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entitled

Computation and Analysis of Effective Permittivity of Thin Film Nanostructures:

An Effective Medium Perspective

by

Abbasali Naseem

Submitted to the Graduate Faculty as partial fulfillment of the
requirements for the Master of Science Degree in Electrical Engineering

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An Abstract of

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This thesis probes the techniques involved in the calculation of effective
permittivity of thin film nanostructures. Stress is given on the calculation of effective
permittivity particularly in the anisotropic environment. Also a detailed investigation of
isotropic and anisotropic mediums is performed with respect to the displacement vector
and electric field vector. The effective permittivity thus calculated can give evidence of
many electrical and optical properties a mixture might possess.

During the research a novel method was discovered, which suggests that the
effective permittivity might be a vector. Such a vector form of the permittivity is
achieved from purely isotropic materials. Thus some anisotropy is achieved by beginning
with pure isotropic materials. Generalization of all the equations for the calculation of
effective permittivity for multiple kinds of inclusions which further makes the mixture
more complex.
We have developed a code for these computations which is intended to be very user friendly. We use an input file as an input to this code. All the results are then stored in an output file. The effect due to the shape of the inclusions is also taken into account with depolarization factors. Also the effect of orientation of the inclusions in space is considered and is introduced with the help for eigen vectors.
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Chapter 1

Introduction

Permittivity is a very important physical quantity that depicts how the electric field affects and how it also affects the dielectric medium that it propagates through\(^1\). The ability of the dielectric material to polarize when the electric field acts on the medium and thereby reduce it is determined by the permittivity. One of the most basic examples is that of a capacitor, whose permittivity if increased allows the same amount of charge to be stored at even smaller electric fields. Enhancement of permittivity is possible by the use of novel materials which can be made using mixtures. Effective permittivity of these mixtures can be calculated using the methods described in this thesis.

1.1 Motivation

Light has proved to be a very useful medium for conveyance of information. Optical fibers guide light signals which carry tremendous amounts of data capable for voice and video communication also, are now being used very widely all over the world. This enormous data carrying volume of the optical fibers has therefore led researchers to believe that photonic devices that engineer and direct visible light and electromagnetic waves would, at a later time substitute the existing electric circuits in microprocessors
and other computer chips. Although the dimensions and performance of photonic devices are bounded by the diffraction limit, the diffraction limit resolution is defined by the diameter of the optical substance and the wavelength of the light. The width of the optical fiber carrying the light waves must be at least half the wavelength of the light\(^2\).

Recently there has been a special stress on the development and miniaturization of optical devices. There has been a turnabout in integrated optical components brought about by the present technologies like the planar waveguides and photonic crystals\(^3\). It was shown experimentally in the 1980’s that having light incident on an interface between a metallic substance and a non-conducting dielectric material, a resonant interaction can be induced between the light waves and free electrons at the surface of the metallic substance. This dielectric material can be a thin film nanostructure which can further be a mixture of several materials. It is therefore important to know the effective permittivity of such a material. We have the oscillations of free electrons on the surface of the metal matching the oscillations of the electromagnetic field at the exterior of the metal, which results in the generation of surface plasmons with a much shorter wavelength\(^4\). Surface plasmons can be defined as the density waves of electrons that propagate along the interface\(^2\). These density waves can be compared to the ripples produced in still water due to disturbance. This phenomenon would permit these plasmons to travel onward nano-scale wires, which are called interconnects, to carry data or information between various parts of a microprocessor. Chip designers have had a very difficult time constructing miniscule electronic circuits that can pass information much faster across the chip. Therefore, designers who wish to design even smaller and faster transistors would consider these plasmonic interconnects to be a huge help.
Other results have shown that if we vary the water content by a percent then we witness a large variation in the effective permittivity. Therefore researchers can have a tight control over the water content for modeling of biological tissues. There have been several controversies of how electromagnetic waves influence biological bodies. The manner in which fields pass or propagate through bodies is governed by the biological properties of the bodies such as permittivity.

1.2 Applications

This emerging field related to the transfer of plasmons in order to carry information has been given the name “plasmonics” by Harry Atwater and his group at the California Institute of Technology in 2000. In the not so far away future, there is a possibility to incorporate plasmonic devices in an extensive variety of instruments. These instruments can be used to enhance the efficiency of light emitting diodes (LED’s), resolution of microscopes and the sensitivity of biological and chemical sensors. There are also some medical applications that have been taken into consideration. For example, the design of very small devices could employ plasmon resonance absorption to destroy cancerous tissues. It is also believed and theorized by some scientists to a certain extent that some plasmonic materials could vary the electromagnetic field surrounding an object to such an extent that it would become invisible. The above mentioned applications have had researchers eagerly study plasmonics as this new and emerging field has the potential to reveal many mysteries of the nanoworld.
1.3 Progress and Scope

Since many years, alchemists and glassmakers have unknowingly utilized the advantageous properties of plasmonic effects when they made stained-glass windows and multi-colored goblets which had small particles of metal in the glass. One of the most famous and popular examples is the “Lycurgus cup”. The Lycurgus cup is a roman goblet which dates as far as the fourth century A.D and changes color because of the excitations of the plasmons due to the metallic particles inside the glass cup. The cup scatters blue and green light, which are comparatively shorter wavelengths of the visible spectrum. On the other hand when a source of light is situated inside the cup, the cup appears to be red in color.

The discovery of “metamaterials” gave another boost to the yet emerging field of plasmonics. Metamaterials are materials having astonishing optical properties due to result of electron oscillation. The term “metamaterial” is used to refer to media which are characterized by both the simultaneously negative values for permittivity and permeability denoted by ,,ε” and ‘μ’ respectively\(^2\). The recent rise in computational power has allowed scientists to accurately simulate the complex electromagnetic fields produced by plasmonic effects. Also, new methods for manufacturing nanoscale structures have made it seem not so impossible to construct and test very small plasmonic devices and circuits.

Metals have been understood to have high optical losses and thus it seems impractical to use metallic substances or structures for the transmission of light signals. The electromagnetic field’s energy is dissipated due to the collision of the oscillating
electrons in the electromagnetic field and the enclosing lattice of atoms. But at the interface of a thin metal film and a dielectric substance, the plasmon losses are much lower as compared to the inside of bulk of a metal. This is due to the fact that the field spreads into a material that is non-conductive and has no free electrons. Therefore, there is no energy dissipation due to collision, since there are no free electrons. Hence, the plasmons are restricted to the metallic surface adjacent to the dielectric and are sandwiched between the dielectric and the metallic layers.

Due to this phenomenon nanoshells are becoming a favorable tool for the treatment of cancer. In 2004, plasmonic nanocells were injected into the bloodstream of mice having cancerous tumors, by Halas and her teammate Jennifer West in Rice University\(^1\). It was found that these injected nanoshells were not toxic. As there was more amount of blood being circulated to the briskly growing tumors in the mice, the nanoshells tended to attach themselves to the cancerous tissues as compared to the healthy tissues. Keeping this in mind, we can also embed nanoshells to antibodies to confirm that they target cancers.

Animal and human tissues are fortunately transparent to radiation at some wavelengths in the infrared region. When laser light near to the infrared region was channeled through the skin of the mice, it was observed that the resonant absorption of energy in the attached nanoshells made the temperature of the cancer tissues to rise from about 37 degrees Celsius to around 45 degrees Celsius. This type of photo-thermal heating destroyed the cancer cells and left the surrounding healthy tissues undamaged.

Recently a new discovery of a “Left Handed Material” has come into realization at the University of California, San Diego. These materials have negative permittivity and
negative permeability simultaneously. This is also an example of metamaterials. Metamaterials again, are those materials which show unusual properties from not their constituents but its structure.

The main reason for the researchers to gain interest in metamaterials is that they can be used to create a structure which has negative refractive index. Almost all materials in nature have positive permittivities and permeabilities. But there are some metals like gold and silver which have negative permittivity at visible wavelengths.
Chapter 2
Isotropic and Anisotropic Media

2.1 Introduction

It has been from the time of Maxwell that transport properties of randomly inhomogeneous materials have been of great intrigue to researchers. The demand of today’s scientific and technological world is the use of novel materials which have unique optical properties that have not been witnessed in the already existing materials. There has always been exhausting amount of research on manufacturing or developing such unique materials or modify the existing materials to exhibit special properties\textsuperscript{8,9,10,11}, with the presence of the available techniques for the preparation of thin films.

The approach in which the properties of these composite thin films are modified is generally a more convenient way because of its ease of implementation. These techniques involving the modification or thin films deposition techniques are namely, evaporation, sputtering and ion beams assisted depositions. These techniques have been proved to be quite successful for preparing composite or inhomogeneous dielectric thin films. Thin films manufactured using the above mentioned techniques have found uses in optical thin film devices.
Cermet films have been developed by the co-deposition of dielectrics with different metals and have found applications in devices for solar energy conversion. Dielectric-Dielectric and Metal-Dielectric composite thin films have been vastly researched upon with special emphasis on their optical properties in the near infrared and solar regions.

The most astonishing fact about these thin metallic films is that they show different optical properties from those of just the bulk metal. These films show very selective absorption and their properties strongly depend on the film structure, for example their thickness. Electron-microscopic results have determined that actual thin films are not parallel sided homogeneous slabs, but they are films having some in-homogeneity like unevenness or some cracks or particles isolated from each other. Experimental results show that when very thin silver films are heated they show a resonance type absorption and whose peak exists at around 435 µm or at longer wavelength. These films are composed of a large number of small particles of silver\textsuperscript{12}. Therefore, there should be no uncertainty in the fact that this kind of deviant behavior can be credited to such “in-homogeneity”. Results from experiments have concluded that thin metallic films can be regarded as a two dimensional aggregate of small rotational ellipsoids\textsuperscript{12,13}. The shape of the ellipsoids influences resonating of the free electron gas bounded within an ellipsoid at particular frequency.
2.2 Electromagnetic Waves in Isotropic Media

An isotropic optical material is one whose properties are independent of the direction of propagation or polarization state of an electromagnetic wave passing through the material\(^{14}\). We have some constitutional relations which hold true for this type of a material.

2.2.1 Governing Equations for Fields and Waves in Isotropic Media

The polarization induced by the electric field of the wave, which is parallel to the electric field is\(^{15}\)

\[
\vec{P} = \epsilon_0 \chi \vec{E} \tag{2.1}
\]

Where, \(\vec{P}\) = Polarization,

\(\vec{E}\) = Electric Field of the wave,

\(\epsilon_0\) = Permittivity of free air,

\(\chi\) = Electric Susceptibility.

Therefore it follows that electric displacement vector of the wave is parallel the electric field given by\(^{15}\)

\[
\vec{D} = \epsilon_0 \vec{E} + \vec{P} \tag{2.2}
\]

Where, \(\vec{D}\) = Electric Displacement Vector.

Therefore substituting equation (2.1) in equation (2.2) we get,
\[ \vec{D} = \varepsilon_0 \vec{E} + \varepsilon_0 \chi \vec{E} \]

\[ \Rightarrow \quad \vec{D} = \varepsilon_0 (1 + \chi) \vec{E} \quad (2.3) \]

or

\[ \vec{D} = \varepsilon_0 \varepsilon_r \vec{E} \quad (2.4) \]

Where \( \varepsilon_r = 1 + \chi \) = Dielectric Constant of a material. For a material which is absorbing or amplifying we have \( \varepsilon_r \) as complex given by

\[ \varepsilon_r = \varepsilon' - i\varepsilon'' \quad (2.5) \]

The refractive index of the material is given by

\[ n = \sqrt{\varepsilon_r} = \sqrt{\varepsilon' - i\varepsilon''} \quad (2.6) \]

Where, \( n = \) Refractive Index. The dielectric constant and therefore the refractive index are related to the frequency of the wave. This phenomenon is known as dispersion and is the cause for a prism to separate white light into its constituent colors.

