Journal of Quantitative Spectroscopy & Radiative Transfer 133 (2014) 579–588

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

Radiative behaviors of crystalline silicon nanowire and nanohole arrays for photovoltaic applications

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ARTICLE INFO

Article history:
Received 20 May 2013
Received in revised form
21 August 2013
Accepted 19 September 2013
Available online 25 September 2013

Keywords:
Radiative property
Nanowire
Nanohole
RCWA
Photovoltaic application

ABSTRACT

The optical absorption of four square arrays of crystalline silicon nanostructures, i.e., circular nanowire array, circular nanohole arrays, square nanowire arrays, and square nanohole arrays, are numerically investigated. The method of rigorous coupled-wave analysis (RCWA) is employed to calculate the absorptivity for the arrays with lattice constant from 100 nm to 1500 nm. The results indicated that the lattice constant is the foremost structural parameter to determine the ultimate efficiency, and the peaks of ultimate efficiencies for the four different nanostructures always appear around the lattice constant of 600 nm. It demonstrates that square nanowire arrays and circular nanohole arrays have great potentials for photovoltaic applications with high ultimate efficiencies and low filling ratios. Moreover, high ultimate efficiencies of all structures can be maintained over a large range of incident angles.

1. Introduction

More and more researchers are convinced that better nano and microphotonics design for photon management inside the solar cell is the key challenge and has a great potential for cost-effective photovoltaic energy conversion [1–5]. As an abundant element on the Earth, silicon is nontoxic and compatible with the semiconductor manufacturing technology [6,7]. Currently, 80–90% of the photovoltaic market is based on crystalline Si solar cells [8,9]. The usage of expensive silicon wafers accounts for more than 40% of the cost of a solar module [8,10,11], which impels the development of the thin film solar cell for reducing material cost. New designs and technologies have been proposed to make up for the relatively low absorption due to smaller thickness, and nanowire arrays and nanohole arrays are one of the most promising ways to address the above issue.

The nanowire arrays have become potential structures for photovoltaic applications since Atwater established the physical model of radial p–n junction nanowire solar cells, in which large aspect-ratio of the structure keeps both large absorption along the incident direction and efficient collection of photon-generated carriers [12]. Hu and Chen [13] first numerically investigated the absorption enhancement in Si nanowire arrays. Their results showed that the nanowire arrays have much lower reflectivity than thin films, while higher absorptivity only occurs in the high-frequency regime (>2 eV). The weak absorption in low frequency (<2 eV) can be attributed to the unusually small nanostructures adopted in their simulations, in which diameters of nanowires are from 50 nm to 80 nm and the lattice constant is fixed at 100 nm. Li et al. [14] numerically optimized the nanostructures of Si nanowire arrays. In their model, the nanowire arrays are based on Si thin film that participates in the multi-reflection and absorption. The results predicted that the ultimate

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http://dx.doi.org/10.1016/j.jqsrt.2013.09.021

efficiency (absorption over the whole incident spectrum) reaches the peak when the lattice constant is around 500 nm. The role of the lattice constant on absorption for nanowire arrays was examined by Lin and Povinelli [7]. The ultimate efficiency increases with the lattice constant from 100 nm to 600 nm, and they interpreted the phenomenon by using the excitation of guided resonance modes in nanowires with large lattice constants. However, the above interpretation cannot properly explain the decline of absorption when the lattice constant gets larger than 600 nm [14,15]. Apart from the aforementioned numerical studies, some experiments have been carried out, and the results also verified the high conversion efficiencies of the nanowire arrays for photovoltaic applications [16–19].

On the other hand, the nanohole arrays (the counterpart of the nanowire arrays) have also received much attention recently. Han and Chen [20] manifested better spectral absorption of circular nanohole arrays than the nanowire arrays, and this is further supported by more numerical studies [21–25] and experimental observations [23–25].

Apart from the above studies for circular nanostructures, Xiong et al. [21] studied the absorption of square nanowire arrays with square nanohole arrays, and the results showed that the square nanohole arrays exhibit higher absorption. Radiative properties of square nanohole arrays and the hybrid nanowire–nanohole arrays (in which nanowires are distributed in each square nanohole) have been studied by Wangyang et al. [15], and results have shown that nanostructures have higher absorption than Si film.

