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Modeling of triangular-shaped substrates for light trapping in microcrystalline silicon solar cells

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ABSTRACT

The influence of triangular grating used as a light trapping structure on the optical wave propagation within thin-film microcrystalline silicon (μc-Si:H) solar cells is investigated. A finite difference time domain (FDTD) approach is used to rigorously solve the Maxwell's equations in three dimensions. We apply two parameters of mean surface roughness (S_a) and slope (k) to define triangular structure and study their influence on the absorption of μc-Si:H. When S_a and k are set to 400 nm and 1, respectively, a largest enhancement of absorption is achieved. The optimum short circuit photocurrent (J_{sc}) of a 1-μm thick μc-Si:H solar cell made on such a textured substrate can reach 27.0 mA/cm^2. The carrier generation rate in the μc-Si:H material is also rigorously analyzed. Finally, we identify some key optical losses in μc-Si:H solar cells and propose for further optimizing the device design.

1. Introduction

Thin-film silicon (TF-Si) based solar cells, for their abundance and nontoxicity of the source materials, flexibility and lightweight, are particularly promising for building integrated photovoltaic (BIPV), household and portable applications [1,2]. The family of TF-Si based solar cells usually includes hydrogenated amorphous silicon (a-Si:H), hydrogenated microcrystalline silicon (μc-Si:H), hydrogenated amorphous silicon-germanium alloy (a-SiGe:H), and associated multi-junction cells. Especially for the μc-Si:H material, it is a well-known material for its narrow bandgap (~1.1 eV) and the low material cost, which has been routinely used as the bottom and middle cell in various multi-junction TF-Si based solar cells [3–7]. But due to its low photo-response in the long wavelength region (600–1100 nm), light trapping is crucial for any μc-Si:H based device to obtain a high photocurrent with reduced thickness. The light trapping performance of a textured substrate can be characterized usually by measuring its reflection and scattering in the far-field. For understanding the nature of light trapping of textured substrate, however, one needs to study the (optical) electrical field and carrier generation rate within the μc-Si:H material. Thus, it is necessary to use numerical methods to solve the Maxwell's equations rigorously.

In this work, a finite difference time domain (FDTD) technique from a commercial FDTD software package (Lumerical Solution, Inc) is used to investigate light propagation in n-i-p type μc-Si:H solar cells fabricated on different triangular grating substrates. The triangular structure is an important structure due to it is resemble to actual surface morphology of various textured substrates used in TF-Si solar cells, such as pyramid-like texture of fluorine-doped tin oxide (SnO_2:F) and boron-doped zinc oxide (ZnO:B) produced by vapor deposition [8,9], crater-like configuration of aluminum doped zinc oxide (ZnO:Al) formed by solution etching technique [10], and textured silver surface formed by high deposition temperature [11]. So, it is valuable to study the influence of triangular grating substrates on the light propagation in μc-Si:H solar cell. Although the triangular gratinged structure has been investigated as a means of light trapping in TF-Si solar cells by optical simulation [12–14], these studies mainly focused on the effect of the triangular structure on the absorption of the μc-Si:H solar cells, with no mention of carrier generation rate distribution and parasitic losses in μc-Si:H solar cells limiting their further optimization.

In this work, we first apply two parameters, the mean surface roughness (S_a) and the slope (k), to define triangular structure and look into the effect of S_a and k on the electric field intensity distribution and absorption of a μc-Si:H solar cell in order to determine the optimal surface geometry. Next, the carrier generation rate in the μc-Si:H absorber under AM 1.5G illumination is calculated over the triangular region. Finally, the optical losses in the solar cell are analyzed and some key losses are identified for further optimizing the device design.

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2. Optical simulation model

Fig. 1(a) and (b) show the cross section of a n-i-p μc-Si:H solar cell deposited on a smooth and a periodic triangular textured substrate, respectively. The configuration of the μc-Si:H solar cell consists six layers: from bottom to top, Ag acting as the conducting and reflection coating layer, a 50 nm ZnO:Al as the dielectric layer, a 20 nm n-μc-Si:H doping layer, a μc-Si:H intrinsic layer, a 10 nm p-μc-Si:H doping layer, and a 70 nm indium tin oxide (ITO) layer acting as the conducting and antireflection coating layer. In this study we define two parameters, i.e. S_a and k in a rectangular coordinate system to describe the triangular surface (See Fig. 1(b)). S_a denotes the roughness of triangular substrate, calculated using the following equation,

$$S_a = \frac{1}{l}\int_0^l kxdx \tag{1}$$

where k is the slope of the triangular surface characterizing the openness of the triangular surface morphology, and l is the shadow length of half period triangular surface on x axis. S_a is varied from 200 nm to 500 nm at an interval of every 100 nm, and k takes four values of 0.5, 1, 2 and 4 respectively.

The wave propagation in a μc-Si:H solar cell is simulated using FDTD. The unit cell surrounded by the orange dashed line in Fig. 1 (b) is selected as the configuration in simulation. The plane wave illumination, as shown in red arrows, is used to simulate the incidence at a normal angle with the amplitude of the incident wave being fixed at 1 V/m. Both upper and lower boundaries used in the simulation are perfectly matched layers (PMLs) while periodic boundary conditions (PBCs) are used for the vertical boundaries.

The real part of refractive indices $n(\lambda)$ and extinction coefficient $k(\lambda)$ of ITO [15], ZnO:Al [16], μc-Si:H [17], n-μc-Si:H [17], p-μc-Si:H [17] and Ag [18] are taken from previous papers. The imaginary part of the permittivity $\varepsilon''(\lambda)=2\varepsilon_0 n(\lambda)k(\lambda)$, where ε_0 is the vacuum dielectric constant. The simulation range is from 350 nm to 1100 nm.

