



The Simulation of the Optical Characteristics of Platinum and Platinum/Silica Nanoparticles

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ABSTRACT

Optical properties of platinum and platinum/silica core/shell nanospheres are studied based on simulation. The numerical simulation results show that optical properties of platinum and platinum/silica core/shell nanospheres are mainly dependent on their sizes and refractive index of environment that's are embedded. The wavelength corresponding to maximum extinction shifts to longer wavelengths as the size of the nanoparticle is increased. The influence of higher-order multipoles is evident for large nanospheres, making the spectra more complex. When the shell thickness of a core/shell particle is decreased, the plasmon resonance shifts to longer wavelengths. This red shift is accompanied by an increase in peak intensity.

Key words: Mie Theory; Nanospheres; Optical Properties; Platinum; Silica.

INTRODUCTION

The search for new functional materials is one of the defining characteristics of modern science and technology. Metal nanoparticles (MNPs), in particular, platinum nanoparticles (PtNs) can possess a wide range of properties that can be used for many practical applications. Nanostructured materials show much interdisciplinary effort. Both chemical and physical properties were found to be fruitful and, in many cases, fascinating in this nanosize range. MNPs are of interest due to their special properties in many aspects, such as catalysis and applications of optical devices. Many physical and chemical

properties of modern materials for electronics, optics, chemical reactions, and other high-tech applications depend closely on the manufacturing process. Synthesis and processing of MNPs pose a number of difficulties, especially in terms of reactivity and agglomeration. The remarkable reactivity of MNPs, which makes them potential candidates, for instance, as catalysts, is associated to their high fraction of surface atoms as compared to conventional bulk materials. In certain applications, a uniform dispersion of nanoparticles is required¹. Also, the light scattering from nanoparticle surface due to the oscillatory motion of nanoparticle electrons. These electrons produce radiation. If the light is absorbed by the nanoparticle,

the energy of the incident light is converted to another form e.g. heat. The optical properties is strongly dependent on size, shape and composition of the particles and medium of nanoparticles are embedded. By modifying these parameters, we can simulate the some optical properties of nanoparticles like scattering, absorbing and extinction (sum of the absorbed and scattered energy) over a wide range of wavelengths. Due to potential technological interests of Pt nanoparticles, the synthesis and study of Pt nanoparticles was a very active field of research during last years. Platinum containing films could be used for enzyme immobilization², optical applications³, and catalytic activity⁴. For instance, the enhanced catalytic activity of Pt Ns plays an important role in the reduction of pollutant gases exhausted from automobiles and thermal ablation⁵⁻⁶. When platinum nanoparticles interact with the light, according to the fluctuation of the electron band on nanoparticle surface, a phenomenon called surface plasmon occurs. Platinum nanoparticles plasmon modes have a high absorption in the ultraviolet and violet spectral region⁷. Also, when a silica and platinum core/shell nanoparticles is used, a sharp plasmon frequency is observed, that can be reduced by changing the diameter of the core and shell. Recently, the strong photostimulated luminescence is obtained from platinum and PVP-capped Pt nanoclusters⁹⁻¹². The main advantage of using spherical geometry of nanoparticles is control of optical properties in a highly predictive state. Also, the optical properties of a material with sphere geometry can be simulated by using the solution of Maxwell's Equations for arbitrary diameter and dielectric constant. Therefore, we uses the Mie theory solution for simulation of the optical properties of platinum and core/shell platinum/silica nanospheres and discuss about their optical properties.

