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Modeling and optimizing the performance of plasmonic solar cells using effective medium theory

M. Piralaee [a,b], A. Asgari [a,c], V. Siahpoush [a]

[a] Research Institute of Applied Physics and Astronomy, University of Tabriz, Tabriz, 51665-163, Iran
[b] Photonics Group, Aras International Campus, University of Tabriz, Tabriz, Iran
[c] School of Electrical, Electronic and Computer Engineering, University of Western Australia, Crawley, WA 6009, Australia

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ABSTRACT

In this paper, the effects of random Ag nanoparticle used within the active layer of Si based thin film solar cell are investigated. To avoid the complexity of taking into account all random nanoparticles, an effective dielectric function for random Ag nanoparticles and Si nanocomposites is used that is the Maxwell–Garnet theory along with Percus–Yevick correction term. Considering the energy reservation law and using the effective dielectric function, the absorbance of the active layer, therefore, the solar cell's maximum short current density is obtained. Also, the maximum external quantum efficiency of the solar cell is obtained using the optimum values for the radius and filling fraction of Ag nanoparticles.

1. Introduction

Solar energy, unlike the fossil fuels, is an endless source of energy for energy consuming life activities. The solar cell is a device which converts electromagnetic energy into electrical energy and the conversion process is based upon the photovoltaic effect [1]. Unfortunately, the cost of electricity generated by a solar cell is higher than one generated using conventional methods, especially in the case of wafer based crystalline silicon (C–Si), which depends on the cost of silicon that is an expensive medium with weak absorbing ability. A simple approach to reduce the cost of these devices is decreasing the volume of used material by fabricating thinner devices. Thin-film solar cells, having thicknesses usually in the range 100–150 μm, are deposited on cheap substrates such as glass, plastic or stainless steel [2]. They are made from a variety of semiconductors including cadmium telluride and copper indium diselenide [3]. On the other hand, silicon is an indirect semiconductor and its absorbance in near-band gap region is ineffective, thus reducing the thickness extremely affects the performance of the device. So, a way to overcome this problem is using the light trapping techniques, in order to increase the absorbance of device [4].

Many light trapping methods have been proposed in order to achieve high efficiency in thin film solar cells, such as: coupling of incident light at the front side, reflection at the back side, intermediate reflectors in multi-junction solar cells, light scattering at rough interfaces, etc. [5]. A novel method that has emerged lately is using of the scattering from noble metal nanoparticles excited at their surface plasmon resonance. Metal nanoparticles are strong scatterers of light at wavelengths near the plasmon resonance, which is due to a collective oscillation of the conduction electrons in the metal [3]. Recently, metallic nanoparticles have been widely used to enhance photovoltaic performance [6–8]. The resonance of metallic nanoparticles strongly depends on size, shape, and spacing of the metallic particles as well as the dielectric properties of the surrounding medium [2]. In most research works, models are based on single nanoparticles, but in particle ensembles additional movement in resonance frequency are expected to occur due to electromagnetic interactions between the nanoparticles [9]. It should mention that, for nanoparticles much smaller than the wavelength of light, the dominant scattering mechanism is Rayleigh scattering [10].

Recently, it has been shown that using the metallic nanoparticles, deposited on the silicon surface, could significantly increase the absorption of light over a broad spectral range, giving rise to a stronger photocurrent response [8]. From experimental point of view, random metal–dielectric nanocomposites are easy to prepare using thin film deposition techniques. But the geometry that nanoparticles randomly distributed through the active layer of solar cell has not studied. In this paper, it has been proposed to use such composites to tune the operational wavelength of a solar

E-mail address: asgari@tabrizu.ac.ir (A. Asgari).

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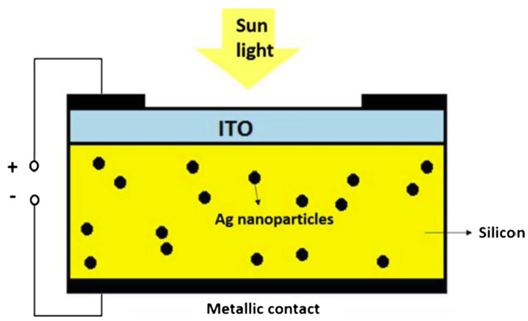

Fig. 1. Schematic structure of random plasmonic solar cell.

cell in a broad spectral range, by just adjusting the random metal nanoparticle's filling fraction and radiuses [11].

2. Model description

The simple schematic cross sectional view of random Ag nanoparticle distributed in silicon solar cell is shown in Fig. 1, where an ITO (indium tin oxide) layer is a transparent anode as the front side of solar cell.

In order to have a comparison between the performances of proposed solar cell with a common thin film silicon solar cell, we investigated the absorption coefficient of silicon and also absorption coefficient of Ag-nanoparticle doped silicon nanocomposite. For the case of bare silicon (without Ag nanoparticles), we have used absorption coefficient calculated from the k-selection rule in the matrix element for a bulk semiconductor, as follows [12]:

$$\alpha\ (\mu\mathrm{m}^{-1}) = \begin{cases} -0.425(\hbar\omega - E_g)^3 + 0.757(\hbar\omega - E_g)^2 \\ \quad - 0.0224(\hbar\omega - E_g) + 10^{-4} \\ \quad (1.1\ \mathrm{eV} < \hbar\omega < 1.5\ \mathrm{eV}) \\ 0.0287\exp[2.72(\hbar\omega - E_g)] \\ \quad (\hbar\omega > 1.5\ \mathrm{eV}) \end{cases} \tag{1}$$

where $\hbar\omega$ is the energy of incident photon and E_g is the band gap energy of silicon.