The wave vector, \( \vec{k} \) is perpendicular to the phasefronts and is by definition perpendicular to the vectors \( \vec{D} \) and \( \vec{B} \). The magnitude and the direction of energy flow are represented by the Poynting vector of the wave. This pointing vector is parallel to the wavevector \( \vec{k} \). The poynting vector is given by

\[ \vec{S} = \vec{E} \times \vec{H} \quad (2.7) \]

The above mentioned is explained by the Figure 2.1. The local direction of \( \vec{S} \) is also called the ray direction. Only for wavefronts is the ray direction the same at all
points on the phasefront. The best way to understand the properties of an optical system is to find out what happens to a ray of light entering the system. It is necessary to understand what happens to the direction of light as it encounters lenses or mirrors, the intensity of light when it crosses an interface, etc.

Where, \( B \) = magnetic field,

\( H \) = magnetic field intensity.

2.2.2 Maxwell’s Equations in Isotropic Media

The Maxwell equations in the isotropic medium are given below,

\[
\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} = -\mu \frac{\partial \vec{H}}{\partial t}
\]

or

\[
\nabla \times \vec{E} = -j\omega \vec{B} = -j\omega \mu \vec{H}
\]  \hspace{1cm} (2.8)
Where, $\mu$ = Magnetic Permeability,

$$\omega = \text{Frequency of time harmonic fields.}$$

$$\nabla \times \vec{H} = \varepsilon \frac{\partial \vec{E}}{\partial t} + \vec{j}$$

or

$$\nabla \times \vec{H} = -j\omega \varepsilon \vec{E} + \vec{j}$$ \hspace{1cm} (2.9)

Where, $\vec{j}$ = Total Current Density.

$$\nabla \cdot \vec{E} = \frac{\rho}{\varepsilon}$$ \hspace{1cm} (2.10)

Where, $\rho$ = Total Charge Density.

$$\nabla \cdot \vec{B} = \nabla \cdot (\mu \vec{H}) = 0$$ \hspace{1cm} (2.11)

### 2.3 Electromagnetic Waves in Anisotropic Media

In anisotropic media, the electric vector of a propagating wave is not in general parallel to its polarization direction and is defined by the direction of its electric displacement vector$^{14,16,17}$. There are two different possible polarization directions that exist for plane waves travelling in a particular direction through an anisotropic medium, and the waves that have these different polarization directions, travel with different velocities. The most common and most important anisotropic media are generally crystalline. These anisotropic mediums have their optical properties closely associated to the various symmetry properties possessed by crystals.
In an isotropic medium, the propagation characteristics of an electromagnetic wave are independent of their direction of propagation. This therefore means that there is no other direction possible in the medium which is different than any other direction. It is obvious then that we cannot just simply categorize liquid crystals as isotropic media, as we can do for gases or liquids, given that there are no externally applied fields present. Such a field would mean the presence of a unique direction in the medium, that of the field. The case of a gas in a magnetic field is fine example to understand the circumstance of an isotropic medium being converted into an anisotropic medium when an external field is applied. This phenomenon occurs because the gas alters the characteristics of polarization of a wave which propagates in the field direction. This very well known phenomenon is known as the “Faraday Effect”.

In an isotropic medium the electric displacement vector and its associated electric field are parallel. Therefore we have the relation

$$\vec{D} = \epsilon_r \epsilon_0 \vec{E}$$  \hspace{1cm} (2.12)

Where $\vec{D}$ = Electric Displacement Vector,
$\vec{E}$ = Associated Electric Field,
$\epsilon_r$ = Scalar dielectric Constant,
$\epsilon_0$ = Permittivity of free air.

Therefore we can also say that the polarization induced by the field and the field itself are parallel to each other. Therefore we have

$$\vec{P} = \epsilon_0 \chi \vec{E}$$  \hspace{1cm} (2.13)
Where, \( \vec{P} \) = Polarization,

\( \chi \) = Electric Susceptibility.

We have followed the assumption in considering materials that are neither absorbing nor amplifying and hence the scalar dielectric constant and the electric susceptibility are real and not complex. We have stated the above equations in section (2.2.1). They have only been rewritten for the ease of comparison between the isotropic and anisotropic media.

It has been noticed and learned that in isotropic media, the orientation of polarization or magnetization is in the same direction as that of the field vector and the responses to fields with different orientations are the same. Therefore a very important conclusion is made here that in isotropic media, the permittivity and the permeability are scalars which may be complex and maybe frequency dependent or nonlinear.

In a number of technically important materials, responses of polarization and magnetization to fields with different orientations may differ, so that the orientation of polarization or magnetization can be in the different direction to that of the field vector as shown in Figure 2.2. These media are known as the “anisotropic media”. For anisotropic media the permittivity and the permeability are tensors or matrices.\(^9\)
2.3.1 Governing Equations for Fields and Waves in Anisotropic Media

The constitutional equations in anisotropic media are given by\(^{16}\)

\[
\vec{D} = \vec{\varepsilon} \vec{E} \tag{2.14}
\]

and

\[
\vec{B} = \vec{\mu} \vec{H} \tag{2.15}
\]

Where, \(\vec{\varepsilon}\) = Tensor Permittivity,

\(\vec{\mu}\) = Tensor Permeability.
The tensor permittivity and tensor permeability are complex and are dependent on the frequency for steady state sinusoidal time varying fields. This implies that all the elements of the permittivity and permeability matrices are complex. It is possible for a medium to be both electric and magnetic anisotropic, but it is common for an anisotropic medium to be either just electric anisotropic or magnetic anisotropic.

If the medium is just electric anisotropic, it is known as $\varepsilon$-anisotropic medium. In such a medium the permittivity $\varepsilon$ becomes a tensor and the permeability $\mu$ remains a scalar. Therefore the governing relations for such a medium become

$$\vec{D} = \varepsilon \vec{E}$$  \hspace{1cm} (2.16)

and

$$\vec{B} = \mu \vec{H}$$  \hspace{1cm} (2.17)

Where,

$$\varepsilon = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix}$$  \hspace{1cm} (2.18)

Similarly, if the medium is just magnetic anisotropic, it is known as $\mu$-anisotropic medium. In such a medium the permeability $\mu$ becomes a tensor and the permittivity $\varepsilon$ remains a scalar. Therefore the governing relations for such a medium become

$$\vec{D} = \varepsilon \vec{E}$$  \hspace{1cm} (2.19)

and

$$\vec{B} = \mu \vec{H}$$  \hspace{1cm} (2.20)
Where,

\[ \tilde{\mu} = \begin{bmatrix} \mu_{xx} & \mu_{xy} & \mu_{xz} \\ \mu_{yx} & \mu_{yy} & \mu_{yz} \\ \mu_{zx} & \mu_{zy} & \mu_{zz} \end{bmatrix} \quad (2.21) \]

Since the permittivity and permeability are tensors in their respective anisotropic mediums, their inverse has similar importance in calculations. The alternative expressions of the constitutional expressions,

for electric anisotropic media are,

\[ \vec{E} = \tilde{\kappa} \vec{D} \quad (2.22) \]

And

\[ \vec{H} = \tilde{\nu} \vec{B} \quad (2.23) \]

Where,

\[ \tilde{\kappa} = \begin{bmatrix} \kappa_{xx} & \kappa_{xy} & \kappa_{xz} \\ \kappa_{yx} & \kappa_{yy} & \kappa_{yz} \\ \kappa_{zx} & \kappa_{zy} & \kappa_{zz} \end{bmatrix} = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{bmatrix}^{-1} \quad (2.24) \]

For magnetic anisotropic media are,

\[ \vec{E} = \kappa \vec{D} \quad (2.25) \]

And

\[ \vec{H} = \tilde{\nu} \vec{B} \quad (2.26) \]

Where,

\[ \tilde{\nu} = \begin{bmatrix} \nu_{xx} & \nu_{xy} & \nu_{xz} \\ \nu_{yx} & \nu_{yy} & \nu_{yz} \\ \nu_{zx} & \nu_{zy} & \nu_{zz} \end{bmatrix} = \begin{bmatrix} \mu_{xx} & \mu_{xy} & \mu_{xz} \\ \mu_{yx} & \mu_{yy} & \mu_{yz} \\ \mu_{zx} & \mu_{zy} & \mu_{zz} \end{bmatrix}^{-1} \quad (2.27) \]
\( \varepsilon \) and \( \mu \) are better known as the permittivity and the permeability tensors respectively.

### 2.3.2 Symmetrical Properties of the Constitutional Tensors

The properties of constitutional tensors will now be explained for passive and lossless media. We have to consider first the poynting vector for that purpose. When the equivalent magnetic charge and equivalent magnetic current are introduced into the Maxwell’s equations, we have\(^{16}\)

\[
\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} - \dot{J}_m
\] (2.28)

Where, \( \dot{J}_m \) = equivalent Magnetic Current Density.

\[
\vec{\nabla} \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \sigma \vec{E} + \vec{J}
\] (2.29)

Where, \( \sigma \) = Conductivity.

\[
\vec{\nabla}.\vec{D} = \rho
\] (2.30)

\[
\vec{\nabla}.\vec{B} = \rho_m
\] (2.31)

Where, \( \rho_m \) = Total Magnetic Charge Density.

Rewriting equations (2.28) and (2.29) in its frequency domain and then writing the complex conjugate of equation (2.29), we get

\[
\vec{\nabla} \times \vec{E} = -j\omega \vec{B} - \dot{J}_m
\] (2.32)

\[
\vec{\nabla} \times \vec{H}^* = -j\omega \vec{D}^* + \sigma \vec{E}^* + \dot{J}^*
\] (2.33)
Now, we have the well known relation for the pointing vector given by \(^{16}\),

\[
\vec{S} = \vec{E} \times \vec{H}
\]  

(2.34)

Where, \(\vec{S}\) gives the magnitude and direction of the power flow per unit area at any point in space and is called as Poynting Vector. The complex form of Poynting Vector can be given by,

\[
\vec{S}^c = \frac{1}{2}(\vec{E} \times \vec{H}^*)
\]  

(2.35)

Where, \(\vec{S}^c\) = Complex Poynting Vector. We also have the well known vector identity given below as

\[
\nabla \cdot (\vec{A} \times \vec{B}) = \vec{B} \cdot (\nabla \times \vec{A}) - \vec{A} \cdot (\nabla \times \vec{B})
\]  

(2.36)

Multiplying both sides of equation (2.35) by \(-\nabla\) we get

\[
-\nabla \cdot \vec{S}^c = -\nabla \cdot \left[ \frac{1}{2}(\vec{E} \times \vec{H}^*) \right]
\]  

(2.37)

Now using the vector identity given by equation (2.36) and substituting in equation (2.37) we get,

\[
-\nabla \cdot \vec{S}^c = \frac{1}{2} \vec{H}^* \cdot (\nabla \times \vec{E}) - \frac{1}{2} \vec{E} \cdot (\nabla \times \vec{H})
\]  

(2.38)

Now using equations (2.32) and (2.33) and applying them to equation (2.38) we have,

\[
-\nabla \cdot \vec{S}^c = j2\omega \left( \frac{\vec{H}^* \cdot \vec{B}}{4} - \frac{\vec{E} \cdot \vec{D}^*}{4} \right) + \sigma \frac{\vec{E} \cdot \vec{E}^*}{2} + \frac{\vec{E} \cdot \vec{j}^*}{2} + \frac{\vec{H}^* \cdot \vec{j}_m}{2}
\]  

(2.39)

Now in source free and non-conducting media, \(\vec{j} = 0\), \(\vec{j}_m = 0\) and \(\sigma = 0\). Therefore now equation (2.39) becomes,
\[ \nabla \cdot \mathbf{\hat{S}}^c = j\omega \left( \frac{\mathbf{E} \cdot \mathbf{D}^*}{2} - \frac{\mathbf{B} \cdot \mathbf{H}^*}{2} \right) \]  

Now the divergence of average pointing vector is

\[ \nabla \cdot \mathbf{\hat{S}}^{Av} = \nabla \left[ \frac{1}{2} \Re(\mathbf{E} \times \mathbf{H}^*) \right] \]

\[ = \frac{1}{2} \Re \left[ j\omega (\mathbf{E} \cdot \mathbf{D}^* - \mathbf{B} \cdot \mathbf{H}^*) \right] \]  

