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Anisotropic optical properties of silicon nanowire arrays based on the effective medium approximation

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ABSTRACT

In search of next-generation solar cells, silicon nanowire arrays have attracted great attention since they are cost-effective and may absorb more light compared to current thin-film silicon solar cells. Theoretical studies using finite-difference time-domain and transfer matrix methods have been performed to investigate the optical properties of silicon nanowire (SiNW) arrays. However, these methods are computationally intensive and require periodic conditions, which may not be satisfied with most fabricated samples. In the present study, an effective medium analysis considering the anisotropic nature of vertically aligned SiNWs is performed to study their optical properties in the wavelength range from 310 nm to 1100 nm, which is of the most importance for solar photovoltaic cells. The effective dielectric functions of the SiNW layer for both ordinary and extraordinary waves are obtained from the Bruggeman approximation. Thin-film optics formulae incorporating the anisotropic wave propagation in uniaxial media are employed to calculate the reflectance and absorptance of the SiNWs on silicon substrates for different polarizations. The effect of geometric parameters such as filling ratio and wire length is investigated. In addition to modeling the directional radiative properties at various angles of incidence, the hemispherical properties are also calculated to understand the light absorption and to facilitate the optimal design of high-performance SiNW solar cells.

1. Introduction

Silicon nanostructures hold promise for achieving higher conversion efficiencies over traditional silicon photovoltaic cells due to enhanced light trapping and photo-carrier collection [1–4]. Arrays of silicon nanowires (SiNWs) have been investigated by researchers owing to the potential of cutting down the cost of solar cells by using less materials and inexpensive fabrication techniques, which could make the implementation of the solar cells at large scale possible [5–7]. Moreover, the potential of achieving high absorption and low reflection with polarization-insensitive, broadband, and omnidirectional characteristics makes SiNWs extremely attractive for harvesting solar energy [8]. Intensive research activities have been devoted to theoretically studying the effect of geometric parameters on the optical properties of SiNWs using the transfer matrix method (TMM) [9,10] and finite-difference time-domain (FDTD) technique [11–13], because both methods could consider the wave effects in SiNWs by solving full-wave vector Maxwell's equations. Hu and Chen [9] numerically modeled the optical absorption of a free-standing periodic SiNW array and found higher absorption in a high-frequency regime compared with thin-film counterparts. Han and Chen [10] designed an asymmetric tapered two-dimensional grating structure, whose absorption approaches the Lambertian limit at normal incidence. Lin and Povinelli [11] reported that significant optical absorption enhancement occurs when the lattice constant is varied from 100 nm to 600 nm with a fixed filling ratio of the SiNWs. Wang and Leu [12] demonstrated enhanced absorption and efficiencies in the silicon nanocone structures over SiNWs with uniform diameters. Bao and Ruan [13] found that the optical absorption in disordered SiNW arrays can be enhanced significantly with random diameter or length but slightly with random position. Recently, Zhang and Ye [14] performed a survey on the silicon nanowire and nanocone structures for solar photovoltaic applications.

In general, TMM and FDTD methods are computationally intensive and require periodic structures, which may not be satisfied with most fabricated samples. On the other hand, effective medium

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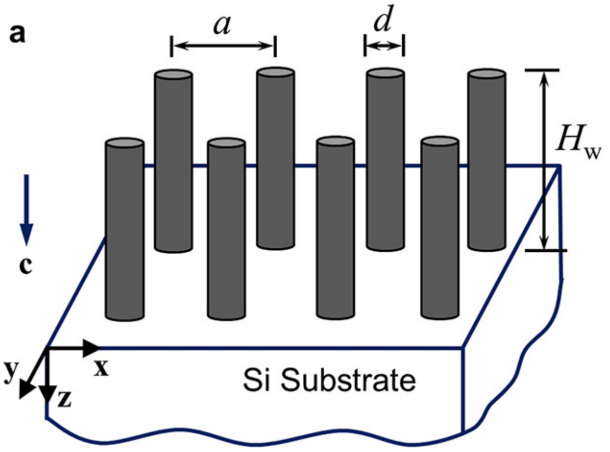
theory (EMT) allows for a rapid first-order prediction [15–17], and has been used to study the optical properties of vertically aligned carbon nanotubes [18–20]. The anisotropic wave propagation has been studied with the aid of EMT inside different uniaxial media such as arrays of inclined metallic nanorods [21,22].

The present work aims at studying optical absorption of SiNW arrays on Si substrates using EMT and an anisotropic optical model. The effective dielectric functions of the SiNW arrays for both ordinary and extraordinary waves are calculated with the Bruggeman approximation. Thin-film optics formulae incorporated with anisotropic wave propagation in uniaxial media are employed to calculate the reflectance and absorptance of the SiNW arrays on silicon substrate for different polarizations. The effects of geometric parameters on the optical properties are discussed. The directional behavior of the absorption is investigated for both polarizations, and the spectral hemispherical absorptance of the composite structure is also presented.

