Project Report

(As a part of the Internal Assessment assignment)

Computation of Optical Properties of Gold Rectangular Nano-Prism using the DDSCAT Code

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1 Introduction

Gold nanoparticles have garnered significant interest due to their unique optical properties, which find applications in various fields such as photonics, sensing, and biomedical imaging. Understanding the optical properties of these nanoparticles is crucial for optimizing their performance in different applications. In this project, we employ the Discrete Dipole Scattering (DDSCAT) code to compute the optical properties of a gold rectangular nano prism.

DDSCAT is a powerful computational tool used to simulate the interaction of electromagnetic waves with particles of arbitrary shape and composition. By representing particles as a collection of polarizable points (dipoles) and solving Maxwell's equations, DDSCAT enables us to study the scattering and absorption of light by particles with diverse shapes and compositions.

Through this project, we aim to investigate how the size and shape of gold rectangular nanoprism affect its extinction, scattering, and absorption properties. By systematically varying the dimensions of the nanoprism, we will generate data for the efficiency factors of absorption, scattering, and extinction. This will allow us to understand how the morphology of the nanoprism influences its interaction with light, which is crucial for various applications such as sensing, imaging, and photothermal therapy.

Absorption efficiency factor:

$$Q_{\mathrm{abs}} = C_{\mathrm{abs}} = \frac{4\pi a^2}{\lambda} Im(m)$$

Scattering efficiency factor:

$$Q_{\mathrm{sca}} = C_{\mathrm{sca}} = \frac{4\pi a^2}{\lambda} Re(m)$$

Extinction efficiency factor:

$$Q_{\mathrm{ext}} = Q_{\mathrm{sca}} + Q_{\mathrm{abs}}$$

2 Procedure

The Fortran code files are compiled to generate the executable program `ddscat.exe`. Initially, to set up the environment for the calculation, the command `ddscat >& ddscat.out &` is executed. This command generates empty output files necessary for the calculation process.

Subsequently, the main DDSCAT calculation is performed using the command `ddscat >& ddscat.log &`. This command generates various ASCII files containing important simulation data.

Finally, the main calculation for the material is executed using the command `./ddscat`. This step completes the DDSCAT simulation process and provides the desired results.

Input Files

1. ddscat.par - The ddscat.par file is an input file that contains parameters for the DDSCAT program. The parameters in the ddscat.par file are as follows:

- **NOTORQ**: Specifies whether to perform torque calculations (NOTORQ = skip, DOTORQ = do calculations).
- **PBCGS2**: Specifies the conjugate gradient method for solving linear equations in PBC calculations.
- **GPFAFT**: Specifies the FFT method for Fast Fourier Transform.
- **GKDLDR**: Specifies the method for solving the electromagnetic scattering problem (DDA method).
- **NOTBIN**: Specifies whether to generate binary output files (NOTBIN = skip, ORIBIN = original, ALLBIN = all output).
- **Initial Memory Allocation**: Initial memory allocation for target generation.
- **RCTGLPRSM**: Specifies the shape of the target (rectangular prism).
- **NCOMP**: Number of dielectric materials.
- **../diel/Au_evap**: File containing the refractive index of the dielectric material.
- **NRFLD**: Specifies whether to calculate additional nearfield (0 = skip, 1 = calculate).
- **TOL**: Error tolerance for the calculation.
- **MXITER**: Maximum number of iterations allowed.

- **GAMMA**: Interaction cutoff parameter for periodic boundary condition (PBC) calculations.
- **ETASCA**: Angular resolution for calculation of ¡cos¿, etc.
- **Vacuum wavelengths**: Wavelengths for calculations.
- **NAMBIENT**: Refractive index of ambient medium.
- **Effective Radii**: Effective radii of the target.
- **Define Incident Polarizations**: Incident polarizations (e01 and orthogonal).
- **IWRKSC**: Specifies which output files to write.
- **Prescribe Target Rotations**: Rotational parameters for the target.
- **First IWAV, IRAD, IORI**: Specify the starting indices for wavelengths, angles, and target orientations.
- **NSMELTS**: Number of elements of S_ij matrix to print.
- **Specify Scattered Directions**: Specifies the scattering planes and their parameters.

2. Au_evap - File containing the refractive index of the dielectric material *Evaporated Gold(Au)* over a range of wavelengths.

