THE ABSORPTION COEFFICIENT AND ABSORPTION CROSS-SECTION OF AN ENSEMBLE OF DIFFERENT SHAPE ELLIPSOIDAL METALLIC PARTICLES, IN DIELECTRIC HOST MATERIAL

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PHYSICS

The undersigned hereby certify that they have read and recommend to the College of Natural Sciences for acceptance a thesis entitled "**The absorption coefficient and absorption cross-section of an ensemble of different shape ellipsoidal metallic particles, in dielectric host material**" by **Samuel Ofocho Dige** in partial fulfillment of the requirements for the degree of **Master of Science in Physics(Condensed matter)**.

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To my family

Table of Contents

Abstract

The effects of particle shape on the polarizability, absorption coefficient, and absorption cross sections of randomly oriented particles as the function of distribution function are studied in the Rayleigh limit. In particular, the validity of the so-called statistical approach are investigated. In this approach it is assumed that the scattering and absorption properties of irregularly shaped particles can be simulated by the average properties of a distribution of simple shapes. Polarizability, absorption coefficient, and the absorption cross sections as functions of distribution function of ellipsoidal metallic particles are compared one another. Moreover, the imaginary part of polarizability, absorption coefficient and absorption cross-section as the function of distribution function are derived analytically. As the result, the imaginary part of polarizability, absorption cross-section and absorption coefficient versus frequency curve of different shapes of nano-ellipsoidal metallic dielectric host materials by varying distribution function parameter (δ) with the constant value of relative phonon damping constant (Γ) are explained. And also by varying relative phonon damping constant (Γ) with the constant value of distribution function parameter (δ) are described. The polarizability, absorption coefficient and absorption cross-section; versus frequency curve with the variation of distribution parameter delta (δ) and damping constant(Γ)are studied graphically. In general, the effect of distribution function parameter (δ) and relative phonon damping constant (Γ) on polarizability, absorption coefficient and absorption cross-section of ellipsoidal metallic particles are discussed briefly by using graphs.

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List of Figures

Chapter 1

General Background

With recent developments of nanoscience and nanotechnology, the correlation of composite properties with nanostructure has become a subject of great interest. As a result, much of work has been focused on nanocomposite materials[1]. Nanocomposite materials have attracted tremendous attention due to their potential applications in photonics, biochemistry, medicine, capacitors, micro fabrications, resonant coupling devices, fuel cells, and so on.

In many astrophysical environments dust is an important component. Radiation interacting with the dust particles can be absorbed, scattered and re-emitted. For the interpretation of infrared spectra of dusty objects it is, therefore, needed to realize the way small particles interact with light. This strongly depends on the size, structure, shape and composition of the dust grains. In this thesis we consider the limiting case of particles very small compared to the wavelength of radiation inside and outside the particle (the Rayleigh limit) and concentrate on how the absorption and scattering properties depend on the shape of the particles. In this thesis all particles are in random orientation.

Calculations of scattering and absorption properties of homogeneous spherical

particles can be done very precisely using the so called Mie theory [2]. Because of this, in most applications of light scattering the particles are considered to be spherical and homogeneous. However, if we observe, for example, pictures of interplanetary dust particles, we see that these particles are not at all spherical and in most cases are inhomogeneous in structure and composition [3]. Also, when we compare the positions of features in the spectra of the mass absorption coefficients of homogeneous spherical particles with the positions of features derived from the spectral energy distributions of different astronomical dusty environments, we find that there is often no satisfactory agreement see example [4, 5],. As a result, it is important to study the absorption and scattering properties of particles that are not homogeneous and not spherical.

For the reason that the solid particles in astrophysical environments are expected to be very irregular in shape, it is very difficult (if not impossible) to characterize the shape of the particles in an appropriate way. Therefore, we employ the idea of a statistical approach as suggested by Bohren and Huffman [6]. In this approach one simulates the scattering and absorption characteristics of irregularly shaped particles by those of a shape distribution of particles with various simple shapes, such as ellipsoids or spheroids. Important tests of this idea have been done by for example [7, 8, 9]. The statistical approach has been extensively applied for ellipsoids in the Rayleigh limit (see [6, 10]). However, it is difficult to calculate scattering by randomly oriented ellipsoids outside the Rayleigh limit. However, for ellipsoids of revolution (spheroids) with moderate aspect ratios calculations of scattering by shape distributions of randomly oriented spheroids of arbitrary size can be performed very well and with sufficient accuracy using the so-called T-matrix method in combination with appropriate approximate methods (see [11]).

One of the main assumptions in the statistical approach is that when we average over a wide range of shapes, the typical characteristics of the separate shapes blend together into something which is independent of the choice of the separate shapes we used for the averaging. If this is true we can indeed simulate a shape distribution of irregular particles by using a distribution of simple shapes.

The outline of this research is organized as follow:

The general background of polarizability, absorption coefficient and absorption cross-section as the function of distribution function for different shapes of ellipsoidal metallic particles are described in chapter one.

Electromagnetic radiation in vacuum as well as in material medium, lorentz model, Drude model, basic mixing rule, statistical approach, Mie theory, T-matrices approach and optimality of spherical shape are reviewed in chapter two.

Material and methodology are described in chapter three. Analytic results for polarizabilty, absorption coefficient, and absorption cross-section as the function of distribution function for different shapes of ellipsoidal metallic particles described in chapter four.

In chapter five we discuss how the results obtained from chapter four can be employed, together with other constraints, to capture the general idea of polarizability, absorption coefficient and absorption cross-section as the function of distribution function for different shapes of ellipsoidal metallic particles.

1.1 Statement of the Problem

The problem of finding the optical cross section of the absorption by small particles are practical importance. It arises in many cases involving interpretation of the results of

optical measurements. In this study we deal with ellipsoidal particles. In an excellent book [6] it was suggested that spectra of particles of any complicated form may be approximated by the appropriately averaged spectra of ellipsoidal particles. Having no intention to discuss this idea here, we would like to note that the case of ellipsoidal particles enables one to consider a broad spectrum of objects, from sharp needles to flat disks. It is also important that an analytical expression for polarizability, absorption coefficient and absorption cross-section of nano-ellipsoids are represented through its distribution funtion parameter and damping constant. Such an expression is convenient for various calculations.

One of the main issues in this study is, therefore, to investigate the polarizability, absorption coefficient and absorption cross-section as the function of distribution function and concentration for such materials. Even though different researches were conducted on this area; the polarizability, absorption coefficient and absorption cross-section of electromagnetic waves as a function of distribution function and concentration were not well realized. So the main focus of this project is to describe the polarizability, absorption coefficient and absorption cross-section of electromagnetic waves in different shapes of nano-ellipsoidal metal in transparent dielectric host material as the function of distribution function.

1.2 Objectives

1.2.1 General objective

The main objective of this study is to understand the polarizability, absorption coefficient and absorption cross-section of metalic ellipsoids as a function of distribution function.

1.2.2   Specific objective

- To determine the imaginary part of polarizablity of an ensemble of ellipsoidal particles as a function of distribution function.

- To determine the absorption coefficient of an ensemble of ellipsoidal particles as a function of distribution function.

- To determine the absorption cross-section of an ellipsoidal particles as a function of distribution function.

1.3   Significance of the Study

The physics of metal-dielectric composites has recently gained attention because of their unique linear and nonlinear optical properties and high application potential as nonlinear media and media for optical data storage. These properties find their application in optics, electronics, optoelectronics and material science. Thus understanding the optical properties such as ellipsoidal metallic nano-particles as a function of distribution function is helpful for characterization of the composite system. Moreover, knowledge of the features of interaction of electromagnetic radiation with composite or disperse materials is crucial for further advances in technology.

1.4   Scope of the study

The scope of the study is limited to the polarizability, absorption coefficient and absorption cross-section of metallic ellipsoids as a function of distribution function in dielectric host media.

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Chapter 2

Literature Review

2.1 Electromagnetic Radiation in Vacuum

The electric and magnetic fields are in phase and mutually perpendicular as a consequence of Maxwell's equations [12]. Physically, Electric field results from electric charges or from time dependent magnetic fields, while magnetic fields result from electric currents or time - dependent electric field. Maxwell's equations can be manipulated to give classical wave equations from the time and space dependence of the electric and magnetic field. A significant achievement of this picture was the relation derived between the speed of light c and the product of the electric permittivity ϵ_0 and magnetic permeability μ_0 of free space:

$$c^2 \mu_0 \epsilon_0 = 1 \tag{2.1.1}$$

Maxwell's equations are postulates that predict about the physical property of light. In vacuum, they are:

$$\vec{\nabla}.\vec{E} = 0 \tag{2.1.2}$$

$$\vec{\nabla}.\vec{B} = 0 \tag{2.1.3}$$

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \tag{2.1.4}$$

$$\vec{\nabla} \times \vec{B} = \mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t} \tag{2.1.5}$$

where, $\epsilon_0 = 8.854 \times 10^{-12} C^2 m^{-1} J^{-1}$, and $\mu_0 = 4\Pi \times 10^{-7} \frac{N}{A^2}$

After some manipulation Maxwell's equations can be recast in the following form to give classical wave equation:

$$\nabla^2 \vec{E} = \epsilon_0 \mu_0 \frac{\partial^2 \vec{E}}{\partial t^2} \tag{2.1.6}$$

$$\nabla^2 \vec{B} = \epsilon_0 \mu_0 \frac{\partial^2 \vec{B}}{\partial t^2} \tag{2.1.7}$$

From the symmetrical relationship between the magnetic and electric field, there are two quantities, the scalar potential ϕ and the vector potential $\vec{A}$, from which $\vec{E}$ and $\vec{B}$ can be derived:

$$\vec{E} = -\nabla\phi - \frac{\partial \vec{A}}{\partial t} \tag{2.1.8}$$

$$\vec{B} = \nabla \times \vec{A} \tag{2.1.9}$$

Hence the vector potential also obeys the classical wave equation,

$$\nabla^2 \vec{A} = \mu_0 \epsilon_0 \frac{\partial^2 \vec{A}}{\partial t^2} \tag{2.1.10}$$

2.2 Electromagnetic Radiation in Material Media

All macroscopic aspects of the static and dynamics of the electromagnetic field of the material media described by Maxwell's equation:

$$\nabla.\vec{D} = \rho_f \tag{2.2.1}$$

9

$$\nabla \cdot \vec{B} = 0 \tag{2.2.2}$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \tag{2.2.3}$$

$$\nabla \times \vec{H} = \vec{J} + \frac{\partial \vec{D}}{\partial t} \tag{2.2.4}$$

where the electromagnetic properties of material media may be taken in to account through relations, $\vec{D} = \epsilon \vec{E}$, $\vec{B} = \mu H$ and $\vec{J} = \sigma \vec{E}$ known as constitutive relations.

