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Numerically investigating the optical properties of plasmonic metallic nanoparticles for effective solar absorption and heating

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ABSTRACT

Solar heating with plasmonic nanoparticles (NPs) has great potential for application in optical storage, solar thermal collectors, and thermo-photovoltaic technologies. The performance of solar thermal conversion applications depends on the NP parameters. Herein, we present a comparative analysis of the solar absorption properties of noble metallic NPs (Au, Ag, Cu, and Al), to determine suitable parameters for effective solar heating by using the finite-difference time-domain method and the finite-element method. Results show that light absorption plays a major role in the interaction of light with the small NP size, small sphericity, or small dielectric constant of the surrounding environment. Au and Cu NPs have higher solar absorption power and absorption ratio. The NP size has little effect on the peak absorption wavelength. A Au sphere smaller than 30 nm has greater solar absorption ability for the solar heating process when considering the absorption power per unit volume. The solar absorption power first increases rapidly and subsequently decreases slightly with increasing dielectric constant, and can become as high as 0.0045 nW when the dielectric constant is 1.33–2.5 in the calculation samples. The solar scattering power and solar absorption power decrease with increasing sphericity, i.e., ranging from cubic to cylindrical and spherical. Finally, simulation results of NP solar heating show that the Au cube obtains a higher maximum temperature than the Au sphere and Au cylinder, which further verifies that Au NPs with low sphericity can significantly enhance solar heating ability in the simulation cases.

1. Introduction

Although the basic interaction between an electromagnetic field and a nanomaterial was understood using the Mie theory several decades ago, light or radiation interaction with nanomaterials has attracted considerable interest in recent years (Sardar et al., 2009). Various nanoparticles (NPs) have been developed for application in the fields of imaging, heat generation (Richardson et al., 2009; Das and Soni, 2016), surface-enhanced sensing (Haes et al., 2005), and especially, light harvesting in solar cells. Among them, the presence of noble metallic (Au, Ag, Cu, and Al) NPs provides an efficient medium to improve solar cell performance due to the efficient excitation of localized surface plasmon resonance (LSPR) oscillation with the light source (Wang et al., 2014; Li et al., 2016), which can be simply seen as a photon greatly captured to the surface of the small NP through the free electrons in the NP when the frequency of the photon is near or equal to the oscillation frequency of the electrons around the surface of the NP, leading to an intense electric field around the NP surface. The LSPR occurs and decays by two ways: one is radiation by radiating its energy, resulting in light scattering, the other is a non-radiative way as a result of photothermal conversion process (Jain et al., 2008). Moreover, the scattering and absorption properties of these noble metal NPs can be enhanced strongly at the resonant frequency due to the LSPR, which lies in the visible and near-infrared regions for Au, Ag, and Cu (Eustis and El-Sayed, 2006).

Compared to common fluids, nanofluids, formed by adding NPs to the base fluid, show better heat transfer and optical properties. Otanicar et al. (2009) experimentally studied the solar absorption ability of four common liquids (water, ethylene glycol, propylene glycol, and Therminol VP-1) in solar thermal applications. Results showed that water obtained the greatest solar absorption ability among the four fluids, absorbing only 13% of the solar energy. It's still too low for the pure medium applied in the solar thermal conversion. Therefore, the solar thermal conversion performance of NPs has been widely investigated in recent decades by many researchers. Much experimental work has also been conducted recently owing to the rapid development of nanotechnology. It was demonstrated that the absorption coefficient of NP suspension is much higher than that of the base liquid for visible to

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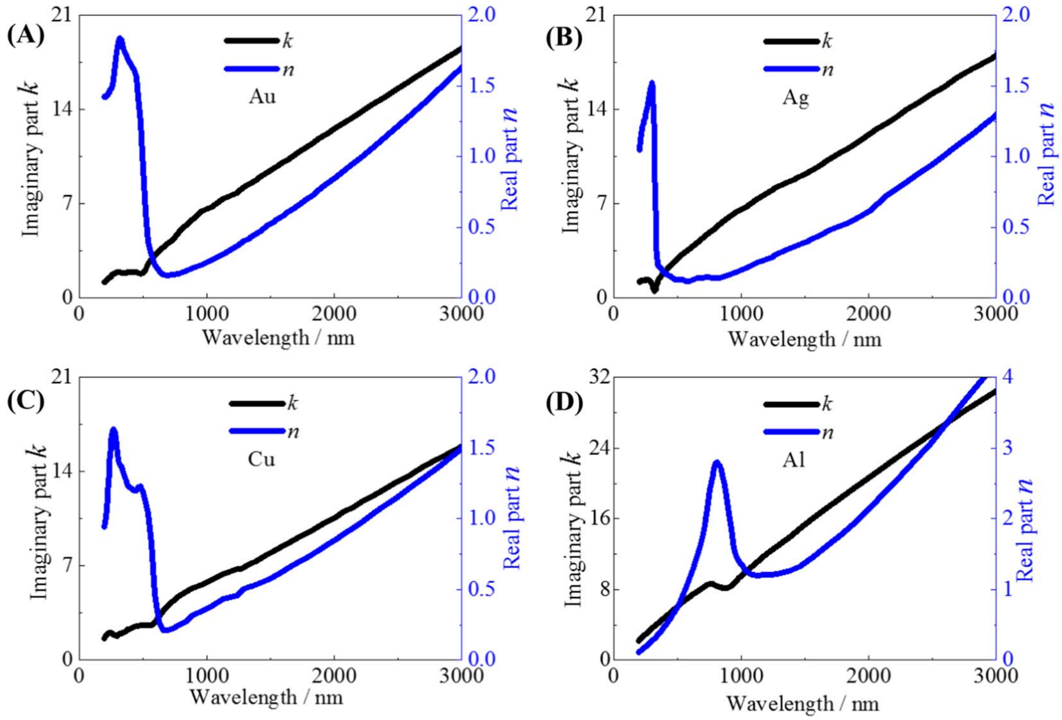