Where, \( \mathbf{\hat{S}}^{Av} = \text{Average Poynting Vector} \),

\( \Re = \text{Real part of. For an arbitrary complex quantity, we have} \)

\[ \Re z = \frac{1}{2} (z + z^*) \]  

Using equation (2.42), equation (2.41) becomes

\[ \nabla \cdot \mathbf{\hat{S}}^{Av} = \frac{1}{4} \left\{ [j\omega (\mathbf{E} \cdot \mathbf{D}^* - \mathbf{B} \cdot \mathbf{H}^*)] + [j\omega (\mathbf{E} \cdot \mathbf{D}^* - \mathbf{B} \cdot \mathbf{H}^*)]^* \right\} \]

\[ = \frac{j\omega}{4} \left[ \mathbf{E} \cdot \mathbf{D}^* - \mathbf{B} \cdot \mathbf{H}^* - \mathbf{E}^* \mathbf{D} + \mathbf{B}^* \mathbf{H} \right] \]  

Substituting equation (2.14) and (2.15) in equation (2.43) we get

\[ \nabla \cdot \mathbf{\hat{S}}^{Av} = \frac{j\omega}{4} \left[ (\mathbf{E} \cdot \mathbf{E}^*) - (\mathbf{B} \cdot \mathbf{H}^*) \mathbf{H}^* - \mathbf{E}^* \cdot \mathbf{E} + (\mathbf{B} \cdot \mathbf{H}) \cdot \mathbf{H}^* \right] \]  

From the knowledge of tensor algebra we have,

\[ \mathbf{\hat{A}} \cdot \bar{\mathbf{a}} \cdot \mathbf{\hat{A}}^* = \mathbf{\hat{A}}^* \cdot \bar{\mathbf{a}}^T \cdot \mathbf{\hat{A}} \]  

Where, \( \bar{\mathbf{a}}^T \) is the transpose of tensor \( \bar{\mathbf{a}} \) and \( \mathbf{\hat{A}} \) is a vector and \( \mathbf{\hat{A}}^* \) is its complex conjugate. Applying this rule in equation (2.45) we get,

\[ \nabla \cdot \mathbf{\hat{S}}^{Av} = \frac{j\omega}{4} \left[ \mathbf{E}^* (\mathbf{\bar{e}}^R - \mathbf{\bar{e}}) \cdot \mathbf{E} + \mathbf{\bar{H}}^* (\mathbf{\bar{\mu}}^R - \mathbf{\bar{\mu}}) \cdot \mathbf{\bar{H}} \right] \]
Where, $\tilde{\varepsilon}^R = \tilde{\varepsilon}^{*T}$ and $\tilde{\mu}^R = \tilde{\mu}^{*T}$

Now in source free and no conducting media we have $\nabla \cdot \tilde{S}^{A\nu} = 0$. This must be true for an arbitrary choice of $\tilde{E}$ and $\tilde{H}$. Therefore we have

$$\tilde{\varepsilon}^R = \tilde{\varepsilon} \quad \text{and} \quad \tilde{\mu}^R = \tilde{\mu}$$

or

$$\tilde{\varepsilon}^{*T} = \tilde{\varepsilon}^* \quad \text{and} \quad \tilde{\mu}^{*T} = \tilde{\mu}^* \quad (2.48)$$

Therefore, we can safely conclude that for anisotropic media, the transpose of the constitutional tensor is the complex conjugate of the tensor itself. Another conclusion can be made here that both the tensors are Hermitian Tensors. For a tensor to be a Hermitian Tensor the diagonal elements are real and the non-diagonal elements have conjugate symmetry. The equations below will give further understanding to what Hermitian Tensors are,

$$\epsilon_{ii} = \epsilon_{ii}^* \quad \text{and} \quad \mu_{ii} = \mu_{ii}^* \quad (2.49)$$

and

$$\epsilon_{ij} = \epsilon_{ji}^* \quad \text{and} \quad \mu_{ij} = \mu_{ji}^* \quad (2.50)$$

### 2.3.3 Reciprocal Media

If in equation (2.50), $\epsilon_{ij}$ and $\mu_{ij}$ are real, then we have,

$$\epsilon_{ij} = \epsilon_{ji} \quad \text{and} \quad \mu_{ij} = \mu_{ji} \quad (2.51)$$

Therefore now the constitutional tensors $\tilde{\varepsilon}$ and $\tilde{\mu}$ are real and now symmetrical tensors. Therefore,

$$\tilde{\varepsilon}^T = \tilde{\varepsilon} \quad \text{and} \quad \tilde{\mu}^T = \tilde{\mu} \quad (2.52)$$
Such media is known as “Reciprocal Media”.

We can rotate the co-ordinate system so that every symmetrical tensor of rank two can be changed to a diagonal tensor. When all the off-diagonal terms of the symmetrical tensor are zero, the tensor is known as a diagonal tensor. Therefore in a diagonal tensor we have

$$\varepsilon_{ij} = 0 \text{ and } \mu_{ij} = 0, \text{ when } i \neq j \quad (2.53)$$

Hence with respect to a given reciprocal medium, by appropriate orientation of the co-ordinate axes permittivity tensor and the permeability tensor can be stated as,

$$\bar{\varepsilon} = \begin{bmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_2 & 0 \\ 0 & 0 & \varepsilon_3 \end{bmatrix} \text{ and } \bar{\mu} = \begin{bmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_2 & 0 \\ 0 & 0 & \mu_3 \end{bmatrix} \quad (2.54)$$

This specially oriented co-ordinate system, in which the permittivity and permeability tensors are a diagonal matrix, is called a “Principle Co-ordinate System”. These three co-ordinate axes of the principle co-ordinate system are known as the “Principle Axes”. When in reciprocal media, $\varepsilon_1 = \varepsilon_2 = \varepsilon_3$ or for that matter $\mu_1 = \mu_2 = \mu_3$ then the reciprocal media becomes the isotropic media.

### 2.3.4 Non-reciprocal Media

If in equation (2.50), $\varepsilon_{ij}$ and $\mu_{ij}$ are imaginary, then we have,

$$\varepsilon_{ij} = -\varepsilon_{ji} \text{ and } \mu_{ij} = -\mu_{ji} \quad (2.55)$$
Therefore, now the constitutional tensors \( \bar{\varepsilon} \) and \( \bar{\mu} \) are not symmetrical tensors. These constitutional tensors cannot be changed or transformed to a diagonal tensor, as in the case of reciprocal media, by the rotation of the co-ordinate system. These constitutional tensors now take the general form of

\[
\bar{\varepsilon} = \begin{bmatrix} \varepsilon_1 & j\varepsilon_4 & j\varepsilon_5 \\ -j\varepsilon_4 & \varepsilon_2 & j\varepsilon_6 \\ -j\varepsilon_5 & -j\varepsilon_6 & \varepsilon_3 \end{bmatrix} \quad \text{and} \quad \bar{\mu} = \begin{bmatrix} \mu_1 & j\mu_4 & j\mu_5 \\ -j\mu_4 & \mu_2 & j\mu_6 \\ -j\mu_5 & -j\mu_6 & \mu_3 \end{bmatrix} \quad (2.56)
\]

Such media is known as “Non-reciprocal Anisotropic Media” or “Gyrotropic Media”. The rotation of the co-ordinate system for non-reciprocal media makes it possible to have the constitutional tensors a simpler form such as

\[
\bar{\varepsilon} = \begin{bmatrix} \varepsilon_1 & j\varepsilon_2 & 0 \\ -j\varepsilon_2 & \varepsilon_3 & 0 \\ 0 & 0 & \varepsilon_3 \end{bmatrix} \quad \text{and} \quad \bar{\mu} = \begin{bmatrix} \mu_1 & j\mu_2 & 0 \\ -j\mu_2 & \mu_3 & 0 \\ 0 & 0 & \mu_3 \end{bmatrix} \quad (2.57)
\]

For non-reciprocal media, this special co-ordinate system is the principle co-ordinate system and the z axis is known as the gyrotropic axis.

### 2.3.5 Maxwell’s Equations in Anisotropic Media

The Maxwell’s equations for electric anisotropic and magnetic anisotropic media are,

<table>
<thead>
<tr>
<th>Electric Anisotropic Media</th>
<th>Magnetic Anisotropic Media</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \nabla \times \vec{E} = -j\omega\bar{\varepsilon}\vec{H} ) \quad (2.58)</td>
<td>( \nabla \times \vec{E} = -j\omega\bar{\mu}.\vec{H} ) \quad (2.62)</td>
</tr>
<tr>
<td>( \nabla \times \vec{H} = -j\omega\bar{\varepsilon}.\vec{E} + \vec{J} ) \quad (2.59)</td>
<td>( \nabla \times \vec{H} = -j\omega\varepsilon\vec{E} + \vec{J} ) \quad (2.63)</td>
</tr>
</tbody>
</table>
As can be seen clearly in the above equations, the electric anisotropic media has the permittivity as the tensor and permeability as a scalar, whereas the magnetic anisotropic media has the permittivity as the scalar and the permeability as a tensor.

2.3.6 Wave Vector and Poynting Vector in Anisotropic Media

As a definition of gradient, we have

\[ \nabla \cdot f = \left[ \frac{\delta}{\delta x} + j \frac{\delta}{\delta y} + k \frac{\delta}{\delta z} \right] f \]  \hspace{1cm} (2.66)

Where, \( f = f_0 e^{-j\vec{k} \cdot \vec{x}} \)

And \( \vec{k} = k_x \hat{i} + k_y \hat{j} + k_z \hat{k} \) is the wave vector, and \( \vec{x} = x \hat{i} + y \hat{j} + z \hat{k} \)

Therefore

\[ \vec{k} \cdot \vec{x} = k_x x + k_y y + k_z z \]  \hspace{1cm} (2.67)

Further operation on equation (2.66) will yield

\[ \nabla \cdot f = f_0 [(-k_x) \hat{i} + (-k_y) \hat{j} + (-k_z) \hat{k}] e^{-j(k_x x + k_y y + k_z z)} \]

\[ = -j f_0 e^{-j\vec{k} \cdot \vec{x}} \]  \hspace{1cm} (2.68)

Comparing equations (2.68) and (2.66) we can see that

\[ \nabla = -j \vec{k} \]  \hspace{1cm} (2.69)

Therefore the Maxwell equation (2.58) can be written as

\[ \vec{k} \times \vec{E} = \omega \vec{B} \quad \text{and} \quad \vec{k} \times \vec{H} = -\omega \vec{D} \]  \hspace{1cm} (2.70)
\[ \mathbf{k} \cdot \mathbf{D} = 0 \quad \text{and} \quad \mathbf{k} \cdot \mathbf{B} = 0 \quad (2.71) \]

It is evident after analyzing the above equations that the wave vector is perpendicular to the plane formed by \( \mathbf{D} \) and \( \mathbf{B} \). This plane is called the DB plane.

The Poynting Vector is given by\(^{16}\)

\[ \mathbf{S} = \frac{1}{2} (\mathbf{E} \times \mathbf{H}) \quad (2.72) \]

Where \( \mathbf{S} \) gives the direction of the power flow. Again we can see that from equation (2.72) \( \mathbf{S} \) is perpendicular to both \( \mathbf{E} \) and \( \mathbf{H} \) and lies in the plane formed by them.