When an external electric field is applied to an insulator, the matter responds with an induced polarization that partially cancels the field due to out side charges. Although the charges in an insulator are not mobile as they are in conductor, an external field has the ability to displace the charges in length of polar bonds [12]. The resulting net dipole moment per unit volume is called the polarization, and in linear electric materials it is proportional to the electric field. If there are N such molecules per unit volume the macroscopic polarization $\vec{P}$ is given by:

$$\vec{P} = N\vec{p} \tag{2.2.5}$$

$$\vec{P} = \epsilon_0 \chi_e \vec{E} \tag{2.2.6}$$

$$\vec{D} = \epsilon_0 (1 + \chi_e) \vec{E} \tag{2.2.7}$$

Similarly, when ordinary matter is placed in an external magnetic field, induced magnetization, $\vec{M}$, the magnetic dipole moment per unit volume, results. Unlike the

polarization $\vec{P}$, the magnetization can either reinforce or oppose the applied field. The bound and free charges in electric polarization are analogous to the bound and free currents in magnetic polarization. The magnetic field $\vec{H}$ is given by:

$$\vec{H} = \frac{\vec{B}}{\mu_0} - \vec{M} \tag{2.2.8}$$

The bound currents are those due to the induced magnetic moments and the alignment of permanent moments, possessed by the atoms molecules that comprise the sample.

$$\vec{M} = \chi_m \vec{E} \tag{2.2.9}$$

$$\vec{B} = \mu_0 (1 + \chi_m) \vec{E} \tag{2.2.10}$$

Applying the curl operation to both sides of Equation (2.2.3), we obtain

$$\nabla \times (\nabla \times \vec{E}) = -\nabla \times \frac{\partial \vec{B}}{\partial t} = \frac{\partial}{\partial t}(\nabla \times \vec{B}) \tag{2.2.11}$$

$$\nabla \times (\nabla \times \vec{E}) = \nabla(\nabla . \vec{E}) - \nabla^2 \vec{E} \tag{2.2.12}$$

$$\nabla(\nabla . \vec{E}) - \nabla^2 \vec{E} = -\mu_0 \frac{\partial^2}{\partial t^2}(\epsilon_0 \vec{E} + \vec{P}) \tag{2.2.13}$$

$$\nabla^2 \vec{E} - \nabla(\nabla . \vec{E}) - \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} = \frac{1}{\epsilon_0 c^2}\frac{\partial^2 \vec{P}}{\partial t^2} \tag{2.2.14}$$

for transverse fields (some times called solenoidal or radiation fields) satisfy,

$$\nabla . \vec{E} = 0 \tag{2.2.15}$$

Transverse equations therefore satisfy the inhomogeneous wave equation,

$$\nabla^2 \vec{E} - \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} = \frac{1}{\epsilon_0 c^2}\frac{\partial^2 \vec{P}}{\partial t^2} \qquad (2.2.16)$$

In classical physics Newton's second law describes the motion of particle. For charged particles in electromagnetic field the force referred to in Newton's second law is the Lorentz force [13],

$$\vec{F} = e(\vec{E} + \nabla \times \vec{B}) \qquad (2.2.17)$$

In equation (2.2.17), the magnetic contribution to the Lorentz force is dropped. Because optical phenomena do not normally involve relativistic particle velocities, we can safely disregard the magnetic force. Under the influence of electromagnetic field the electron experiences a Lorentz force, and the equation of the force without considering the damping force consequently, the equation of motion is,

$$m\frac{d^2 \vec{x}}{dt^2} = e\vec{E}(\vec{r}, t) - K_s \vec{x} \qquad (2.2.18)$$

When a field is applied, each atoms electron is displaced by some $\vec{x}$ from its original position. Thus each atom has a dipole moment,

$$\vec{p} = e\vec{x} \qquad (2.2.19)$$

If the density of atoms is denoted by N, then the density of dipole moment is,

$$\vec{P} = N\vec{p} = Ne\vec{x} \qquad (2.2.20)$$

The Maxwell's equations (2.2.16) tell us how the electric field $\vec{E}$ depends up on the dipole moment density $\vec{P}$ of the medium. Newton's equation (2.2.17) tells us how the electron displacement $\vec{x}$ depends upon the $\vec{E}$. Equation (2.2.20) connects these basic equations by relating $\vec{P}$ to $\vec{x}$. The electron oscillator model thus ties together

the Maxwell's equations with Newton's law of motion. Solutions of these coupled equations will provide the model's predictions about the mutual interaction of light and matter. For linearly polarized wave the electric field at the position of the atom has the form,

$$\vec{E}(z,t) = \hat{\epsilon}E_0 \cos(\omega t - kz) \tag{2.2.21}$$

where, E_0 is the amplitude and $\hat{\epsilon}$ is a unit vector in x-direction. If the electric field in equation (2.2.21) is to be a solution of coupled Maxwell-Newton equations, it must be the driving field in the Newton equation (2.2.18),

$$\frac{d^2\vec{x}}{dt^2} + \omega_0^2\vec{x} = \hat{\epsilon}\frac{e}{m}E_0 \cos(\omega t - kz) \tag{2.2.22}$$

This equation has the solution,

$$\vec{x} = \hat{\epsilon}\left(\frac{\frac{e}{m}E_0}{\omega_0^2 - \omega^2}\right) \cos(\omega t - kz) \tag{2.2.23}$$

The dipole moment can also be described by polarizablity,

$$\vec{p} = e\vec{x} = \alpha(\omega)\vec{E} \tag{2.2.24}$$

Relating equations (2.2.22), (2.2.23) and (2.2.24) the polarizablity is given by,

$$\alpha(\omega) = \frac{e^2}{m}\frac{1}{\omega_0^2 - \omega^2} \tag{2.2.25}$$

Thus the dipole moment density is,

$$\vec{P} = \hat{\epsilon}\left(\frac{\frac{Ne^2}{m}}{\omega_0^2 - \omega^2}\right)E_0 \cos(\omega t - kz) \tag{2.2.26}$$

This solution for the polarization provides the source term on the right hand side of the Maxwell equation (2.2.16),

$$\left(-k^2 + \frac{\omega^2}{c^2}\right)\hat{\epsilon}E_0 \cos(\omega t - kz) = -\frac{N_\alpha(\omega)\omega^2}{\epsilon_0 c^2}\hat{\epsilon}E_0 \cos(\omega t - kz) \tag{2.2.27}$$

To satisfy this equation k must satisfy a more general dispersion relation

$$k^2 = \frac{\omega^2}{c^2}(1 + \frac{N_\alpha}{\epsilon_0}) = \frac{\omega^2}{c^2} n^2(\omega) \qquad (2.2.28)$$

$$n(\omega) = (1 + \frac{\frac{Ne^2}{m\epsilon_0}}{\omega_0^2 - \omega^2})^{1/2} \qquad (2.2.29)$$

In the presence of damping force equation (2.2.22) can be modified as,

$$\frac{d^2\vec{x}}{dt^2} - \gamma\frac{dx}{dt} + \omega^2\vec{x} = \hat{\epsilon}\frac{e}{m}E_0[\cos(\omega t - kz) - i\sin(\omega t - kz)] \qquad (2.2.30)$$

where γ in equation (2.2.30) is the damping constant.

$$\vec{x}(t) = \Re\hat{\epsilon}\frac{\frac{e}{m}E_0 e^{-i(\omega t - kz)}}{\omega_0^2 - \omega^2 - i\gamma\omega} \qquad (2.2.31)$$

The polarizablity in damping case is complex and given by,

$$\alpha(\omega) = \frac{\frac{e^2}{m}}{\omega_0^2 - \omega^2 - i\gamma\omega} \qquad (2.2.32)$$

The complex nature of polarizablity leads to the complexity of the index of refraction.

$$n^2(\omega) = 1 + \frac{\frac{Ne^2}{m\epsilon_0}}{\omega_0^2 - \omega^2 - i\gamma\omega} = [n\Re(\omega) + in\Im(\omega)]^2 \qquad (2.2.33)$$

The electric field is given by,

$$\vec{E} = \hat{\epsilon}E_0 e^{-i(\omega t - kz)} \qquad (2.2.34)$$

But the wave vector is,

$$k = \frac{w}{c}[n\Im(\omega) - in\Im(\omega)] \qquad (2.2.35)$$

Then,

$$\vec{E} = \hat{\epsilon}E_0 e^{\frac{-w}{c}n\Im(\omega)z} e^{-i[\omega t - \frac{\omega z}{c}n\Im(\omega)]} \qquad (2.2.36)$$

14

The intensity is proportional to the square of the amplitude of the electric field and given by

$$I(\omega) = I_0 e^{-\sigma(\omega)z} \tag{2.2.37}$$

$\sigma(\omega)$is the absorption coefficient or extinction coefficient, and is given by,

$$\sigma(\omega) = 2[n\Im(\omega)]\frac{w}{c} = \frac{Ne^2}{\epsilon_0 mc}\frac{\gamma\omega^2}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2} \tag{2.2.38}$$

2.3   The Lorentz model

Near the beginning of this century H. A. Lorentz developed a classical theory of optical properties in which the electrons and ions of matter were treated as simple harmonic oscillators (i.e., "springs") subject to the driving force of applied electromagnetic fields. The results obtained therefrom are formally identical to those of quantum-mechanical treatments, although various quantities are interpreted differently in the classical and quantum-mechanical theories. As most of us are more comfortable thinking in classical terms, it is fortunate that we may do so without doing violence to the correct results. This undoubtedly explains why the Lorentz model remains so useful, not only in guiding our intuition, but also in quantitatively analyzing experimental data. Following Lorentz, we take as our microscopic model of polarizable matter a collection of identical, independent, isotropic harmonic oscillators. We shall later generalize to more than one kind of oscillator and to anisotropic oscillators. An oscillator with mass $\mathbf{m}$ and charge $\mathbf{e}$ is acted upon by a linear restoring force $\mathbf{Kx}$, where $\mathbf{K}$ is the spring constant (stiffness) and $\mathbf{x}$ is the displacement from equilibrium; a damping force $b\dot{x}$, where b is the damping constant and $\dot{x}$ is the first derivative of displacement with respect to time; and a driving force produced by the local electric field E_{1ocal} (magnetic forces may usually be neglected compared with electrical forces).

We neglect radiation reaction in which the equation of motion of such an oscillator is

$$m\ddot{x} + b\dot{x} + kx = eE_{local} \tag{2.3.1}$$

The local field E_{local} "seen" by a single oscillator and the macroscopic field E, which is an average over a region containing many oscillators, are different in general. However, we shall ignore this difference because it does not affect our simple model of optical constants, and proper treatment of the local field would be a fruitless digression at this point. A good elementary discussion of the local field is given in Kittel (1971, pp. 454-458). The electric field is taken to be time harmonic with frequency ω. As in previous chapters, we shall deal with the complex representations of the real time-harmonic quantities. The solution to (2.3.1) is composed of a transient part, which dies away because of damping, and an oscillatory part with the same frequency as the driving field. We shall be interested only in the oscillatory part

$$x = \frac{(e/m)E}{\omega_0^2 - \omega^2 - i\gamma\omega} \tag{2.3.2}$$

where $\omega_0 = k/m$ and $\gamma = b/m$. If $\gamma \neq 0$, the proportionality factor between x and E is complex; therefore, the displacement and field are not, in general, in phase. In order to discuss the consequences of this phase difference, we write the displacement as $Ae^{i\Theta}(eE/m)$, where the amplitude A and phase angle Θ are

$$A = \frac{1}{[(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2]^{1/2}}$$

$$\Theta = \tan^{-1}\frac{\gamma\omega}{\omega_0^2 - \omega^2} \tag{2.3.3}$$

16

Given the response of a single oscillator to a time-harmonic electric field, the optical constants appropriate to a collection of such oscillators readily follow. The induced dipole moment $\mathbf{p}$ of an oscillator is $e\mathbf{x}$. If $\Re$ is the number of oscillators per unit volume, the polarization $\mathbf{P}$ (dipole moment per unit volume) is $\Re\mathbf{p}= \Re e\mathbf{x}$, and from (2.3.2) we have

$$\mathbf{p} = \frac{\omega_p^2}{\omega_o^2 - \omega^2 - i\gamma\omega}\varepsilon_0\mathbf{E} \tag{2.3.4}$$

where the plasma frequency is defined by $\omega_p^2 = \Re e^2/m\varepsilon_0$. Equation (2.3.4) is a particular example of the constitutive relation [6]. Therefore, the dielectric function for our system of simple harmonic oscillators is

$$\epsilon = 1 + \chi = 1 + \frac{\omega_p^2}{\omega_o^2 - \omega^2 - i\gamma\omega} \tag{2.3.5}$$

with real and imaginary parts are respectively,

$$\epsilon' = 1 + \chi' = 1 + \frac{\omega_p^2(\omega_0^2 - \omega^2)}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2} \tag{2.3.6}$$

$$\epsilon'' = \chi'' = \frac{\omega_p^2\gamma\omega}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2} \tag{2.3.7}$$

The proof is lengthy, although straightforward, and will be omitted here, but it can be shown by direct substitution and integration that χ' and χ'' satisfy the Kramers-Kronig relation.

