

# Scattering, Absorption and Extinction Properties of Al/TiO<sub>2</sub> Core/Shell Nanospheres

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## Abstract

The Al/TiO<sub>2</sub> core/shell nanoparticles can be used as coating materials in many industrial applications. In this article, we simulated the optical extinction, absorption and scattering properties of Al and Al/TiO<sub>2</sub> nanoparticles. Results show that optical properties of Al/TiO<sub>2</sub> core/shell nanoparticles are highly dependent on many factors such as size, index of environment, intrinsic properties, and surface chemistry. The Al/TiO<sub>2</sub> nanoparticles have especial optical properties in the absorption, extinction and scattering cross section area spectrum. These especial properties can be used in various application of industry. Also, according to the optical properties of Al/TiO<sub>2</sub> nanospheres, best result for these structures, is that the core diameter and shell thickness being equal, because of high scattering occurred in the wide band of visible spectrum.

**Keywords:** Absorption, Extinction, Mie Theory, Optical Properties, Scattering

## 1. Introduction

Nanotechnology is an area of scientific research due to the high potential applications in defense-industry, optical devices, media-recorder, and electronic devices. Aluminum nanoparticles have been researched and used in industrial, because of their interesting properties due to the increased reactivity as compared with particle. The Al nanoparticles morphology is spherical and they appear as black or grey-black nanopowder. Aluminum nanoparticles are very reactive, so experimental circumstance must also be taken to protect the nanopowder from moisture, heat, and sunlight<sup>1</sup>. We can use aluminum nanoparticles in vacuum and stored in a cool and dry room. Also, Aluminum nanoparticles are very effective catalysts. When we add Al nanoparticles into solid rocket fuel, it helps improve stability, speed and heat combustion<sup>2</sup>. The aluminum nanoparticles can be increased

the burning rate of solid propellant, 7-25 times higher than larger particle sizes. Another part of this study is the titanium dioxide that has been used for shell material. Titanium dioxide is the best material for optical application because of their special scattering, absorbing and extinction properties. Scientists discovered the photovoltaic property of TiO<sub>2</sub><sup>3</sup>. They have been researched on the electronic structure, catalytic reactivity and surface property of TiO<sub>2</sub>. In this article, we simulated the optical properties of Aluminum/Titanium dioxide core/shell nanospheres. We used the solution of Maxwell's equations for spherical particles using Mie-Gans theory. A history about Mie's theory can be found in<sup>4-10</sup>, which was written in 2008 at the occasion of the centenary anniversary of Mie's original publication. According to this theory, we calculate the optical cross section area, used MATLAB 2012 software, such as the extinction, absorption and scattering cross sectional area for

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Aluminum/Titanium dioxide core/shell nanoparticles at different diameter and shell thickness.

## 2. Simulation Method

In this study, we focused on the optical properties of Aluminum/Titanium dioxide core/shell nanoparticles. For this reason, to compute the cross section area diagrams (scattering, absorbing and extinction curves) Mie Coefficients  $a_n$  and  $b_n$  of coated spheres can be used like that for homogeneous spheres by following formulas<sup>11</sup>:

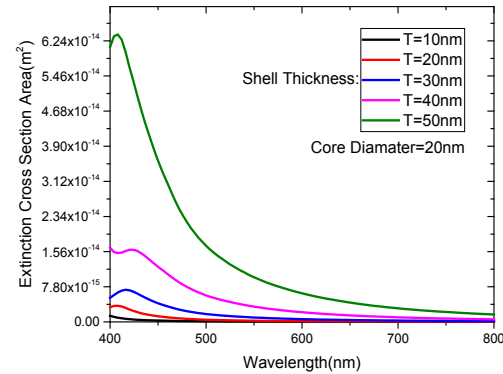
$$a_n = \frac{\left( \frac{\beta_n^0}{m_2} + \frac{n}{y} \right) \psi_n(y) - \psi_{n-1}(y)}{\left( \frac{\beta_n^0}{m_2} + \frac{n}{y} \right) \xi_n(y) - \xi_{n-1}(y)} \quad (1)$$

$$b_n = \frac{\left( m_2 \beta_n^0 + \frac{n}{y} \right) \psi_n(y) - \psi_{n-1}(y)}{\left( m_2 \beta_n^0 + \frac{n}{y} \right) \xi_n(y) - \xi_{n-1}(y)} \quad (2)$$

