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Role of 2-D periodic symmetrical nanostructures in improving efficiency of thin film solar cells

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ABSTRACT

We systematically investigated several different nanostructures in crystalline silicon (c-Si) thin film solar cells and then proposed a brand-new structure with two dimensional (2-D) periodic dielectric cylinders on the top and annular metal columns on bottom surface to enhance the optical harvesting. The periodic symmetrical nanostructures affect the solar cell efficiency due to the grating diffraction effect of dielectric columns and surface plasmon polaritons (SPPs) effect induced by metal nanostructures at the dielectric–metal interface. About 52.1% more optical absorption and 33.3% more power conversion efficiency are obtained, and the maximum short current reaches to 33.24 mA/cm^2.

1. Introduction

In recent years, solar energy is deeply researched to take the place of conventional energy sources such as fossil oil in the future. The most promising device in sunlight utilization is solar cell which can translate solar energy to electricity directly. Nowadays, c-Si-based solar cells are still playing the most important role in the solar cell products due to the mature manufacturing technology and relatively high conversion efficiency. Facing to the future, thin film solar cells with thinner absorbing layer only about hundreds of nanometers thick are proposed by researchers [1–4]. As we know, the solar cell's efficiency is affected by two important aspects, one is the optical harvesting ability and the other is the charge carrier collection efficiency. The thinner active layer could reduce the production cost and make charge carriers easier to reach the electrodes before recombined. However, light energy in the absorption layer is exponential damping with propagating distance in dielectric materials, so too thin c-Si layer also makes the optical harvesting more difficult and lots of photons escape out of the absorber without being completely absorbed, which cause the loss of light energy. The optical loss in solar cells involves the original light reflection on top surface and the transmission from bottom. To solve this problem, researchers have adopted numerous methods. Various nanostructures are widely applied on solar cells for anti-reflection coatings, light trapping absorbers, back reflectors and so on [5–10]. 1-D sub-wavelength gratings are widely used as the anti-reflection layer in the applications [11], which has been used for ultra-broadband and omnidirectional anti-reflection in many aspects owe to the grating diffraction effects. However, the 1-D structures are limited by the incident polarization, they are more sensitively to transverse magnetic (TM) mode incidence rather than transverse electric (TE) mode, therefore, some 2-D structures such as period photonic crystals are proposed [12–15]. In 2-D periodic nanostructures, the structure is symmetrical, hence, no TE or TM mode needs to be considered when the light is normal incident. Surface plasmon polaritons (SPPs) effect induced by metal nanostructures or nano-particles is also introduced to enhance the optical absorption and solar cell efficiency [16–19]. In order to maximum the solar cell efficiency, we combined the diffraction and SPPs effect together to get more optical harvesting in this article. We proposed some structures to reduce the reflection on the top surface and trapping light energy on the bottom and then compared those 1-D and 2-D periodical nanostructures. We proved the structure with top cylinder and bottom annular column is our best choice and specific explanations on the role of nanostructures is presented. Finite-difference time domain (FDTD) method is used to simulate and optimize the nanostructures in our research.

2. Theoretical model

2.1. Analysis methods

The optical properties of thin-film solar cells including reflection, transmission, absorption and electromagnetic field intensity are evaluated through the finite-difference time domain (FDTD) algorithm. FDTD simulation simply takes Maxwell's equations and

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evolves them over time within some finite computational region, essentially performing a kind of numerical experiment, which is widely adopted for rigorous electromagnetic propagation calculation [20]. The optical position-dependent absorption per unit volume $A(\lambda, \vec{r})$ could be obtained by spatial distribution of the electric field intensity according to, [21]

$$A(\lambda, \vec{r}) = \frac{\omega(\lambda)}{2}\varepsilon_0 \mathrm{Im}(\varepsilon(\lambda)) \iiint \left|E(\lambda, \vec{r})\right|^2 dv, \tag{1}$$

where $\omega(\lambda)$ is the angular frequency of the incoming wave, ε_0 and $\mathrm{Im}(\varepsilon(\lambda))$ are respectively the vacuum permittivity and the imaginary part of material relative permittivity, $E(\lambda, \vec{r})$ represents the electric field intensity.

The global optical absorption measurement of solar cells covers a broad waveband from 300 nm to 1100 nm, where the upper limit corresponding to the band gap of c-Si material, and the average optical absorptivity A is calculated by the following equations:

$$A = \frac{\int_{\lambda\, min}^{\lambda\, max} A(\lambda) I_{AM1.5}(\lambda) d\lambda}{\int_{\lambda\, min}^{\lambda\, max} I_{AM1.5}(\lambda) d\lambda}, \tag{2}$$

where $A(\lambda)$ is the optical absorptance of the whole structure at the incident wavelength λ and $I_{AM1.5}(\lambda)$ is the standard solar irradiance spectrum of AM1.5G, the optical absorption rate is the average value for TE and TM polarizations.

