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RESEARCH ARTICLE - PHYSICS

Calculation of Extinction Cross Section For Core- Shell Nanostructures Using COMSOL Multiphysics

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Abstract

Using COMSOL Multiphysics software, SiO_2@Pt and SiO_2@Cu spherical core shell were modeled. For both composites, the sphere radius was constant (60 nm) and the thickness of both shells were changed from 5 to 20 nm. The model was used to simulate wavelength dependent optical properties including absorption, scattering, and extinction cross sections. The resonance wavelength for absorption, scattering and extension cross section decreases with increasing thickness for both the core shell structure. All resonance wavelength values for SiO_2@Pt are less than that for SiO_2@Cu. Exact control over shell thickness modifies the kinetics of electromagnetic interactions at the nanoscale in and adjusts optical density. By paving the path for the construction of innovative nanoscale devices with unique optical properties, the discoveries pave the door for future advancements in nanotechnology. The cross section of absorption and scattering related to the three types of LSPR is then discussed. It is discovered that extinction is dominated by absorption when the shell thickness is smaller, with a small crossover occurring as the shell thickness increases from absorption dominance to scattering dominance.

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Keywords: COMSOL, nanosphere, core, shell, Plasmon.

Introduction

We are now able to explore the intriguing world of the nano-world, which was previously unattainable due to significant advancements in the manufacturing and manipulation of items on the nanoscale scale during the past few decades [1]. The exchange of light and electrons on the outside of nanoparticles is one of their main characteristics. When the frequency of the incident photon is in tune with the collective oscillations of electrons on the nanoparticle's surface, a phenomenao called surface plasmon resonance takes place at a certain wavelength of light [2]. Light-excited electron oscillations are the source of the excitation of LSPs inside the NPs. Consequently, the excitation of the LSPs will result in a partial extinction of light energy. An indicator of a particle's absorption efficiency for incident light is its scattering cross-section. The absorption cross section primarily depends on the NPs' radius and correlates to the geometrical section. The incident light is also scattered by NPs in addition to being absorbed. To investigate the relationship between light and NPS, another metric the scattering cross section must be taken into account. The extinction cross-section, which is relevant to this work, is the total of the scattering and absorption cross-sections. Absorption is more significant than scattering for very small particles, but scattering becomes more significant than absorption when the particle's radius is similar to the wavelength of light [3]. the material, shape, and spacing between the particles all affect the optical characteristics of LSPR in nanoparticle systems. Since core-shell nanoparticles have not been investigated before, we are examining how the size of the core and shell as well as the type of material affect the RIS and spectrum of these nanostructures [4].

The geometrical shape, dimensional size, composition of the nanostructure, and local surroundings of the nanoparticle all have a significant impact on the LSPR spectrum parameters (amplitude, spectral position, and width) (Baida et al. 2009, Billaud et al. 2008[5]. Depending on their structure, metal nanoparticles' optical response can be analyzed using a variety of theoretical techniques. The optical characteristics of various metallic nanoparticles with spherical shape are accurately reproduced by the Mie theory , which is an exact solution of light scattering by a sphere [6]. Absorption, scattering, and extinction cross sections for nanoparticles of various sizes and shapes can be predicted thanks to COMSOL Multiphysics' accurate simulations of particle geometry and the dielectric environment. For parametric research that would be challenging or time-consuming to do experimentally, the program offers a flexible platform. This study is mainly concerned with important optical characteristics, such as plasmon resonance, absorption, scattering, and extinction cross-sections, and how these vary depending on the geometry of nanoparticles [7]. Interest in using plasmon resonant nanoparticles and nanostructures for optical and photonic applications, and more recently, biomedical applications, has increased due to their remarkable optical qualities and recent developments in nanoparticle synthesis, conjugation, and assembly [8,9]. which increases optical absorption and scattering at that wavelength. The nanoparticles' size, shape, and the surrounding media are some of the variables that affect the LSPR response [10].

