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# Optical properties of a grating-nanorod assembly structure for solar cells



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## ABSTRACT

This paper proposes a grating-nanorod assembly structure that can be applied to silicon solar cells. The optical properties of the assembly structure are examined by applying the finite difference time domain method in the 300–1100 nm wavelength region, where the average spectral absorptance of the structure can reach 0.955. This high absorptance is attributed to guided mode resonance and microcavity effect. The transient and steady-state magnetic field distribution of the structure reveals the underlying mechanisms of such extraordinary phenomena. Absorptance is further investigated at different diameters and lengths of the nanorod component. The effects of incident angle on absorptance are also discussed. The solar cells of the structure can yield an optimum conversion efficiency of 25.91%. Thus, the proposed structure can be applied to silicon solar cells.

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## 1. Introduction

Solar photovoltaic technologies have been extensively investigated because of their potential in solving energy crises and environmental problems. Solar cells have been applied since the 1950s [1]. Many kinds of solar cells with increasing absorptance and conversion efficiency have also been explored over the past 50 years [2–5]. With unique effects, micro-nano structures are usually applied to enhance the absorptance and conversion efficiency of solar cells [6,7]. For instance, solar cells of a silicon material are often used for practical applications because of their low costs and convenient manufacturing. With the development of micro-nano technology, micro-nano structures of solar cells have been examined to improve solar energy absorption. Grating and nanowire are two commonly used micro-nano structures applied to solar cells.

The optical properties of the grating structure of solar cells have been numerically investigated in the visible and near-infrared spectrum regions [8–10]. One-dimensional gratings have also been explored to achieve high absorptance by using a rigorous coupled wave analysis (RCWA) method and a finite difference time domain (FDTD) method [11–13]. The absorptance is then enhanced by guided mode resonance, slow Bloch mode resonance, or other types of resonance. To increase absorptance, researchers examined gratings with sidewalls and periodic grating defects and proposed

dual and complex gratings [6,14–17]. The increased absorptance is attributed to the ability of grating sidewalls and defect positions to trap more light and to exhibit microcavity resonance.

The optical properties of solar cells have been improved with a nanowire structure. The optical properties of silicon nanowire solar cells have also been investigated by employing transfer matrix method (TMM) and by applying effective medium theory [18–20]. Likewise, the optical properties of nanowires with different parameters and structures have been examined with TMM, RCWA, and finite element method [21–25]. The increased absorptance can also be attributed to multiple scattering, wave interference, coupling effects, wave-guided resonance, Fabry-Perot resonances [26], and Bloch resonance modes. A novel dual-diameter nanopillar with a high absorptance in certain wave regions has been proposed to improve further the performance of the nanopillar structure; high absorptance can be achieved through waveguide excitation [27]. In addition, optical properties of silicon and ZnO/CdTe core/shell nanowire arrays are compared to obtain the largest short-circuit current density [28].

To increase the absorptance of a broadband, Geldmeier et al. [29] developed a grating-nanocube assembly by employing multiple-plasmonic resonance. A multiplicative enhancement is attributed to two resonances that demonstrate a high average absorption, as calculated by the FDTD method. The cylinder-annular hybrid nanostructure is proposed to improve efficiency of solar cells [30]. Other composite structures [31,32] have also been investigated. Grating and nanowire exhibit a high spectral absorptance in different wave bands. A grating groove is usually hundreds of nanometers in depth, and a nanowire is commonly thousands of nanometers in length.

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An assembly structure that combines one-dimensional grating at the bottom with the nanorod at the top is proposed in this study to cover the surface of silicon solar cells and thus achieve high absorbance and reduce the surface thickness of solar cells. The optical properties of the assembly structure are investigated in the 300–1100 nm wave region by using the FDTD method. The absorbance and conversion efficiency of the assembly, grating, and nanorod structures are compared to demonstrate the improved performance of the assembly structure. The spectral absorbance of the assembly structure is then examined on the basis of different diameters and lengths of the nanorod component. The effects of different incident angles on the absorbance of the assembly structure are also explored.

## 2. Geometric model and theory

### 2.1. Geometric model

Fig. 1 shows the silicon grating-nanorod assembly structure on a semi-infinite silicon substrate for solar cells. The one-dimensional grating with vertically aligned nanorods at the top is located on the substrate. The periods of grating and nanorod structures are equal to  $\Lambda$ . The grating width and depth are denoted by  $W$  and  $h$ , respectively. The nanorod diameter  $d$  and length  $L$  vary across time, but the cross-sectional center of the nanorod remains in the middle of the grating ridge. The filling ratios of the grating structure and the nanorod structure are defined as  $f_1 = W/\Lambda$  and  $f_2 = \pi d^2/(4\Lambda^2)$ , respectively. The optical properties of the assembly structure are investigated by using the FDTD method in the 300–1100 nm wave region. The boundary conditions are periodic in the  $X$  and  $Y$  directions, and perfectly matched layer in the  $Z$  direction in the three-dimensional FDTD simulation. Note that the semi-infinite silicon substrate could be assumed to be  $150 \mu\text{m}$ . Because the transmittance of silicon bulk with thickness of  $150 \mu\text{m}$  is negligible in wavelength range from 300 to 1100 nm. Even if the thickness of silicon bulk is  $100 \mu\text{m}$ , the transmittance is less than 0.01 in most wavelength range. In addition, the substrate thickness is  $160\text{--}240 \mu\text{m}$  for most standard crystalline cells [33]. And the thickness of substrate has little effect on the physical mechanisms occurring in the grating and nanorod components.