Simulation Method

Important physical quantities can be obtained from the previous scattered fields. One of these is the cross section, which can be defined as the net rate at which electromagnetic energy (W) crosses the surface of an imaginary sphere of radius r centered on the particle divided by the incident irradiance (I_i). To quantify the rate of the electromagnetic energy that is absorbed (W_{abs}) or scattered (W_{sca}) by the diffuser, the absorption (C_{abs})

or scattering cross sections (C_{sca}) can be defined. Where

$$C_{abs} = \frac{W_{abs}}{I_i}, \quad C_{sca} = \frac{W_{sca}}{I_i}, \quad \dots(1)$$

The sum of these is the extinction cross section:

$$C_{ext} = C_{sca} + C_{abs} \quad \dots(2)$$

Which gives an idea of the amount of energy removed from the incident field due to scattering and/or absorption generated by the particle. These parameters can be expressed as a function of the Mie coefficients as follows

$$C_{sca} = \frac{W_{sca}}{I_i} = \frac{2\pi}{k^2} \sum_{n=1}^{\infty} (2n+1) (|a_n|^2 + |b_n|^2) \dots(3)$$

$$C_{ext} = \frac{W_{ext}}{I_i} = \frac{2\pi}{k^2} \sum_{n=1}^{\infty} (2n+1) \text{Re}(a_n + b_n) \dots(4)$$

$$C_{abs} = C_{ext} - C_{sca} \quad \dots(5)$$

By dividing these cross sections by the geometrical cross area of the particle projected onto a plane perpendicular to the incident beam, G , we obtain the scattering, extinction and absorption efficiencies. For a sphere, $G = \pi R^2$, and the expressions for the efficiencies become:

$$Q_{sca} = \frac{C_{sca}}{G} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1) (|a_n|^2 + |b_n|^2) \quad \dots(6)$$

$$Q_{ext} = \frac{C_{ext}}{G} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1) \text{Re}(a_n + b_n) \quad \dots(7)$$

$$C_{abs} = C_{ext} - C_{sca} \quad \dots(8)$$

RESULTS AND DISCUSSION

Researchers determined the dielectric functions of copper, platinum and gold and due to the small correction below R_{3} nm, in this work, these dielectric functions used to described the optical properties of platinum nanoparticles¹⁰.

According to these data, we can provide the optical properties of a nanosphere as functions of the particle diameter and the medium refractive index n_m .

The optical properties of platinum nanospheres are highly dependent on the nanosphere diameter. The extinction cross section area spectra of 10 sizes of platinum nanospheres are displayed in the Figure. 1. The identical mass concentrations for these nanospheres is 0.05 mg/mL. Smaller platinum nanospheres primarily absorb light and have peaks near 504 nm (Figure.2). All spectra have a high resonance at visible spectrum, caused by the collective oscillations of the electron on platinum nanoparticles surface. The wavelength

corresponding to maximum extinction shifts to longer wavelengths (red shift) as the particle diameter increases (Figure.3), while larger spheres exhibit increased scattering and have peaks that broaden significantly and shift towards longer wavelengths (known as red-shifting) and generally lies to the near infra-red. High light scattering of the larger spheres due to have larger optical cross sections.

The optical properties of platinum nanospheres also depend on the refractive index near the nanoparticle surface. As the refractive index near the nanoparticle surface increases, the nanoparticle extinction spectrum shifts to longer wavelengths. Practically, this means that the

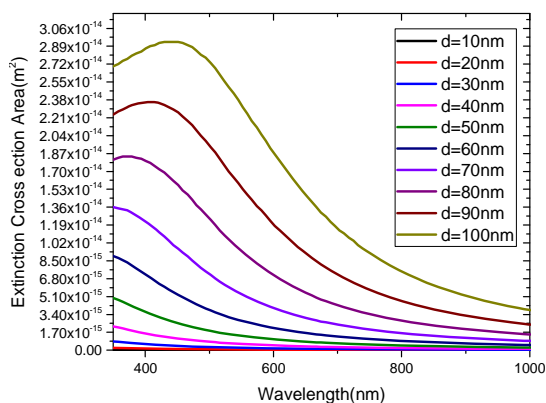


Fig. 1: Extinction cross section area for platinum nanospheres of varying diameter. Refractive index of medium is 1.33.

