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Role of nanocone and nanohemisphere arrays in improving light trapping of thin film solar cells

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ABSTRACT

A new crystalline silicon solar cell with Si nanocone arrays on the top and Al nanohemisphere arrays on bottom surface were proposed. The light-trapping ability were systematically studied by COMSOL Multiphysics. The nanocone arrays benefit light-trapping by introducing gradient change of refractive index and coupling the incoming light into optical modes. The metallic nanohemisphere arrays affect the light-harvesting by surface plasmon polaritons (SPPs) and scattering effect. The numerical simulations show that the optimal parameters for the periodic nanocone arrays are 350 nm in diameter and 1.1 of the pitch/diameter ratio. The optimal parameters for the nanohemisphere arrays are 160 nm in diameter, 1.3 of the pitch/diameter ratio respectively. Eliminating the Ohmic Loss in metallic nanohemisphere, a 700 nm thick silicon solar cell with the combination of these two nanostructures will contribute an average absorption of 72.928% and a 33.311 mA/cm^2 short circuit photocurrent density in the wavelength of 310–1127 nm.

1. Introduction

With the decreased storage of traditional resources, global energy crisis poses great challenges to our human beings worldwide. Solar energy has successfully attracted the attention in the new energies that emerged, for it's clean, renewable and inexhaustible [1,2]. Solar cells are increasingly popular as they excel at harvesting energy directly from sunlight, and silicon remains a dominant position in photovoltaic cells. The high cost and low conversion efficiency are two main problems for solar cells. The solution lies in improving the conversion efficiency and reducing the cost [3]. Thin film solar cells are more favorable for the better flexibility, lighter weights, cheaper processing and ease of integration. At the same time, they bring the incomplete absorption of the incoming light. The commercial SiNx anti-reflection coating layer (ARC) together with the micrometer-scale random pyramidal texturing creates almost-perfect, broadband ARC effect. However, it's not applicable for thin film solar cells of a several hundred meters [4]. The light trapping in thin film solar cells can be improved by introducing various structures, such as nanostructures at front/back surface, back-reflectors, antireflection coatings, photonic crystals, etc [5,6]. Nanocone is commonly used to boost light harvesting for their unique optical properties and compatibility with inexpensive fabrication techniques [7–10]. Many kinds of nanocones were reported, such as nanocone in truncated and parabola shapes [11]. Surface plasmon polaritons (SPPs) of metal nanoparticles is another popular candidate to trap more light into solar cells. The commonly used method to form metal nanoparticles were evaporation of a thin metal film followed by annealing, which leads to distributed particles with a roughly hemispherical shape. K. R. Catchpole verified that hemispherical particles lead to much higher path length enhancements than spherical particles owing to enhanced near-field coupling [12]. F.J. Tsai pointed out that Al nanoparticles showed the most efficient absorption enhancement among Au, Ag, Al. Compared with other metal particles, Al nanoparticles, with abundant reserves and low price, are more likely to prevent light from escaping and reflecting [13]. But few investigations have explored the combination effect of the nanocone and Al nanohemisphere. In this paper, rigorous optical simulations were carried out by COMSOL Multiphysics to investigate thin film solar cells patterned with nanocone arrays on the top and Al nanohemisphere arrays on bottom surface. The results reveal that the combined nanoastructures dedicate great performance in light trapping and have the potential to be a new alternative in light trapping.

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2. Methods

COMSOL Multiphysics, is a finite element software which is capable of coupling different complicated physical fields into one model. Maxwell equations were introduced to rigorously simulate electromagnetic wave propagation through the models. Periodic boundary condition (PCB) was introduced in the lateral direction of the individual nanoparticle to simulate the inter-particle coupling between neighbor nanoparticles as well as the single particle [14,15]. Standard solar radiation (AM 1.5G) was used. Perpendicular incident light of TE and TM wave were calculated separately and the mean value of the two was regarded as the final results [16]. With the band gap of Si around 1.1 eV, simulations were carried out at the wavelength range of 310–1127 nm with a 5 nm step size. The average optical absorption is labeled as *OA*. The short circuit photocurrent density J_{sc} is defined as [17]

$$J_{sc} = \int_{310\text{nm}}^{\lambda_g} I(\lambda)A(\lambda)\frac{e\lambda}{hc}d\lambda \tag{1}$$

where λ_g is the corresponding wavelength of the Si band gap, i.e. 1127 nm, $I(\lambda)$ is the standard solar irradiance spectrum of AM1.5G, $A(\lambda)$ is the optical absorption of the structure at the wavelength λ, e is the elementary charge, h is the Planck constant, c is the velocity of light in vacuum.

As is schematically depicted in Fig. 1, four kinds of models were devised for comparative analysis. They are solar cells with a traditional 67 nm thick Si_3N_4 ARC layer [15], the nanocone arrays, the nanohemisphere arrays and the combination of these two nanostructures respectively. The corresponding parameters were clearly labeled. *D* was the diameter and its step size was 50 nm. The pitch *P* represented the distance between the centers of two nanostructures. We defined *f* as the ratio of pitch and diameter and its step size was 0.5.

