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Effects of silver nanoparticles size and shape on light scattering

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ABSTRACT

The scattering from metal nanoparticles near their localized surface plasmon resonance is a promising way to increase the light absorption in solar cells. In this article, we investigate the light scattering of silver (Ag) nanoparticles on the microcrystalline silicon (μc-Si) substrate with various sizes and shape by finite element method. The results show that large spherical particles lead to enhanced scattering efficiency, whereas reduced coupling efficiency. The scattering cross section and coupling efficiency are very sensitive to the shape of the particles. Compared with spherical particles, hemispherical and cylindrical particles show much lower and broader scattering cross section, containing two surface plasmon resonance modes, and much higher coupling efficiency at longer wavelengths. However, with the increase in the longitudinal size (or height) of the particles, the coupling efficiency decreases, especially at shorter wavelengths, due to backscattering by the longitudinal resonance mode. Finally, we simulate the absorption enhancement in μc-Si thin film solar cells by Ag nanoparticle arrays with various shape. These results will be useful for enhancing performance of the μc-Si thin film solar cells by optimizing the light-trapping design.

1. Introduction

Metallic nanoparticles (MNPs) have attracted much interest for their unique optical properties and promising applications in surface enhanced Raman scattering, biosystems, information storage, as well as solar cells [1–3]. The confined geometry of nanoparticles allows the direct excitation of localized surface plasmon resonances (LSPRs), which can result in strong light scattering and strong enhancement of electromagnetic field around the particles [4]. It has been shown experimentally [5,6] and numerically [7,8] that MNPs deposited on the front surface of solar cells can enhance their light-absorption efficiently.

LSPRs excited in MNPs decay either radiatively (scattering) or via an electron-hole pair cascade (absorption). The scattering and absorption cross section are key properties, which contain valuable information and vary with the composition, size, shape and dielectric environment of MNPs [9,10]. Langhammer et al. [11] reported based on their experiments that absorption dominates the scattering cross section for small Ag, Au, Pt, and Pd nanodisks (diameters $D < 100$ nm), and for $D > 100$ nm absorption still dominates for Pt and Pd nanodisks, while scattering dominates for Au and Ag. Tanabe [12] calculated the optical radiation efficiency (or scattering efficiency) of 11 kinds of spherical MNPs in the air, and found that Ag, Al, Au and Cu have much higher scattering efficiency than the other metals. Recently the scattering cross section of Ag–Cu, Ag–Au,

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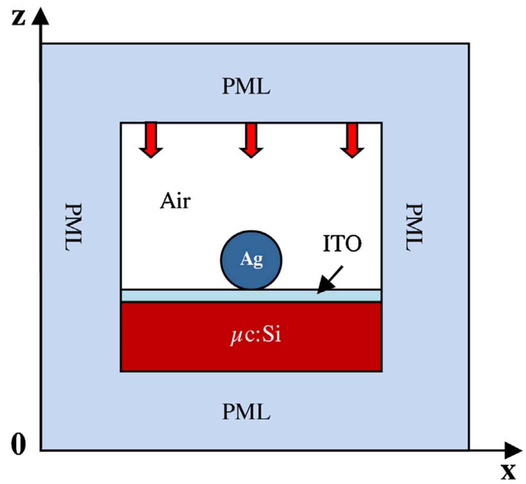

Fig. 1. Schematic cross-section of 3D numerical model used for this study (not to scale). Ag nanoparticle studied is placed on μc-Si with a 20 nm thick ITO spacer layer.

and Au–Cu alloy nanoparticles has been reported based on Mie theory [13]. For the design of plasmonic solar cells, it is crucial to systematically study the scattering properties of nanoparticles located on substrates (not in the air or in a homogenous medium). Firstly, a large scattering cross section is needed for the wavelengths at which transmission losses become significant. Secondly, the parasitic absorption in the particles, wasted as heat, should be minimized. In addition, the coupling efficiency, defined as the fraction of scattered light that is directed into the substrate [14], and the scattered electric field intensity distribution are of particular importance.

In the noble MNPs, Ag is the most popular material for plasmonic application since it has the strongest plasmon resonance with low absorption in the visible region. In this work, we present a numerical simulation on light scattering properties of a single Ag nanoparticle located on the microcrystalline silicon (μc-Si) substrate. The effects of particle size and shape on the normalized scattering and absorption cross section, scattering efficiency and coupling efficiency are discussed in detail. The simulation results will be useful in the light-trapping design of μc-Si thin film solar cells.

2. Simulation method

We use the commercial COMSOL multiphysics software package based on finite-element method (FEM) to investigate the light scattering of Ag nanoparticles. Fig. 1 shows a schematic cross-section of three dimensions (3D) numerical model used for this study. In this configuration, a single Ag nanoparticle is placed on a semi-infinite microcrystalline (μc-Si) substrate covered with a 20 nm thick indium-tin-oxide (ITO) layer, and a plane electromagnetic wave with the wavelength range from 300 nm to 1100 nm normally incidents on the particle from the top side. Here, μc-Si substrate is supposed to be semi-infinite so that the light incident into the substrate is completely absorbed. In order to simulate a single particle and infinitely extended air and μc-Si substrate, all regions above are surrounded by perfectly matched layer (PML). The minimum division mesh size is 2 nm around the particle, and the maximum mesh size of an individual dielectric region is set to be one tenth the shortest wavelength in material. The dielectric constant of μc-Si is obtained from our measurement data. The refractive indices of Ag particle are obtained from Ref. [15] and fixed refractive index 1.7 is used for ITO.

In this simulation, we use the well-known scattered-field formula, in which the total electromagnetic field is divided into an unperturbed part and a scattered part. The scattered power is calculated by integrating the Poynting vector of the scattered field over an artificial sphere or box surrounding the nanoparticle. The scattered power can be separated into the power scattered into the air and the power scattered into the substrate by integrating over the relevant parts. The coupling efficiency, that is the fraction of light scattered forward into the substrate, F_{sub}, is defined as the power scattered into the substrate divided by the total scattered power. The normalized scattering cross section Q_{sca}, is calculated by dividing the scattered power by the incident intensity and by the geometrical cross section of the particle. The normalized absorption cross section Q_{abs} is evaluated in the same manner as Q_{sca} by integrating the Poynting vector for the total field over volume of the particle, then divided by the incident intensity and by the geometrical cross section of the particle. Scattering efficiency η_{sca} is defined as the normalized scattering cross section divided by the normalized extinction cross section which is the sum of Q_{sca} and Q_{abs}.

3. Results and discussion

Fig. 2(a) and (b) shows the normalized scattering and absorption cross section respectively, for spherical Ag particles on μc-Si substrate with radius R varying from 50 nm to 125 nm. We can observe that for the nanoparticle with $R = 50$ nm the