Although a number of research have been done in this field, they usually: either how the geometry of the nanoparticle affects optical properties [11] or how temperature affects these properties [12]. For example, changes in shape change the particle's scattering and absorption cross-sections and the wavelength of LSPR.

The ability of a nanoparticle to absorb energy from an incident electromagnetic wave and transform it into heat is represented by its absorption cross section (σ_{abs}). Particle size and incident light wavelength are two examples of material parameters that affect it [13]. It is computed using equation 1:

$$\sigma_{abs}=4\cdot w_{abs}/I_{np}\ (m^2) \qquad (1)$$

Where: w_{abs} is the total power dissipation, I_{np} is the irradiance power.

Similarly, the nanoparticle's scattering cross section (σ_{sca}) indicates its capacity to redirect light in various directions without absorbing it. It is dependent upon the size and form of the particle. Equation 2 gives it:

$$\sigma_{sca}=4\cdot w_{sca}/I_{np}\ (m^2) \qquad (2)$$

Where: w_{sca} the total power scattered .

The overall loss of light intensity from both absorption and scattering is represented by the nanoparticle's extinction cross section (σ_{ext}); see equation 3:

$$\sigma_{ext}=\sigma_{abs}+\sigma_{sca} \quad (m^2) \qquad (3)$$

Therefore, the current study reveals that the directional pattern may be tuned at the designated resonance wavelengths by accurately altering the core size and shell thickness, as well as by selecting the right material combination for the core and shell[14]. Furthermore, it is now simpler to simulate and forecast the behavior of such complex systems because to developments in computational tools. One effective technique for simulating the optical characteristics of NPs is the simulation program COMSOL Multiphysics [15]. In this study, we employ COMSOL Multiphysics to model a range of nanoparticle forms, including core-shell structures, while methodically altering their sizes[7]. Therefore, the extinction cross-section of core-shell nanostrucres can be calculated with high accuracy using COMSOL Multiphysics simulations ,with a clear influence of both material type and layer thickness on the optical extinction behavior.

Method

Understanding surface plasmon phenomena requires the modeling and simulation of optical properties for core-shell nanoparticles. An analytical model based on an approximate Mie theory is presented in this study. It is built using the Finite Element Method (FEM) in COMSOL Multiphysics software[16].
Wavelength-dependent optical characteristics, including absorption, scattering, and extinction cross sections, were simulated using this model. To improve the accuracy of the results, far-field calculations were also performed on the Perfectly Matched Layer's (PML) inner boundary. The geometric model for a spherical core shell is displayed in Figure (1).

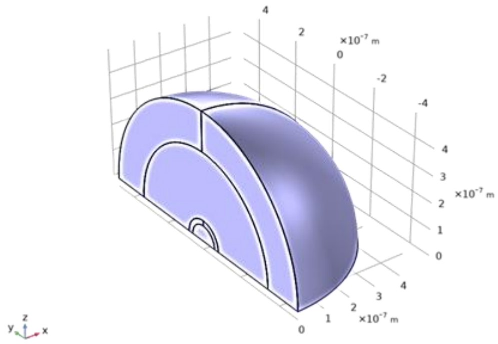

Figure (1) The geometrical model

Results and discussions

In Figure (2-A), a significant increase in the absorption peak is observed as the thickness of the copper shell (t_shell) decreases. At a shell thickness of 5 nm, a sharp absorption peak appears near the wavelength of 800nm, indicating strong Surface Plasmon Resonance (SPR) effects. As the shell thickness increases, the absorption peak shifts towards shorter wavelengths and its intensity decreases. A second peak appears in the absorption curve of the SiO_2@Cu structure at a wavelength of approximately 1000 nm, exhibiting higher absorption intensity than the othershell thicknesses. This indicates the influence of the thin copper shell on absorption in this spectral region. The emergence of this peak is attributed to the Surface Plasmon Resonance (SPR) phenomenon, which is affected by the size and thickness of the copper shell. The reduced thickness leads to a change in the distribution of electromagnetic fields on the surface. Moreover, the absorption in the Near-Infrared (NIR) range makes this nanostructure promising for applications such as biosensing and photothermal therapy.

