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Original Article

Simulation-based Study on Light Absorption Enhancement in Silicon Thin Films Via Nanoparticles

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Abstract: Solar energy is one of the most promising and widely adopted renewable energy sources due to its abundance and sustainability. In recent decades, significant progress has been made in developing photovoltaic (PV) cells with enhanced efficiency using a variety of materials and device architectures. While many next-generation PV technologies are still under development, silicon-based solar cells remain dominant due to their maturity, stability, and cost-effectiveness. This study investigates a simulation-based approach to enhance the optical absorption of silicon thin films by incorporating nanoparticles. The primary goal is to improve absorption in the near-infrared (NIR) region, where silicon typically exhibits limited efficiency. The optical properties of the films are modeled using modified Maxwell–Garnett-Mie theory, based on the effective medium approximation (EMA), which describes the macroscopic attributes of the nanoparticle–integrated composites. We explore different types of nanoparticles, volume fractions, and material combinations to analyze their impact on light absorption. Numerical simulations are carried out to evaluate the absorption spectra of these nanocomposites with silicon thin film as the host matrix. The results demonstrate the potential of nanoparticle-enhanced films to improve light trapping and absorption, offering a viable route toward more efficient silicon-based solar cells.

Keyword: silicon thin film, Maxwell-Garnett-Mie theory, effective medium approximation, near-infrared absorption.

1. Introduction

Thin-film silicon solar cells are attracting significant attention due to their flexibility, low cost, and promising potential for enhanced performance. Despite these advantages, a key weakness remains

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silicon's low absorption coefficient [1, 2]. To overcome this limitation, various light-trapping methods have been proposed to boost efficiency while simultaneously reducing material volume.

Among these methods, metallic nanoparticles effectively enhance light absorption via plasmon resonances, which in turn increase the optical path length through scattering, particularly near the resonance wavelength [2, 3]. The optical properties of these nanoparticles, including their plasmon resonance and scattering effects, are highly tunable and dependent on their size, shape, material, and the surrounding medium [3-5]. Giving the complex interactions involved, accurately predicting the optical characteristics of these composite materials is challenging. To address this, the effective medium approximation (EMA) offers a powerful solution by modeling the macroscopic properties of the composite without explicitly describing each individual nanoparticle [5-7].

The widely used Maxwell-Garnett (MG) theory, a popular EMA, is limited in that it does not explicitly account for nanoparticle size and is only valid when particle sizes are much smaller than the incident wavelength [4, 8]. To address these limitations, size-dependent extensions have been developed. Among them, the Maxwell-Garnett-Mie (MGM) theory, introduced by Doyle, has been widely adopted to enhance light absorption in nanocomposites [9]. However, previous studies have not systematically identified the optimum nanoparticle radius–volume fraction combination that maximizes absorption. To the best of our knowledge, this is the first study that provides a comprehensive evaluation of nanoparticle types, sizes, and volume fractions relative to a pure silicon active layer, and proposes the optimal design parameters (radius and volume fraction) for maximizing absorption efficiency for each material.

2. Design and Simulation

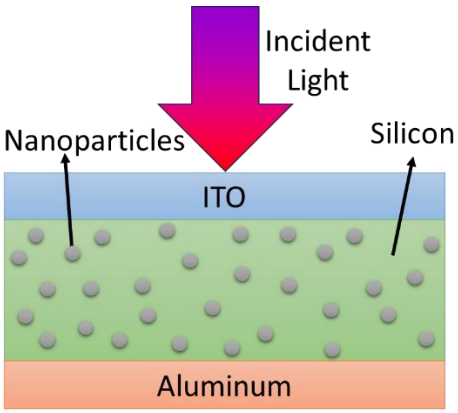

Figure 1. The proposed structure for simulation.

As the thickness of the active layer in solar cells is reduced, the optical path length also decreases, which in turn leads to a low absorption efficiency, particularly at longer wavelengths. Due to this practical consideration, a thin film structure was chosen for our study. Figure 1 shows a simple thin-film solar cell structure, where light is perpendicularly incident. This configuration consists of thin-film indium tin oxide (ITO) (88 nm) and aluminum (20 nm) layers acting as electrodes, with a silicon layer (100 nm) sandwiched in between. These thickness values were chosen based on our preliminary simulations and prior research, with additional reference to the literature from other groups [10, 11]. We examine the effect of embedding gold (Au), silver (Ag), and copper (Cu) nanoparticles of varying sizes and volume fractions into the silicon matrix on its light absorption. These metals were selected as

embedded nanoparticles due to their optical properties, specifically their strong surface plasmon resonances and light scattering capabilities, which depend on the optical constants of the surrounding medium and their sizes [12]. All refractive index data were obtained from ANSYS Lumerical software, with the exception of ITO which was not provided and instead obtained from [10].