We have used the Lorentz–Drude model for describing the dielectric function of Ag nanoparticles, which has a good promising coincidence with experimental data. i.e., Lorentz–Drude model unlike the Drude model, takes into account of both intraband and interband transitions. In fact, the Lorentz–Drude model is able to describe all resonances in the blue-end and provide an accurate fit with the real dielectric function of silver, over the whole frequency range of interest. The dielectric function in Lorentz–Drude model is expressed as

$$\varepsilon(\omega) = \varepsilon_\infty + \sum_{k=0}^{K} \frac{f_k \omega_p^2}{\omega_k^2 - \omega^2 + i\omega\Gamma_k} \tag{2}$$

where ε_∞ is the optical dielectric constant at infinite frequency (for isotropic plasma-like metals = 1), k is the number of oscillators with frequency ω_k, and f_k and Γ_k are strength and damping constant, respectively, and ω_p is the plasma frequency [13].

The propagation of electromagnetic wave and its scattering in a medium with heterogeneity in its dielectric properties, has been a fundamental problem for many years [14]. On the other hand, the dielectric function is one of the most important quantities describing the optical properties of a medium [15]. Analytical investigation of a random two component system requires computing the exact local fields inside the composite and their environs, caused by the inhomogeneities, using a first principle approach, i.e. Maxwell's equations. In the general case of a spatially random structure, solving this problem analytically appears as a formidable task. These difficulties have led numerous groups to study the partial differential equations for local fields, using different computational techniques [16]. An alternative way is to use effective medium theory (EMT). EMT defines an effective dielectric function for a composite material in terms of dielectric function of its components and their geometrical arrangement [11] and it could be applied for localized surface plasmons occurring in metal nanoparticles [17–21].

Over the last century, numerous effective medium theories have been proposed. Maxwell–Garnett (MG) expressions are the most successful expression to explain the effective behavior of a composites. MG effective medium theory provides a simple model for calculating the macroscopic optical properties of materials with a dilute inclusion of spherical nanoparticles. Also, it includes the dipolar interaction between particles, through the averaged Lorentz local field [17,22,20]. However, the Percus–Yevick equation is an improved representation of the pair distribution function for appreciable concentration of nanoparticles [23].

We consider a slab consists of N spherical metal nanoparticles that are randomly distributed in silicon. An electric field in 'z' direction is applied to the slab. In the case of isolated inclusions embedded in a dielectric matrix, the Maxwell–Garnett formula reads as

$$\frac{\varepsilon_{eff} - \varepsilon}{\varepsilon_{eff} + 2\varepsilon} = f_s \frac{\varepsilon_s - \varepsilon}{\varepsilon_s + 2\varepsilon} \tag{3}$$

where ε_{eff} is the effective dielectric function, ε is the dielectric function of the embedding medium, ε_s is the dielectric function of the metal nanoparticles and f_s is the filling fraction of metal in the composite [4]. The induced dipole moment of ith scatterer can be expressed as

$$P_i = \hat{z}\frac{4\pi a^3(\varepsilon_s - \varepsilon)/(\varepsilon_s + 2\varepsilon)}{1 - f_s(\varepsilon_s - \varepsilon)/(\varepsilon_s + 2\varepsilon)} E \tag{4}$$

where a is the radius of nanoparticles and E is the applied electric field. Calculating the scattered field from the ith scatterer, the total scattered intensity, and total scattered power and dividing it to the input power, the effective dielectric function is obtained as

$$\varepsilon_{eff} = \varepsilon\left\{\left(\frac{1 + 2f_s(\varepsilon_s - \varepsilon)/(\varepsilon_s + 2\varepsilon)}{1 - f_s(\varepsilon_s - \varepsilon)/(\varepsilon_s + 2\varepsilon)}\right) + i2f_s k^3 a^3 \left|\frac{(\varepsilon_s - \varepsilon)/(\varepsilon_s + 2\varepsilon)}{1 - f_s(\varepsilon_s - \varepsilon)/(\varepsilon_s + 2\varepsilon)}\right|^2 \{1 + L/N\}\right\} \tag{5}$$

where k is the wavenumber, and L is expressed as

$$L = \frac{N^2}{V}\,\mathrm{Re}\left\{\int drg(r)e^{ik.r}\right\} \tag{6}$$

In which V is the volume containing the scatterers, and $g(r)$ is known as the pair distribution function in the position 'r'. In Percus–Yevick approximation, L is shown as [24]

$$L = N\left[\frac{(1-f)^4}{(1+2f)^2} - 1\right] \tag{7}$$

Considering the effective medium dielectric function ε_{eff}, the reflectance and transmittance for normal incident light, can be written as [8]

$$R = \left|\frac{(-1 + \varepsilon_{eff})[-1 + e^{4iak\sqrt{\varepsilon_{eff}}}]}{e^{4iak\sqrt{\varepsilon_{eff}}}(-1 + \varepsilon_{eff})^2 - (1 + \varepsilon_{eff})^2}\right|^2$$
$$T = \left|\frac{4\varepsilon_{eff} e^{2iak(-1+\sqrt{\varepsilon_{eff}})}}{e^{4iak\sqrt{\varepsilon_{eff}}}(-1 + \varepsilon_{eff})^2 - (1 + \varepsilon_{eff})^2}\right|^2 \tag{8}$$