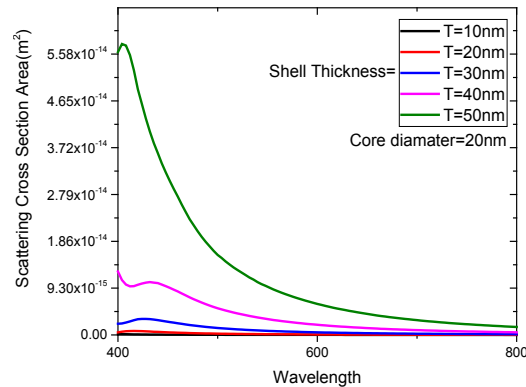
$$\beta_n^0 = \frac{D_n(m_2 y) - \left[ \frac{A_n \chi'_n(m_2 y)}{\psi_n(m_2 y)} \right]}{1 - \left[ \frac{A_n \chi'_n(m_2 y)}{\psi_n(m_2 y)} \right]} \quad (3)$$

## 3. Results and Discussion

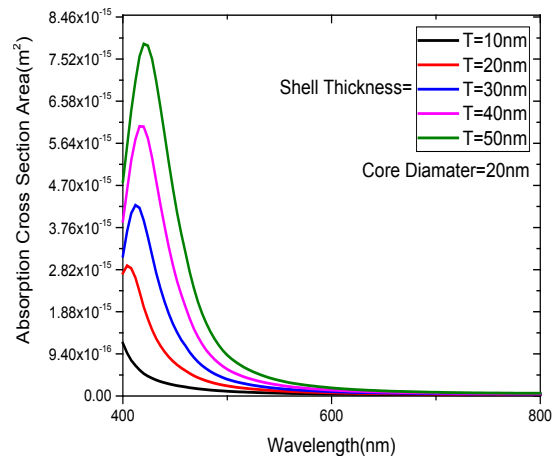
The optical properties of Al/TiO<sub>2</sub> nanospheres are highly relative on the nanospheres diameter. The absorption, extinction and scattering cross section area diagrams of Al/TiO<sub>2</sub> core/shell nanospheres with core diameter of 20 nm at various shell thickness (10-50 nm) are displayed in the Figure 1, Figure 2 and Figure 3. The Al/TiO<sub>2</sub> core/shell nanospheres scatter the light and have peaks near 400 nm (Figure 3). All spectra have a pick resonance at visible spectrum, caused by the oscillations of the nanosphere electrons on the surface. If the core diameter is constant and shell thickness is increased, scattering and extinction cross section curves are exponential and peaks at visible spectrum (Figure 2 and Figure 3). According to the Figure 4, when the core diameter and shell thickness is equal, we can see picks in the curves of optical properties. Also, if the core diameter and shell thickness is kept constant at 50 nm, the optical properties spectrum with a peak at visible area occurred. As the shell thickness is increased, the peaks arise to the high.