The region of high absorption at frequencies around ω_0 gives rise to an associated region of high reflectance provided, of course, that the oscillator parameters are such that $k >> 1$ in this region. The high reflectance allows little light to get past the bounding surface of the material, and that which does is rapidly attenuated.

On both sides of the resonance region n increases with increasing frequency, which is called normal dispersion. Only in the immediate vicinity of the resonance frequency

does n decrease with frequency, so-called anomalous dispersion. Such a reversal of dispersion, if it occurred in transparent regions, would provide a much-needed material for designing color-corrected lenses. Unfortunately, anomalous dispersion occurs only in regions of high absorption where no appreciable light is transmitted.

The maximum value of $\epsilon^{''}$ occurs approximately at ω_0 provided that $\gamma << \omega_0$. For frequencies in the neighborhood of ω_0 the dielectric functions (2.3.6) and (2.3.7) may be approximated by with real and the imaginary parts are respectively

$$\epsilon^{'} \simeq 1 + \frac{\omega_p^2(\omega_0 - \omega)/2\omega_0}{(\omega_0 - \omega)^2 + (\gamma/2)^2} \tag{2.3.8}$$

$$\epsilon^{''} \simeq \frac{\gamma\omega_p^2/4\omega_0}{(\omega_0 - \omega)^2 + (\gamma/2)^2} \tag{2.3.9}$$

It is obvious from (2.3.9) that the maximum value of $\epsilon^{''}$ is approximately $\omega_p^2/\gamma\omega_0$ and the width of the bell-shaped curve $\epsilon^{''}(\omega)$ is γ (i.e., $\epsilon^{''}$ falls to one-half its maximum value when $\omega_0 - \omega = \pm\gamma/2$). If we set the derivative of (2.3.8) with respect to the variable $\omega_0 - \omega$ equal to zero, it follows that the extreme values of $\epsilon^{'}$, $\epsilon^{'}_{max} = 1 + \epsilon^{''}_{max}/2$ and $\epsilon^{'}_{min} = 1 - \epsilon^{''}_{max}/2$, occur at $\omega = \omega_0 - \gamma/2$ and $\omega = \omega_0 + \gamma/2$, respectively. These properties of a narrow Lorentzian line are very helpful in quickly visualizing the shape of $\epsilon(\omega)$ from the parameters of (2.3.5).

For solid materials, the Lorentz model describes the resonant frequencies and damping for characteristic frequencies of the molecules of the medium. Around the resonance, a very strong dispersion takes place [6].

2.4   Drude Model

For metals, there is no spring to connect free electrons to ions, so $\omega_0=0$. From the Lorentz model, we get

$$\varepsilon_r = 1 - \frac{\omega_p^2}{\omega^2 + i\gamma\omega} \tag{2.4.1}$$

The real and the imaginary parts are respectively,

$$\varepsilon_r' = 1 - \frac{\omega_p^2}{\omega^2 + \gamma^2} \tag{2.4.2}$$

and

$$\varepsilon_r'' = \frac{\omega_p^2\gamma}{\omega(\omega^2 + \gamma^2)} \tag{2.4.3}$$

These results are called Drude model. Generally, $\omega_p > \gamma$. If $\omega > \omega_p$, we can see that $\varepsilon_r'' > 0$, which means that $k > 0$. At high frequency, there is no absorption. A metal becomes transparent! The reason is that at this frequency, the electrons in the metal cannot react fast to the incident electrical field. For metals, the Drude model can be used to model their free-electron type behavior [6].

2.5   Basic Mixing and Maxwell Garnett Formula

This section presents the basic principle how the simplest mixing formula, so-called Maxwell Garnett rule, can be derived. The mixture to be analyzed consists of the background medium where spherical inclusions are embedded. The two components composing the mixture are often called phases. The environment phase can also be termed matrix or host, and the inclusion phase as guest.

- **Polarizability of a Dielectric Sphere**
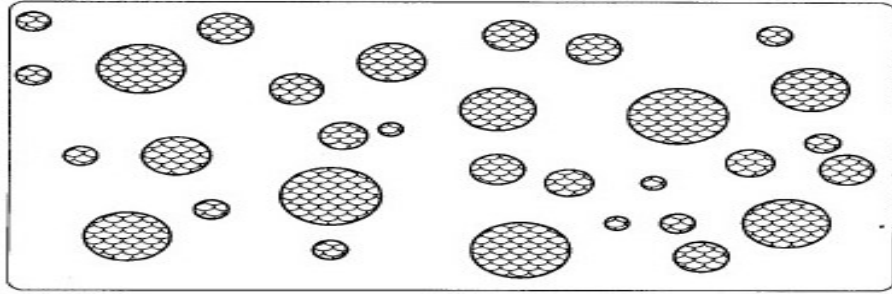
Figure 2.1: A simple mixture: spherical inclusions in a homogeneous background medium. The permittivity of the inclusions is ε_i and that of the environment ε_e.

The polarizability of an inclusion is a measure for its response to an incident electric field. The polarizability of a particle α is the relation between the dipole moment p that is induced in the inclusion by the polarization, and the external electric field E_e:

$$p = \alpha E_e \tag{2.5.1}$$

For a sphere the polarizability is easy to calculate. It is proportional to the internal field within the inclusion, its volume, and the dielectric contrast between the inclusion and the environment. Since the electric field E_i induced in a sphere in a uniform and static external field E_e is also uniform, static, and parallel to the external field [14],

$$E_i = \frac{3\varepsilon_e}{\varepsilon_i + 2\varepsilon_e} E_e \tag{2.5.2}$$

the polarizability can be written immediately:

$$\alpha = V(\varepsilon_i - \varepsilon_e) \frac{3\varepsilon_e}{\varepsilon_i + 2\varepsilon_e} \tag{2.5.3}$$

where the permittivities of the inclusion and its environment are denoted by ε_i and ε_e, respectively. The volume of the sphere is V. Note that the polarizability is

20

a scalar quantity. This is because the inclusion material is isotropic and its shape is spherically symmetric.

- **Clausius-Mossotti Formula**

Now that the polarizability of a single sphere is known, the effective permittivity of a mixture can be calculated as a function of the number density of the spheres in the background medium with permittivity ε_e. The effective permittivity is the relation between the external field and the average electric flux density $< D >$:

$$< D >= \varepsilon_{eff} E_e = \varepsilon_e E_e + < P > \tag{2.5.4}$$

where the average polarization $< P >$ is connected to the dipole moment density in the mixture:

$$< P >= np \tag{2.5.5}$$

and here n is the number density of dipole moments p in the mixture.

In a mixture, especially when it is dense, one cannot assume the field exciting one inclusion to be the external field E_e. The surrounding polarization increases the field effect and has to be taken into account [15]. The field that excites one inclusion E_L is often called as the local field or Lorentzian field. It is dependent on the shape of the inclusion [16], and for a sphere it is

$$E_l = E_e + \frac{1}{3\varepsilon_e} P \tag{2.5.6}$$

where $\frac{1}{3}$ is the depolarization factor of the sphere. Combining this equation with $p = \alpha E_L$ leaves us with the average polarization, and then the effective permittivity can be written see equation (2.5.4):

$$\varepsilon_{eff} = \varepsilon_e + \frac{n\alpha}{1 - n\alpha/(3\varepsilon_e)} \tag{2.5.7}$$

21

The equation can often be seen in the form

$$\frac{\varepsilon_{eff} - \varepsilon_e}{\varepsilon_{eff} + 2\varepsilon_e} = \frac{n\alpha}{3\varepsilon_e} \qquad (2.5.8)$$

This relation carries the name $Clausius - Mossotti$ formula, although it deserves the label $Lorenz - Lorentz$ formula as well [17]. The dilute mixture approximation can be written by taking the limit of small n:

$$\varepsilon_{eff} \approx \varepsilon_e + n\alpha \qquad (2.5.9)$$

- **Maxwell Garnett Mixing Rule**

The mixing process can affect strongly the dispersive characteristics of materials. For example, if metal spheres are mixed in non-dispersive environment, the mixture becomes a Lorentz-medium with resonant behavior.

In practical applications quantities like polarizabilities and scatterer densities are not always those most convenient to use. Rather, one prefers to play with the permittivities of the components of the mixture. When this is the case, it is advantageous to combine Clausius-Mossotti formula with the polarizability expression equation (2.5.3). Then we can write

$$\frac{\varepsilon_{eff} - \varepsilon_e}{\varepsilon_{eff} - 2\varepsilon_e} = f\frac{\varepsilon_i - \varepsilon_e}{\varepsilon_i - 2\varepsilon_e} \qquad (2.5.10)$$

where $f = nV$ is a dimensionless quantity called the volume fraction of the inclusions in the mixture. This formula is called Rayleigh mixing formula. Note that because only the volume fraction and the permittivities appear in the mixture rule, the spheres need not be of the same size if only all of them are small compared to the wavelength.

Perhaps the most common mixing rule is the Maxwell Garnett formula which is the Rayleigh rule (2.5.10) written explicitly for the effective permittivity:

$$\varepsilon_{eff} = \varepsilon_e + 3f\varepsilon_e \frac{\varepsilon_i - \varepsilon_e}{\varepsilon_i + 2\varepsilon_e - f(\varepsilon_i - \varepsilon_e)} \tag{2.5.11}$$

This formula is in wide use in very diverse fields of application. The beauty of the Maxwell Garnett formula is in its simple appearance combined with its broad applicability. It satisfies the limiting processes for vanishing inclusion phase

$$f \to 0 \Rightarrow \varepsilon_{eff} \to \varepsilon_e \tag{2.5.12}$$

and vanishing background

$$f \to 1 \Rightarrow \varepsilon_{eff} \to \varepsilon_i \tag{2.5.13}$$

The perturbation expansion of the Maxwell Garnett rule gives the mixing equation for dilute mixtures ($f << 1$):

$$\varepsilon_{eff} = \varepsilon_e + 3f\varepsilon_e \frac{\varepsilon_i - \varepsilon_e}{\varepsilon_i + 2\varepsilon_e} \tag{2.5.14}$$

- **Random Mixture**

If, on the other hand, all the ellipsoids in the mixture are randomly oriented, there is no longer any macroscopically preferred direction. The mixture is isotropic and the effective permittivity ε_{eff} is a scalar:

$$\varepsilon_{eff} = \varepsilon_e + \varepsilon_e \frac{\frac{f}{3}\sum_{j=x,y,z} \frac{\varepsilon_i - \varepsilon_e}{\varepsilon_e + N_j}}{1 - \frac{f}{3}\sum_{j=x,y,z} \varepsilon_e + N_j \frac{\varepsilon_i - \varepsilon_e}{\varepsilon_e + N_j}} \tag{2.5.15}$$

2.6   T-matrix approach

Waterman's T-matrix method [18, 19, 20] is one of the most widely used method for calculating electromagnetic scattering properties of nonspherical particles. It is specially suitable for axisymmetric homogeneous particles [21] and can be efficiently applied to ensembles of randomly oriented particle systems [22, 23].