For SiO2@Pt, Figure (2-B) shows the absorption cross-section has high valuesat short wavelengths (in the ultraviolet range) and gradually decreases as the shell thickness decreases. The absorption peak at shorter wavelengths is associated with electronic transitions in the energy bands of platinum and their interaction with surface plasmons. Additionally, increasing the shell thickness modifies the boundary conditions of free electrons, affecting the surface plasmon frequency and consequently shifting the peak to shorter wavelengths [17,18].

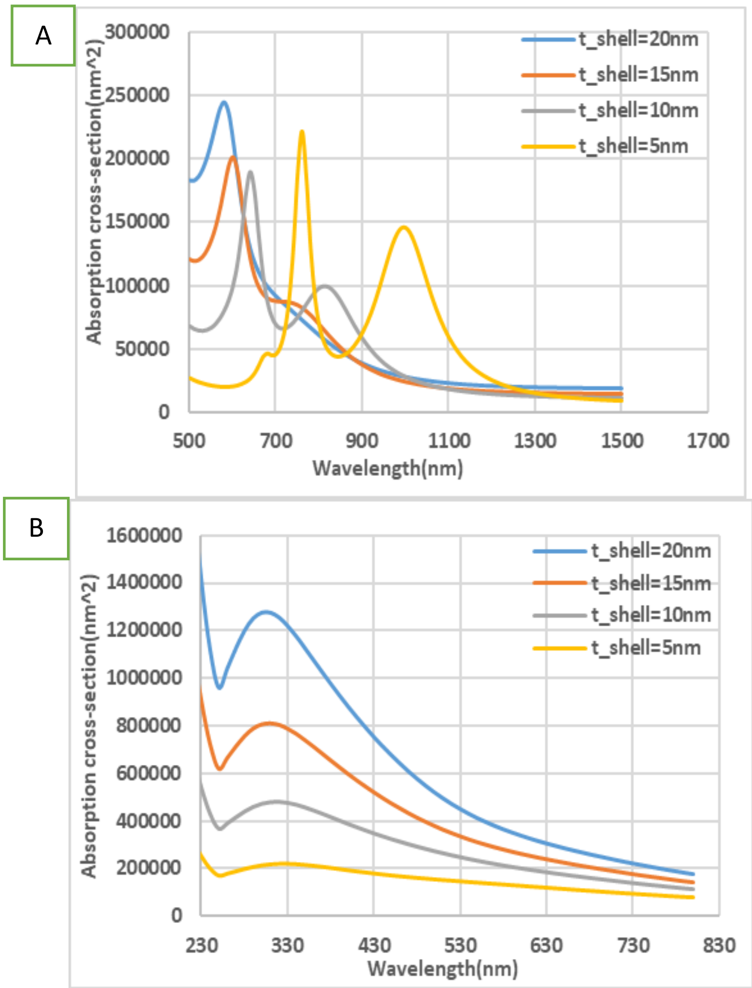

Figure (2) Absorption cross section for: A- SiO_2@Cu, and B- SiO_2@Pt

The scattering peak becomes more distinct at larger thicknesses (15 and 20 nm), suggesting that particles with thicker shells reflect and scatter light more effectively, see Figure (3-A). These peaks also shift towards longer wavelengths as the thickness decreases.

For SiO_2@Pt, the scattering cross section shows high values at shorter wavelengths and gradually decreases as the shell thickness increases. According to Mie Theory of light scattering by nanoparticles, scattering is strongly dependent on the particle size relative to the wavelength of light. When the particle size (or shell thickness) increases, stronger scattering occurs at shorter wavelengths because the wavelength becomes more comparable to the particle dimensions, enhancing both forward and backward scattering [10].

