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Enhancing absorption properties of composite nanosphere and nanowire arrays by localized surface plasmon resonance shift

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ABSTRACT

Nanoparticles with nonmetallic core and metallic shell can improve the spectral solar absorption efficiency for traditional working fluids, due to the localized surface plasmon resonance (LSPR) effect exists at the surfaces of these core-shell composite nanoparticles. In this work, the effect of geometry and material, and hence the LSPR effect, on the optical absorption properties of core-shell nanostructures was numerically demonstrated by the finite difference time domain method. The nanostructures were formed by varying the inner and outer radii of the composite nanospheres and nanowires and by changing the particle spacing for their arrays. The result indicates that varying the inner radius itself can tune the absorption efficiency factors of the nanostructures monotonously, while an optimal outer radius may exist for maximizing the absorption efficiency factors. It also shows that varying the inner radius itself can widen the absorption spectrums for the arrays, but the absorptance tends to increase with decreasing inner radius or particle spacing. Meanwhile, the second absorption peaks may be observed for nanowires or nanosphere/nanowire arrays, which can be tuned by the resonance shifts induced by the change of either inner or outer radius and hence the LSPR effect. The coupled LSPR effect under studied can be efficiently utilized for tuning the optical absorption properties of nanoparticles used in many applications including photothermal conversion, and perspective also exists for many other applications including surface-enhanced Raman spectroscopy (SERS) enhancement.

Introduction

Nanofluid has been proposed for efficient photothermal application because of its unique thermal and optical absorption properties [1,2]. An efficiency improvement up to 5–28.3% can be obtained using nanofluids in non-concentrating direct absorption solar collectors [2–4]. It was shown that the efficiency improvements are significantly influenced by factors such as particle material, size, shape and volume fraction [5]. When the incident electron oscillation frequency equals to the frequency of metal nanoparticles, there exists the localized surface plasmon resonance (LSPR) effect at the nanoparticle surface, which could significantly enhance the optical absorption efficiency [6–8]. This effect is obviously influenced by the particle size, material and structure and could be efficiently utilized for tuning the radiative properties of plasmonic nanofluids used in photothermal application.

Core-shell nanospheres can be widely used in many industrial applications including nonlinear optics, photo-chemical transformation and nanosensing [9,10]. In our previous investigation [11], some typical composite nanospheres (with Si or SiC core and Au, Ag, Cu or Al shell) are numerically investigated for the LSPR effect existing at the particle surfaces on the thermal and optical properties of water-based plasmonic nanofluids. The results show that the structure itself can influence simultaneously the average and the near-field radiative properties of the composite nanospheres and thus the nanofluids. It is meaningful to study how these factors, especially the structure, influence the optical absorption properties of composite nanoparticles. Recently, nanostructures such as nanowire arrays have also drawn much attention for enhancing the optical absorption due to the augmented light trapping in the far-field [12–14]. However, further enhancement of the radiation cannot be achieved due to the inherently narrow band of surface modes induced by resonances [15]. Core-shell composite nanowire has different properties from that of single-component nanowire and can be good candidate for this enhancement [16], which needs for investigation on their absorption properties.

The optical absorption efficiency can be accurately calculated by the well-known Mie's theory for single-component nanoparticles

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Nomenclature

LSPR	localized surface plasmon resonance
FDTD	finite difference time domain
PML	perfectly matched layer
r_1	inner radius (m)
r_2	outer radius (m)
$\boldsymbol{E}$	electric field intensity
$\boldsymbol{H}$	magnetic field intensity
Δx	spatial step in x axis
Δy	spatial step in y axis
Δz	spatial step in z axis
Δt	time step
c	light speed ($m \cdot s^{-1}$)
C_{abs}	absorption cross section (m^2)
C_{sca}	scattering cross section (m^2)
Q_{abs}	absorption efficiency factor
Q_{sca}	scattering efficiency factor
A	cross-sectional area (m^2)
h	longitudinal length (m)
d	spacing (m)

Greek symbols

μ	permeability
ε	permittivity
σ	conductivity
λ	wavelength (m)