In Waterman's T-matrix approach [18], both the incident and the scattered time-independent electric fields $E_{inc}(r)$, $E_{sca}(r)$ are expanded in vector spherical harmonics [24] M_{mn}, N_{mn}:

$$E_{inc}(r) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [a_{mn} Rg M_{mn}(kr) + b_{mn} Rg N_{nm}(kr)] \tag{2.6.1}$$

$$E_{inc}(r) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [p_{mn} Rg M_{mn}(kr) + q_{mn} Rg N_{nm}(kr)] \tag{2.6.2}$$

The linearity of Maxwell's equations enables us to relate the scattered (p_{mn}, q_{mn}) and incident (a_{mn}, b_{mn}) field coefficients by means of a transition (T) matrix:

$$p_{mn} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [T^{11}_{mnm'n'} a_{m'n'} + T^{12}_{mnm'n'} b_{m'n'}] \tag{2.6.3}$$

$$q_{mn} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [T^{21}_{mnm'n'} a_{m'n'} + T^{22}_{mnm'n'} b_{m'n'}] \tag{2.6.4}$$

The T matrix elements depend on the particle (size, shape, composition, and orientation) but not on the nature of the incident and scattered fields, so they need to be calculated only once and then averaged for all directions of incidence and scattering, which equals to averaging on particle orientation. It is usually calculated for the so-called natural reference frame of the particle, and can be written in compact notation

24

as

$$T = -B * A^{-1} = \begin{pmatrix} T^{11} & T^{12} \\ T^{21} & T^{22} \end{pmatrix} \tag{2.6.5}$$

For a two-layered axisymmetric object (characterized by refractive indices m_1 for core and m_2 for shell), the T matrix is given by [25]

$$T = -[B_2 + BB_2 * T_1] * [A_2 + AA_2 * T_1]^{-1} \tag{2.6.6}$$

where T_1 is the transition matrix for the inner layer, as derived in the homogeneous case [25, 26], with relative refractive indices m_1/m_2, (inner), 1 (outer) and incident radiation wave number $k_0 m_2$. The matrices B_2, A_2 are such that $-B_2 * (A_2)^{-1}$ is the T-matrix for the outer layer, with inner and outer indices $(m_2, 1)$. Finally, the matrix BB2 is the same as B_2, except that the Bessel functions of the first kind with argument kr are replaced by Hankel functions with the same argument; the same applies to the AA_2 and A_2 matrices.

Once the T matrix is calculated for the particle in its natural reference frame (with the z-axis along the axis of symmetry), cross sections can be computed. For an axisymmetric particle, the T matrix divides itself into m smaller, independent sub-matrices. The expressions for extinction and scattering cross sections are [22]

$$C_{ext} = \frac{2\pi}{k^2} Re \sum_{n=1}^{\infty} \sum_{m=-n}^{n} (T_{mnn}^{11} + T_{mnn}^{22}) \tag{2.6.7}$$

$$C_{sca} = \frac{2\pi}{k^2} \sum_{i,j=1}^{2} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} \sum_{m=0}^{min(n,n')} (2 - \delta_{mo}) |T_{mnn'}^{ij}|^2 \tag{2.6.8}$$

25

2.7 The statistical approach

The method described in this thesis provides a strong argument in favor of the main assumption of the statistical approach, namely that the optical properties of an ensemble of irregularly shaped particles can be represented in a statistical sense by the average properties of an ensemble of particles with the same composition, but with simple shapes. We have proved that for the absorption properties of particles in the Rayleigh domain, the statistical approach has an analytical basis given by the form-factor distribution. This implies that the average absorption cross section of an ensemble of arbitrarily shaped and arbitrarily oriented particles can be represented by a shape distribution of spheroidal particles with the same composition and in a fixed orientation.

We note that the form-factor distribution only provides the absorption cross sections, and not the scattering properties of small particles. It is in general not possible to find a distribution of spheroidal particles that gives both the absorption and the scattering cross section of an ensemble of arbitrarily shaped particles for every value of the refractive index. For an ensemble of ellipsoidal particles there is a relation between the scattering and the absorption cross section which is independent of the shape of the ellipsoids and is given by ([27])

$$C_{sca} = \frac{k^3 V |m^2 - 1|^2}{6\pi Im(m^2)} C_{abs} \qquad (2.7.1)$$

2.8 Mie theory and the quasi-static approximation

The first description of the optical properties of spherical entities was provided by Mie [28]. In the frame of electrodynamics, an exact solution of Maxwell's equations

was given in spherical coordinates. The resulting scattering and extinction efficiencies are given by

$$Q_{sca} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1)(|a_n|^2 + |b_n|^2) \tag{2.8.1}$$

$$Q_{ext} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1)Re(a_n| + |b_n) \tag{2.8.2}$$

where a_n and b_n are the Mie coefficients in terms of spherical Bessel functions. The size parameter x = ka is a function of the sphere radius 'a' and the wave vector $k = \frac{2\pi\sqrt{\varepsilon_m}}{\lambda}$, with $\frac{\lambda}{\sqrt{\varepsilon_m}}$ the wavelength in the medium surrounding the particles. The efficiencies Q are equal to the cross sections C, normalised to the (effective) particle cross section πa^2. Energy conservation provides the absorption efficiency through

$$Q_{ext} = Q_{abs} + Q_{sca}, \text{or } C_{est} = C_{abs} + C_{sca} \tag{2.8.3}$$

For the calculation of the Mie coefficients and efficiencies in equations (2.8.1) and (2.8.2), the Matlab functions by Mätzler [29, 30] are used. For the smallest particles, the extinction is fully determined by absorption; scattering is negligible. For larger spheres, the overall extinction increases while scattering becomes considerably more important.

For particles much smaller than the wavelength of the light, the optical properties can be described within the quasi-static approximation. In fact, this dipole approximation is equal to the first order Mie calculation, obtained by only considering the n = 1 term in equations (2.8.1) and (2.8.2). The absorption and scattering cross sections in the quasi-static regime are given by

$$C_{abs} = kIm(\alpha) \tag{2.8.4}$$

$$C_{sca} = \frac{k^4}{6\pi}|\alpha|^2 \tag{2.8.5}$$

where α is the single particle polarisability. Energy conservation (2.8.3) yields the extinction cross section C_{ext}. For a spherical gold particle with radius a, the polarisability α_{sph} in equations (2.8.4) and (2.8.5) is given by the $Claussius - Mossotti$ equation, taking into account only dipolar contributions

$$\alpha_{sph} = 4\pi a^3 \frac{\varepsilon_{Au} - \varepsilon_m}{\varepsilon_{Au} + 2\varepsilon_m} \tag{2.8.6}$$

with ε_m the dielectric function of the host medium. For spheres much smaller than the wavelength there is indeed a one-to-one correspondence with the Mie theory. However, for larger spheres the quasi-static approximation is no longer valid; it does not accurately represent the optical properties of the particle.

With the exception of a few limiting cases, such as that of an infinitely long cylinder, Mie theory can not be employed to calculate light scattering and absorption for non-spherical particles. However, within the quasi-static approximation, valid for small particles, introduction of a geometrical factor enables determination of optical properties of prolate and oblate ellipsoidal particles. In many papers, metallic nanorods are treated as prolate ellipsoids, for which the polarisability can be described by introducing depolarisation factors L_x in equation (2.8.6):

$$\alpha_x = \frac{4\pi}{3}ab^2 \frac{\varepsilon_{Au} - \varepsilon_m}{\varepsilon_m - L_x(\varepsilon_{Au} - \varepsilon_m)} \tag{2.8.7}$$

The long and short radii of the ellipsoid are represented by a and b, respectively, with the aspect ratio defined as $Z = \frac{a}{b}$. For incident light with the polarisation direction parallel and perpendicular to the long axis of the nanorod, x=a or x=b,

respectively. Inserting a=b and $L^x = \frac{1}{3}$ for a sphere, equation (2.8.7) is equal to equation (2.8.6).

The depolarisation factor for a prolate ellipsoid along the long axis is given by

$$L_a = \frac{1 - e^2}{e^2}(\frac{1}{2e}\ln(\frac{1-e}{1+e}) - 1) \tag{2.8.8}$$

with the eccentricity $e = \sqrt{1 - \eta^2}$. Since the sum rule $\sum L_x = 1$ holds, the depolarization factor perpendicular to the ellipsoid axis is found to be $L_b = \frac{(1-L_a)}{2}$. In the present work we are considering randomly oriented nanorods, for which the overall polarizability is equal to the average over the three principal orientations: $\langle \alpha \rangle = \frac{1}{3}\alpha_a + \frac{2}{3}\alpha_b$, where α_a and α_b are the longitudinal and transverse polarisabilities, respectively.

Finally, to obtain the efficiency factors Q from the cross sections C for ellipsoidal particles, C is normalised by the effective particle cross section πa_{eff}^2 with the effective radius given by $a_{eff} = (ab^2)^{\frac{1}{3}}$.

2.9 The Absorption Coefficient

Measurement of the absorption of light is one of the most important techniques for optical measurements in solids. In the absorption measurements, we are concerned with the light intensity $I(z)$ after traversal of a thickness z of material as compared with the incident intensity I_0, thereby defining the absorption coefficient $\alpha_{abs}(\omega)$:

$$I(z) = I_0 e^{-\alpha_{abs}(\omega)z} \tag{2.9.1}$$

Since the intensity $I(z)$ depends on the square of the field variables, it immediately follows that

$$\alpha_{abs}(\omega) = 2\frac{\omega\tilde{\kappa}(\omega)}{c} \tag{2.9.2}$$

29

where the factor of 2 results from the definition of $\alpha_{abs}(\omega)$ in terms of the light intensity, which is proportional to the square of the fields. This expression tells us that the absorption coefficient is proportional to $\tilde{\kappa}(\omega)$, the imaginary part of the complex index of refraction (extinction coefficient), so that $\tilde{\kappa}$ is usually associated with power loss. We note that equation (2.9.2) applies to free carrier absorption in semiconductors in the limit $\omega\tau \gg 1$, and $\omega \gg \omega_p$

We will now show that the frequency dependence of the absorption coefficient is quite different for the various physical processes which occur in the optical properties of solids [15]. We will consider here the frequency dependence of the absorption coefficient for:

1. **Free carrier absorption**

    (a) typical semiconductor $\alpha_{abs}(\omega) \sim \omega^{-2}$

    (b) metals at low frequencies $\alpha_{abs}(\omega) \sim \omega^{\frac{1}{2}}$

1. **Direct interband transitions**

    (a) form of absorption coefficient $\alpha_{abs}(\omega) \sim \frac{(\hbar\omega - E_g)^{\frac{1}{2}}}{\hbar\omega}$

    (b) conservation of crystal momentum $\alpha_{abs}(\omega) \sim \omega^{\frac{1}{2}}$

    (c) relation between m* and momentum matrix element

    (d) form of $\alpha_{abs}(\omega)$ for direct forbidden transition $\alpha_{abs}(\omega) \sim \frac{(\hbar\omega - E_g)^{\frac{3}{2}}}{\hbar\omega}$

1. **Indirect interband transitions**

    (a) form of absorption coefficient $\alpha_{abs}(\omega) \sim (\hbar\omega - E_g \pm \hbar\omega_q)^2$

    (b) phonon absorption and emission processes $\alpha_{abs}(\omega) \sim \omega^{\frac{1}{2}}$

2.10 Optimality of the spherical shape

Within the framework of electrostatics, what is the particle shape that attains minimal orientation-averaged magnitude of the induced dipole moment, while keeping volume (mass) and the dielectric function fixed? To that end, let us consider ellipsoidal particles. Let the three principal axes of a dielectric ellipsoid be along x, y and z directions. We shall use an analytic solution in the notation as given in Bohren and Huffman [6] but "renormalized" so that the vacuum permittivity is set to unity (see also [31, 32]). When the ellipsoid is placed in external electric field $\vec{E} = E_1 \hat{x} + E_2 \hat{y} + E_3 \hat{z}$, components of the induced dipole moment of the ellipsoid are given as follows (ε_r= relative permittivity):

$$pi = 4\pi abc \frac{\varepsilon_r - 1}{3 + 3Li(\varepsilon_r - 1)} Ei \tag{2.10.1}$$

where a, b and c are the principal semi-axes, and $L_i s$ are the associated depolarization coefficients of the dielectric ellipsoids [6, 31].

