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A numerical study on effects of surrounding medium, material, and geometry of nanoparticles on solar absorption efficiencies

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ABSTRACT

Effects of surrounding medium, materials (including core–shell configuration) and geometry (size and shape) of nanoparticles on solar energy absorption are studied numerically by employing Mie theory and finite-difference time-domain method. It is shown that nanoparticles, having a high absorption peak in the visible region and a broad absorption band in the wavelength range of 300–1100 nm, have a high solar energy absorption efficiency factor. The resonance wavelength, the absorption peak, and the absorption band of nanoparticles play important roles in enhancing the solar absorption efficiency factor of single nanoparticles.

1. Introduction

It is known that metallic nanoparticles possess unique optical properties when interact with electromagnetic waves [1]. In particular, the localized surface plasmon resonance (LSPR) effect at the surface of metallic nanoparticles is known to enhance the absorption and scattering efficiencies of the nanoparticle at a specific wavelength, promoting its photothermal conversion process [2]. For this reason, nanoparticles have been widely used as biochemical sensors and detectors in medical fields [3,4]. In 2012, Neumann et al. [5] demonstrated experimentally that it was feasible to generate vapor from nanofluids containing SiO_2-Au particles instantaneously under the sun after focusing because of LSPR effects. Their experiments have received a great deal of attention [6–8] because of its potential applications in sterilization, desalination, sewage treatment, etc. [9–11]. In addition to nanofluids, layers containing nanoparticles have also been demonstrated as absorbers of solar energy for solar vapor generation [12–14]. More recently, two new approaches for vapor generation heated by sunlight have been proposed: one by adding an insulating layer to reduce heat dissipation [15] and another by making the best of plasmon resonance of Al nanoparticles to enhance the solar absorption of the media [16]. Both of these two methods can produce clean steam with only one sun.

Optical properties of metallic nanoparticles are strongly sensitive to their materials, sizes, shapes, as well as dielectric properties of surrounding medium, compositions, and the temperature of the nanoparticles [17–20]. On the other hand, non-metallic absorbing nanoparticles are known to have broadband absorption spectra, even though the optical absorptivity is not so high [21]. It has been found that metallic nanoparticles with non-metallic core, such as Si, SiO_2, Co, and brown carbon [20–23], can broaden their absorption spectra and flexible tune the plasmon resonance wavelengths [21,24]. Graphene, one of the most popular materials, has also been used to optimize the optical properties of gold nanoparticles [25,26]. In addition, optical properties of different shapes of nanoparticles, such as nanospheres, nanorods, nanoprisms, nanowires, and nanostars, have been studied either numerically or experimentally [27–30]. However, it should be pointed out that the solar absorption property of single nanoparticles has not been well studied in details in the past. Although Lv et al. [31] have done some calculations on solar absorption property of core-shell nanoparticles, the fact that they used the quasi-static approximation for simplification of the Mie theory limited the scope of their investigations. Recently, Xuan et al. [32,33] also demonstrated experimentally absorption enhancement with TiO_2-Ag core-shell nanofluids, and studied theoretically the plasmonic resonance absorption of TiO_2-Ag nanoparticles for solar energy harvesting. However, effects of different parameters on solar absorption of an individual nanoparticle need to be further examined theoretically.

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In this paper, a numerical study based on traditional Mie theory [34–37] and finite-difference time-domain (FDTD) method [38] is carried out to investigate effects of size, shape, material, component and the dielectric constant of the surrounding medium on solar absorption efficiency factor (SAEF) of an individual nanoparticle. Mechanisms of SAEF enhancement of a single nanoparticle are also discussed in details by using the optical properties of nanoparticles concerned. The results obtained from the present study provide fundamental information and guideline to fabricate nanoparticles for enhancement in solar energy harvesting.

2. Calculation of Q_{solar}

The SAEF Q_{solar} of a single nanoparticle can be calculated according to the following equation [21]:

$$Q_{solar} = \frac{\int_{\lambda_1}^{\lambda_2} Q_{abs}(\lambda) I_{AM1.5}(\lambda) d\lambda}{\int_{\lambda_1}^{\lambda_2} I_{AM1.5}(\lambda) d\lambda} \tag{1}$$

where $I_{AM1.5}$ is the solar spectral irradiance at air mass 1.5 [39], and $Q_{abs}(\lambda)$ is the absorption efficiency factor (AEF) which is the ratio of absorption cross section ($C_{abs}(\lambda)$) and the cross-sectional area of the particle. In order to calculate the AEF of an arbitrary nanoparticle, the nanoparticle is usually regarded as a sphere with the effective volume of the sphere equal to the volume V of the particle [40]. Then, the calculation of $Q_{abs}(\lambda)$ for a nanoparticle of arbitrary shape can be obtained from

$$Q_{abs} = C_{abs}/\pi r_{eff}^2 \tag{2}$$

where C_{abs} is the absorption cross section of the nanoparticle, r_{eff} is the effective radius of the nanoparticle. According to the definition, for spherical nanoparticle, it is the radius of the nanoparticle.

Since water strongly absorbs solar energy in the wavelength range longer than 1100 nm, so we just focus on the wavelength range of 300–1100 nm. Eq. (1) is a weighted integration of the SAEF over the wavelength region considered (i.e., 300–1100 nm), normalized with respect to the total solar energy in the same wavelength range. The calculation of C_{abs} in Eq. (2) will be discussed next.