Fig. 1. Refractive index of Au, Ag, Cu, and Al as a function of wavelength, obtained from the result of Palik (1998).

near-infrared wavelengths (Kameya and Hanamura, 2011). Various materials have been used in direct solar energy collectors to enhance the absorption of light (Otanicar et al., 2010; Yousefi et al., 2012; Saidur et al., 2012). The solar thermal efficiencies of a graphite nanofluid (0.01 vol%) and an Al_2O_3 nanofluid (0.5 vol%) were 122.7% and 117.5% of the traditional solar surface absorbing collector, respectively, which showed that nanofluids have good ability to absorb solar radiation (Luo et al., 2014). Zhang et al. (2014) proposed and validated a novel idea of using plasmonic NPs to improve the solar thermal conversion efficiency. Experimental results showed that gold NPs had excellent photothermal conversion capability compared to other reported materials. Besides these experimental results, Paris et al. (2012), Pustovalov et al. (2015) investigated the absorption and scattering characteristics of metal NPs in terms of possible application to solar cells. Xuan's group (Duan and Xuan, 2014; Xuan et al., 2014) calculated the absorption properties of random Al/CdS nanoshell suspensions and studied the optical properties of both TiO_2/Ag composite NPs and water-based nanofluids composed of different NPs for the solar radiation spectrum. The results revealed that absorption enhancement was affected by the LSPR effect. Hence, the optical absorption of the TiO_2/Ag plasmonic nanofluid was remarkably enhanced experimentally.

The absorption ability of nanofluids is affected by NP size, material, shape, and the environment medium, which is important for solar energy absorption (Jain et al., 2006; Noguez, 2007; Hao et al., 2007). Therefore, it is important to select suitable NP parameters for solar energy harvesting and conversion. For example, compared with nanospheres, nanowire could provide an important test platform for the investigation of selected fundamental issues in sensitized solar cell photoanodes (Chen et al., 2012b). In fact, the solar absorption capabilities of NPs in a plasmonic system can significantly affect the solar photothermal conversion performance (Chen et al., 2016). However, a comparative analysis of optimal parameters of metallic NPs for solar thermal conversion has rarely been accurately characterized and most work has focused on direct experimental measurements. Herein, our aim is to provide a thorough analysis to investigate the optimal parameters of NPs for solar thermal applications. The optical properties of NPs were calculated, and then, their interaction with solar radiation was investigated to optimize the NP parameters for solar absorption and conversion.

2. Methods

2.1. Optical property calculation

One of the most commonly used methods for numerically solving Maxwell's equations is the finite-difference time-domain (FDTD) method, originally introduced by Yee (1966). The basic idea is to use a Yee cell to transform Maxwell's equations into a set of linear algebraic equations that can be solved numerically. With the introduction of the perfect matching layer boundary conditions and other algorithmic developments, FDTD has become a well-accepted method for solving electromagnetic wave interactions with nanostructures and near-field thermal radiation due to its flexibility and accuracy, especially for nanostructures with arbitrary shapes.

Based on this method, the propagation of electromagnetic waves within the NP can be simulated, which can be described by Maxwell's equations (Taflove and Hagness, 2005):

$$\varepsilon\frac{\partial \overrightarrow{E}}{\partial t} = \nabla \times \overrightarrow{H} - \overrightarrow{J} \tag{1}$$

$$\mu\frac{\partial \overrightarrow{H}}{\partial t} = -\nabla \times \overrightarrow{E} \tag{2}$$

$$\overrightarrow{J} = \sigma\overrightarrow{E} \tag{3}$$

where E and H are electric and magnetic fields, respectively, J is current density, ε and μ are permittivity and permeability of the medium, respectively, and σ is conductivity. These equations are solved on the discrete grids by replacing all derivatives with finite-difference expressions. In the present study, the FDTD method was employed to calculate the optical properties for main NPs. For nanostructures with strong plasmonic interactions between a metal and dielectric, care must be taken to select the proper solver, boundary conditions, mesh sizes, and conformal techniques. During a computational process, the new

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