For the special cases of prolate and oblate spheroids, the depolarization factors are given by

$$L_1 = L_2 = \frac{g(e)}{2e^2} \left[\frac{\pi}{2} - \arctan g(e) \right] - \frac{g^2(e)}{2}$$

$$L_3 = 1 - 2L_1 \tag{2.10.2}$$

Where $g(e) = \sqrt{\frac{1-e^2}{e^2}}$

$$L = \frac{1 - e^2}{e^2} \left(-1 + \frac{1}{2e} \log \frac{1+e}{1-e} \right)$$

$$L_2 = L_3 = \frac{1 - L_1}{2} \tag{2.10.3}$$

31

Then, the associated polarizabilities are given by [6]:

$$\alpha_i = 4\pi abc \frac{\varepsilon_r - 1}{3 + 3L_i(e_r - 1)} \tag{2.10.4}$$

and the orientation-averaged polarizability is

$$\alpha = \frac{4\pi abc}{3(\varepsilon_r - 1)} \frac{1}{3} \sum_{i=1}^{3} \frac{1}{1 + L_i(\varepsilon_r - 1)} \tag{2.10.5}$$

while the orientation-averaged polarizability, normalized per volume (a_n), is

$$\alpha_n = (\varepsilon_r - 1) \frac{1}{3} \sum_{i=1}^{3} \frac{1}{1 + L_i(\varepsilon_r - 1)} \tag{2.10.6}$$

The coefficient of $\frac{1}{3}$, arising from orientation averaging, merits an explanation. Polarizability is a 2nd rank tensor, linking the external electric field and the induced dipole moment vectors. Equation (2.10.1) above is a special (diagonal) case, written in the principal axes of the ellipsoid. Orientation-averaged tensor is an isotropic one so its components do not change with coordinate rotations (there are rank 0 and 2 isotropic tensors but not rank 1). But 2nd rank isotropic tensor has the form αI where $I \equiv diag(1, 1, 1)$ is the identity matrix and α is the orientation-averaged polarizability. One can find a by observing that the only scalar invariant at one's disposal is the tensor trace(Tr). As Tr(I)= 3, (1/3) delivers normalization. The question of tensor isotropy is rather subtle in this context, as it yields scalar polarizabilities not only for a sphere but also for any 2nd rank isotropic tensor shapes such as Platonic polyhedra(see also some what cryptic remarks at the very conclusion of [33]. However,this is not so for spheroids until orientation-averaging is performed.

To gain physical insight for the respective roles of geometry and electrostatics, we examine the transparent (Rayleigh–Gans) limit. To that end, define dielectric contrast as

$$\delta \equiv \varepsilon_r - 1 \tag{2.10.7}$$

We can rewrite the average polarizability per volume of dielectric ellipsoid interms of δ. Then, upon expanding in Taylor series for $\delta << O(\delta^3)$, equation (2.10.6) yields the orientation-averaged polarizability per volume

$$\alpha_n \cong \frac{\delta}{3}\left[\ 3 - \delta(L_1 + L_2 + L_3) + \delta(L_1^2 + L_2^2 + L_3^2)\ \right] \tag{2.10.8}$$

Using the constraint

$$g\left(\ L_1, L_2, L_3\ \right) = L_1 + L_2 + L_3 = 1 \tag{2.10.9}$$

which holds for ellipsoids at all aspect ratios,we obtain

$$\alpha_n \cong \frac{\delta}{3}\left[\ 3 - \delta + \delta^2(L_1 + L_2 + L_3)\ \right] \tag{2.10.10}$$

which, for the sphere, reduces to $\alpha_{n,sphere} \cong \left(\frac{\delta}{3}\right)\left[\ 3 - \delta + \frac{\delta^2}{3}\ \right]$. We now introduce the spheroidal access as $\alpha_n \equiv \frac{\alpha_{n,spheroid}}{\alpha_{n,sphere}}$. Adding and subtracting $\frac{\delta}{3}$ in the numerator of α_r then yield the following equation: $\alpha_r = 1 + \frac{\delta^2(L_1^2+L_2^2+L_3^2-\frac{1}{3})}{3-\delta+\frac{\delta^2}{3}}$

$$\approx 1 + \frac{\delta^2(L_1^2 + L_2^2 + L_3^2 - \frac{1}{3})}{3} \tag{2.10.11}$$

The separation of the geometrical $(L_1^2 + L_2^2 + L_3^2 - \frac{1}{3})$ and the electrical δ^2 effects is now evident and appears to be a new insight. What shape attains minimal α_n? The question reduces to finding the minimum of $L_1^2 + L_2^2 + L_3^2$, subject to the constraint (2.10.9). A general proof is given below, but an appealing geometrical argument can now be given for spherical optimality, based on an isoperimetric inequality. Interpret the constraint (2.10.9) as afixed perimeter of a rectangular solid, whose surface area, which is twice the quantity $L_1^2 + L_2^2 + L_3^2$, is the one to optimize. As the minimal surface area of all rectangular blocks of a given perimeteris that of acube,i.e., $L_1 =$

$L_2 = L_3 = 13$ in the space of depolarization factors, in real space the sphere delivers optimal shape.

For the special case of a conducting ellipsoid, components of the dipole moment are given by

$$P_i = \frac{E_i V}{4\pi L_i} \tag{2.10.12}$$

where i=1,2 and 3, V is volume of the ellipsoid and L_i is the depolarization coefficient of the conducting ellipsoid. Then, the polarizability is $\alpha_i = V/4\pi L_i$ and the orientation-averaged polarizability per volume is

$$\alpha_n = \frac{1}{12\pi}\left(\frac{1}{L_1} + \frac{1}{L_2} + \frac{1}{L_3}\right) \tag{2.10.13}$$

Coated particles are ubiquitous in applications, example, [34, 35]. Next, we pose the optimal shape question about coated spheroids, apparently for the first time. Is the concentric spherical configuration still the optimal one? To that end, using the coated ellipsoid analytic solution, [6], we write the components of polarizability of a coated confocal ellipsoid as

$$\alpha_i = \frac{V\left((\varepsilon_2 - 1)\left[\varepsilon_2 + (\varepsilon_1 - \varepsilon_2)(L_i^{(1)} - fL_i^{(2)}) \right] + f\varepsilon_2(\varepsilon_1 - \epsilon_2) \right)}{\left[\varepsilon_2 + (\varepsilon_1 - \varepsilon_2)(L_i^{(1)} - fL_i^{(2)}) \right]\left[1 + (\varepsilon_2 - 1)L_i^{(2)} \right] + fL_i^{(2)}\varepsilon_2(\varepsilon_1 - \varepsilon_2)} \tag{2.10.14}$$

where V is total volume of the ellipsoid, f is the ratio of volume of inner ellipsoid per total volume, ε_1 and ε_2 is the relative permittivity of the inner and outer ellipsoids, superscript(1) and (2) denotes inner and outer, respectively. Then, the orientation-averaged polarizability per volume of the coated ellipsoid is

$$\alpha_n = \frac{1}{3}\sum_{i=1}^{3} \frac{\left((\varepsilon_2 - 1)\left[\varepsilon_2 + (\varepsilon_1 - \varepsilon_2)(L_i^{(1)} - fL_i^{(2)}) \right] + f\varepsilon_2(\varepsilon_1 - \epsilon_2) \right)}{\left[\varepsilon_2 + (\varepsilon_1 - \varepsilon_2)(L_i^{(1)} - fL_i^{(2)}) \right]\left[1 + (\varepsilon_2 - 1)L_i^{(2)} \right] + fL_i^{(2)}\varepsilon_2(\varepsilon_1 - \varepsilon_2)} \tag{2.10.15}$$

34

Along with the evident spherical optimality ,they also include the monotonic dependence on the aspect ratio. Also shown, for comparison, is the relative spheroidal surface area. It can now be readily understood why the geometric case is the intermediate one between the conducting and the dielectric one: as the relative permittivity approaches unity, spheroidal excess disappears at all aspect ratios. Note that the results hold for confocal coated spheroids, regardless of the sign of $\delta_\varepsilon = \varepsilon_2 - \varepsilon_1$.

In passing, we note that the minimum at the spherical value of $\rho = 1$ is smooth for all curves so that in the near- spherical expansion, the first non-zero term in the aspect ratio is quadratic. Also, note that no qualitative change in the plot would occur, if one were to move from ρ to δ_ρ, defined by $\rho = 1 + \delta_\rho$ and subtract off unity from all abscissa values. Now, quadratic dependence in δ_ρ implies 4th order dependence in eccentricity as $\varrho \approx [2(\rho - 1)]^{1/2}$ (we used the prolate expression as an example). Calculations show that this is, indeed, the case, e.g., eccentricity expansions of the relative surface area of oblate and prolate spheroids, respectively, are $O(\varrho^4)$ and contain even powers as follows:

$$S_r \cong 1 + \frac{2e^4}{45} + \frac{136e^6}{2835} + \frac{131e^8}{2835} + \frac{12224e^{10}}{280665} + ... \qquad (2.10.16)$$

$$1 + \frac{2e^4}{45} + \frac{116e^6}{2835} + \frac{101e^8}{2835} + \frac{8764e^{10}}{280665} + ... \qquad (2.10.17)$$

We now proceed to the scattering cross-sections. As the orientation-averaged absorption cross-sections scale with the product of the imaginary part of relative permittivity and the arithmetic average of principal polarizabilities (example, see equaation (2.10.1) [6, 36], respectively), shape optimization proceeds exactly as for

polarizabilities. Therefore, we next consider the orientation-averaged scattering cross-section, given by [6]

$$< C_{sca} >= \frac{k^4}{18\pi}(|\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2) \tag{2.10.18}$$

Substituting for the polarizability from equation (2.10.4) into the above equation, we obtain

$$< C_{sca} >= \frac{k^4(4\pi abc)^2(\varepsilon_r - 1)^2}{18\pi} \sum_{i=1}^{3}[(\frac{1}{1 + L_i(\varepsilon_r - 1)})^2] \tag{2.10.19}$$

Similarly, substituting the polarizability of a conducting ellipsoid in equation (2.10.18), for the scattering cross section of conducting ellipsoid we obtain

$$< C_{sca} >= \frac{k^4 V^2}{228\pi^2}(\frac{1}{L_1^2} + \frac{1}{L_2^2} + \frac{1}{L_3^2}) \tag{2.10.20}$$

For the coated ellipsoid case, the average scattering cross section is

$$< C_{sca} >= \frac{k^4 V^2}{18\pi} \sum_{i=1}^{3}(\frac{((\varepsilon_2 - 1)[\varepsilon_2 + (\varepsilon_1 - \varepsilon_2)(L_i^{(1)} - fL_i^{(2)})] + f\varepsilon_2(\varepsilon_1 - \epsilon_2))}{[\varepsilon_2 + (\varepsilon_1 - \varepsilon_2)(L_i^{(1)} - fL_i^{(2)})][1 + (\varepsilon_2 - 1)L_i^{(2)}] + fL_i^{(2)}\varepsilon_2(\varepsilon_1 - \varepsilon_2)})^2 \tag{2.10.21}$$

We have been able to prove spherical optimality of polarizabilities and cross-sections for the conducting and dielectric spheroids. We use dielectric ellipsoid family to illustrate the proof by employing the method of Lagrange multipliers.