Therefore we can summarize that

\[ \mathbf{k} \perp \mathbf{D}, \quad \mathbf{k} \perp \mathbf{B}, \quad \mathbf{S} \perp \mathbf{E} \quad \text{and} \quad \mathbf{S} \perp \mathbf{H} \]

When \( \mathbf{D} \parallel \mathbf{E} \) and also, \( \mathbf{B} \parallel \mathbf{H} \), the direction of the wave vector and the pointing vector is same. Isotropic media exhibit such behavior. Figure 2.3 shows the ray diagrams in order for simplicity in understanding. In the case when \( \mathbf{D} \) is not parallel to \( \mathbf{E} \), then \( \mathbf{S} \) is also not parallel to \( \mathbf{k} \). The angle between \( \mathbf{D} \) and \( \mathbf{E} \) is equal to that between \( \mathbf{S} \) and \( \mathbf{k} \). Such media is called electric-anisotropic media. In such a media \( \mathbf{B} \parallel \mathbf{H} \) and hence \( \mathbf{D}, \mathbf{E}, \mathbf{S} \) and \( \mathbf{k} \) are coplanar and normal to both \( \mathbf{B} \) and \( \mathbf{H} \). Similarly, in magnetic-anisotropic media \( \mathbf{B} \) is not parallel to \( \mathbf{H} \) and \( \mathbf{S} \) is also not parallel to \( \mathbf{k} \). Therefore \( \mathbf{D} \parallel \mathbf{E} \) and hence \( \mathbf{B}, \mathbf{H}, \mathbf{S} \) and \( \mathbf{k} \) are coplanar and normal to both \( \mathbf{D} \) and \( \mathbf{E} \). It can be concluded from this discussion in an anisotropic media \( \mathbf{S} \) is not necessarily parallel to \( \mathbf{k} \).
2.4 Elements of the Permittivity Tensor

Let the finite uniform dc magnetic field be in z-direction. For finite electric fields, the Newton-Lorentz equation is given as

\[ \text{Eq 2.3 Tree Diagram summarizing different media and their relations} \]

\[ 2.4 \text{ Elements of the Permittivity Tensor} \]
\[
\frac{d\vec{v}}{dt} = -\frac{e}{m} (\vec{E} + \vec{v} \times \vec{B}) \quad (2.73)
\]

Where, \( \vec{v} \) = electron velocity. We can write \( \frac{d}{dt} \) as \( j\omega \). Therefore equation (2.73) becomes

\[
j\omega \vec{v} = -\frac{e}{m} (\vec{E} + \vec{v} \times \vec{B})
\]

\[
=> \quad j\omega (v_x \hat{e}_x + v_y \hat{e}_y + v_z \hat{e}_z) = -\frac{e}{m} [(E_x \hat{e}_x + E_y \hat{e}_y + E_z \hat{e}_z) + (v_x \hat{e}_x + v_y \hat{e}_y + v_z \hat{e}_z) \times (B_0 \hat{e}_z)]
\]

\[
= -\frac{e}{m} [(E_x \hat{e}_x + E_y \hat{e}_y + E_z \hat{e}_z) + (-v_x B_0 \hat{e}_y + v_y B_0 \hat{e}_x)]
\]

\[
= -\frac{e}{m} [\hat{e}_x (E_x + v_y B_0) + \hat{e}_y (E_y - v_x B_0) + \hat{e}_z E_z] \quad (2.74)
\]

Therefore from above equation we can write,

\[
j\omega v_x = -\frac{e}{m} E_x - \frac{e}{m} v_y B_0 \quad (2.75)
\]

\[
j\omega v_y = -\frac{e}{m} E_y + \frac{e}{m} v_x B_0 \quad (2.76)
\]

\[
j\omega v_z = -\frac{e}{m} E_z \quad (2.77)
\]

\[
j\omega v_x = -\frac{e}{m} E_x - \omega_c v_y \quad (2.78)
\]

\[
j\omega v_y = -\frac{e}{m} E_y + \omega_c v_x \quad (2.79)
\]

\[
j\omega v_z = -\frac{e}{m} E_z \quad (2.80)
\]

Where, \( \omega_c = \frac{e}{m} B_0 \), is the angular cyclotron frequency. Using equation (2.79) to substitute the value of \( v_y \) in equation (2.78), we get

\[
v_x = -j\omega \left( \frac{e}{m} \right) E_x + \omega_c \left( \frac{e}{m} \right) E_y \over \omega_c^2 - \omega^2 \quad (2.81)
\]
Similarly now substituting the value of \( v_x \) from equation (2.81) in equation (2.79) we get,

\[
v_y = -\omega_c \left( \frac{e}{m} \right) E_x - j\omega \left( \frac{e}{m} \right) E_y \frac{\omega_c^2 - \omega^2}{\omega^2 - \omega^2}
\]

(2.82)

From equation (2.80) we have

\[
v_z = \frac{j \left( \frac{e}{m} \right) E_z}{\omega}
\]

(2.83)

Now the Charge Density is given by\(^9\)

\[
\mathcal{q} = -\mathcal{q}_0 + \tilde{\mathcal{q}} \quad \text{where} \quad \tilde{\mathcal{q}} = \mathcal{q}_1 e^{j(\omega t - \vec{k} \cdot \vec{x})}
\]

Where \( \tilde{\mathcal{q}} \) is the a.c. component and \( \mathcal{q}_0 \) is the d.c. component. It is assumed that the d.c. component is much more greater than the a.c. component, i.e. \( \mathcal{q}_0 \gg \tilde{\mathcal{q}} \), so that the cross products of a.c. components can be neglected. Current density is given by

\[
\vec{j} = \mathcal{q} \vec{v} = (-\mathcal{q}_0 + \tilde{\mathcal{q}}) \vec{v}
\]

\[
\approx -\mathcal{q}_0 \vec{v}
\]

(2.84)

Using equation (2.84) in equations (2.81), (2.82) and (2.83) we get,

\[
J_x = \frac{j\omega \mathcal{q}_0 \left( \frac{e}{m} \right) E_x - \omega_c \mathcal{q}_0 \left( \frac{e}{m} \right) E_y}{\omega_c^2 - \omega^2}
\]

(2.85)

\[
J_y = \frac{\omega_c \mathcal{q}_0 \left( \frac{e}{m} \right) E_x + j\omega \mathcal{q}_0 \left( \frac{e}{m} \right) E_y}{\omega_c^2 - \omega^2}
\]

(2.86)

\[
J_z = \frac{-j\mathcal{q}_0 \left( \frac{e}{m} \right) E_z}{\omega}
\]

(2.87)
Multiplying and dividing the right hand sides of equations (2.85), (2.86) and (2.87) by $\varepsilon_0$ we get,

\[
J_x = \frac{j\omega\varepsilon_0\omega_p^2 E_x - \omega_c\varepsilon_0\omega_p^2 E_y}{\omega_c^2 - \omega^2}
\]

\[
J_y = \frac{\omega_c\varepsilon_0\omega_p^2 E_x + j\omega\varepsilon_0\omega_p^2 E_y}{\omega_c^2 - \omega^2}
\]

\[
J_z = \frac{-j\varepsilon_0\omega_p^2 E_z}{\omega}
\]

Where, $\omega_p = \sqrt{\frac{e^2}{m}\left(\frac{\varepsilon_0}{\varepsilon_0}\right)}$ which is the angular plasma frequency\textsuperscript{16}.

Let us write the Maxwell’s equation for the curl of $\vec{H}$.

\[
\vec{\nabla} \times \vec{H} = j\omega\varepsilon_0 \vec{E} + \vec{j} = j\omega\varepsilon_0 \vec{E} = j\omega \vec{D}
\]

\[
\Rightarrow \quad \vec{D} = \varepsilon_0 \vec{E} - \frac{j}{\omega} \vec{j}
\]

Decomposing equation (2.91) into its three components respectively we get,

\[
D_{x,y,z} = \varepsilon_0 E_{x,y,z} - \frac{j}{\omega} J_{x,y,z}
\]

Substituting equations (2.88), (2.89) and (2.90) in equation (2.92) we get,

\[
D_x = \varepsilon_0 \left(1 + \frac{\omega_p^2}{\omega_c^2 - \omega^2}\right) E_x + j\varepsilon_0 \left(\frac{\omega_p^2}{\omega_c^2 - \omega^2}\right) E_y
\]

\[
D_y = -j\varepsilon_0 \left(\frac{\omega_p^2}{\omega_c^2 - \omega^2}\right) E_x + \varepsilon_0 \left(1 + \frac{\omega_p^2}{\omega_c^2 - \omega^2}\right) E_y
\]

\[
D_z = \varepsilon_0 \left(1 - \frac{\omega_p^2}{\omega_c^2 - \omega^2}\right) E_z
\]
From equations (2.93), (2.94) and (2.95) it is evident that

\[
\ddot{\varepsilon} = \begin{bmatrix}
\varepsilon_1 & j\varepsilon_2 & 0 \\
-j\varepsilon_2 & \varepsilon_1 & 0 \\
0 & 0 & \varepsilon_3
\end{bmatrix}
\]

\[
\begin{bmatrix}
\varepsilon_0 \left(1 + \frac{\omega_p^2}{\omega_c^2 - \omega^2}\right) & j\varepsilon_0 \left(\frac{\omega_p^2}{\omega_c^2 - \omega^2}\right) & 0 \\
-j\varepsilon_0 \left(\frac{\omega_p^2}{\omega_c^2 - \omega^2}\right) & \varepsilon_0 \left(1 + \frac{\omega_p^2}{\omega_c^2 - \omega^2}\right) & 0 \\
0 & 0 & \varepsilon_0 \left(1 - \frac{\omega_p^2}{\omega^2}\right)
\end{bmatrix}
\]

(2.96)

Where,

\[
\varepsilon_1 = \varepsilon_0 \left(1 + \frac{\omega_p^2}{\omega_c^2 - \omega^2}\right)
\]

\[
\varepsilon_2 = \varepsilon_0 \left(\frac{\omega_p^2}{\omega_c^2 - \omega^2}\right)
\]

\[
\varepsilon_3 = \varepsilon_0 \left(1 - \frac{\omega_p^2}{\omega^2}\right)
\]
Chapter 3

The Effective Medium Theory

3.1 Response of Dielectric Materials

Dielectrics or dielectric materials are materials which do not conduct electricity. But the most important property of dielectrics is their capability to store electrical energy rather than not conducting it. This property of dielectric materials is measured by the dielectric constant or the permittivity. Actually, the permittivity is far more a higher level invention to describe approximately the electric response of matter. There is a large amount of study and physics involved in this calculation.

Matter is although considered to neutral in average in terms of its electric character, but is composed of charged elements at the atomic level. It consists of negatively charged electrons orbiting around a positively charged nucleus. The ideal dielectric does not permit the free flow of these electrons by the applied electric field. Instead, the force exerted by the applied electric field displaces the electrons from their equilibrium position. This situation also includes a restoring force which tries to restrict the electrons to their undisturbed position. The resultant force from these two forces decides the final static picture, which also determines the net displacement of positive
charges in the direction of the applied electric field and that of negatively charged electrons in the opposite direction. This separation between the positively and negatively charged particles is equivalent to a dipole moment as shown in the Figure 3.1. Also another measure is achieved which is the polarizability which depends on the dipole moment and the applied electric field.

![Figure 3.1 Dipole moment is proportional to the Electric Field](image)

$\vec{p} = \alpha \vec{E}$

Where, $\vec{p}$ = Dipole Moment,

$\vec{E}$ = Electric Field,

There can be different types of polarizations since the charge distribution in matter is of different types.

In the isotropic case, the response of matter to electrical excitation is linear and spatially local. This phenomenon takes place when the polarizable quantities in matter such as the atom is exposed to the applied electric field and the dipole moment is established in such a manner that it is linearly dependent on the electric field given by,

$\vec{p} = \alpha \vec{E}$

(3.1)
\[ \alpha = \text{Polarizability}. \]

The above situation is quite simple and in practical cases, there are materials which exhibit different properties when exposed to similar kind of arrangement.

As discussed in the previous chapter, anisotropy brings in the need for a dependency in direction, for the dielectric response with the electric field. Therefore, now we cannot express the dipole moment as in equation (3.1) as a product of the electric field and the scalar polarizability. Even if anisotropy is assumed the linear form of the above equation can be kept by replacing the scalar polarizability with a dyadic or a tensor polarizability. Hence the components of the dipole moment have to be calculated through matrix expansion of the polarizability dyadic. An example for the anisotropy to arise can be from geometrical effects. These geometrical effects in micro-structures cause the charge to get collected much easily in some directions and polarization can get difficult if the applied direction of the electric field is in some other direction.