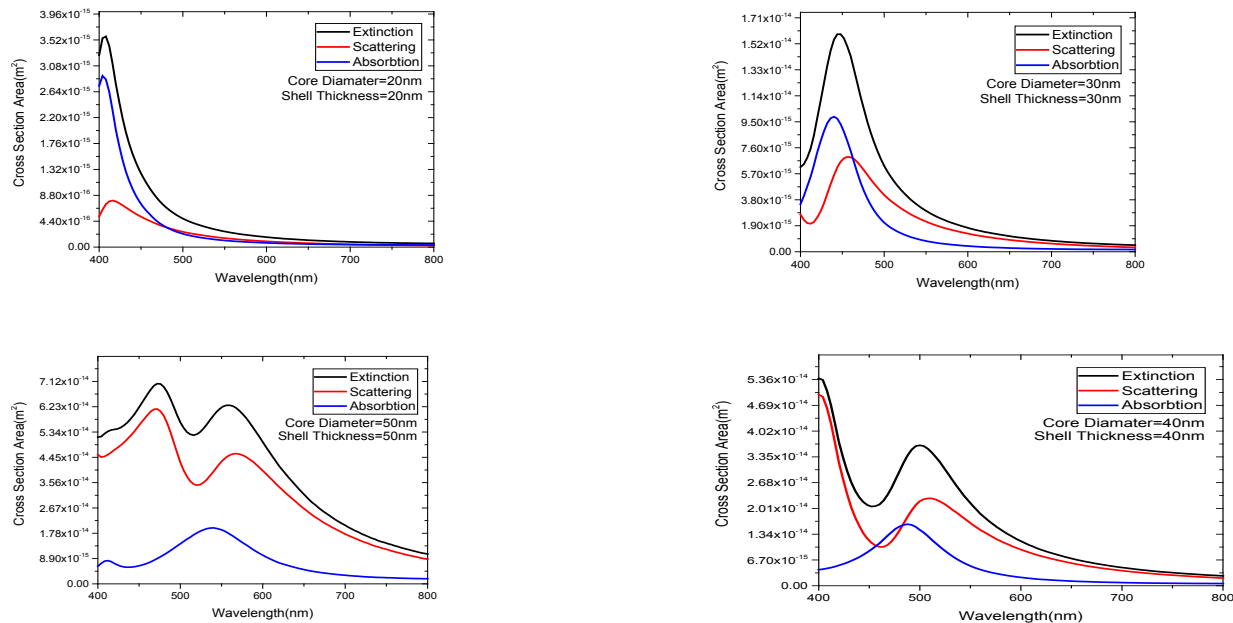
**Figure 1.** Extinction cross section area for Al/TiO<sub>2</sub> core/shell nanospheres at varying thickness shell.



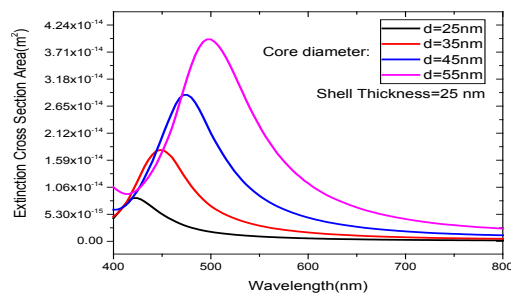
**Figure 2.** Scattering cross section area for Al/TiO<sub>2</sub> core/shell nanospheres at varying thickness shell.



**Figure 3.** Absorption cross section area for Al/TiO<sub>2</sub> core/shell nanospheres at varying thickness shell.



**Figure 4.** Cross section area for Al/TiO<sub>2</sub> Nanospheres (core diameter and shell thickness are equal).



**Figure 5.** Extinction cross section area for Al/TiO<sub>2</sub> core/shell nanospheres at varying core diameter.

Figure 5 shows the extinction cross sectional area for Al/TiO<sub>2</sub> core/shell nanospheres at different core diameter. The shell thickness is kept constant at 25 nm. The spectrum with a peak at visible area. As the core diameter is increased, the peaks arise to the high and become wider. Thinning the shell layer produces a high increase in polarization at the sphere boundary, which yields the more intense extinction peaks.

## 4. Conclusion

The Al/TiO<sub>2</sub> nanospheres have interesting optical properties due to the result of absorption, extinction and scattering cross section area curves. These optical proper

ties can be used in various applications of military and optical devices. Also, according to the optical properties of Al/TiO<sub>2</sub> nanospheres, one of the useful choices of these structures is that the core diameter and shell thickness being equal, because of high scattering occurred in the wide band of visible spectrum.

## 5. References

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