Consider the space of depolarization factors, spanned by L_1, L_2 and L_3. While varying ellipsoidal shapes, the relative permittivity is held constant and the objective function is

$$F(L_1, L_2, L_3) = \sum_{1}^{3} \frac{1}{1 + L_i(\varepsilon_r - 1)} \tag{2.10.22}$$

with the constraint in (2.10.9). Following the method of Lagrange multipliers, we write

$$\vec{\nabla}F(L_1, L_2, L_3) = \lambda\vec{\nabla}g(L_1, L_2, L_3) \tag{2.10.23}$$

36

Then, we get

$$\frac{\partial}{\partial L_i} \frac{1}{1 + L_i(\varepsilon_r - 1)} \qquad (2.10.24)$$

for i=1, 2, 3. In so far as this Equation is invariant w.r.t. interchange of labels, that is, completely symmetric in L_1, L_2, and L_3, it follows that $L_1 = L_2 = L_3$, delivers the minimum and $L_i = 1/3$ is obtained from the constraint 2.10.9. This represents spherical depolarization factors. We used the same method to establish spherical optimality for equations (2.10.13), (2.10.19) and (2.10.20).

Chapter 3

Materials and Methodology

3.1 Materials

The study is purely theoretical. An intensive survey of literature from published articles, books, thesis and dissertation will be carried out based on the project title. MATLAB and MATHEMATICA software's and computers are additional instruments used to accomplish this project.

3.2 Methodology

3.2.1 Analytical

In this thesis one of the method or approach used to solve the problem is analytical method i.e, polarizability, absorption coefficient and absorption cross-section of different shape ellipsoidal metallic particles as the function of distribution function.

3.2.2 Computational (graphical)

To interpret the result and to observe the effect of distribution function for different shapes nano ellipsoidal metals of polarizability, absorption cross-section and absorption coefficient are employed computational and graphical methods.

Chapter 4

Absorption Coefficient, scattering and absorption cross-section of an ensemble of ellipsoidal particles

4.1 Introduction

The absorption and scattering properties of small particles are very important in both astronomical and atmospheric remote sensing applications. The interaction of light with particles much smaller than the wavelength of radiation has been studied first by Lord Rayleigh [37] who described from basic physical rules the color and polarization of the light from the sky. When studying the detailed spectral properties of the interaction of particles with light, we have to consider the effects of particle size, shape and composition. In this thesis we discuss the effects of shape and composition of homogeneous particles, while taking the particle sizes to be in the Rayleigh domain, i.e. much smaller than the wavelength both inside and outside the particle.

When considering the possibilities for computing the optical (i.e. the absorption and scattering) properties of small particles there are two extreme approaches one can take. The first approach is to assume the particles are homogeneous in composition

and spherical in shape, which allows us to perform fast and simple computations of its interaction with light using Mie theory [38]. The second extreme is to make a model of the particle in an exact way, and perform numerical calculations to obtain its optical properties. This can be done using, for example, the T-matrix method [39, 40]. The first approach is fast, and provides insight into the physics and effects that play a role in the interaction of light with small particles [41]. However, due to the perfect symmetry of homogeneous spheres, resonance effects may occur, for example, at particular values of the refractive index, that are not seen in realistically shaped natural particles. This limits the applicability of this approach. The second approach allows us to reproduce details in the observed properties of irregular particles. The main drawback is, however, that the computational demand of most numerical techniques available to compute the optical properties of realistically shaped particles, is high. If we wish to consider a large collection of various particle compositions, sizes or wavelengths, one can resort to a third method, the statistical approach. In the statistical approach one simulates the average optical properties of an ensemble of irregularly shaped particles by the average properties of an ensemble of particles with simple shapes. These simple shapes guarantee computations of the optical properties to be relatively fast. In addition, by choosing a broad distribution of simple shapes, we can get rid of the resonance effects which can occur when using homogeneous spheres. The statistical approach is proven useful for, for example, computing absorption spectra of small forsterite grains [42], and for calculating the degree of linear polarization for small quartz particles [43].

4.2 Absorption coefficient and scattering cross-section

For an assembly of particles having different ellipsoidal shapes the absorption coefficient can be described as

$$\beta = N\langle C_{abs}\rangle = Nk\langle V\rangle Im\langle\alpha\rangle \tag{4.2.1}$$

with k, the wave vector, N, is the number of particle concentration, $\langle V\rangle$ the ensemble average volume and $Im\langle\alpha\rangle$ is the imaginary part of an ensemble of shape distribution ellipsoid.

For ellipsoids of different shapes the effective absorption cross-section is

$$\langle C_{abs}\rangle = \int\int C_{abs}^{(n)} f(l_1, l_2) dl_1 dl_2 \tag{4.2.2}$$

where

$$\langle C_{abs}^{(n)}\rangle = \frac{1}{3}kVIm\left[\ \sum_{i=1}^{3}\frac{\epsilon-1}{1+l_i(\epsilon-1)}\ \right]$$

, $f(l_1, l_2)$ is the particle shape distribution.

That is $f(l'_1, l'_2)dl'_1 dl'_2$ sets a polarizability sampled ellipsoid from an ensemble have the depolarization factors l_1 from $l'_1 + dl'_1$ and l_2 from $l'_2 + dl'_2$ and the third dipolarization factor can simply determined the distribution function f must be normalized to unity[44]:

$$\int\int f(l_1, l_2) dl_1 dl_2 = 1 \tag{4.2.3}$$

The departure of ellipsoids from strictly spherical shape are equiprobable. However, narrowing the range of deviations considered seems quite natural for a very wide class of actual particle ensembles. As the result the domain of integration in equation (4.2.3) is an isosceles right angled triangle in the $l_1 - l_2$ co-ordinates. The ellipsoid depolarization factor l_i vary with in the domain of integration from $\frac{1}{3} - \frac{1}{3}\delta$ to $\frac{1}{3} + \frac{2}{3}\delta$

41

with δ is the legs of triangle. According to this assumption, the ellipsoid shape distribution function takes the form:

$$f(l_1, l_2) = f_\delta = \frac{2}{\delta^2}\chi\left(l_1 - \frac{1}{3} + \frac{1}{3\delta}\right)\chi\left(l_2 - \frac{1}{3} + \frac{1}{3\delta}\right)\chi\left(-l_1 + \frac{1}{3} + \frac{2}{3\delta}\right)\chi(-l_2 + \frac{1}{3} + \frac{2}{3\delta})$$

$$(4.2.4)$$

Where χ is Heaviside unit function. It should be noted here that passage to the limit $\delta \to 0$ corresponds to degeneration of ellipsoids into spheres; in this case the distribution function $f(l_1, l_2)$ becomes the Dirac delta function: $f(l_1, l_2) = \delta(l_1 - 1/3, l_2 - 1/3)$. With the above assumptions made, the effective absorption cross-section $\langle C_{abs} \rangle$ for an ensemble of ellipsoid is

$$\langle C_{abs} \rangle = \frac{2}{3\delta^2}k\langle V \rangle Im \int_{\frac{1}{3}(1-\delta)}^{\frac{1}{3}(1+2\delta)} dl_1 \int_{\frac{1}{3}(1-\delta)}^{\frac{1}{3}(2+\delta)-l_1} dl_2 \left[\sum_{i=1}^{2} \frac{\epsilon-1}{1+l_i(\epsilon-1)} + \frac{\epsilon-1}{1+(1-l_1-l_2)(\epsilon-1)} \right]$$

$$(4.2.5)$$

The solution of double integral is

$$\langle \alpha \rangle = \frac{2}{3\delta^2}k\langle V \rangle Im \left[\left(\frac{1}{\epsilon-1} + \frac{1}{3} + \frac{2}{3\delta}\right) \ln\left(\frac{\frac{1}{\epsilon-1}+\frac{1}{3}+\frac{2}{3\delta}}{\frac{1}{\epsilon-1}+\frac{1}{3}-\frac{1}{3\delta}}\right) - \delta \right] \qquad (4.2.6)$$

From equation (4.2.6); effective absorption cross-section becoms,

$$\langle C_{abs} \rangle = \frac{2}{3\delta^2}k\langle V \rangle Im \left[\left(\frac{1}{\epsilon-1} + \frac{1}{3} + \frac{2}{3\delta}\right) \ln\left(\frac{\frac{1}{\epsilon-1}+\frac{1}{3}+\frac{2}{3\delta}}{\frac{1}{\epsilon-1}+\frac{1}{3}-\frac{1}{3\delta}}\right) \right] \qquad (4.2.7)$$

for $\delta = 1$,

$$\langle C_{abs} \rangle = k\langle V \rangle Im \left(\frac{2\epsilon}{\epsilon-1} \ln \epsilon \right)$$

is uniform distribution of ellipsoidal shape.

Taking the imaginary part of equation (4.2.5) we get

$$Im\langle \alpha \rangle = \frac{2}{\delta^2}\left\{ \frac{1}{2}\frac{\epsilon'-1}{(\epsilon'-1)^2+\epsilon''^2} \ln\left(y_1^2 + y_2^2 \right) + \left(\frac{\epsilon'-1}{(\epsilon'-1)^2+\epsilon''^2} + \frac{1}{3} + \frac{2}{3\delta} \right)\left[\pi\chi\left(\frac{-y_2}{y_1}\right) + \arctan\left(\frac{y_2}{y_1}\right) \right] \right\}$$

$$(4.2.8)$$

42

where

$$y_1 = \frac{\left(\frac{\epsilon'-1}{(\epsilon'-1)^2+\epsilon''^2} + \frac{1}{3} + \frac{2}{3\delta} \right)\left(\frac{\epsilon'-1}{(\epsilon'-1)^2+\epsilon''^2} + \frac{1}{3} - \frac{1}{3\delta} \right) + \frac{\epsilon''^2}{((\epsilon'-1)^2+\epsilon''^2)^2}}{\left(\frac{\epsilon'-1}{(\epsilon'-1)^2+\epsilon''^2} + \frac{1}{3} - \frac{1}{3\delta} \right)^2 + \left(\frac{\epsilon''}{(\epsilon'-1)^2+\epsilon''^2} \right)^2}$$

$$y_2 = \frac{\left(\frac{\epsilon''}{(\epsilon'-1)^2+\epsilon''^2} \right)\left(\frac{1}{\delta} \right)}{\left(\frac{\epsilon'-1}{(\epsilon'-1)^2+\epsilon''^2} + \frac{1}{3} - \frac{1}{3\delta} \right)^2 + \left(\frac{\epsilon''}{(\epsilon'-1)^2+\epsilon''^2} \right)^2}$$

In equation (4.2.8) imaginary part of logarithmic function is not uniquely defined. However, the average value of polarizability $\langle \alpha \rangle$ being a definite integral and uniquely defined. To resolve this contradiction if in necessary to take the principal value of logarithmic function. Accordingly the phase of logarithmic function changes by π when its argument pass over zero. As the result equation (4.2.8) becomes

$$Im\langle \alpha \rangle = \frac{1}{\delta}\left[\pi\chi(\tfrac{-y_2}{y_1}) + \arctan(\tfrac{y_2}{y_1}) \right] \tag{4.2.9}$$

For an ensemble of shape distributed ellipsoids, the Lorentz type of dielectric function

$$\epsilon(\omega) = \frac{\epsilon_\infty(\omega_{LT}^2 - \tilde{\omega}^2 - \imath\tilde{\omega}\tilde{\Gamma})}{(1 - \tilde{\omega}^2 - \imath\tilde{\omega}\tilde{\Gamma})} \tag{4.2.10}$$

where ϵ_∞ is the high-frequency (background) permittivity; $\omega_{LT} = \frac{\omega_L}{\omega_T}$, where ω_L and ω_T are the frequencies of the longitudinal and transverse optical phonons, respectively; $\tilde{\omega} = \frac{\omega}{\omega_T}$ is the relative frequency; and $\tilde{\Gamma} = \frac{\Gamma}{\omega_T}$ is the relative phonon damping constant.

