the waveguide to guide some specific wavelengths into the absorbing layer. But when the period is larger than specific value, the enhancement drops quickly. In general, the design of larger degrees of angles enhances light conversion efficiency for all range of incident wavelengths and periods. Considered of two parts, we have been mentioned, for the entire spectrum (300 nm-1100 nm), that the conversion efficiency was calculated to be 24.13%, 36.22%, 37.18%, 37.31%, 36.22%, and 32.69% for the



Fig. 4. (a) and (b) Absorption distribution with period of 500 nm, duty ratio of 0.2, and angle of 75° for wavelength of 400 and 720 nm, respectively. (c) and (d) Electronic field distribution of different shapes which from left to right are triangular, tented, and concave, with the wavelength of 720 nm for angle equal to 30 and 80°, respectively.

solar cell on a smooth substrate, and with triangular structures of 60° of period 100, 300, 500, 700, 900 nm, respectively. As result, careful design of the period is necessary considering of both antireflection and diffraction.

Fig. 3(c) shows that the duty ratio smaller than 0.5 enhances conversion more strongly than ratios larger than 0.5 for the wavelength range from 300 to 600 nm, especially for fairly flat $(0-30^{\circ})$ surface. But these flat surfaces did not reduce as much reflection as larger angles did. As a result, when applying smaller duty ratios, whose main influence is to reduce the reflection for high-energy wavelengths, the enhancement of efficiency at small angles can be significant. On the other hand, for duty ratios larger than 0.5, the influence of profile angle due to its better trapping of the shorter wavelengths tends to be more crucial. For the longer wavelengths in Fig. 3(d), a small duty ratio does not have as much influence as shorter wavelengths. After the influence of better enhancement by duty ratio of 0.4, it only changes slightly. Thus the influence of the angle at larger duty ratios tends to become more significant than small ratios. Wavelengths for red and infrared region in the light spectrum passing though the triangle profile would be diffracted into lateral path, so the amount of absorbing material, duty ratio, decides how much light will be absorbed. However, a small duty ratio can form a refractive index matching layer to reduce the reflection and to increase light intensity into the structure for most of the spectrum. This explains why small duty ratios have higher efficiency and why the efficiency does not increase as the duty ratio becomes larger. Furthermore, the angle of triangle profile will influence the best utilization of the diffraction, scattering of light, and reduction of reflectance. In short, if the angle is not large enough, reducing the duty ratio will enhance the efficiency mainly because of anti-reflection. In addition, we can observe that increasing angle of triangular profile can enhance the conversion efficiency for both shorter and longer wavelengths. As the discussed above, by increasing the angle of the profile, the efficiency can be enhanced as well. For example, when the angle is 84°, the efficiency can reach 40.07%, the enhancement 65.15% compared to flat amorphous silicon solar cell.

After discussing the parameters in the profile, we focus on the shapes of the profiles. The absorption distributions of different shapes with the same average nanowire thickness of 1000 nm with period of 500 nm, duty ratio of 0.2, and angle of 75° are shown in Fig. 4(a) and (b). Short



Fig. 5. Conversion efficiency versus angle for triangular, tented, and concave types NWs. Two point at the 0° area are the conversion efficiency of the flat structure with/without NWs, and one point at the 75° is the triangular structure without NWs.

wavelength light absorbed very quickly by the NWs, especially at sharper parts of the profiles. Although the position of higher enhancement differs from one to another, the nanowire profiles have similar influence on the absorption for short wavelength light. However, the concave profile with the small angle has more significant influence than others, because the sharper part of a concave profile with a small angle seems more obvious to reduce reflection. In addition, the absorptance distribution of long wavelength light in the a-Si nanowires appeared in different positions, and the pattern of the absorptance distribution is similar to ripples. The concave profile have higher absorption enhancement since it has the better effective refractive index match between air and NWs.

Fig. 4 shows the electric field distributions in the three kinds of NWs (triangular, tented, and concave). The concave profile shows stronger enhancement of electric field than the triangular profile, especially at the sharpest part, and the tented profile demonstrates the weakest enhancement due to the larger reflectance of the tented NWs almost twice that of the concave NWs.