The dipole moment is one of the main contributors to the electrostatic energy, when the matter is macroscopically neutral. Therefore it is evident that in neutral materials and when a homogeneous electric field is applied, the energy density is due to the dipole moments. However due to more random and complex real materials we cannot conclude the above statement for higher order multi-poles.
3.2 Fundamentals of the Effective Medium Theory

It is now time to start closing down to the concepts effective medium theory while considering heterogeneous media. We will start with the explanation of the simplest model of a dielectric mixture and then move on to more complexities and generalizations to the formulae and theories. We will start by embedding isotropic dielectric spheres in an environment which is also isotropic and dielectric as shown in Figure 3.2. The embedded isotropic and dielectric spheres are also known as “inclusions” and are often referred to as the “guests”. The isotropic dielectric environment is also popularly referred to as the “host” or the “matrix”.

![Figure 3.2 Simplest form of Dielectric Mixture. Dielectric Spheres are the “Guests” or the “Inclusions” in the Dielectric Background called “Host” or “Matrix”](image)

This mixture can be viewed macroscopically so that only the averages are taken into consideration, and therefore a macroscopic permittivity can be associated with the mixture. This macroscopic permittivity or also known as the effective permittivity can be
calculated if both the permittivities of the embedded inclusions and the dielectric host environment are known. Calculation of this effective permittivity is far from trivial and an appropriate formula needs to derived, which takes into account all possible factors affecting the calculation.

We will derive the basic rule for mixing of such above mentioned permittivities, which is known as the “Maxwell Garnett Formula”. We will then generalize this basic mixing rule for more complex geometries. The advantage of deriving the basic formula first is that the formula retains its mathematical form after generalizations.

### 3.3 Maxwell Garnett Formula for Dielectric Spherical Inclusions in a Dielectric Host

The Clausius-Mossotti relation also known as the Lorentz-Lorentz relation is mostly a student’s only connection with local field effects and the fundamental theory of the dielectric response of matter. The main step of the derivation is replacing the microscopic model, which consists of a simple cubic lattice of polarizable points, with a dielectrically equivalent homogeneous solid. To acquaint us with the idea of a local field, we use an imaginary cavity to express the microscopic polarizability of a lattice point as a function of the macroscopic observable, the dielectric function. Also a very important conclusion is reached making us realize that intuitively it is expected that the neighboring dipoles will contribute most strongly to the local field but actually contribute nothing.
Some problems may arise due to the fact that if the same formalism is applied to low symmetry configurations like some linear molecules, for which the assumption of a spherical cavity may not hold true.

There is a very simple reason for which this kind of confusion occurs. Usually the case in electrodynamics which is also evident in thermodynamics is that the length scales of laboratory probes are usually far larger than the length scales that describe a system on the microscopic or in most cases the atomic level, which is the level at which these interactions actually occur. Therefore laboratory probes actually measure the average of macroscopic responses. In this manner we will have to calculate macroscopic dielectric function in terms of the microscopic parameters. This calculation generally consists of involvement of two distinct steps. One of the steps is to calculate or compute the microscopic problem as accurately as possible. The second step consists of taking suitable averages of the microscopic solution from the first step to compute the macroscopic quantity\(^{18}\).

It was long ago realized by researchers and thermodynamicists the usefulness of trying to put in use the above prescription. The first step in the prescription incorporated the implementation of a large amount of equations, for example for each molecule of a gas we would require six such equations for the microscopic parameters. Therefore the importance of the second step was emphasized which first defined the macroscopic averages also known as observable quantities such as pressure, temperature or entropy and then establishing dependencies amongst them with the microscopic or unobservable parameters. Such dependencies among observable or macroscopic averages are also noticed in Maxwell’s equations which stress on the relationships between the
electromagnetic fields $\vec{E}$, $\vec{D}$, $\vec{H}$ and $\vec{B}$, as shown by the equations (2.8) – (2.11) and (2.58) – (2.65). Especially the relations $\vec{D} = \varepsilon \vec{E}$ and $\vec{B} = \mu \vec{H}$ are of prime importance because the dielectric function $\varepsilon$ and the permeability $\mu$ enter through the constitutive relations. These parameters represent the microscopic reaction of a physical system to an external field entirely. This approach is quite adequate for the purpose in electrodynamics. But if one wishes or needs to know the origin of dielectric response functions, then the microscopic aspects cannot be ignored.

One of the most basic approaches in thermodynamics which give stress on the macroscopic average is the treatment of simple cubic lattice in standard textbooks. This treatment considers the simple cubic lattice of point dipoles an ideal model of the local field problem. One needs to start by considering the effective permittivity or the dielectric function of a homogeneous solid and solve the microscopic problem only enough to establish a connection between the dielectric function and the polarizability of its microscopic constituents respectively.

### 3.3.1 The Basic Model

We will go through the standard treatment for the spherical cavity assumption. We will consider the arrayed sites $r = R_i$ at which points the polarizability is to be calculated. This simple cubic lattice is assumed to have its center at the co-ordinate origin. The Figure 3.3 gives us much better idea of the model and the scenario.
3.3.2 The Field at the Origin

Let us assume the material to be spatially homogeneous. Therefore a uniform applied field will produce a dipole moment per unit volume which are related to each other by the expressions\textsuperscript{19}

\[
\vec{D} = \epsilon_{eff} \vec{E} \tag{3.2}
\]

\[
= \vec{E} + 4\pi \vec{P} \tag{3.3}
\]
Where, $\epsilon_{eff} = \text{Effective Dielectric Permittivity or the dielectric function of the spatially homogeneous material,}$

$\vec{E} = \text{Uniform Applied Field,}$

$\vec{P} = \text{Dipole Moment per unit Volume.}$

It is of our utmost necessity that we relate the polarizability of the dipole at the coordinate origin with the dielectric function. It is therefore important to consider factors such as the discrete nature of the lattice at the origin as well as the dipoles neighboring the origin. The approximation of assuming a homogeneous material also holds true for the case when these neighboring dipoles are at large enough distances from the dipole at the origin.

Figure 3.4 Spherical Boundary showing the separation in the Lattice between the Macroscopic and Microscopic Phases. $\vec{E}_{Loc}$ is the Field at the center of the Cavity.
Let us assume the lattice constant of the lattice to be \(\alpha\) and draw a spherical boundary with the radius as the lattice constant. This spherical boundary will divide the lattice into two phases which are the homogeneous (macroscopic) and the discrete (microscopic) phases. This discussion can be more easily understood from Figure 3.4.

Hence it is quite obvious that the field at the center of the cavity is equal to the sum of the uniform applied field and the contribution from the polarization of the uniform region outside the boundary and also let us not forget, the contributions given by the neighboring dipoles in the cavity. The integral over the boundary charge can be done explicitly\(^\text{20,21}\),

\[
\vec{E}_{loc} = \vec{E} + \frac{4\pi}{3} \vec{P} + \sum_i \vec{E}(\vec{p}, -\vec{R}_i) \tag{3.4}
\]

Where, \(\vec{E}_{loc}\) = The field at the origin of the cavity,

\(\vec{P}\) = Polarization or Dipole moment per unit volume,

\(\vec{E}(p, r)\) = The electric field at \(\vec{r}\) of a dipole \(\vec{p}\) located at the origin.

Expression (3.4) is restricted to those \(\vec{R}_i\) within the cavity.

3.3.2.1 The Electric field at each Dipole

The electrostatic potential is given by\(^\text{20}\),

\[
\Phi(\vec{r}) = \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d^3r' \tag{3.5}
\]

Using Taylor’s expansion formula we have,

\[
\frac{1}{|\vec{r} - \vec{r}'|} = \frac{1}{r} + \frac{\vec{r}' \cdot \vec{r}}{r^3} \tag{3.6}
\]
Substituting equation (3.6) in (3.7) we have,

\[ \Phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \left[ \int \frac{1}{r} \rho(\vec{r}') d^3r' + \frac{\vec{r}}{r^3} \cdot \int \rho(\vec{r}') \vec{r}' d^3r' \right] \]

\[ = \frac{1}{4\pi\varepsilon_0} \left[ \frac{Q}{r} + \frac{\vec{r} \cdot \vec{p}}{r^3} \right] \quad (3.7) \]

Where, \( Q = \) Net charge on the system = \( \int \rho(\vec{r}') d^3r' \),

\[ \vec{p} = \) Dipole moment = \( \int \rho(\vec{r}') \vec{r}' d^3r' \).

Let us assume that the net charge on the system \( Q \) be zero.

Therefore,

\[ \Phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \left[ \frac{\vec{r} \cdot \vec{p}}{r^3} \right] \quad (3.8) \]

Also, we have the Electric field given by\(^{15}\),

\[ \vec{E} = -\nabla \Phi \quad (3.9) \]

\[ = -\nabla \left[ \frac{1}{4\pi\varepsilon_0} \left( \frac{\vec{r} \cdot \vec{p}}{r^3} \right) \right] \]

\[ = -\frac{1}{4\pi\varepsilon_0} \nabla \left( \frac{\vec{r} \cdot \vec{p}}{r^3} \right) \quad (3.10) \]

Now,

\[ \nabla f = \vec{n}_r \frac{\partial f}{\partial r} + \vec{n}_\theta \frac{\partial f}{\partial \theta} + \vec{n}_\phi \frac{\partial f}{\partial \phi} \quad (3.11) \]

\[ \vec{r} \cdot \vec{p} = |\vec{r}| |\vec{p}| \cos \theta \]

\[ = rp \cos \theta \quad (3.12) \]

Substituting equations (3.11) and (3.12) in equation (3.10) we get,

\[ \vec{E} = -\frac{1}{4\pi\varepsilon_0} \nabla \left( \frac{p \cos \theta}{r^2} \right) \]
We can write

\[
\vec{\rho} = \vec{\rho} \cdot \vec{n}_r \vec{n}_r + \vec{\rho} \cdot \vec{n}_\theta \vec{n}_\theta
\]

\[
= p \cos \theta \vec{n}_r - p \sin \theta \vec{n}_\theta
\]  

(3.14)

Substituting equation (3.14) in (3.13) we get

\[
= \frac{1}{4\pi \epsilon_0 r^3} [\vec{n}_r 2p \cos \theta \vec{n}_\theta r^3 - \vec{n}_\theta p \sin \theta]
\]

\[
= \frac{1}{4\pi \epsilon_0 r^3} [3(\vec{\rho} \cdot \vec{n}_r) \vec{n}_r - \vec{\rho}]
\]

(3.15)

Expression (3.15) is Gaussian units. Converting it into M.K.S. units we get

\[
\vec{E} = \frac{1}{4\pi \epsilon_0} \frac{3(\vec{\rho} \cdot \vec{r}) \vec{r} - \vec{\rho}}{r^3}
\]  

(3.16)

If we calculate the sum then the contributions from all dipoles on a given shell

\[|\vec{R}_i|\] cancel identically for the simple cubic lattice.

Therefore equation (3.4) becomes,

\[
\vec{E}_{loc} = \vec{E} + \frac{4\pi}{3} \vec{\rho}
\]  

(3.17)
3.3.3 The Internal Field and the Dipole Moment in a Dielectric

Our basic aim is to calculate the electric field inside a sphere of homogeneous dielectric material when it is placed in an uniform electric field as shown in Figure 3.5 below.

Let us begin with the general solution of linear combination of separable solutions given by equation below and then we will move on to the boundary conditions required.

\[
\Phi(r, \theta) = \sum_{l=0}^{\infty} \left( A_l r^l + \frac{B_l}{r^{l+1}} \right) P_l(\cos \theta)
\]  

(3.18)

Where, \( A \) and \( B \) are two arbitrary constants to be expected in a second order differential equation.