Taking the equation of (4.2.10), the real and imaginary parts are respectively

$$\epsilon'(\omega) = \frac{\epsilon_\infty\left[\left(\omega_{LT}^2 - \tilde{\omega}^2 \right)\left(1 - \tilde{\omega}^2 \right) + \tilde{\omega}^2\tilde{\Gamma}^2 \right]}{\left(1 - \tilde{\omega}^2 \right)^2 + \tilde{\omega}^2\Gamma^2} \tag{4.2.11}$$

$$\epsilon''(\omega) = \frac{\epsilon_\infty\left[\tilde{\omega}\tilde{\Gamma}\left(\omega_{LT}^2 - 1 \right) \right]}{\left(1 - \tilde{\omega}^2 \right)^2 + \tilde{\omega}^2\Gamma^2} \tag{4.2.12}$$

43

Let

$$A = \frac{1}{\epsilon - 1}$$

$$\langle \alpha \rangle = \frac{2}{\delta^2} \left[\left(A + \tfrac{1}{3} + \tfrac{2}{3\delta} \right) \ln \left(\frac{A + \frac{1}{3} + \frac{2}{3\delta}}{A + \frac{1}{3} - \frac{1}{3\delta}} \right) - \delta \right] \tag{4.2.13}$$

Similarly with equation (4.2.5) the absorption cross-section is given by

$$\langle C_{abs} \rangle = k \langle V \rangle Im \left[\int_{\frac{1}{3}(1-\delta)}^{\frac{1}{3}(1+2\delta)} dl_1 \int_{\frac{1}{3}(1-\delta)}^{\frac{1}{3}(2+\delta)-l_1} dl_2 \left[\sum_{i=1}^{3} \frac{\epsilon - 1}{1 + l_i(\epsilon - 1)} + \sum \frac{\epsilon - 1}{1 + (1 - l_1 - l_2)(\epsilon - 1)} \right] \right] \tag{4.2.14}$$

From equation (4.2.1) and (4.2.13)

$$\langle C_{abs} \rangle = \frac{2}{\delta^2} k \langle V \rangle Im \left[(A + \tfrac{1}{3} + \tfrac{2}{3\delta}) \ln(\frac{A + \frac{1}{3} + \frac{2}{3\delta}}{A + \frac{1}{3} - \frac{1}{3\delta}}) \right] \tag{4.2.15}$$

Also let $A_1 = \frac{\epsilon' - 1}{(\epsilon' - 1)^2 + \epsilon''^2}$ and $A2 = \frac{-\epsilon''}{(\epsilon' - 1)^2 + \epsilon''^2}$

$$Im \langle \alpha \rangle = \frac{1}{\delta} \left[\pi \chi(\tfrac{-z_2}{z_1}) + \arctan(\tfrac{z_2}{z_1}) \right] \tag{4.2.16}$$

where

$$z_1 = \left(\frac{(A_1 + \frac{1}{3} + \frac{2}{3\delta})(A_1 + \frac{1}{3} - \frac{1}{3\delta}) + A_2^2}{(A_1 + \frac{1}{3} - \frac{1}{3\delta})^2 + A_2^2} \right)$$

and

$$z_2 = \left(\frac{\frac{A_2}{\delta}}{(A_1 + \frac{1}{3} - \frac{1}{3\delta})^2 + A_2^2} \right)$$

The results of $Im(\langle \alpha \rangle)$ calculations for the ellipsoids having typical oscillator parameters of ZnO is ($\epsilon_\infty = 8.5$, $\omega_{LT} = 1.1$, and $\tilde{\Gamma} = 0.002$). From Fig. (4.1-4.6) for different values of distribution function parameter (δ) and the relative phonon damping constant (Γ) are labeled. One can see that this parameter affects both the half-width and the symmetry (i.e., the form of polarizability, absorption coefficient and absorption cross section versus frequency curve), as well as the position of polarizability,

absorption coefficient and absorption cross-section values at this peak. Usually, the reststrahlen spectral region is rather narrow. For minimum values of distribution function parameter (δ) and the relative phonon damping constant (Γ), polarizability, absorption coefficient and absorption cross section versus frequency curve values are maximum and vice versa. So one has to allow for possible considerable distortion of the absorption spectra that is due to the spectral characteristic of the instrument used. We place special emphasis on the effect of distribution function parameter (δ) and the relative phonon damping constant (Γ) on the polarizability, absorption coefficient, and absorption cross-section.
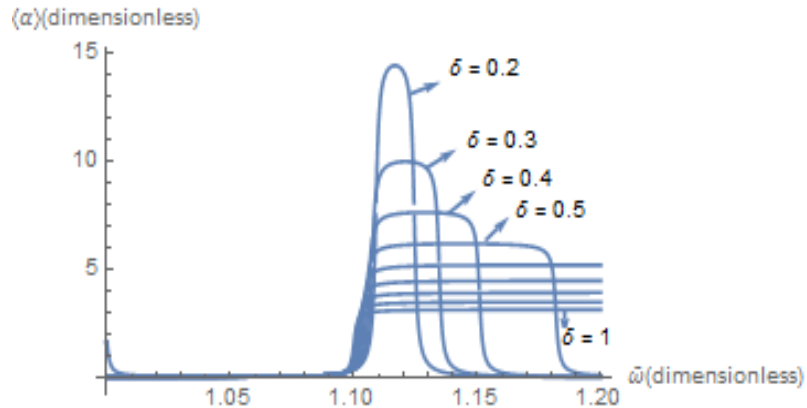

Figure 4.1: Imaginary part of the nondimensional effective polarizability $Im\langle\alpha\rangle$ versus relative frequency ($\tilde{\omega}$). The parameter (δ) of the ellipsoidal-shape distribution is 0.2, 0,3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, and 1.0.

From the Fig. (4.1) is polarizability (α) versus relative frequency curve with different values of distribution function parameter delta (δ). If the polarizability (α) of different shapes of nano ellipsoidal metallic particles are increased, the distribution function parameter delta (δ) of those different shapes of nano ellipsoidal metallic particles are decreased. From this idea one can conclude that polarizability (α) versus

frequency curve with different values distribution function parameter delta (δ); polarizability (α) is inversely proportional to the distribution function parameter delta (δ).
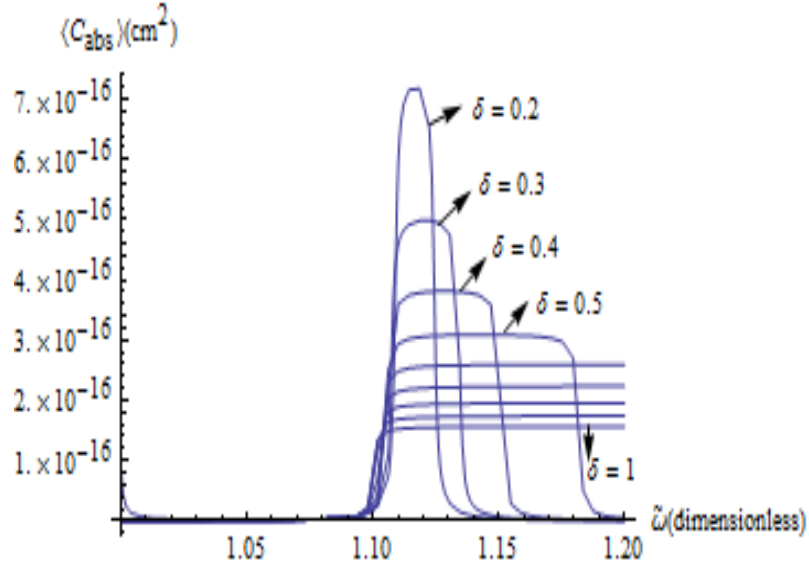

Figure 4.2: Absorption cross-section (C_{abs}) versus relative frequency ($\tilde{\omega}$). The parameter (δ) of the ellipsoidal-shape distribution is 0.2, 0,3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, and 1.0.

From the Fig. (4.2) is absorption cross-section (C_{abs}) versus relative frequency curve with different vales of distribution function parameter delta (δ). If the absorption cross-section (C_{abs}) of different shapes of nano-ellipsoidal metallic particles are increased, the distribution function parameter delta (δ) of those different shapes of nano ellipsoidal metallic particles are decreased. From this idea one can conclude that absorption cross-section (C_{abs}) versus relative frequency curve with different values of distribution function parameter delta (δ); absorption cross-section (C_{abs}) is inversely proportional to the distribution function parameter delta (δ).
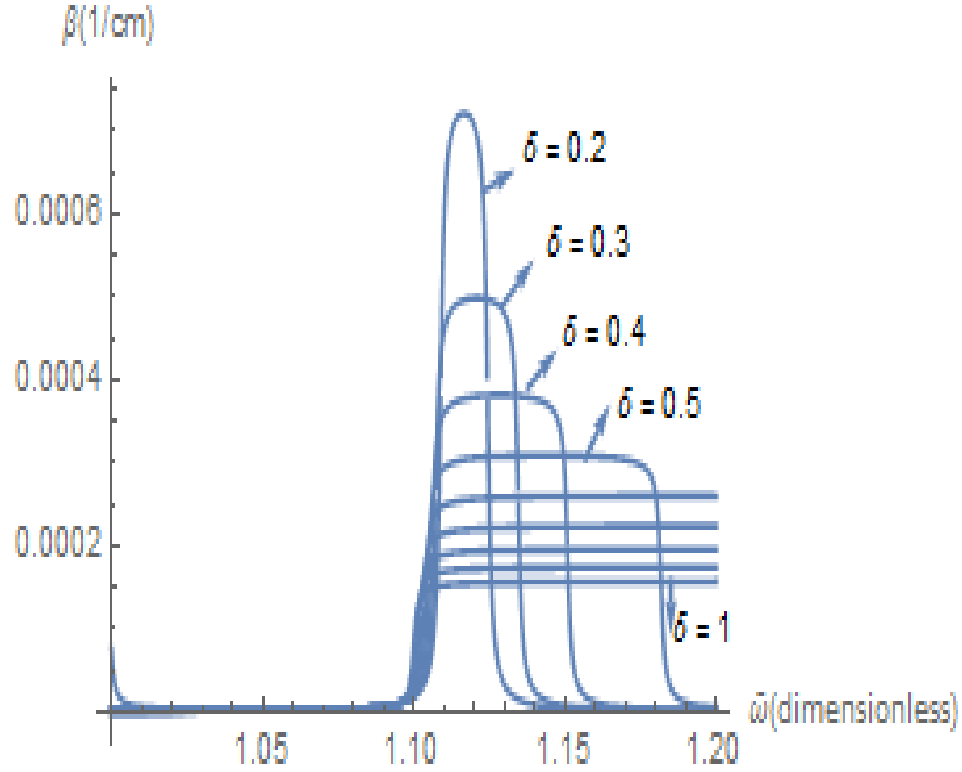
46

Figure 4.3: Absorption coefficient (β) versus relative frequency ($\tilde{\omega}$). The parameter (δ) of the ellipsoidal-shape distribution is 0.2, 0,3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, and 1.0.