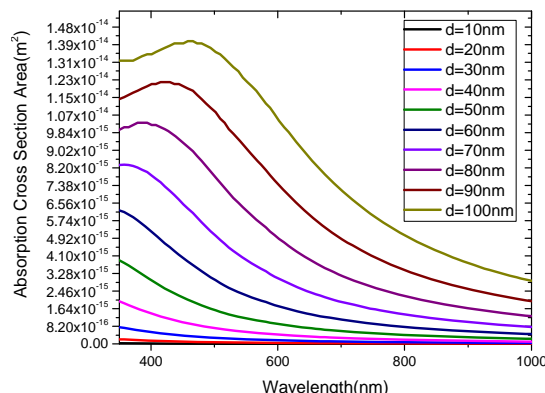


Fig. 2: Absorption cross section area for 10 sizes platinum nanospheres of varying diameter. Refractive index of medium is 1.33

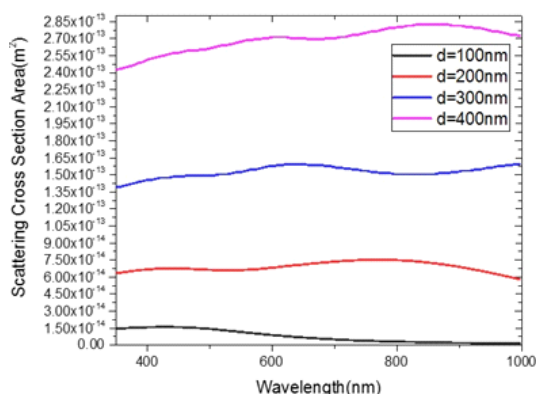


Fig. 3: Scattering cross section area for spherical platinum nanoparticles of varying radii. Refractive index of medium is 1.33

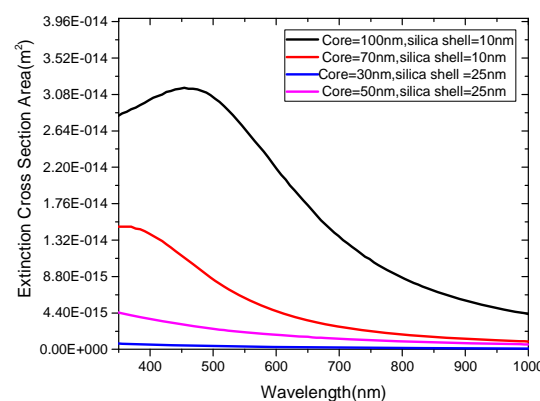


Fig. 4: Extinction cross section area of core/shell nanoparticles. The core is platinum and the shell is silica

nanoparticle extinction peak location will shift to shorter wavelengths (blue-shift) if the particles are transferred from water ($n=1.33$) to air ($n=1.00$), or shift to longer wavelengths if the particles are transferred to oil ($n=1.5$). Increasing the refractive index from 1 to 1.33 results in an extinction peak shift of over 75 nm, moving the peak from the ultraviolet to the visible region of the spectrum. When embedded in high index materials, the extinction cross section is substantially increased. Figure. 4 shows the extinction for platinum/silica core/shell nanospheres with different sizes. The spectrum with a peak at 482 nm is the extinction from a platinum sphere with a diameter of 100 nm. As the shell thickness is decreased, the peaks shift to the red and become more intense. Increasing the ratio of core diameter to total diameter causes the peak to shift red. Thinning the shell layer produces a large increase in polarization at the sphere boundary, which yields the more intense extinction

peaks. The same general trends are observed when the nanoparticle size is increased.

CONCLUSION

The optical properties of spherical platinum and platinum/silica core/shell nanospheres can be found by modifying the physical dimensions. The thickness and diameter of the nanospheres are extremely important and play an important role in the intensity and placement of the plasmon resonances. If platinum spherical nanospheres get larger, the peaks broaden and shift to longer wavelengths. Higher-order modes also become important, making the extinction spectrum more complex. The platinum/silica core/shell nanospheres display a red shift and an increase in intensity of extinction as the shell size is decreased. The magnitude of the shift is highly dependent on the shell thickness.

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