The frequency-dependent dielectric function of metallic nanoparticles is governed by both interband and intraband electron transitions. In bulk metals, the interband transition can often be neglected due to the absence of energy band gap, so the dielectric function is primarily contributed by the intraband transition [13]. However, in nanoparticles, confinement effects arise because the electron mean free path is limited by the particle size, which significantly influences the intraband contribution to the dielectric function [4, 14]. The resulting frequency (ω)- and size (R)-dependent dielectric function of the nanoparticles (ε_{np}) is given by:

$$\varepsilon_{np}(\omega, R) = \varepsilon_m(\omega) + \frac{\omega_p^2}{\omega^2 + i\omega\gamma} - \frac{\omega_p^2}{\omega^2 + i\omega\left(\gamma + C\frac{v_f}{R}\right)} \quad (1)$$

where $\varepsilon_m, \omega_p, \gamma, v_f$ are the dielectric function of bulk metal, plasma frequency, electron damping constant and Fermi velocity, respectively. C is a constant related to the scattering process of electron within the particle, has a value between 0.75 – 1 depending on the nanoparticle shape and its surrounding medium. In this paper, C is assumed to be 1 for spherical inclusions according to [13]. The wavelength value of incident light for this simulation will be between a fixed range of 200-1450 nm.

The MG calculates the effective dielectric function (ε_{eff}) of the composite medium from the Clausius–Mossotti relation [6, 7, 15, 16]:

$$\frac{\varepsilon_{eff} - \varepsilon_h}{\varepsilon_{eff} + 2\varepsilon_h} = \frac{v}{R^3}\alpha(R) \quad (2)$$

where ε_h, v are the dielectric function of the host medium and volume fraction of the inclusions.

Nanoparticle inclusions will be polarized under the effect of external electric field, the polarizability can be expressed as:

$$\alpha(R) = R^3 \frac{\varepsilon_{np} - \varepsilon_h}{\varepsilon_{np} + 2\varepsilon_h} \quad (3)$$

Substituting (3) for (2), we obtain the general Maxwell–Garnett theory:

$$\varepsilon_{eff} = \varepsilon_h \frac{2v(\varepsilon_{np} - \varepsilon_h) + \varepsilon_{np} + 2\varepsilon_h}{2\varepsilon_h + \varepsilon_{np} - v(\varepsilon_{np} - \varepsilon_h)} \quad (4)$$

Similarly, the effective permeability can be obtained through a similar method, and the effective refractive index can then be calculated using $n_{eff} = \sqrt{\varepsilon_{eff}\mu_{eff}}$. However, the difference between the results with and without permeability is negligible for non–magnetic metallic nanoparticles and will not be considered in this paper. It is important to note that the effective dielectric function in the MG theory does not explicitly depend on the size of the nanoparticles within the host medium. For this reason, MG theory is only applicable when the nanoparticle sizes are much smaller than the wavelength of the incident light [8]. To address this limitation, we utilize the MGM theory, which modifies the polarizability to include Mie scattering effects:

$$\alpha(R) = \frac{3i\lambda^3}{16\pi^3\varepsilon_h^{\frac{3}{2}}} a_1(R) \quad (5)$$

a_1 is the first Mie coefficient, given by:

$$a_1(R) = \frac{m\psi_1(mx)\psi_1'(x) - \psi_1(x)\psi_1'(mx)}{m\psi_1(mx)\xi_1'(x) - \xi_1(x)\psi_1'(mx)} \tag{6}$$

where ψ_1 and ξ_1 are the Riccati–Bessel functions of the first order, m is the ratio of the refractive index of the inclusions (n_{np}) to that of the host medium (n_h), i.e., $m = n_{np}/n_h$. And $x = k_h R = n_h \frac{2\pi}{\lambda} R$, also known as the size parameter of the nanoparticles. k_h is the wavenumber of the host medium.