From the Fig. (4.3) is absorption coefficient (β) versus relative frequency curve with different values of distribution function parameter delta (δ). If the absorption coefficient (β) of different shapes of nano ellipsoidal metallic particles are increased, the distribution function parameter delta (δ) of those different shapes of nano ellipsoidal metallic particles are decreased. From this idea; one can conclude that absorption coefficient (β) versus relative frequency curve with different values of distribution function parameter delta (δ), absorption coefficient (β) is inversely proportional to the distribution function parameter delta (δ).
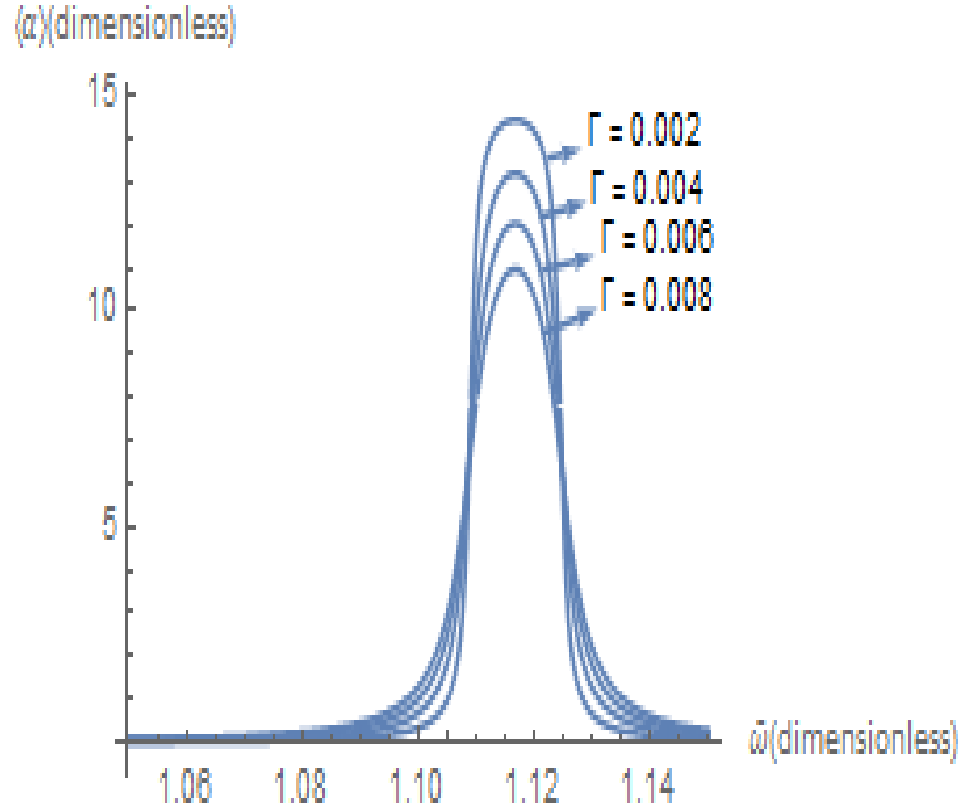
47

Figure 4.4: Imaginary part of the nondimensional effective polarizability $Im\langle\alpha\rangle$ versus relative frequency ($\tilde{\omega}$). The parameter of relative phonon damping constant (Γ) of the ellipsoidal-shape distribution is 0.002, 0.004, 0.006, and 0.008.

From the Fig. (4.4) is polarizability (α) versus relative frequency curve with different values of relative phonon damping constant (Γ). If the polarizability (α) of different shapes of nano ellipsoidal metallic particles are increased, the relative phonon damping constant (Γ) of those different shapes of nano ellipsoidal metallic particles are decreased. From this idea; one can conclude that polarizability (α) versus relative frequency curve with different values of relative phonon damping constant (Γ); polarizability (α) is inversely proportional to relative phonon damping constant (Γ).
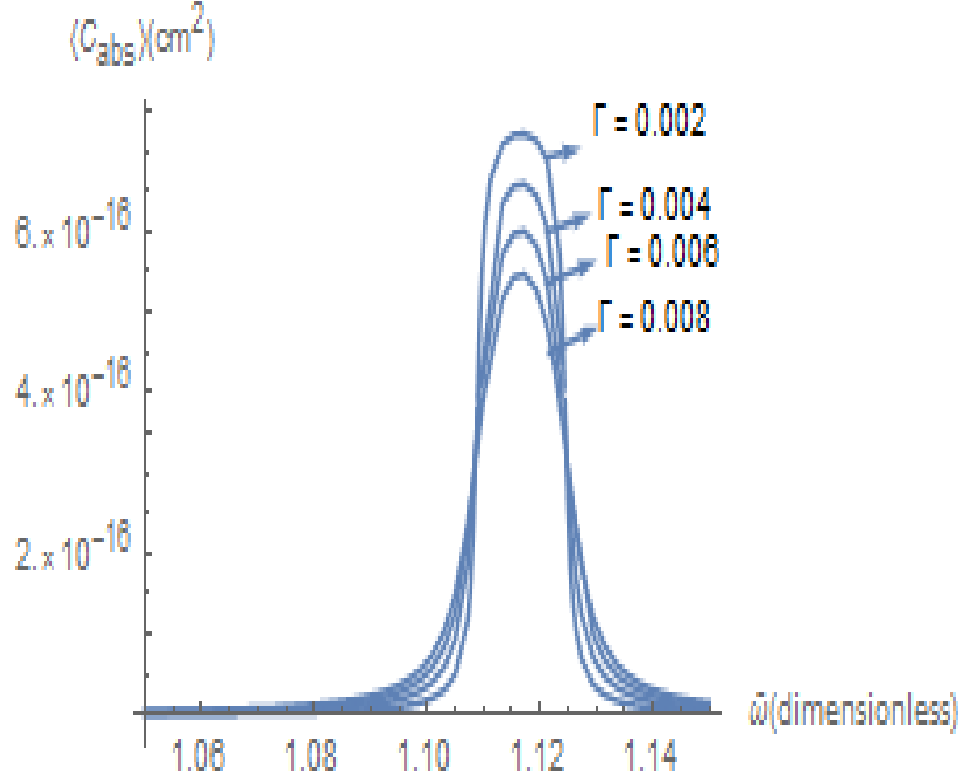
Figure 4.5: Absorption cross-section (C_{abs}) versus relative frequency ($\tilde{\omega}$). The parameter of relative phonon damping constant (Γ) of the ellipsoidal-shape distribution is 0.002, 0.004, 0.006, and 0.008.

From the Fig. (4.5) is absorption cross-section (C_{abs}) versus relative frequency curve with different values of relative phonon damping constant (Γ). If the absorption cross-section (C_{abs}) of different shapes of nano ellipsoidal metallic particles are increased, the relative phonon damping constant (Γ) of those different shapes of nano ellipsoidal metallic particles are decreased. From this idea; one can conclude that absorption cross-section (C_{abs}) versus relative frequency curve with different values of relative phonon damping constant (Γ), absorption cross-section (C_{abs}) is inversely proportional to relative phonon damping constant (Γ).
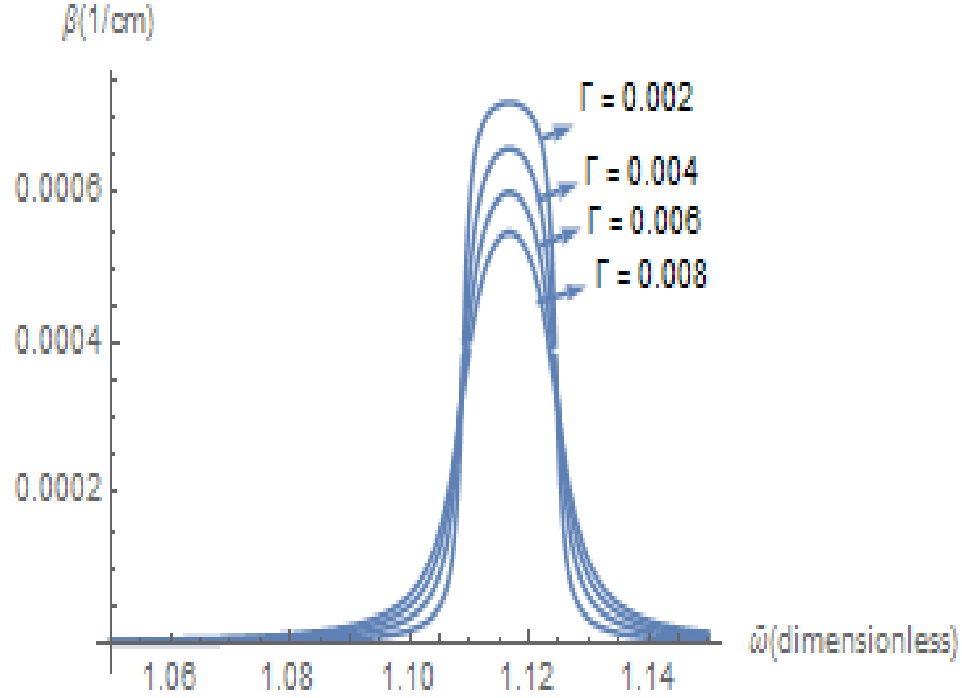
Figure 4.6: Absorption coefficient (β) versus relative frequency ($\tilde{\omega}$). The parameter of relative phonon damping constant (Γ) of the ellipsoidal-shape distribution is 0.002, 0.004, 0.006, and 0.008.

From the Fig. (4.6) is the absorption coefficient (β) versus relative frequency curve with different values of relative phonon damping constant (Γ). If the absorption coefficient (β) of different shapes of nano ellipsoidal metallic particles are increased, relative phonon damping constant (Γ) of those different shapes of nano ellipsoidal metallic particles are decreased. From this idea; one can conclude that the absorption coefficient (β) versus relative frequency curve with different values of relative phonon damping constant (Γ), absorption coefficient (β) is inversely proportional to relative phonon damping constant (Γ)

Chapter 5

Conclusion

In this study; polarizability, absorption coefficient and absorption cross-section of an ensemble of different shapes of nano-ellipsoidal metallic particles in the dielectric host media are focused. Shape effects in scattering and absorption cross-section as the function of distribution function by randomly oriented particles small compared to the wavelength have been investigated. First; imaginary part of polarizability as the function of distribution function for different shapes of nano-ellipsoidal metallic particles in the dielectric host media are derived analytically. Depending on analytic expression of polarizibility; the absorption cross-section and absorption coefficients are calculated. Using those relations; polarizability, absorption cross-section and absorption coefficient versus relative frequency curve; either by varying distribution function parameter (δ) with constant value of relative phonon damping constant (Γ) or by varying reative phonon damping constant (Γ) with constant value of distribution function parameter (δ) are described. From this idea one can conclude that, it is possible to calculate the average polarizability, absorption coefficient and absorption cross section for different shapes of nano-ellipsoidal metal as the function of distribution function.

The variation of polarizability, absorption coefficient and absorption cross-section for different shapes of nano-ellipsoidal dielectric composite media are due to the changes in distribution function parameter (δ) and relative phonon damping constant (Γ). As the result; polarizability, absorption coefficient and absorption cross section versus relative frequency curve , as well as the position of their peak value are analyzed. If the distribution function parameter and relative phonon damping constant decreased; polarizability, absorption coefficient and absorption cross section are increased and the reststrahlen spectral region is rather narrowed.

In general, polarizability, absorption coefficient and absorption cross section of nono-ellipsoida metals are affected by distribution function parameter and relative phonon damping constant.

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