Output Files

After the execution of the program, the following output files are generated:

- **ddscat.log -** Log file containing general information about the calculation process.
- **mtable -** Summary of the dielectric constant used in the calculations.
- **qtable -** Summary of the orientationally-averaged values of $Q_{\rm ext}$, $Q_{\rm abs}$, $Q_{\rm sca}$, $g(1)$, $\langle\cos^2(\theta_s)\rangle$, $Q_{\rm bk}$, and $N_{\rm sca}$.
- **qtable2 -** Summary of the orientationally-averaged values of $Q_{\rm pha}$, $Q_{\rm pol}$, and $Q_{\rm cpol}$.
- **wxxxryyyori.avg -** this file contains Q values and scattering information averaged over however many target orientations have been specified.
- **wxxxryyykzzz.sca -** Files containing the scattering cross-sections for each scattering direction if `IWRKSC=1` is specified in `ddscat.par`.

The file **ddscat.out** may contain minimal information and be empty. The file **ddscat.log_000** will contain any error messages generated and a running report on the progress of the calculation, including the creation of the target dipole array.

3 Post-Processing and Analysis

After the completion of the DDSCAT simulation, the file **qtable** is generated, containing the extinction (Q_{ext}), absorption (Q_{abs}), and scattering (Q_{sca}) efficiency factors over the wavelength range.

Data Analysis

Using the data from the **qtable** file, we perform post-processing and analysis to generate graphs of wavelength (λ) versus Q_{ext}, Q_{abs}, and Q_{sca}. These graphs allow us to study the variation of the optical properties with wavelength for various effective radii of the gold rectangular nano-prism.

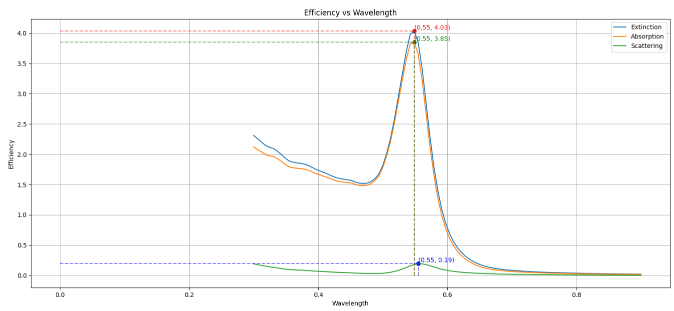

Figure 1: Efficiency for Gold Rectangular Prism with an effective radius of 20 nm

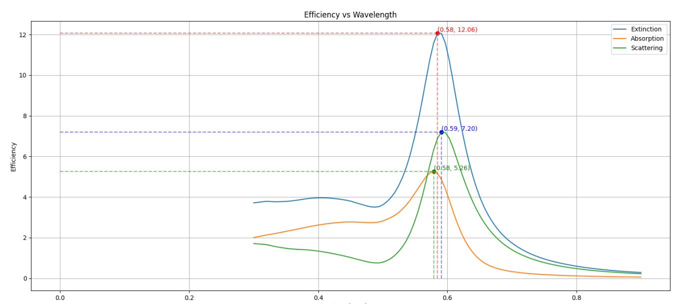

Figure 2: Efficiency for Gold Rectangular Prism with an effective radius of 50 nm

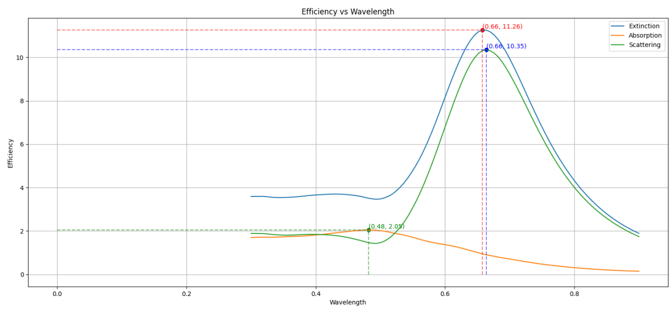

Figure 3: Efficiency for Gold Rectangular Prism with an effective radius of 75 nm

4 Results

After plotting the graphs, we noted down the peak wavelength (λ) on the x-axis for each effective radius [20 nm, 50 nm, 75 nm]. *The peak wavelength for scattering is 550 nm, 590 nm, and 660 nm. The peak wavelength for absorption is 550 nm, 580 nm, and 489 nm. The peak wavelength for extinction is 550 nm, 580 nm, and 660 nm respectively.* We note the peak wavelength for each efficiency and then plot it with R_{eff}, and notice the trend between effective radius vs peak wavelength.