However, the effective absorbed photon energy is larger than the band gap of c-Si, and a photon could produce an electric–hole pair only. The rest energy is transformed to heat, so the optical absorption is not equal to the photovoltaic conversion efficiency. Therefore, to translate the optical absorption ability to electricity performance, we define the maximum achievable short circuit photocurrent density $J_{sc\, max}$ and the maximum real power conversion efficiency η_{max} as: [22]

$$J_{sc\, max} = \frac{e}{hc} \int_{\lambda\, min}^{\lambda\, max} \lambda A(\lambda) I_{AM1.5}(\lambda) d\lambda, \tag{3}$$

$$\eta_{max} = \frac{e \cdot E_g}{hc} \cdot \frac{\int_{\lambda\, min}^{\lambda\, max} \lambda A(\lambda) I_{AM1.5}(\lambda) d\lambda}{\int_{\lambda\, min}^{\lambda\, max} I_{AM1.5}(\lambda) d\lambda}, \tag{4}$$

where e is the elementary charge, h the Planck constant, c the light velocity in vacuum, E_g is the band gap of c-Si fixed at 1.11 eV [23], and we assume the carrier collection efficiency is 1 without considering the surface recombination in this condition.

2.2. Basic structure design

The basic specific structure is shown in Fig. 1, 2-D periodic symmetrical nanostructures are placed on the top and bottom surface. From front to back, the c-Si nanorods, c-Si absorber layer and metal reflector layer with nanostructures. The front nanostructures are introduced as window layer, c-Si nanorods consisting of a square lattice could reduce the original reflection than more light streams into the active layer, meanwhile, the c-Si nanostructures could also absorb parts of solar energy to produce electro–hole pairs. Then, the middle active layer is the core part of solar cell where most of charge carriers are generated. C-Si is chosen as the absorbing material in our research considering the cost and industrial feasibility. On the bottom, silver (Ag) film is widely used due to its excellent reflecting capacity and electroconductibility, and nanostructures consisted of annular column arrays are introduced on it. The metal reflector is used to scatter and reflect light that has not been absorbed by c-Si layer in single-pass absorption back into the active layer for another absorption process. The metal nanostructure also induces SPPs effect on the interface of dielectric and metal materials to trap light in the absorbing layer, extremely improving the optical absorption.

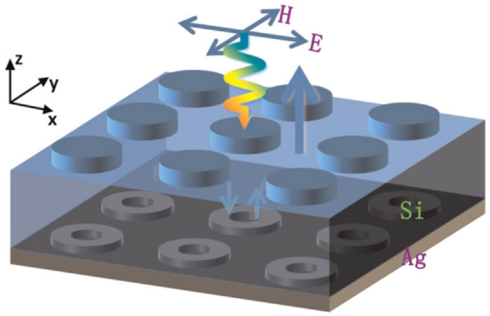

Fig. 1. Specific structure of thin film solar cells with 2-D periodic symmetrical nanostructures on both top and bottom surfaces.

3. Simulations and discussion

In the FDTD numerical simulations, plane waves are normally incident from the top of thin film solar cells, the top and bottom boundary conditions are perfectly matched layer (PML) while periodic conditions are applied in x and y directions. To simplify the simulation, we calculated only one period of the structure. The optimized structure parameters are as follows, the period P is 220 nm, the height of c-Si nanorods h is 100 nm and the diameter d is 154 nm with the fill factor (d/P)0.7. The thickness of active layer t_1 is only 500 nm and $t_2 = 100$ nm is thick enough for silver back reflector to completely eradicate light transmission. The bottom annular column height h_0 is 50 nm, with the same period $P_0 = 220$ nm. The outer diameter $d_{out} = 154$ nm and the inner diameter $d_{in} = 77$ nm with the annular fill factor (d_{in}/d_{out}) is 0.5.

3.1. Antireflection nanostructures

Firstly, we analyze the antireflection function on top surface only. We suppose that the c-Si layer is thick enough for absorption and no light could reflect from back side in this condition. The top reflection on the air and c-Si interface is the first step that light works on solar cells, it directly decides the amount of photons that flow into the active layer. We designed several different nanostructures on top surface, and Fig. 2(a) is the diagram of the surface morphology seen from top, respectively the 1-D gratings, 2-D square nanorods, cylinders and annular columns consisting of square lattice, and the last one is the cylinder arrays with a triangular lattice. Fig. 2(b)–(e) are the comparisons of reflection spectrum results on different nanostructures. Fig. 2(b) compares the reflection on flat film, 1-D gratings and 2-D square nanorods arrays consisting of a square lattice with the same period 220 nm and fill factor 0.7. On the flat film, the reflection follows the Fresnel reflection law, simply related to the real part of material refractive index. When 1-D gratings are induced, the grating diffraction effect reduces the top reflection obviously which are presented by the green and red curves, respectively representing the TM incidence and average value for TE and TM polarizations. The average value is more close to the flat reflection while the TM reflection is similar to the 2-D square nanorods. The results confirm that the polarization dependency of 1-D structures limits the antireflection effect while no polarization needs to be considered in 2-D periodic structures due to the symmetry on x–y plane. Fig. 2(c) is the results of different 2-D structures with square nanorods, cylinders and annular columns consisting of square lattice. We found that the light reflection is sharply dropped from square nanorod to cylinder in the short wavelength range. The cylinder structure