3. Results and discussion

To find out the light trapping performance of different substrates, the cross-section of electric field profiles in a unit cell of the μc-Si:H layer of 1-μm thick for wavelength 800 nm is calculated and displayed in Fig. 2. Fig. 2(flat) shows the field profiles on the flat back reflector (BR). Due to low absorption coefficient of μc-Si:H for longer wavelength, a large fraction of light is reflected from BR and leading to the formation of standing wave in μc-Si:H layer. On textured substrates, however, the optical field intensity varies greatly according to the roughness and the shape of triangles.

As is seen from Fig. 2(a)–(d) where S_a is kept at 200 nm but with varying k values. When k =0.5 (Fig. 2(a)), the electric field is much stronger than other three cases, owing to the enhancement of scattering and diffraction. As the slope increases from 0.5 to 4.0, the field strength decreases noticeably. When k reaches 4, there is almost no scattering enhancement in the μc-Si:H absorber layer. For a higher surface roughness S_a of 400 nm, the electric field shows an interesting change with the slope k. It increases first (Fig. 2(e)), reaching a maximum (Fig. 2(f)), and then decreases (Fig. 2(g)-(h)). At k=4, the field strength is the smallest with compared to other three cases. Apparently, the light scattering and diffraction are much weaker in this case.

With the established electric field parameters, we can now calculate power absorption P_{abs}, which is calculated from the following equation,

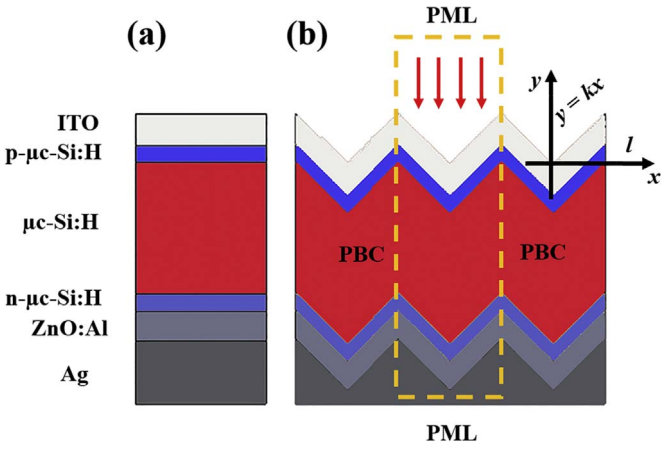

Fig. 1. Schematic sketch of a μc-Si:H n-i-p solar cell (a) on a flat back reflector and (b) with periodically triangular textured substrate. The unit cell surrounded by the orange dashed line in (b) is selected as the configuration in simulation. S_a can be calculated using Eq. (1) in a x-y rectangular coordinate system as show in (b). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

$$P_{abs} = \frac{1}{2}\int_V \omega(\lambda)|E(\varphi,\lambda)|^2\varepsilon''(\lambda)dV \tag{2}$$

where λ is wavelength, $\omega(\lambda)$ the angular frequency of incident light, $\varepsilon''(\lambda)$ the imaginary part of the permittivity, φ the space coordinate and $E(\varphi,\lambda)$ the electric field. The optical absorbance of μc-Si:H can be then obtained by P_{abs}/P_{in}, where P_{in} is the total incident power. Fig. 3(a)–(d) shows the simulated absorbance spectra in the 1-μm thick μc-Si:H layer for different S_a and k values. For comparison, the absorbance for the case of the specular substrate is also presented. It is seen that, in the short wavelength region (350–600 nm), the μc-Si:H absorber shows the lowest absorbance on the flat Ag/ZnO:Al substrate, caused by lack of light trapping. When k is increased from 0.5 to 4.0, the absorbance increases in all four different S_a cases.

On the other hand, in the long wavelength region (600–1100 nm), the absorbance curves show a more complicate behavior. It is seen from Fig. 3(a) that, where S_a=200 nm, the absorbance decreases with increasing k from 0.5–4. As S_a increases (Fig. 3(b)–(d)), the average absorbance of μc-Si:H reaches a maximum at k=1. In general, the absorbance on all textured substrates is higher than that on the flat BR.

In order to compare the enhancement of μc-Si:H cell absorption accurately at different triangular substrates, the short circuit current density, J_{sc}, is then calculated from the absorbance P_{abs}/P_{in} assuming 100% carrier collection by the following equation

$$J_{sc} = e\int \frac{\lambda}{hc}\frac{P_{abs}}{P_{in}}I_{AM1.5}d\lambda \tag{3}$$

where $I_{AM1.5}$ is the reference solar spectral irradiance, h the Plank constant, and c the speed of the light.

Fig. 4 shows the J_{sc} calculated as a function of k for varying S_a over a wavelength range of 350–1100 nm. The J_{sc} for a flat substrate is represented as the dash line in graph. As it is seen from Fig. 4, regardless of S_a, the J_{sc} initially increases as k increases from 0.5 to 1 and reaches a maximum at k=1. It then decreases with further increasing k. It is interesting to note that variation of J_{sc} with k is affected by S_a. When k is below 1, the J_{sc} decreases with increasing S_a. However, for $k \geq 1$, the J_{sc} exhibits an increase with increasing S_a from 200 nm to 400 nm, it then decreases for $S_a > 400$ nm. When S_a and k reach 400 nm and 1 respectively, the highest J_{sc} of 27.0 mA/cm^2 is achieved in μc-Si:H, which is an enhancement by 7.1 mA/cm^2 (or a relative increase by 35.6%) in