By using this modified polarizability, we derive a more accurate ε_{eff} that explicitly depends on both the nanoparticle size and volume fraction. This is achieved by substituting the new polarizability expression (5) into the original MG equation (2):

$$\frac{\varepsilon_{eff} - \varepsilon_h}{\varepsilon_{eff} + 2\varepsilon_h} = \frac{v}{R^3} \frac{3i\lambda^3}{16\pi^3 \varepsilon_h^{\frac{3}{2}}} a_1(R) \tag{7}$$

Let the right side be $A(R)$, we finally obtain:

$$\varepsilon_{eff} = \varepsilon_h \frac{1 + 2A(R)}{1 - A(R)} \tag{8}$$

We performed simulations using ANSYS Lumerical to evaluate light absorption in the 200–1450 nm wavelength region for configurations in which the silicon layer includes Cu, Ag, and Au nanoparticles. The parameters of these nanoparticles are based on prior research [2, 3, 12] and are listed in Table 2. The radius of the particles was systematically investigated at 1 nm, 5 nm, 10 nm, and 20 nm, while the volume fractions were set to 0.01, 0.05, and 0.1 respectively. Note that the volume fractions are dimensionless, since they are defined as the ratio of the total nanoparticles volume to the total volume of the Si matrix.

Table 1. Simulation parameters for nanoparticles

	Cu	Ag	Au
ω_p (10^{16} rad/s)	1.307	1.276	1.376
γ (10^{14} rad/s)	1.660	1.215	1.170
v_f (10^6 m/s)	1.570	1.390	1.400

3. Results and Discussion

From the simulated reflectivity (R^*), transmittivity (T) and effective refractive index, we can calculate the absorption:

$$A = 1 - R^* - T \tag{9}$$

Figure 2 shows that for a volume fraction of 0.01, integrating nanoparticles generally increases absorption compared to pure silicon. A notable absorption spike between 700–1100 nm indicates enhanced light scattering and trapping. For Ag, the enhancement is slight at $R = 1$ nm but significant at $R = 5$ nm, peaking around 800 nm. As the radius increases, the peak red-shifts, with 10 nm particles showing maximum enhancement. Au nanoparticles exhibit a similar trend but with a slightly red-shifted enhancement range. Cu nanoparticles show the most prominent absorption increase, peaking at $R = 1$ and $R = 5$ nm before decreasing with larger radii. For all materials, the enhancement peak red-shifts as the radius increases.