\( P_l(x) = \) Legendre Polynomial where,
\[ P_1(x) = 1, \]
\[ P_2(x) = x, \]
\[ P_3(x) = (3x^2 - 1)/2. \]

If we assume that at the interface there are absolutely no surface charges, we can use the boundary condition

\[ \vec{D}_{\text{in}} = \vec{D}_{\text{out}} \]
\[ \epsilon \vec{E}_{\text{in}} = \epsilon_0 \vec{E}_{\text{out}} \]
\[ \epsilon \frac{\partial \Phi_{\text{in}}}{\partial r} = \epsilon_0 \frac{\partial \Phi_{\text{out}}}{\partial r} \]  \hspace{1cm} (3.19.1)

Where, \( \epsilon = \) permittivity of dielectric sphere,

\( \epsilon_0 = \) permittivity of medium outside the sphere which is air.

Another boundary condition arises from the tangential component of the electric field given by,

\[ \vec{E}_{\text{in}} = \vec{E}_{\text{out}} \]
\[ \Phi_{\text{in}} = \Phi_{\text{out}} \]  \hspace{1cm} (3.19.2)

As we move away from the dielectric sphere the electric field \( \vec{E}_{\text{out}} = \vec{E} = \vec{E} \hat{z} \) goes on reducing. Therefore the potential outside the dielectric sphere also goes on decreasing and is given by,

\[ \Phi_{\text{out}} \to -\epsilon_0 r \cos \theta \]  \hspace{1cm} (3.19.3)

The electric field \( \vec{E}_{\text{out}} = \vec{E} \hat{z} \) has been chosen by us in the direction parallel to the z axis for a specific reason. It is possible choose the “principal axes”, which in our case is the z axes, in such a way that the off diagonal terms of the tensor become zero. Therefore
the orientation of the axes is very crucial in deciding all the elements in the tensor. Now in equation (3.18), for the potential inside the dielectric sphere we have $B = 0$.

$$\Phi_{\text{in}}(r, \theta) = \sum_{l=0}^{\infty} A_l r^l P_l(\cos \theta)$$  \hspace{1cm} (3.20)

And for outside the sphere we have $A = 0$

$$\Phi_{\text{out}}(r, \theta) = \sum_{l=0}^{\infty} \frac{B_l}{r^{l+1}} P_l(\cos \theta)$$  \hspace{1cm} (3.21)

Substituting the condition given by equation (3.19.3) in equation (3.21) we get

$$\Phi_{\text{out}}(r, \theta) = \left[ \sum_{l=0}^{\infty} \frac{B_l}{r^{l+1}} P_l(\cos \theta) \right] - E_0 r \cos \theta$$  \hspace{1cm} (3.22)

Applying boundary condition from equation (3.19.2) to equations (3.20) and (3.22), we get

$$\sum_{l=0}^{\infty} A_l r^l P_l(\cos \theta) = \left[ \sum_{l=0}^{\infty} \frac{B_l}{r^{l+1}} P_l(\cos \theta) \right] - E_0 r \cos \theta$$

For $l \neq 1$ we have $P_l(\cos \theta) = \cos \theta$. Substituting in above equation we have

$$A_l r^l = \frac{B_l}{r^{l+1}} - E_0 r$$

For $l = 1$

$$A_1 r = \frac{B_1}{r^2} - E_0 r$$  \hspace{1cm} (3.23)

Now applying boundary condition from equation (3.19.1) in equations (3.20) and (3.22) we get,

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\[
\epsilon \frac{\partial}{\partial r} \left[ \sum_{l=0}^{\infty} A_l r^l P_l(\cos \theta) \right] = \epsilon_0 \frac{\partial}{\partial r} \left\{ \sum_{l=0}^{\infty} \frac{B_l}{r^{l+1}} P_l(\cos \theta) \right\} - E_0 r \cos \theta
\]

\[
\epsilon \sum_{l=0}^{\infty} l A_l r^{l-1} P_l(\cos \theta) = \epsilon_0 \left[ \sum_{l=0}^{\infty} \frac{-B_l(l+1)}{r^{l+2}} P_l(\cos \theta) \right] - E_0 \cos \theta
\]

Again for \( l \neq 1 \) we have

\[
\epsilon l A_l r^{l-1} = \epsilon_0 \left[ \frac{-B_l(l+1)}{r^{l+2}} - E_0 \right]
\]

For \( l = 1 \)

\[
\epsilon A_1 = \epsilon_0 \left[ \frac{-2B_1}{r^3} - E_0 \right]
\]
(3.24)

Substituting the value of \( A_1 \) from equation (3.23) in equation (3.24) and solving for \( B_1 \) we get

\[
B_1 = \left[ \frac{\epsilon - \epsilon_0}{\epsilon + 2\epsilon_0} \right] r^3 E_0
\]

\[
B_1 = \left[ \frac{\epsilon_r - 1}{\epsilon_r + 2} \right] r^3 E_0
\]
(3.25.1)

Similarly,

\[
A_1 = \left[ -\frac{3}{\epsilon_r + 2} \right] E_0
\]
(3.25.2)

From equation (3.20) and for \( l = 1 \) we have

\[
\Phi_{in}(r, \theta) = A_1 r P_1(\cos \theta)
\]

\[
= \left[ -\frac{3}{\epsilon_r + 2} \right] E_0 r \cos \theta
\]

Converting the above equation into the xyz co-ordinate system we get,

\[
\Phi_{in}(r, \theta) = \left[ -\frac{3}{\epsilon_r + 2} \right] E_0 z
\]
(3.26)
Therefore we can now calculate the electric field inside the dielectric sphere from the well known relation,

\[ \vec{E}_{\text{in}} = -\nabla \Phi_{\text{in}} \]

\[ \vec{E}_{\text{in}} = \frac{3}{\varepsilon_r + 2} \vec{E}_0 = \frac{3}{\varepsilon_r + 2} \vec{E} \quad (3.27) \]

Similarly,

\[ \Phi_{\text{out}}(r, \theta) = \left[ \frac{\varepsilon_r - 1}{\varepsilon_r + 2} \right] \frac{r^3}{r^2} E_0 \cos \theta - E_0 r \cos \theta \]

Now outside the sphere the potential is equal to the applied field and the field of an electric dipole at the origin with dipole moment,

\[ \vec{p} = \left[ \frac{\varepsilon_r - 1}{\varepsilon_r + 2} \right] r^3 \vec{E}_0 = \left[ \frac{\varepsilon_r - 1}{\varepsilon_r + 2} \right] r^3 \vec{E} \quad (3.28) \]

### 3.3.4 The Effective Medium Theory

In the above section we showed the relation between the internal electric field and the external electric field for one dielectric sphere. Our interests require more than one or in fact any number of such dielectric spheres be embedded in another medium which in our case up till now has been air. If we have many such small metallic or ferromagnetic spheres in surrounding space we have to also consider the effect due to the regular field \( \vec{E} \) and also the forces due to the nearby or neighboring spheres. Therefore now because we have more than one dielectric sphere in the surrounding and we also have to incorporate the effect of nearby spheres equation (3.28) will change to\textsuperscript{21,22,23}
\[ p = \left( \frac{\varepsilon_r - 1}{\varepsilon_r + 2} \right) r^3 \vec{E}_{loc} \]  

(3.29)

Where the \( \vec{E}_{loc} \) is given by equation (3.17) and the theory of replacing \( \vec{E} \) with \( \vec{E}_{loc} \) to incorporate the effects of nearby spheres is explained by the theory given to derive \( \vec{E}_{loc} \).

Now if there are \( n \) spheres or inclusions per unit volume we have

\[ \vec{p} = n \vec{p} \]  

(3.30)

Where, \( n = 1/a^3 \) and \( a \) is the lattice constant.

Now let us substitute equation (3.30) and equation (3.29) in equation (3.17)

\[ \vec{E}_{loc} = \vec{E} + \frac{4\pi}{3} n \left[ \frac{\varepsilon_r - 1}{\varepsilon_r + 2} \right] r^3 \vec{E}_{loc} \]

Again replacing the value of \( \vec{E}_{loc} \) from the above equation in equation (3.29) and then the polarization or dipole moment per unit volume in equation (3.30) becomes,

\[ \vec{p} = n \left[ \frac{\varepsilon_r - 1}{\varepsilon_r + 2} \right] r^3 \vec{E} \]  

(3.32)

Now from the well known relation we have

\[ \vec{D} = \varepsilon_r \vec{E} \]

\[ = (1 + 4\pi \chi_e) \vec{E} \]

\[ = \vec{E} + 4\pi \vec{P} \]  

(3.33)

\[ \therefore \epsilon_r \vec{E} = \vec{E} + 4\pi \vec{P} \]

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Now substituting equation (3.32) in equation (3.34)

\[ \epsilon_{r'} = 1 + 4\pi n \frac{\left[ \frac{\epsilon_r - 1}{\epsilon_r + 2} \right] r^3 \tilde{E}^{-1}}{1 - \frac{4\pi}{3} n \left[ \frac{\epsilon_r - 1}{\epsilon_r + 2} \right] r^3} \]

Now the volume of a sphere is given by \( V = 4\pi r^3 / 3 \). Therefore \( f = nV \) is the volume fraction of the inclusions or the spheres. Let us substitute this in the above equation. We are allowed to this because \( r \) is nothing but the radius of the spheres. If there were spheres of different radii they would have been treated as different types of inclusions with the spheres having the same radius being treated as of one type. So far, in our discussion we have not yet extended our approach to different types of inclusions. We will deal with this type of situation a little later.

\[ \epsilon_{r'} = 1 + \frac{3f \left[ \frac{\epsilon_r - 1}{\epsilon_r + 2} \right]}{1 - f \left[ \frac{\epsilon_r - 1}{\epsilon_r + 2} \right]} \]  

(3.35)

We have to realize that so far in our derivation we have considered that the dielectric spheres are embedded in air. So as per our previous discussions the host medium can be considered to be air with permittivity \( \epsilon_0 \). Now if we want to embed the dielectric spheres in another dielectric material having permittivity \( \epsilon_h \) and if the dielectric spheres have permittivity \( \epsilon_1 \) then it follows that now \( \epsilon_r = \epsilon_1 / \epsilon_h \) and therefore \( \epsilon_{r'} = \epsilon_{eff} / \epsilon_h \), where \( \epsilon_{eff} \) becomes the effective permittivity of the material which is the combination of the permittivities of the dielectric inclusions and the host material.

Therefore equation (3.35) becomes
Equation (3.35) can be used to calculate the effective permittivity of a mixture, where the host and the inclusion permittivities are known, the volume fraction of the inclusions are known. The above formula is restricted for the calculation of the effective permittivity only when the embedded dielectric inclusions in the host medium are spherical. The above formula has also other popular forms when on simplifying gives the following result,

$$
\frac{\varepsilon_{\text{eff}} - \varepsilon_h}{\varepsilon_{\text{eff}} + 2\varepsilon_h} = f \frac{\varepsilon_1 - \varepsilon_h}{\varepsilon_1 + 2\varepsilon_h}
$$

(3.36)

This equation is well known as Maxwell Garnett Effective Medium expression. In the next chapters, our attempt will be to generalize the above equation for multiple types of inclusions. There will also be discussions and implementations of other factors on the above equation which greatly influence the accuracy of the effective permittivity.
Chapter 4
Bruggeman’s Effective Medium Theory
and
Depolarization Factors

4.1 Maxwell Garnett Formula for Multiple Types of Spherical Inclusions

In this section we will attempt to derive the Maxwell Garnett formula for multiple types of inclusions embedded in the host medium and also try to generalize it. We will see the changes we have to incorporate in the expression for internal field of a dielectric and also the dipole moment. Therefore it is also obvious that we will have to take into account the polarization caused by both such types of inclusions and introduce them into the expressions that we require to calculate the effective permittivity. This approach is fairly simple and straightforward, but very meaningful, if one has understood all the concepts required to derive the Maxwell Garnett expression in the previous chapter. The inclusions will still remain spherical but their sizes will be treated of different types. We will first start with just two inclusions and then generalize it for any number.
4.1.1 The Internal Field and the Dipole Moment in a Dielectric of each Inclusion

Let us assume that now we have two spherical inclusions placed in a uniform electric field and that both the dielectric spheres are of different sizes as shown in Figure 4.1 below.

\[ E_{in1} = \frac{3}{\varepsilon_r + 2} E \]  \hspace{1cm} (4.1.1) \\
\[ E_{in2} = \frac{3}{\varepsilon_{r2} + 2} E \]  \hspace{1cm} (4.1.2)

Figure 4.1 Two Dielectric Spheres of different types placed in an Uniform Electric Field

The two dielectric spheres will have two different internal electric fields produced in them given by,
Where, $\vec{E}_{in1}$ = Internal Electric Field in Dielectric Sphere 1,

$\vec{E}_{in2}$ = Internal Electric Field in Dielectric Sphere 2,

$\epsilon_{r1} = \epsilon_1/\epsilon_h$ = Permittivity of Dielectric Sphere 1,

$\epsilon_{r2} = \epsilon_2/\epsilon_h$ = Permittivity of Dielectric Sphere 2.