Subscripts

1	inner
2	outer
abs	absorption
sca	scattering

[17]. For core-shell composite nanoparticles, such as nanosphere and nanowire, the optical absorption properties can usually be approximated by the finite difference time domain (FDTD) method, which can simulate the propagation of electromagnetic waves in arbitrary structures [18,19]. For example, Gray et al. [20] analyzed the spectral absorption properties and the extinction efficiency of silver nanowires and manifested that the absorption peaks were red-shifted with increasing radius. Some other metal materials were used for studying the LSPR effect excited at the particle surfaces, and strong absorption peaks were observed for core-shell nanospheres due to the induced resonance [21–24]. Besides the effect of materials, the geometry of nanoparticle or the spatial distribution of nanoparticle array may play an important role in altering the absorption peaks.

In this paper, core-shell composite nanoparticles, including nanospheres, nanowires, and their arrays, are numerically studied for the effect of plasmon resonance shifts on the optical absorption properties. The theoretical basis of the FDTD method will be introduced and the relationship between the spectral absorption characteristics and the thickness of each layer will then be given by computational analysis for the composite nanospheres and nanowires. The absorptance for composite nanosphere and nanowire arrays with different radii and particle spacing will also be calculated for comparison.

Numerical method

The FDTD method is based on the Maxwell's equations of electrodynamics. It converts the time-domain differential equations to finite differential equations and thus treat easily with nanoparticles consisting of different shapes of media without complex progressive approximation or the Green's functions [25,26]. For isotropic media, the Maxwell's equations are given as:

$$\nabla \times \boldsymbol{E} = -\mu \frac{\partial \boldsymbol{H}}{\partial t} \tag{1}$$

$$\nabla \times \boldsymbol{H} = \varepsilon \frac{\partial \boldsymbol{E}}{\partial t} + \sigma \boldsymbol{E} \tag{2}$$

where $\boldsymbol{E}$ and $\boldsymbol{H}$ are the electric and magnetic field intensities, μ and ε are respectively the permeability and permittivity of the medium, and σ is the conductivity. In Cartesian coordinates, the corresponding differential equations can be expressed as:

$$\left.\begin{aligned} \frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} &= -\mu \frac{\partial H_x}{\partial t} \\ \frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} &= -\mu \frac{\partial H_y}{\partial t} \\ \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} &= -\mu \frac{\partial H_z}{\partial t} \end{aligned}\right\} \tag{3}$$

and

$$\left.\begin{aligned} \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} &= \varepsilon \frac{\partial E_x}{\partial t} + \sigma E_x \\ \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} &= \varepsilon \frac{\partial E_y}{\partial t} + \sigma E_y \\ \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} &= \varepsilon \frac{\partial E_z}{\partial t} + \sigma E_z \end{aligned}\right\} \tag{4}$$

The field components of the partial derivative of time and coordinates in the above equations can be represented by the differences, i.e., Δx, Δy and Δz represent the spatial step in the computational grids of the coordinates, Δt represents the time step, and any component of $\boldsymbol{E}$ or $\boldsymbol{H}$ in function of space and time can be written as follows:

$$F(i\Delta x, j\Delta y, k\Delta z, n\Delta t) = F^n(i,j,k) \tag{5}$$

where i, j, k and n are all integers. Fig. 1 shows schematically the electric and magnetic fields in a grid. The time is calculated by a half of the time-step alternately in the calculation process [27]. The spatial discretization is set as $\Delta x = \Delta y = \Delta z = \delta$. The new field value for each grid depend on its value at the previous time step and the values of neighbor grids at the previous half time-step. Consequently, the electric and magnetic field values can be calculated at each time-step through these operations. One of the differential equations for the electric field can thus be expressed as:

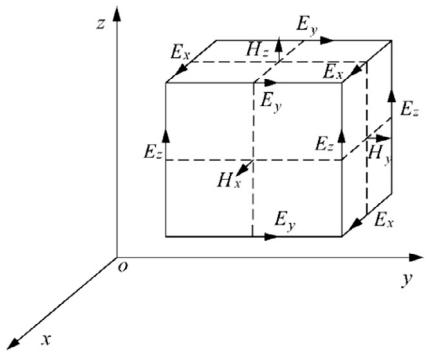

Fig. 1. Field components in the computational grids.