Using Discrete Dipole Approximation studying optical properties of materials

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Unique Paper Code: 32221501

Paper Title: Electromagnetic Theory

Submitted on: October 24, 2023

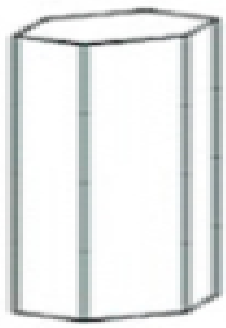
B.Sc(H) Physics Sem VI

Submitted to: Dr. Kuldeep Kumaar

Introduction

In this project we study optical properties of Niobium of shape nano rod using Discrete Dipole Approximation[2]. we studied focus on absorption, extinction and scattering of Electromagnetic waves by calculating absorption spectrum efficiency factor and scattering efficiency factor along with extinction efficiency factor. We also plot the variation of mentioned factors with change in effective radius[3] and refractive indices.

Shape



[1]

Figure 1: Nano Rod Shape

Refractive Index

Medium	Refractive Index
Air	1
Water	1.3
Glycerin	1.4
Glass	1.5

Procedure

- First of all, we download the refractive index data[5] for the selected material.
- Make ddcsat.par file after finding the dimensions and shape of the material.
- The wavelength range in the ddcsat.par file should be in the range of data available .

Calculation of affective radius and shape parameters of nanorod

$$\text{Shape Parameter 1} = \frac{L}{D}$$

$$\text{Shape Parameter 2} = \frac{D}{d}$$

$$\text{Shape Parameter 3} = 1$$

Where L = Length of rod, d = inter dipole spacing, D = Diameter of rod

$$V = \pi \times (\frac{D}{2})^2 \times L$$

$$\text{Affective Radius} = (\frac{3 \times V}{4 \times \pi})^{\frac{1}{3}}$$

In our case, we have taken affective radius of Niobium nano rod 45nm [4] and length of rod (10-20)nm [3]

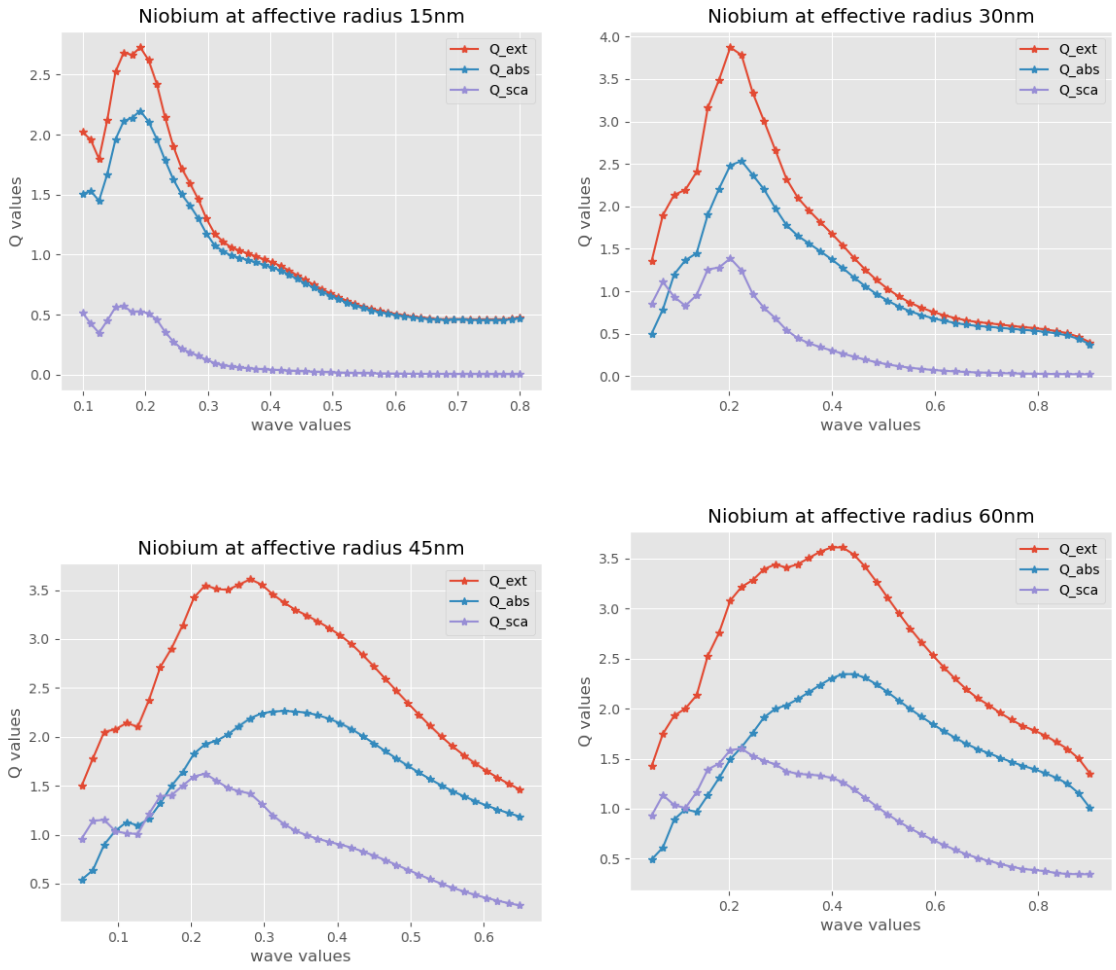
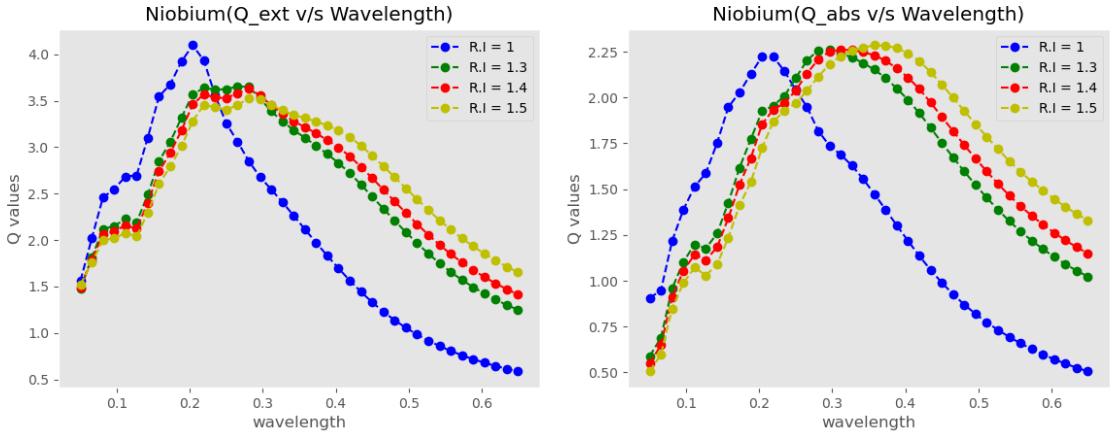