Even though some works have been carried out, the research is still at infant stage, and results are far incomplete to draw a conclusion. The research progress in the nanostructure arrays benefits from the improvement of nano- and micro-processing technology as well as the ability of computers [26]. The previous research on nanowire and nanohole arrays mainly concentrated on small lattice constants (<600 nm) [7,13,15,17–21,24,25,27–29]. Now the processing technology to make silicon nanostructure arrays [16,23,30–33] with large lattice constants has become available, and this warrants the study to examine the relationship between lattice constants and the optical behavior, particularly for the larger lattice constants. Also, square nanostructure arrays are rarely studied in the open literatures, but how the shape (square or circular) of nanostructures influences the optical absorption needs to be answered. In addition, large angle tolerances of the nanowire and nanohole arrays were demonstrated by some researchers [7,13–15,20], however, the underlying physical behaviors are not discussed in any published papers, particularly for the phenomenon of the optical absorption enhancement within a small incident angle. Furthermore, the reason why the optical absorption strongly depends on polarization of the incident wave in the large incident angle needs to be studied. In this paper, the optical behaviors of four different nanostructures are investigated. Parametric analysis has been performed for the radiative properties, namely, the effects of lattice constants, shape of nanostructures, incident angle and polarization, which have been examined and discussed. Finally, this paper predicts ideal candidate nanostructures with high absorption, low filling ratio and a large angle tolerance for a great potential in solar energy harvesting.

2. Models and method

Fig. 1 illustrates models of square lattice periodic arrays to simulate in this paper, which include square nanowire arrays (a), square nanohole arrays (b), circular nanowire arrays (c) and circular nanohole arrays (d). The incident light illuminates the *xy*-plane, as the gray arrows shown in Fig. 1. Nanostructures consist of square nanowires and nanoholes with width w, respectively, while circular nanowires and nanoholes with diameter d. The period of square lattice is called lattice constant L and it varies from 100 nm to 1500 nm. The thickness of nanostructures h is fixed at 2.33 μm, since the value is compatible with the thickness of thin silicon solar cells [34,35] and it would be convenient to compare our results with Refs. [7,13,15,21]. Filling ratio of nanostructures is defined as

$$f_{\mathrm{SNW}}=\frac{w^2}{L^2},\ f_{\mathrm{SNH}}=1-\frac{w^2}{L^2},\ f_{\mathrm{CNW}}=\frac{\pi d^2}{4L^2},\ f_{\mathrm{CNH}}=1-\frac{\pi d^2}{4L^2} \tag{1}$$

where subscripts SNW, SNH, CNW and CNH stand for square nanowire arrays, square nanohole arrays, circular nanowire arrays and circular nanohole arrays, respectively. Here filling ratio varies from 0.22 to 0.78 by considering the minimal filling ratio (when d is equal to L for circular nanohole arrays) and the maximal filling ratio (when d is equal to L for circular nanowire arrays).

The optical constants of crystalline silicon used in this paper is illustrated in Fig. 2(a) [36]. It is convenient to neglect the difference of optical constants between the doped silicon and the intrinsic silicon if both p-type and n-type regions are lightly doped at frequencies above the band gap [37]. The calculated frequency range is from 1 eV to 4 eV by the consideration of the band gap of crystalline (1.1 eV) and the ASTM air mass 1.5 direct and circumsolar spectrum in Fig. 2(b) where the spectral irradiance is negligibly small above photon energy 4 eV [38]. The ultimate efficiency for evaluating the optical absorption across the whole solar spectrum is given by [39]

$$\eta=\frac{\int_{311\ \mathrm{nm}}^{\lambda_g} I(\lambda)A(\lambda)_{\lambda_g}^{\lambda}\mathrm{d}\lambda}{\int_{311\ \mathrm{nm}}^{4000\ \mathrm{nm}} I(\lambda)\mathrm{d}\lambda} \tag{2}$$

where λ is the wavelength, $I(\lambda)$ is the spectral irradiance of AM 1.5 direct and circumsolar spectrum, $A(\lambda)$ is the absorptivity and $\lambda_g=1130$ nm is the wavelength corresponding to the band gap. The lower limit 311 nm of integral corresponds to the maximal photon energy 4 eV, and the upper limit 4000 nm of integral in the denominator is the maximal wavelength available in the table of AM 1.5 solar spectrum.

There are different numerical methods for calculating the reflectivity, absorptivity and transmittivity of periodic arrays such as transfer matrix method (TMM) [7,13,20,21], finite-difference time-domain method (FDTD) [24,25,29], rigorous coupled-wave analysis (RCWA) [15,27], finite element method (FEM) [14,40,41] and discrete dipole