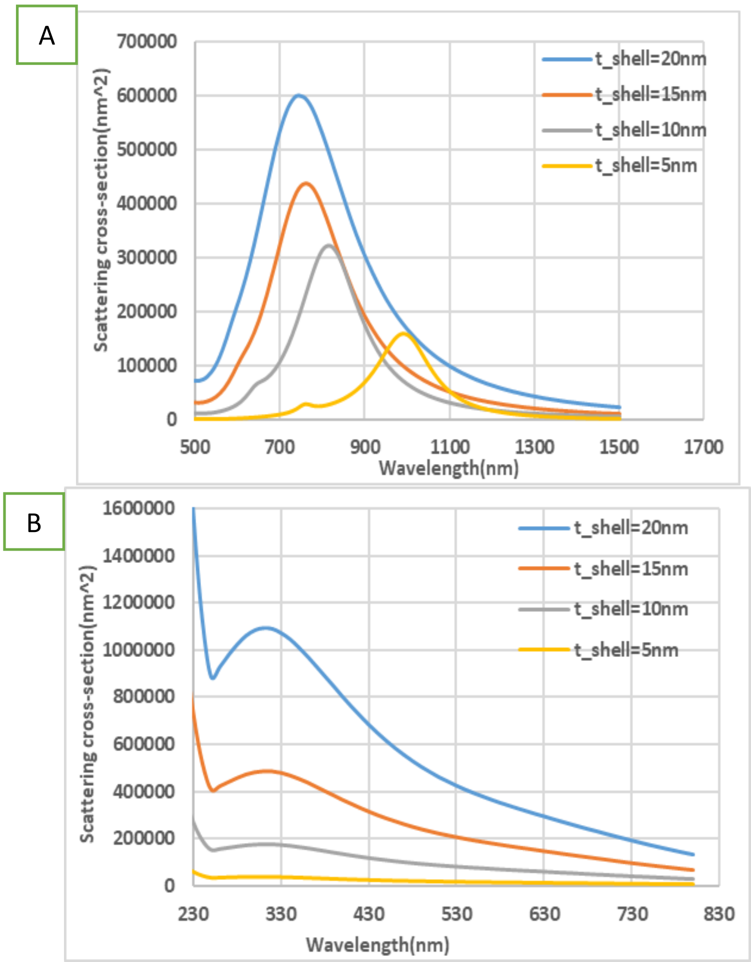

Figure (3) Scattering cross section for: A- SiO_2@Cu, and B- SiO_2@Pt

For SiO_2@Cu sample, Figure (4-A), the extinction (the sum of absorption and scattering) reflects the trends observed in the previous Figures (2-A) and (3-A). The 20 nm shell thickness shows the highest extinction value due to the combination of moderate absorption and strong scattering. The thin copper shell (5 nm) enhances absorption due to surface plasmon resonance, while the thicker shell enhances scattering. This behavior can be utilized in optical applications such as optical sensors or photonics to enhance absorption or scattering at specific wavelengths.

For SiO_2@Pt sample, Figure (4-B), the extinction cross-section shows distinct peaks at shorter wavelengths, then gradually decreases similarly to absorption and scattering. The peaks become more pronounced and shift to shorter wavelengths as the shell thickness increases. Additionally, the overall extinction increases with thicker shells due to the enhancement of both absorption and scattering. At shorter wavelengths, absorption dominates due to the influence of free electrons in platinum, while scattering contributes less. As the wavelength increases, absorption gradually decreases, and scattering becomes relatively more dominant. Increasing the shell thickness enhances both absorption (due to increased free electron density) and scattering (due to larger physical dimensions of the particles). Controlling the shell thickness is an effective tool for tuning the optical properties of nanoparticles, making them suitable for a wide range of applications, including photocatalysis, bioimaging, and nanophotonic technologies [18-20].