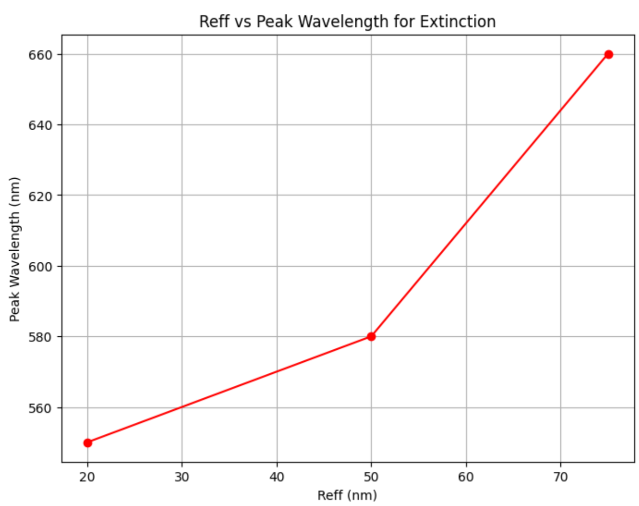

Figure 4: Peak Wavelength for Extinction efficiency factor parameter effective radius

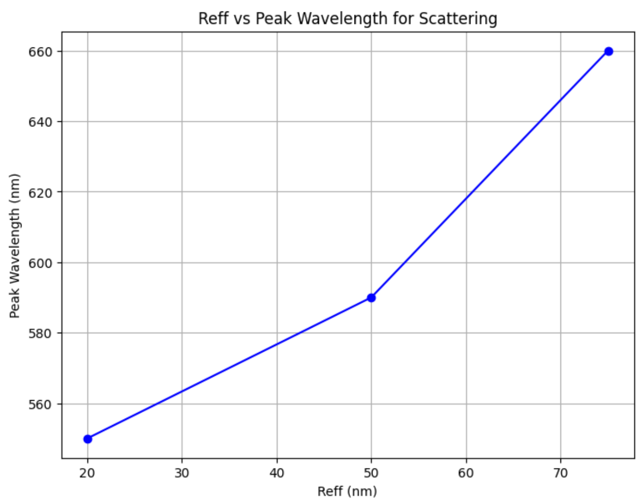

Figure 5: Peak Wavelength for Scattering efficiency factor parameter effective radius

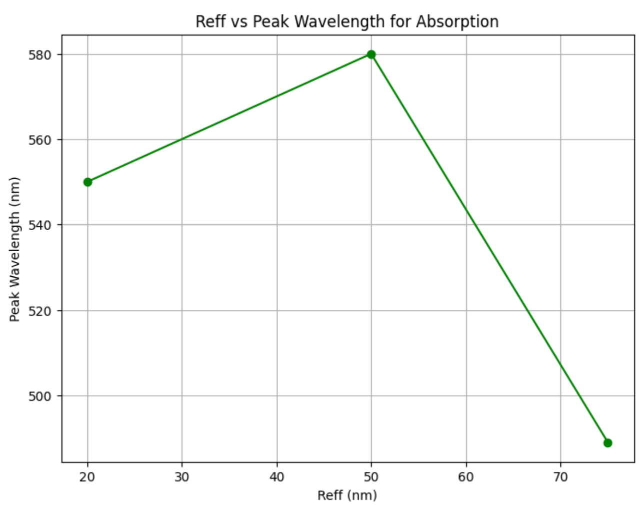

Figure 6: Peak Wavelength for Absorption efficiency factor parameter effective radius

5 Conclusion

we observe that the efficiency factor is increasing for Extinction and Scattering with the effective radius. However, we notice an unexpected decrease in the Absorption efficiency factor for a 75 nm effective radius. After plotting the graphs, we noted down the peak wavelength (λ) on the x-axis for each effective radius [20 nm, 50 nm, 75 nm]. We then plotted the peak wavelength for each efficiency against the effective radius (R_{eff}) and observed the trend of effective radius versus peak wavelength.

5.1 Possible Factors Contributing to the Unexpected Decrease in Absorption Efficiency

1. **Plasmon Resonance Shift**: Gold nanoparticles exhibit plasmon resonance, but at 75 nm, the resonance peak might shift unfavorably, reducing absorption efficiency.

2. **Interference Effects**: Increased scattering and interference between incident and scattered light may divert energy away from absorption.

3. **Surface-to-Volume Ratio**: As the effective radius increases, the surface-to-volume ratio decreases, affecting the interaction with light and possibly reducing absorption.

4. **Increased Reflectance**: Larger particles may exhibit increased internal reflection, leading to higher reflectance and lower absorption.

5. **Shape Effects**: The geometry of rectangular nano prisms may lead to different optical behaviors, affecting absorption efficiency differently than extinction and scattering.

The unexpected drop in absorption efficiency when using gold nanoparticles with a 75 nm effective radius indicates that there's a complex relationship between their size, shape, and material properties. By conducting advanced simulations, theoretical analyses, and experimental studies, we can gain a better understanding of these factors. This understanding is vital for improving the design of gold nanoparticles for different applications. There's still plenty of room for further research to uncover and utilize these complexities to enhance the performance of gold nanoparticles in real-world applications.

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