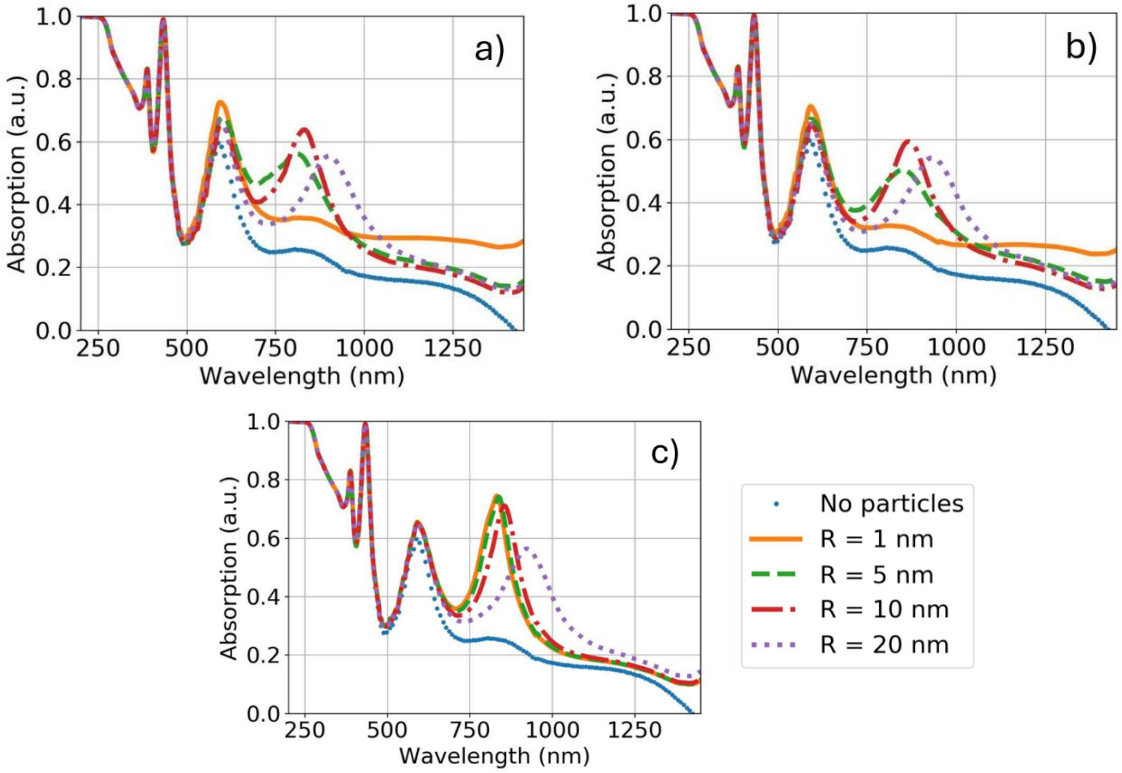

Figure 2. Absorption spectra of the simulated structure with embedded nanoparticles of different materials (a) Ag, (b) Au, (c) Cu, at fixed volume fraction of 0.01 and varying radii.

Figures 3 and 4 present the results for volume fractions of 0.05 and 0.1, respectively. As expected, increasing the volume fraction generally increases absorption due to greater scattering. However, the results show that increasing the volume fraction can shift the peak absorption wavelength, indicating the existence of an optimal radius-volume fraction combination for maximizing absorption. For instance, the maximal absorption near 1000 nm is achieved with a radius of 20 nm and a volume fraction of 0.05 for all materials, or alternatively with Ag/Au at a radius of 5 nm and a volume fraction of 0.1.

The variation in absorption amplitudes can be explained by the radius dependence of the dielectric function, which introduced plasmon resonances at 750–1000 nm range. This effect, combined with multiple scattering and reflection processes at high volume fractions, contributes to the overall absorption enhancement. The red shift phenomenon observed as the radius increases is consistent with dynamic depolarization effect, explained by [4].

This demonstrates that the optical properties of these nanoparticles can be tuned to achieve a specific absorption amplitude and range by carefully selecting the type of particle as well as its radius and volume fraction. For a high absorption target, a volume fraction greater than 0.05 is recommended. For absorption at longer wavelengths, particles with a radius larger than 5 nm are sufficient, although 1 nm particles can also be effective if the volume fraction is high (Figure 4.). Overall, the observed results and phenomena are in good agreement with previous studies, for example, the absorption graph with silver particles in [17] shares a similar absorption peak at around 1000 nm. In future studies, multiple types of particles can be implemented simultaneously to obtain a more diverse enhancement.

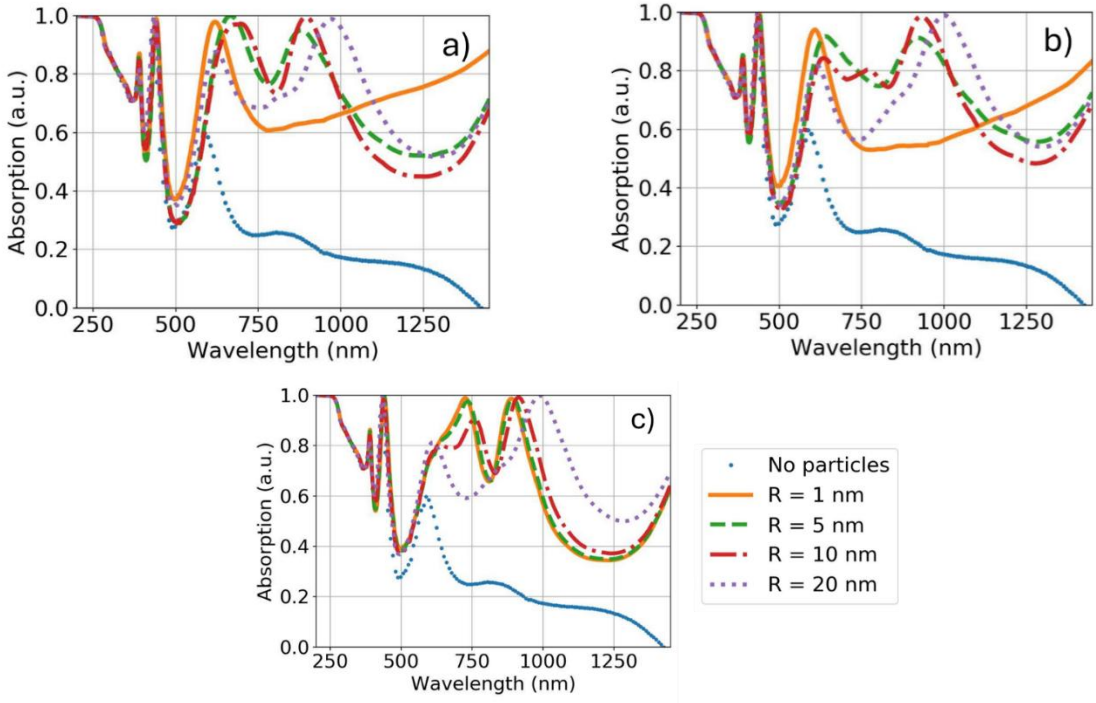

Figure 3. Absorption spectra of the simulated structure with embedded nanoparticles of different materials (a) Ag, (b) Au, (c) Cu, at fixed volume fraction of 0.05 and varying radii.