Figure 2: From the above graphs we can see that in absorption spectrum with increase in effective radius the peak shifts towards lower wavelength value that means it is following blue shift unlike this Extinction and Scattering spectrum shows Red shift.



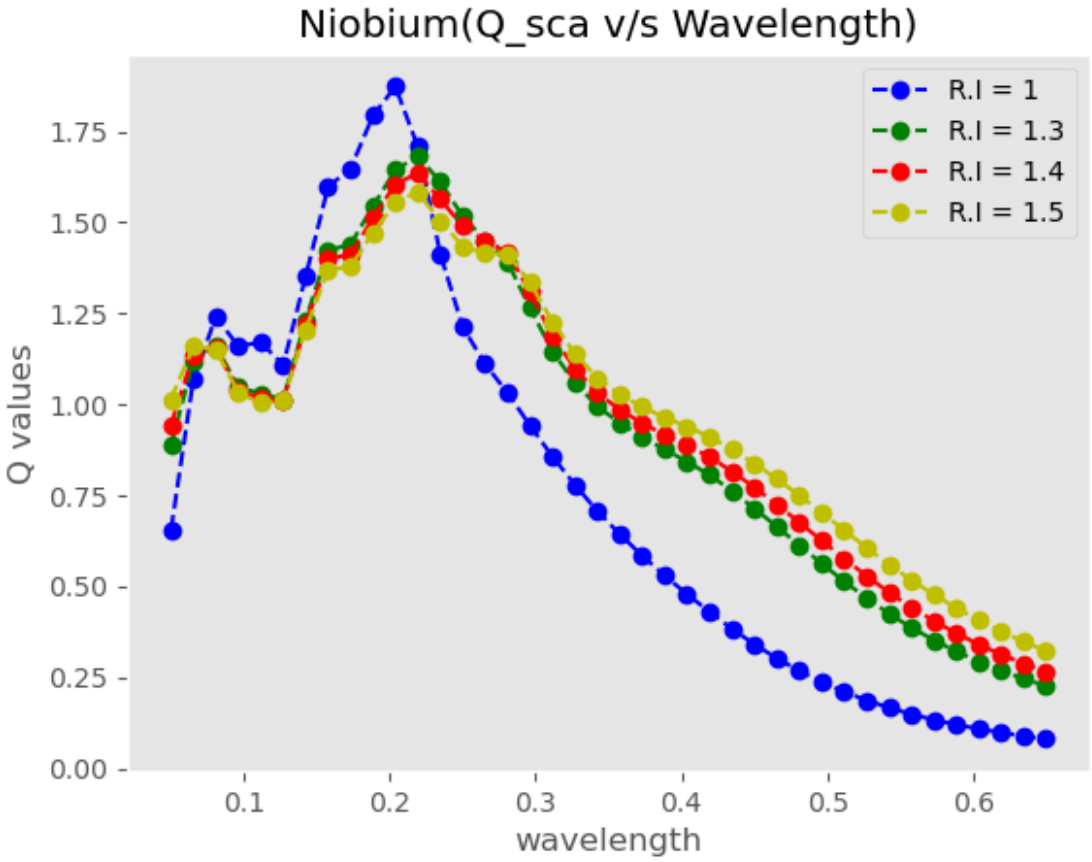
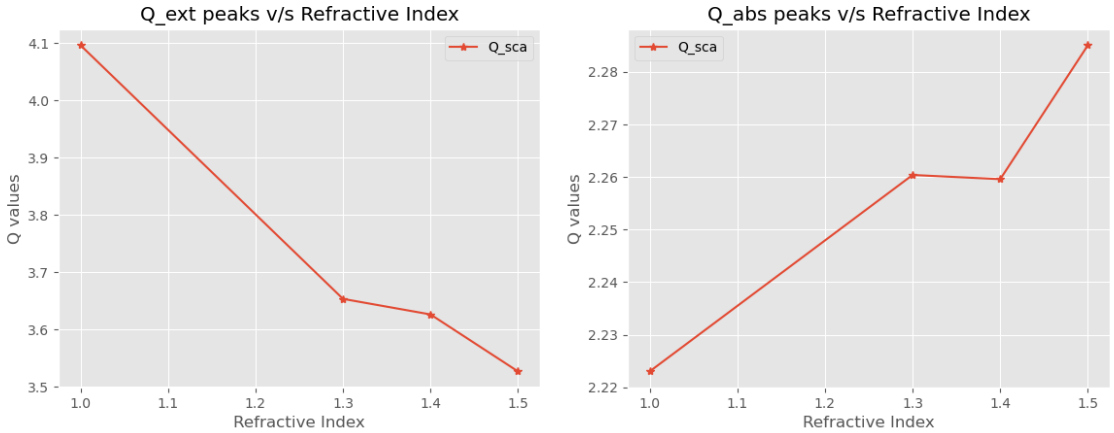