The manufacture of grating-nanorod assembly structure is similar to that of grating-nanocube assembly [29]. The grooves in a silicon substrate are first manufactured by using electron beam

lithography. After that, a filling layer is crammed into grooves of gratings. Furthermore, silicon nanorods are synthesized by using growth catalyst Au, vapor-liquid-solid (VLS) method [34] on gratings in which the large-area silicon wire arrays can be vertically created in precisely size and position [35,36]. Finally, the filling layer of grooves in gratings is rinsed.

### 2.2. Conversion efficiency

In order to quantify the overall absorption performance of solar cells with different micro-nanostructures in the solar spectrum, the conversion efficiency is calculated. Here the conversion efficiency is defined as the ratio of the electric power out cell with respect to the total incident power. The conversion efficiency is calculated as follows [37]:

$$\eta = \frac{V_{oc} J_{sc} FF}{P_{in}} \quad (1)$$

Where  $V_{oc}$  is open-circuit voltage,  $J_{sc}$  short-circuit current density,  $FF$  fill factor,  $P_{in}$  the power from the sun light incident on the solar cell on unit area. We assume that each photon absorbed by solar cell surface can only produce one electric-hole pair. One of these photons contributes only an energy equal to the energy gap to produce one electric-hole pair.

The short-circuit current density  $J_{sc}$  can be given [38]:

$$J_{sc} = q\Phi \quad (2)$$

Where  $q$  ( $> 0$ ) is the electron charge,  $\Phi$  is the photon flux corresponding to AM1.5 standard [39], the latter parameter is related to the absorbance, structure and material of solar cell and incident spectrum. The energy incident to the surface of solar cells cannot be completely absorbed due to reflection, so the spectral irradiance needs to be modified by the absorbance. Note that the absorbance, within nanorod, grating and substrate, is obtained from  $\alpha = 1 - R$  where  $R$  is reflectance obtained by the FDTD method, and the transmittance can be negligible due to the infinite substrate. In addition, the surface recombination is not considered by assuming the carrier collection efficiency to be unity.

For the ideal solar cell, the open-circuit voltage  $V_{oc}$  can be obtained by using the short-circuit current density  $J_{sc}$  and the dark saturation current density  $J_0$  [38]:

$$V_{oc} = \frac{kT_c}{q} \ln \left( 1 + \frac{J_{sc}}{J_0} \right) \quad (3)$$

Where  $k$  is the Boltzmann constant (unit is J/K),  $T_c$  is solar cell temperature that is assumed to be equal to the ambient temperature (i.e., 300 K).

The dark saturation current density is given by a semi-empirical expression:

$$J_0 = 1.5 \times 10^9 \exp \left( -\frac{E_g}{k_B T_c} \right) \quad (4)$$

Where  $k_B$  is the Boltzmann constant (unit is eV/K),  $E_g$  is the energy gap of silicon that is 1.12 eV in the ambient temperature.

For the ideal solar cell, the fill factor  $FF$  depends only upon  $\nu_{oc} = V_{oc}/(kT_c/q)$  when  $\nu_{oc} > 10$ . It is given by an approximate expression with an excellent accuracy [1]:

$$FF = \frac{\nu_{oc} - \ln(\nu_{oc} + 0.72)}{\nu_{oc} + 1} \quad (5)$$

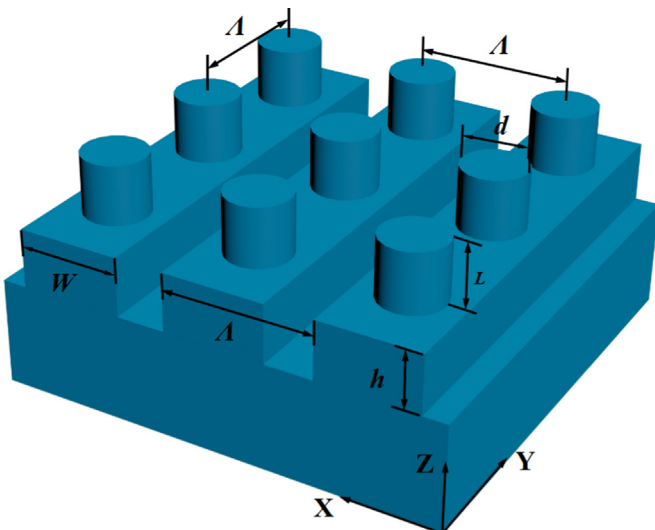


Fig. 1. Schematic of the grating-nanorod assembly structure.

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