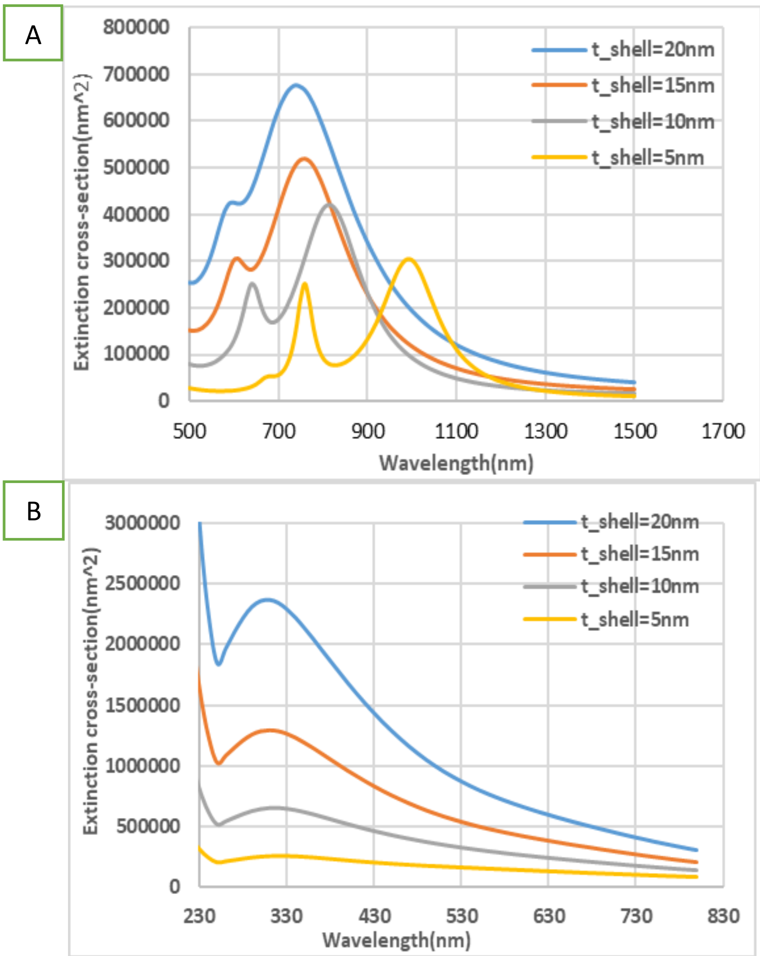

Figure (3) Extinction cross section for: A- SiO2@Cu, and B- SiO2@Pt

The above results are summarized in the following Tables

Table (1) Resonance wavelengths for SiO_2@Cu composite

Radius of SiO2 Core (nm)	Thickness of Cu shell (nm)	Resonance Wavelength (nm) of		
		Extinction cross section	Scattering cross section	Absorption cross section
60	20	740	740	580
60	15	760	760	600
60	10	810	820	640
60	5	990	990	760

Table (2) Resonance wavelengths for SiO_2@Pt composite

Radius of SiO_2 Core (nm)	Thickness of Pt shell (nm)	Resonance Wavelength (nm) of		
		Extinction cross section	Scattering cross section	Absorption cross section
60	20	310	310	300
60	15	310	310	310
60	10	320	310	320
60	5	320	310	320

Conclusions

At shorter wavelengths, absorption was the dominant contributor due to the oscillation of free electrons and the influence of surface plasmons. As the wavelength increased, scattering became the primary factor influencing extinction, indicating a shift in electromagnetic interaction mechanisms. These findings underscore the critical role of shell thickness in fine-tuning the optical response of core-shell nanostructures paving the way for advanced application such as efficient photocatalysis, high-resolution bioimaging And nanophotonics.

The study shows that exact control over shell thickness modifies the kinetics of electromagnetic interactions at the nanoscale in addition to adjusting optical density. These discoveries pave the way for future developments in nanotechnology and represent a significant step toward the creation of novel nanoscale devices with tailored optical characteristics. Temperature-dependent properties should be included in modeling to provide a more accurate representation of how nanostructures work in practical situations. It is also recommended to look at how different environmental media, including air, water, or biological fluids, impact the extinction cross-section, especially for biomedical and sensing applications.

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