The conversion efficiency of various type NWs are shown in Fig. 5. We found that the concave profile tends to have higher efficiency than other shapes among varied angles. It can be assumed that the shape with sharp corner, such as the concaved profile, has the better anti-reflection ability, because the gradient of refractive index can reduce the reflectance while the light entering the structure. The refractive index mismatch of the triangular NWs is larger than that of the concave NWs, when the light is transmitting through the interface between air and NWs, and the reflectance of triangular NWs is slightly larger than that of concave NWs. The investigation shows that the optical characteristics match well with the reference data. There is about 28% efficiency in the case of 800 nm thick substrate with a 1000 nm nanowire array [18], which is the same as in our study. The nanowire with periodic shaped profile in our design has the same advantages with the randomlength NW arrays [19], both of which can significantly reduce reflection and enhance absorption. The difference between the random-length NWs and profiled NWs is, the lengths of the randomlength NWs are picked from 1 to 2 μ m with a uniform probability distribution, and the lengths of the profiled NWs are a set of optimized heights. Moreover, the total average thickness in our study of 1500 nm provides higher efficiency, over 33%, for all shapes and using fewer raw materials. Although influence of the shape is not as significant as other parameters, the shapes with sharp corner seem to have better conversion efficiency, which can apply to other PV solar cell designs.

The efficiency enhancement of shaped profile for TM waves is higher than that for TE waves. Considering both TE and TM polarization of light wave, the conversion efficiency of the nanowires with optimized parameters are calculated in Table 1. The efficiency enhancement of shaped profile for TM waves is higher than that for TE waves. In the optimized case under TM polarization condition, the efficiency of NWs having a period of 700 nm, duty ratio of 0.6, and concave shape with 75° profile can reach 40.76%. Compared to the other cases (flat case, flat NW, and period of

| (%) | P = 700 nm, r = 0.2, 75 deg. | P = 500 nm, r = 0.2, 75 deg. | Flat case | flat NW <i>r</i> = 0.6, | P = 700 nm, 75 deg. w/o NW |
|--------------------------------|------------------------------------|------------------------------------|-----------|----------------------------|----------------------------------|
| Conversion efficiency (TM) | 40.6567 | 38.9874 | 24.2652 | 26.9600 | 32.2056 |
| Conversion efficiency (TE) | 36.0324 | 35.54036 | 24.2652 | 26.9400 | 31.5723 |
| Conversion efficiency | 38.3903 | 37.2639 | 24.2652 | 26.9500 | 31.8889 |
| Enhancement of optimal case | - | 3.0227 | 58.2113 | 42.4500 | 20.3875 |

TABLE 1

Conversion efficiency and enhancement of optimal cases

700 nm without NW) in Table 1, the efficiency is improved by 68.165%, 51.209%, and 26.602%, respectively. Finally, the total conversion efficiency of NWs with the optimized parameter (P = 700 nm, r = 0.2, concave shape with 75°) can be improved by 58.21%, 42.45%, and 20.38%, compared to those of the flat case, flat NW, and period of 700 nm without NW, respectively.

4. Conclusion

This study has investigated optical characteristics for the structure of an a-Si thin film with a periodic shaped profile formed by nanowires and optimized parameters including period, duty ratio, and angle of unit cell and the shape of the profile for optimal results of light absorption and conversion efficiency. It is found that smaller duty ratio and period play an important role in decreasing the reflection and enhancing light absorption within the absorber layer, owing to better effective refraction index matching layer and better light trapping mechanism. Furthermore, light trapping is mainly dominated by period and angle. Steeper angles and shaped profiles all enhance efficiency in the solar cell, especially when the profile shapes are sharper. This study compares the efficiency of three designs: flat solar cell without nanowires of 1500 nm of 24.26%, a flat absorbing layer of 500 nm decorated with nanowires of 1000 nm with unvaried height of 27.01%, and a periodic triangular substrate without nanowires of average thickness of 1500 nm of 33.56%. It is found that the light absorption and conversion efficiency are enhanced both for TE and TM waves with the introduction of a periodic shaped nanowire grating in a-Si thin- film solar cells. Finally, the enhancement of conversion efficiency both occurs in TE and TM polarizations. The photovoltaic conversion efficiency of the solar cell with triangular profile can be increased by 58.21%, 42.45%, and 20.38% compared to those with flat surface, equal-thickness nanowires, and periodic triangular textures, respectively.

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