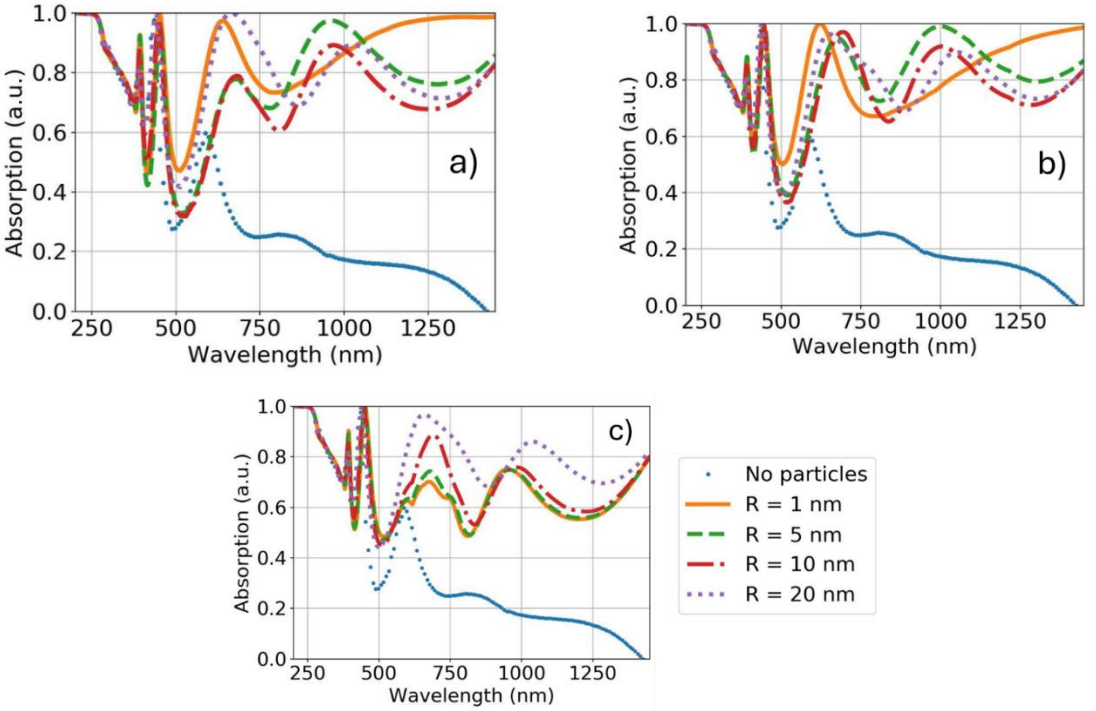

Figure 4. Absorption spectra of the simulated structure with embedded nanoparticles of different materials (a) Ag, (b) Au, (c) Cu, at fixed volume fraction of 0.1 and varying radii.

4. Conclusion

In this paper, we have successfully utilized the Maxwell–Garnett–Mie theory and simulations to predict the optical properties of a nanocomposite structure consisting of metallic nanoparticles embedded within a silicon host medium. Our study demonstrates that by systematically adjusting the radius and volume fraction of the nanoparticles, the light absorption of the composite can be significantly enhanced and tailored to specific wavelength regions. Composites with 1 nm radius Ag nanoparticles show a strong absorption enhancement at wavelengths greater than 1000 nm, and this enhancement increases linearly with the volume fraction. A similar behavior is observed for composites with Au nanoparticles. For composites with Cu nanoparticles, the effect of particle size on absorption enhancement at wavelengths greater than 600 nm is not significant when radius varies from 1 nm to 10 nm across all volume fractions. A Cu volume fraction of 0.05 provides the largest absorption enhancement compared to other volume fractions, while for Ag and Au nanoparticles, the optimum fraction is 0.1. These findings allow for the optimization of the structure of highly tunable solar cells that can absorb light across a broad range of wavelengths.

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