Consequently the dipole moment of each spherical dielectric inclusion will be,

$$\vec{p}_1 = \left[\frac{\epsilon_{r1} - 1}{\epsilon_{r1} + 2}\right] r_1^3 \vec{E}$$

(4.2.1)

$$\vec{p}_2 = \left[\frac{\epsilon_{r2} - 1}{\epsilon_{r2} + 2}\right] r_2^3 \vec{E}$$

(4.2.2)

Where, $\vec{p}_1$ = Dipole Moment of Spherical Dielectric Inclusion 1,

$\vec{p}_2$ = Dipole Moment of Spherical Dielectric Inclusion 2.

### 4.1.2 The Polarization in each Dielectric Sphere

If we also consider the number of each kind or type of inclusions as shown in the Figure 4.2, then the polarization

$$\vec{P}_1 = n_1 \vec{p}_1$$

(4.3.1)

$$\vec{P}_2 = n_2 \vec{p}_2$$

(4.3.2)

Where, $\vec{P}_1$ and $\vec{P}_2$ is the Polarization caused by Dielectric Spheres of type 1 and 2,

$n_1$ and $n_2$ are the number of dielectric spheres of each kinds, 1 and 2.
Therefore, equations (4.2.1) and (4.2.2) we get,

\[
\vec{p}_1 = n_1 \left[ \frac{\varepsilon_{r1} - 1}{\varepsilon_{r1} + 2} \right] r_1^3 \vec{E} 
\]

\[
\vec{p}_2 = n_2 \left[ \frac{\varepsilon_{r2} - 1}{\varepsilon_{r2} + 2} \right] r_2^3 \vec{E} 
\]

4.1.3 The Effective Medium Theory

Like we did in the previous chapter, we need to incorporate the effects caused by just not the external electric fields but also the polarization caused by the nearby dipoles. Only this will not be enough, polarization from nearby dielectric spheres will also have to taken account of.

Therefore the equations (4.4.1) and (4.4.2) will have to incorporate the field at the center which already takes care of such an effect.

\[
\vec{p}_1 = n_1 \left[ \frac{\varepsilon_{r1} - 1}{\varepsilon_{r1} + 2} \right] r_1^3 \vec{E}_{loc} 
\]
Now for two dielectric spheres the equation (3.17) will become

$$\vec{E}_{loc} = \vec{E} + \frac{4\pi}{3} \vec{P}_1 + \frac{4\pi}{3} \vec{P}_2$$  \hspace{1cm} (4.6)

By simplification we have,

$$\vec{E}_{loc} = \frac{\vec{E}}{1 - \left[ \frac{4\pi}{3} \frac{n_1}{n_1} \frac{\left( \frac{\varepsilon_{r1} - 1}{\varepsilon_{r1} + 2} \right)}{r_1^3} + \frac{4\pi}{3} \frac{n_2}{n_2} \frac{\left( \frac{\varepsilon_{r2} - 1}{\varepsilon_{r2} + 2} \right)}{r_2^3} \right]}$$  \hspace{1cm} (4.7)

Using equation (4.7) in equations (4.5.1) and equation (4.5.2) we have

$$\vec{P}_1 = \frac{n_1 \left( \frac{\varepsilon_{r1} - 1}{\varepsilon_{r1} + 2} \right) r_1^3 \vec{E}}{1 - \left[ \frac{4\pi}{3} \frac{n_1}{n_1} \frac{\left( \frac{\varepsilon_{r1} - 1}{\varepsilon_{r1} + 2} \right)}{r_1^3} + \frac{4\pi}{3} \frac{n_2}{n_2} \frac{\left( \frac{\varepsilon_{r2} - 1}{\varepsilon_{r2} + 2} \right)}{r_2^3} \right]}$$  \hspace{1cm} (4.8.1)

$$\vec{P}_2 = \frac{n_2 \left( \frac{\varepsilon_{r2} - 1}{\varepsilon_{r2} + 2} \right) r_2^3 \vec{E}}{1 - \left[ \frac{4\pi}{3} \frac{n_1}{n_1} \frac{\left( \frac{\varepsilon_{r1} - 1}{\varepsilon_{r1} + 2} \right)}{r_1^3} + \frac{4\pi}{3} \frac{n_2}{n_2} \frac{\left( \frac{\varepsilon_{r2} - 1}{\varepsilon_{r2} + 2} \right)}{r_2^3} \right]}$$  \hspace{1cm} (4.8.2)

Now equation (3.34), for two types of inclusions will become

$$\varepsilon_{r'} = 1 + 4\pi \left[ \vec{P}_1 + \vec{P}_2 \right] \cdot \vec{E}^{-1}$$  \hspace{1cm} (4.9)

From equation (4.8.1) and (4.8.2) we have

$$\varepsilon_{r'} = 1 + \frac{3f_1 \left( \frac{\varepsilon_{r1} - 1}{\varepsilon_{r1} + 2} \right) + 3f_2 \left( \frac{\varepsilon_{r2} - 1}{\varepsilon_{r2} + 2} \right)}{1 - \left[ f_1 \left( \frac{\varepsilon_{r1} - 1}{\varepsilon_{r1} + 2} \right) + f_2 \left( \frac{\varepsilon_{r2} - 1}{\varepsilon_{r2} + 2} \right) \right]}$$

Where, $f_1$ and $f_2$ are the Volume Fractions of inclusion type 1 and 2.

Now we can rewrite the above equation as
This equations looks like this because \( \epsilon_r' = \frac{\epsilon_{eff}}{\epsilon_h} \) and \( \epsilon_{r1} = \epsilon_1/\epsilon_h \) and \( \epsilon_{r2} = \epsilon_2/\epsilon_h \). The above equation can also be written as

\[
\frac{\epsilon_{eff} - \epsilon_h}{\epsilon_{eff} + 2\epsilon_h} = f_1 \frac{\epsilon_1 - \epsilon_h}{\epsilon_1 + 2\epsilon_h} + f_2 \frac{\epsilon_2 - \epsilon_h}{\epsilon_2 + 2\epsilon_h}
\] (4.11)

4.1.4 Generalization of the Maxwell Garnett Equation for Multiple Types of Spherical Inclusions

It is quite obvious how the generalization of the Maxwell Garnett Equation comes about. It is very important for us to remember that this generalization only applies to spheres as inclusions.

\[
\epsilon_{eff} = \epsilon_h + 3\epsilon_h \sum_{i=1}^{\text{types of inclusions}} f_i \frac{\epsilon_i - \epsilon_h}{\epsilon_i + 2\epsilon_h}
\] (4.12)

Or

\[
\frac{\epsilon_{eff} - \epsilon_h}{\epsilon_{eff} + 2\epsilon_h} = \sum_{i=1}^{\text{types of inclusions}} f_i \frac{\epsilon_i - \epsilon_h}{\epsilon_i + 2\epsilon_h}
\] (4.13)

The above two equations can be used to calculate the effective permittivity for any number of types of dielectric spherical inclusions embedded in dielectric host. We will later attempt to even further generalize the above two formulae. We will introduce the depolarization factors which tend to significantly influence the values of the effective permittivity.
4.2 Bruggeman’s Effective Medium Theory

Let us again consider the equation (4.11) as it is important for our discussion further.

\[
\frac{\varepsilon_{\text{eff}} - \varepsilon_h}{\varepsilon_{\text{eff}} + 2\varepsilon_h} = f_1 \frac{\varepsilon_1 - \varepsilon_h}{\varepsilon_1 + 2\varepsilon_h} + f_2 \frac{\varepsilon_2 - \varepsilon_h}{\varepsilon_2 + 2\varepsilon_h}
\]  

(4.14)

In the above expression if we put \( \varepsilon_h = \varepsilon_2 \), we get the Maxwell Garnett Equation for calculating the effective permittivity when only one type dielectric spheres are embedded in the host. This is very simple to understand as the second type of dielectric spheres in the above expression become a part of the host material.

Now in the above equation if \( f_1 > f_2 \) then we would opt that \( \varepsilon_h \) would be equal to \( \varepsilon_1 \). However the resulting \( \varepsilon_{\text{eff}} \) values are different for each of these two options. Bruggeman’s effective medium theory gives a solution for such a dilemma\textsuperscript{24}. His suggestion was to not give any preference to either phase to be host or the inclusion phase. He proposed that inclusions should be considered as being embedded in the effective medium itself. This theory suggests replacing \( \varepsilon_h \) with \( \varepsilon_{\text{eff}} \) in the above equation. Therefore, the left hand-side of the above equation vanishes and we get an expression as shown below,

\[
0 = f_1 \frac{\varepsilon_1 - \varepsilon_{\text{eff}}}{\varepsilon_1 + 2\varepsilon_{\text{eff}}} + f_2 \frac{\varepsilon_2 - \varepsilon_{\text{eff}}}{\varepsilon_2 + 2\varepsilon_{\text{eff}}}
\]  

(4.15)

The above equation is known as the Bruggeman Effective Medium Expression or the effective medium approximation. In the above equation \( \varepsilon_2 \) can be considered as the
permittivity of the host and the volume fraction \( f_2 = 1 - f_1 \) is nothing but the volume fraction of the host. In this manner the Bruggeman expression does not give preference to either of the two dielectric materials to be the host or the inclusion phase.

There has been an interest in finding out the differences between the Maxwell Garnett Formula and the Bruggeman’s Effective Medium Approximation\(^{25,26}\). These differences are generally based on the fundamentals in terms of the microstructure of the composite material. It was found that the configuration that the Maxwell Garnett Formula follows is that the inclusion phase is completely surrounded by the host medium. Whereas, the Bruggeman approximation comes up from an aggregate model where the particles of the inclusion phase 1 and inclusion phase 2 are mixed on a random basis and hence no special consideration is given to the host. Each volume fraction of all inclusion phases are to be considered.

Therefore we can now wisely say that Bruggeman made a significant improvement to the Maxwell Garnett theory\(^ {27} \). Other names for the Bruggeman Formula, found in many textbooks are “Polder Van Santen Formula”\(^ {28} \), “De Loor Formula”\(^ {29} \) and “Bottcher Formula”\(^ {30} \). Therefore it would be safe to write the generalized equation,

\[
\sum_{i=1}^{n} f_i \frac{\varepsilon_i - \varepsilon_{eff}}{\varepsilon_i + \varepsilon_{eff}} = 0
\]

(4.16)

Where, \( n \) is the number of type of spherical inclusions.
4.3 Depolarization Factors

Up till now all the discussions have involved only spherical inclusions being embedded in the host medium. It is now time to relax the assumption of the inclusions only being spherical. Let us now move onto more practical cases. Also, in order to know more about how the microscopic geometry and the specifics of surface area effect the response of material and dielectric scatterers, it is important to take into account the factors influenced by the particle size and shape effects of the embedded inclusions.

One of the shapes which can be used for the generalization of all shapes is an ellipsoid as shown in the Figure 4.3. The advantage of using an ellipsoid is that many shapes can be formed by choosing the semi-axes appropriately. In our case the semi-axes are given by \(a_x\), \(a_y\) and \(a_z\). Ellipsoids serve the purpose of having a simple geometry and therefore the dipole moment of such homogeneous objects can be written in a closed form. This happens because the internal field in such a homogeneous ellipsoid also remains constant if the applied electric field is also constant.