Figure 3: From above graphs we can clearly see that with increase in refractive index the peak shifts towards higher wavelength.



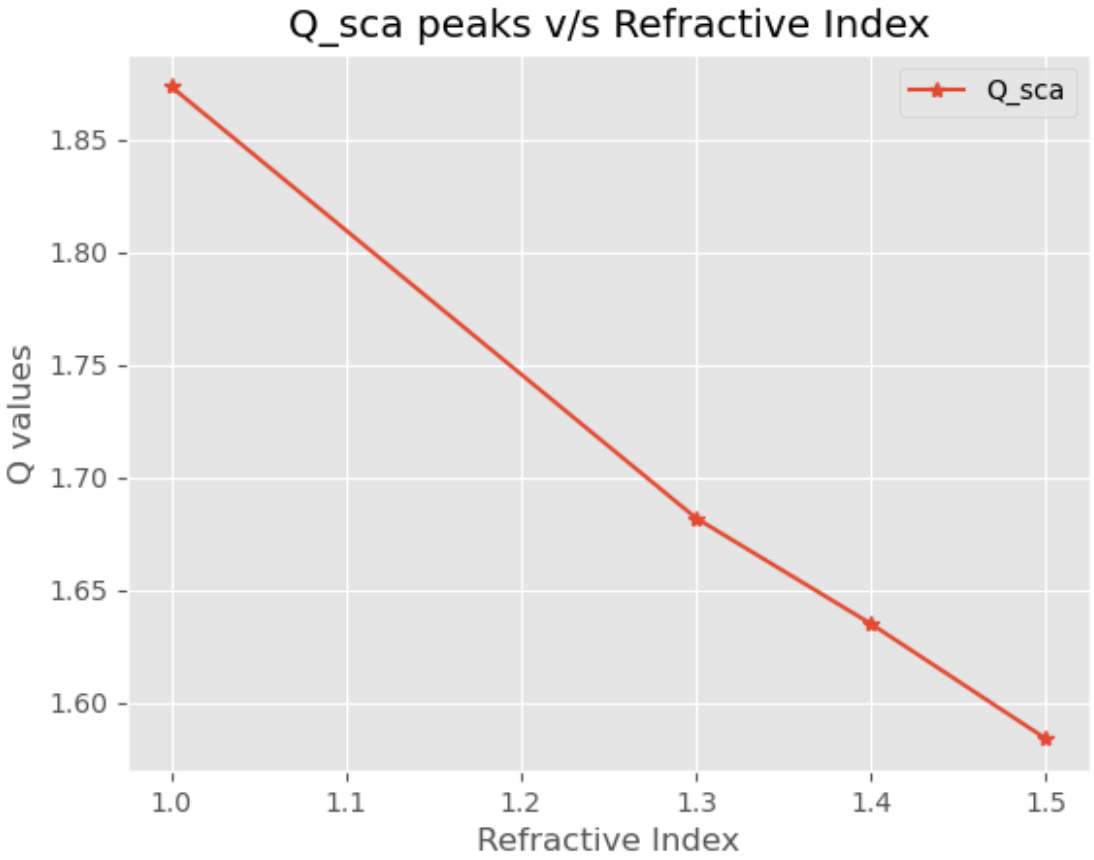


Figure 4: From above graphs we can clearly see that with increase in refractive index the peak values of absorption spectrum increases and scattering decreases.

References

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