3. Results and discussion

3.1. Analysis of thin film solar cells with nanocone arrays on the top

To investigate the light-trapping property of the nanocone arrays on the top of the cell (Fig. 1(b)), the diameter (*D*) and the ratio (*f*) were varied respectively, from 100 nm to 400 nm for *D* and from 1 to 3 for *f*. The calculated average absorption of per model were shown in Fig. 2(a), different colors represent different absorption rates and the values can be read from color bar the on the right. The better enhancement parameters focus on the diameter range of 300–360 nm and 1–1.2 for the variable *f*. To further optimize the simulation, the step size was altered more precisely, i.e.10 nm for *D* and 0.1 for *f*. The set of parameter, $D=350$ nm, $f=1.1$, $P=385$ nm, were proved to be the best one in this given situation.

It's reported that the high reflection originates from the mismatch between the refractive index of the air and the solar cell [5]. The nanostructures bring forth the gradient change of the refractive index and ease the mismatch between the two refractive indexes, which reduce the reflection on the top and finally promote the absorption greatly [18]. According to the Effective Medium Theory, nanoarray structure can be equivalent to a layer of uniform medium with a refractive index of n_{eff}. Consider the equation below [19]:

$$n_{eff,j} = \left[f_j n_{Si}^2 + (1-f_j)n_{air}^2 + \frac{\pi^2}{3}\left(\frac{P}{\lambda}\right)^2 f_j^2(1-f_j)^2\left(n_{Si}^2 - n_{air}^2\right) \right]^{1/2} \tag{2}$$

where n_{eff} is the effective index of refraction, f_j stands for the filling fraction which can be easily got through the geometrical relationship, n_{si} is the refractive index of silicon at different wavelengths, n_{air} is the refractive index of the air ($n_{air}=1$), *P* is the pitch, λ represents the wavelength of incident light. The effective index of refraction at wavelength of 500 nm is described in Fig. 2(b). Referring to the graph, we know that gradient change of refractive index arises between the thickness of 700–900 nm, where the nanocone array is.

What is more, the nanocone arrays facilitate the incoming light to couple into optical modes in the Si layer. Fig. 3 visualizes the intensity distribution of the time-averaged TE polarized electric field within the models. In Fig. 3(a), obvious interference fringes appear in the Si substrate at 680 nm. The layered distribution of the electric field stems from Fabry–Perot resonance [20]. The field distribution of Fig. 3(b) shows the periodic intensity variations in the Si layer at the wavelength of 795 nm, which is the characteristic of the guided resonances. The guided resonances result from the phase-matched coupling of the normally incident plane and waveguided mode of the Si layer [6].

3.2. Analysis of thin film solar cells with nanohemisphere arrays on bottom surface

Similarly, we investigated the optimal parameters for nanohemisphere arrays on bottom surface (Fig. 1(c)). Referencing to Fig. 4(a), the average absorption varies corresponding to different *D* and *f*. The better enhancement parameters focus on the diameter range of 135–170 nm and 1.3–1.7 for the variable *f*. The absorption value is found to be maximum at 58.015% ($D=160$ nm, $f=1.3$, $P=208$ nm), while its counterpart, solar cell of 700 nm thick with a 67 nm Si_3N_4 ARC reaches to 34.256%.

As the plasmon resonance propagates along the interface between metal and semiconductor, the electromagnetic field is localized at the interface. What is more, it results in large scattering cross sections, even exceeding their geometrical cross sections [21]. The scattering effect of the nanostructures enables the

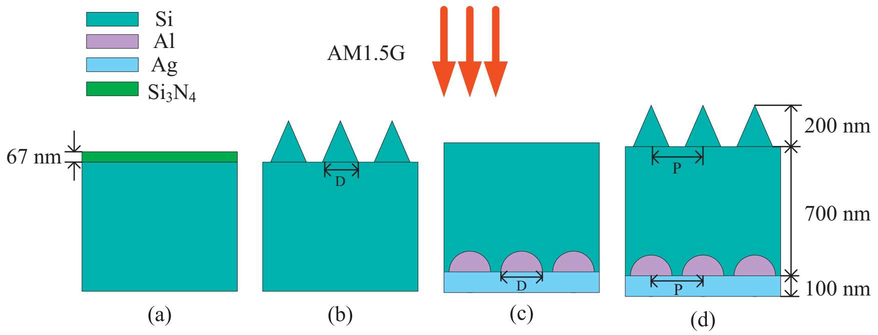

Fig. 1. The 67 nm thick Si_3N_4 ARC on the surface (a), Si nanocone arrays on the top (b), Al nanohemisphere arrays on bottom surface (c), nanocone arrays on the top and Al nanohemisphere arrays on bottom surface(d). The thickness of all silicon substrates is 700 nm.