2. Theoretical model

2.1. Effective medium theory

Consider a layer of vertically aligned SiNW array with a thickness of H_w on a semi-infinite Si substrate, as shown in Fig. 1(a). The average spacing between SiNWs is a, and the diameter of each SiNW is d. The medium surrounding the SiNW is air. The volume filling ratio f is given by $f = \pi d^2/(4a^2)$. It should be noted that the assumption that the Si substrate can be treated as opaque is a good one because the penetration depth of Si is usually small, except at wavelengths close to the indirect bandgap (around 1.1 μm wavelength). EMT is a homogenization method for characterizing the optical properties of an inhomogeneous medium with different material constituents based on the field average method [15]. The basic assumption is that the characteristic geometric dimensions are much smaller than the wavelength of the electromagnetic waves. Therefore, as long as the nanowires are vertically aligned and the diameter is much smaller than the wavelength, the variations in diameter and spacing do not affect the predicted dielectric function for fixed filling ratio (f). This is very different from the full-wave simulation, which assumes periodic geometries and identical diameters of the SiNWs. The interest of this study is to determine the radiative properties of the effective homogeneous SiNW layer, as illustrated in Fig. 1(b), to be discussed in Section 2.2.



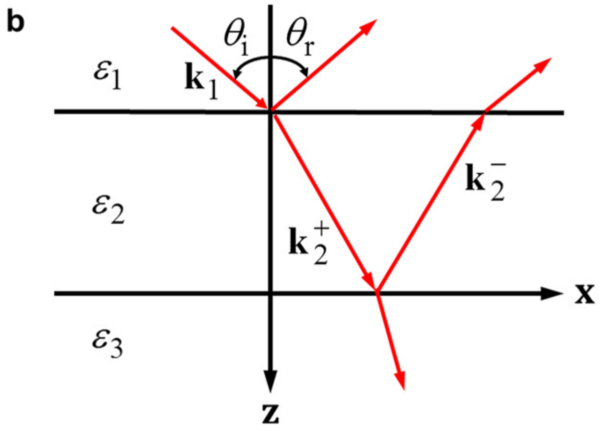


Fig. 1. (a) Schematic of the SiNW array on a silicon substrate, noting that "**c**" stands for the optical axis; (b) depiction of wave propagation in a three layer structure used in the model, where medium 2 is a uniaxial medium whose optical axis is parallel to the z axis.

The Maxwell–Garnett (MG) [16] and Bruggeman (BR) [17] approximations are two effective medium theories that are widely used. The MG approximation assumes one constituent as the host and all other constituents as embedded grains that are spatially separated, and therefore, it is valid for dilute systems (i.e., low volume fractions of the filling constituents). On the other hand, the BR approximation treats all constituents equally as grains imbedded in an otherwise homogenous "effective" medium which is assumed to possess the average properties of the composite. Due to the relatively large volume fractions considered, the BR approximation is adopted in the present study. The effective dielectric function ε_eff of the SiNW layer can be calculated by solving [15].

$$\frac{(1-f)\left(\varepsilon_\mathrm{air}-\varepsilon_\mathrm{eff}\right)}{\varepsilon_\mathrm{eff}+g\left(\varepsilon_\mathrm{air}-\varepsilon_\mathrm{eff}\right)}+\frac{f\left(\varepsilon_\mathrm{Si}-\varepsilon_\mathrm{eff}\right)}{\varepsilon_\mathrm{eff}+g\left(\varepsilon_\mathrm{Si}-\varepsilon_\mathrm{eff}\right)}=0 \tag{1}$$

where ε_air and ε_Si are the dielectric functions of air and bulk Si, respectively. The depolarization factor g in Eq. (1) depends on the geometry and polarization. Assuming that the length-to-diameter aspect ratio, H_w/d, is greater than 20, the SiNWs can be treated as infinitely long. In this case, $g_\mathrm{E}=0$ and $g_\mathrm{O}=0.5$, where the subscripts "E" and "O" represent extraordinary and ordinary waves, respectively [21]. Therefore, the effective dielectric function depends on the polarization of the incident plane waves. Such a uniaxial medium can be characterized by two major dielectric functions: one is the extraordinary ε_2E (when the electric field is parallel to the optical axis) and the other is the ordinary ε_2O (when the electric field is perpendicular to the optical axis). Both of them are complex and wavelength-dependent. Usually, lightly doped crystalline Si is used in solar cell applications. The dielectric function of single-crystal Si is obtained from the optical constants using the updated table and equations in Vol. 3 of Palik's handbook series [23].

2.2. Wave propagation in a uniaxial medium

Fig. 1(b) schematically illustrates the wave propagation through a uniaxial layer for either polarization as well as multiple reflections occurring in medium 2. The incidence is from air (medium 1) and note that medium 3 is assumed to extend to infinity. As mentioned previously, the nanowire array can be treated as a uniaxial medium whose optical axis **c** is parallel to the z axis. Wave propagation inside the uniaxial layer (medium 2) is different for different polarized incident waves [21,22]. For s-polarized incident waves or TE waves, the electric field **E** is perpendicular to