2.1. Spherical nanoparticles

Fig. 1 shows a homogenous spherical core-shell nanoparticle (where the core is indicated in black color) with inner radius of r_1 and the shell with outer radius of r_2. The extinction, scattering and absorption cross sections C_{ext}, C_{sca} and C_{abs} of a core-shell nanoparticle can be calculated based on the Mie theory [34–37] as:

$$C_{ext} = \frac{2\pi}{k^2}\sum_{n=1}^{\infty}(2n+1)Re(a_n + b_n) \tag{3}$$

$$C_{sca} = \frac{2\pi}{k^2}\sum_{n=1}^{\infty}(2n+1)(|a_n|^2 + |b_n|^2) \tag{4}$$

$$C_{abs} = C_{ext} - C_{sca} \tag{5}$$

$$a_n = \frac{\psi_n(x_2)[\psi_n'(m_2x_2) - A_n\chi_n'(m_2x_2)] - m_2\psi_n'(x_2)[\psi_n(m_2x_2) - A_n\chi_n(m_2x_2)]}{\xi_n(x_2)[\psi_n'(m_2x_2) - A_n\chi_n'(m_2x_2)] - m_2\xi_n'(x_2)[\psi_n(m_2x_2) - A_n\chi_n(m_2x_2)]} \tag{6}$$

$$b_n = \frac{m_2\psi_n(x_2)[\psi_n'(m_2x_2) - B_n\chi_n'(m_2x_2)] - \psi_n'(x_2)[\psi_n(m_2x_2) - B_n\chi_n(m_2x_2)]}{m_2\xi_n(x_2)[\psi_n'(m_2x_2) - B_n\chi_n'(m_2x_2)] - \xi_n'(x_2)[\psi_n(m_2x_2) - B_n\chi_n(m_2x_2)]} \tag{7}$$

with

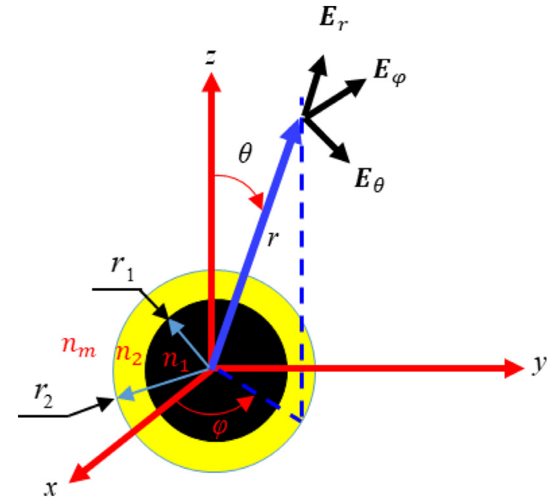

Fig. 1. Schematic of the Mie theory for spherical nanoparticles.

$$A_n = \frac{m_2\psi_n'(m_1x_1)\psi_n(m_2x_1) - m_1\psi_n(m_1x_1)\psi_n'(m_2x_1)}{m_2\psi_n'(m_1x_1)\chi_n(m_2x_1) - m_1\psi_n(m_1x_1)\chi_n'(m_2x_1)} \tag{8}$$

$$B_n = \frac{m_2\psi_n'(m_2x_1)\psi_n(m_1x_1) - m_1\psi_n(m_2x_1)\psi_n'(m_1x_1)}{m_2\chi_n'(m_2x_1)\psi_n(m_1x_1) - m_1\chi_n(m_2x_1)\psi_n'(m_1x_1)} \tag{9}$$

where $k = 2\pi n_m/\lambda$ is the wave number in the medium surrounding the nanoparticle, m_i is the ratio of refractive index of the core ($i = 1$) and shell ($i = 2$) n_i to that of the surrounding medium n_m; $x_i = kr_i$ with inner radius r_1 and outer radius r_2; ψ_n, ξ_n and χ_n are the Riccati-Bessel functions, where $\chi_n = i(\xi_n - \psi_n)$ and n is the order of the Riccati-Bessel functions, while $i = \sqrt{-1}$. If $m_1 = m_2$, then $A_n = B_n = 0$, the reduced equations of (3)–(9) are for a homogeneous sphere. All the calculations of the Mie theories were performed at discrete points in the wavelength range from 300 nm to 1100 nm. The complex dielectric functions of gold and brown carbon used in this calculation were given by Olmon [41] and Alexander [42], respectively, while dielectric functions for the rest of the materials were taken from the data measured by Palik [43].

2.2. Other geometries

The calculation of the AEF of non-spherical nanoparticles can be performed according to Eq. (2), where the absorption cross section (C_{abs}) of non-spherical nanoparticles can be obtained from Maxwell equations using the FDTD method [38], which has been regarded as one of the most powerful methods for computing optical properties of particles with an arbitrary shape.

3. Results and discussion

All calculations were carried out under the condition of having the same surface area equals to a sphere with a radius of 50 nm except in Section 3.2 to explore size effects. Because of the small penetration depth of the water at the wavelengths longer than 1100 nm, numerical calculations of AEF and SAEF were both performed in the wavelength range of 300–1100 nm, which occupies 76.1% of the total solar energy. All nanoparticles were surrounded by water (with n_m = 1.33) except for the investigation on the effect of the surrounding medium in Section 3.3.