The amplitude of the internal electric field is linear to the applied external field but there is clearly a dependence of the internal electric field on the permittivity of the ellipsoidal inclusion and a specific shape parameter known as the “Depolarization Factor”.
If the semi-axes as shown above are in the three orthogonal directions then the depolarization factors in the $a_x$, $a_y$ and $a_z$ directions are respectively given by equations (4.17), (4.18) and (4.19) respectively.

$$N_x = \frac{a_x a_y a_z}{2} \int_0^\infty \frac{ds}{(s + a_x^2)(s + a_y^2)(s + a_z^2)}$$

(4.17)

$$N_y = \frac{a_x a_y a_z}{2} \int_0^\infty \frac{ds}{(s + a_y^2)(s + a_x^2)(s + a_z^2)}$$

(4.18)

$$N_z = \frac{a_x a_y a_z}{2} \int_0^\infty \frac{ds}{(s + a_z^2)(s + a_x^2)(s + a_y^2)}$$

(4.19)

The condition that the three depolarization factors of the ellipsoid is

$$N_x + N_y + N_z = 1$$

(4.20)

An example of depolarization factors for a structure where ellipsoids can be used is a sphere which has three equal depolarization factors $1/3$. This can be achieved by
keeping the three semi-axes in the above equations equal (for spheres \( a_x = a_y = a_z \)) and then calculating their respective depolarization factors.

Various closed form expressions for equations (4.17), (4.18) and (4.19) are found in textbooks\(^{31,32,33,34}\).

For Prolate Spheroids where \( a_x > a_y = a_z \) we have

\[
N_x = \frac{1 - e^2}{2e^3} \left[ \ln \left( \frac{1 + e}{1 - e} \right) - 2e \right] \tag{4.21}
\]

And

\[
N_y = N_z = \frac{1}{2} (1 - N_x) \tag{4.22}
\]

Where, \( e = \sqrt{1 - (a_y^2/a_x^2)} \) and is known as the eccentricity.

Similarly for Oblate Spheroids where \( a_x < a_y = a_z \) we have

\[
N_x = \frac{1 + e^2}{e^3} (e - \tan^{-1} e) \tag{4.23}
\]

And

\[
N_y = N_z = \frac{1}{2} (1 - N_x) \tag{4.24}
\]

The eccentricity is the same as that for prolate spheroids.

For a general ellipsoid with three different semi-axes the corresponding depolarization factors can be calculated from equations (4.17) – (4.19). We have developed a program in C Language for calculating the depolarization factors. The discussions although on the program will be done in subsequent chapters.
4.4 Maxwell Garnett Equation for Random Shapes

The Maxwell Garnett Equation only takes into account the spherical nature of the inclusion. We can also extend this theory to involve many other different shapes like discs or needles by choosing the appropriate semi-axes values and then calculating the depolarization factors.

4.4.1 The Internal Electric Field in a General Ellipsoid

Let us imagine a general ellipsoid like the one shown in figure 4.3 and place it in a uniform electric field instead of a dielectric sphere as in figure 3.5. The dipole moment vector has a different direction than that of the applied electric field vector. Rather, the electric field creates three components of the dipole moment vector in three principal axes directions in alignment with the field.

Therefore, the internal electric field in a general ellipsoid placed in an uniform electric field in each respective x, y and z direction is

\[
\vec{E}_{ix,y,z} = \frac{\epsilon_h}{\epsilon_h + N_{x,y,z}(\epsilon_1 - \epsilon_h)} \vec{E}_{x,y,z}
\]  

(4.25)

Where \(\vec{E}_{ix,y,z}\) and \(\vec{E}_{x,y,z}\) is the internal field vector and the applied uniform field vector in x, y and z directions respectively.

It can be seen from the above equation that if we replace \(N_{x,y,z}\) with 1/3 (for a sphere \(N_{x,y,z} = 1/3\)) we will get the same equation when we calculated the internal electric field for a dielectric sphere placed in a uniform applied field.
4.4.2 The Dipole Moment and Polarizability

Similarly we have to include the depolarization factors into the dipole moment equation.

\[ \vec{p}_{x,y,z} = \left[ \frac{(\varepsilon_1 - \varepsilon_h)}{\varepsilon_h + N_{x,y,z}(\varepsilon_1 - \varepsilon_h)} \right] \frac{a_x a_y a_z}{3} \vec{E} \] (4.26)

We also have the expression

\[ \vec{p}_{x,y,z} = \alpha_{x,y,z} \vec{E} \]

Where \( \vec{p}_{x,y,z} \) and \( \alpha_{x,y,z} \) are the dipole moments and polarizabilities in x, y and z directions respectively and \( r^3 \) is replaced by \( a_x a_y a_z \). We can therefore write

\[ \alpha_{x,y,z} = \left[ \frac{(\varepsilon_1 - \varepsilon_h)}{\varepsilon_h + N_{x,y,z}(\varepsilon_1 - \varepsilon_h)} \right] \frac{a_x a_y a_z}{3} \]

\[ = \frac{1}{4\pi} V \left[ \frac{(\varepsilon_1 - \varepsilon_h)}{\varepsilon_h + N_{x,y,z}(\varepsilon_1 - \varepsilon_h)} \right] \]

Where \( V = (4\pi/3) a_x a_y a_z \) = volume of the general ellipsoid.

The above equation is in Gaussian Units. If we want to convert it into M.K.S. units we have to replace \( 1/4\pi \) with \( \varepsilon_0 \). But we have \( \varepsilon_0 = \varepsilon_h \)

\[ \alpha_{x,y,z} = V \left[ \frac{\varepsilon_h (\varepsilon_1 - \varepsilon_h)}{\varepsilon_h + N_{x,y,z}(\varepsilon_1 - \varepsilon_h)} \right] \] (4.27)

After converting equation (4.25), it will look the same as it is now. From this point onwards we will convert all equations in the M.K.S. units.
4.4.3 The Effective Medium Theory

We are assuming the random orientation of ellipsoidal inclusions in host medium. To understand this situation more clearly let us consider the example of a fluid background material when there is no external force orienting the inclusions. Then it is very clear that any previous anisotropy of the ordered mixture will be totally washed away. The mixture therefore becomes isotropic and hence the effective permittivity becomes a scalar. In such a case it has to be assumed that one third of each polarizability component gives equal compensation to the macroscopic polarization density. We will apply this formalism when we substitute the total polarization in equation (3.33).

Therefore we can write the polarization to be

\[
\vec{p} = n \vec{p}_{x,y,z} = n \vec{\alpha}_{x,y,z} \cdot \vec{E} = n \left( \frac{\alpha_x + \alpha_y + \alpha_z}{3} \right) \vec{E}
\]

\[
= n V \frac{1}{3} \left( \left[ \frac{\epsilon_h (\epsilon_1 - \epsilon_h)}{\epsilon_h + N_x (\epsilon_1 - \epsilon_h)} \right] + \left[ \frac{\epsilon_h (\epsilon_1 - \epsilon_h)}{\epsilon_h + N_y (\epsilon_1 - \epsilon_h)} \right] + \left[ \frac{\epsilon_h (\epsilon_1 - \epsilon_h)}{\epsilon_h + N_z (\epsilon_1 - \epsilon_h)} \right] \right) \vec{E}
\]

\[
\vec{p} = \frac{f}{3} \sum_{j=x,y,z} \left[ \frac{\epsilon_h (\epsilon_1 - \epsilon_h)}{\epsilon_h + N_j (\epsilon_1 - \epsilon_h)} \right] \vec{E}
\]

(4.28)

It is now time to apply the effective medium theory as we did in previous derivations. As in spheres it is analogous to apply the same treatment for ellipsoids with the inclusion of the depolarization factors.

\[
\vec{p} = \frac{f}{3} \sum_{j=x,y,z} \left[ \frac{\epsilon_h (\epsilon_1 - \epsilon_h)}{\epsilon_h + N_j (\epsilon_1 - \epsilon_h)} \right] \vec{E}_{loc}
\]

(4.29)

It is now time to calculate \( \vec{E}_{loc} \) using equation (3.17). But let us convert it from Gaussian Units to M. K. S. Units.
Now let substitute the value of $\vec{E}_{loc(x,y,z)}$ in equation (4.29)

\begin{equation}
\vec{\tilde{E}} = \vec{E} + \frac{N_{x,y,z}}{\epsilon_h} \vec{p}
\end{equation}

\begin{equation}
\vec{E}_{loc(x,y,z)} = \frac{\vec{E}}{1 - \frac{N_{x,y,z}}{\epsilon_h} f \sum_{j=x,y,z} \frac{\epsilon_h (\epsilon_1 - \epsilon_h)}{\epsilon_h + N_j (\epsilon_1 - \epsilon_h)}}
\end{equation}

\begin{equation}
\vec{E}_{loc(x,y,z)} = \frac{\vec{E}}{1 - \frac{\frac{f}{3} j=x,y,z} N_j (\epsilon_1 - \epsilon_h)} \frac{\epsilon_h (\epsilon_1 - \epsilon_h)}{\epsilon_h + N_j (\epsilon_1 - \epsilon_h)}
\end{equation}

Now let substitute the value of $\vec{E}_{loc(x,y,z)}$ in equation (4.29)

\begin{equation}
\vec{p} = \frac{\frac{f}{3} j=x,y,z} N_j (\epsilon_1 - \epsilon_h) \frac{\epsilon_h (\epsilon_1 - \epsilon_h)}{\epsilon_h + N_j (\epsilon_1 - \epsilon_h)} \vec{E}
\end{equation}

The total polarization can therefore be written as the one third of the sum of each polarizability components as shown above.

Now converting equation (3.33) into M. K. S. Units

\begin{equation}
\epsilon_{eff} = \epsilon_h + \vec{p}, \vec{E}^{-1}
\end{equation}

Now substituting equation (4.33) in equation (4.34) we have,

\begin{equation}
\epsilon_{eff} = \epsilon_h + \frac{\frac{f}{3} j=x,y,z} N_j (\epsilon_1 - \epsilon_h) \frac{\epsilon_h (\epsilon_1 - \epsilon_h)}{\epsilon_h + N_j (\epsilon_1 - \epsilon_h)} \vec{E}
\end{equation}

It is possible to identify the similarity between equation (3.35) and (4.35) with a very important difference. Both formulas are used to calculate the effective permittivity in which one type of inclusions are embedded in the host medium, except of the fact that equation (3.35) is used when the inclusions are only spheres and equation (4.35) is for general ellipsoidal inclusions whose semi-axes can be set to achieve the appropriate
shape. Therefore, depolarization factors greatly help us in the generalization of the Maxwell Garnett Formula for many shapes.

4.4.4 Generalization for Multiple Types of Inclusions

We have reached to the point that it is now important for us to generalize equation (4.35) for multiple types of inclusions. This is done exactly in the same manner as we generalized for multiple types of inclusions in the case of spheres in previous sections of this chapter. Hence following the same mannerism adopted in section (4.1), it is possible to reach to the formula given below.

\[
\varepsilon_{\text{eff}} = \varepsilon_h + \frac{\sum_{i=1}^{\text{types of inclusions}} \left( \sum_{j=x,y,z} f_i \frac{\varepsilon_i (\varepsilon_j - \varepsilon_h)}{\varepsilon_h + N_{ij} (\varepsilon_i - \varepsilon_h)} \right)}{1 - \sum_{i=1}^{\text{types of inclusions}} \left( \sum_{j=x,y,z} f_i \frac{N_{ij} (\varepsilon_i - \varepsilon_h)}{\varepsilon_h + N_{ij} (\varepsilon_i - \varepsilon_h)} \right)} \tag{4.36}
\]

Therefore now we have completed the isotropic case. We have generalized the Maxwell Garnett Formula for random shapes and number of types of inclusions. In the next chapter we will discuss the Maxwell Garnett Formula in anisotropic medium and will attempt to make generalizations and understand its limitations.
Chapter 5

Advanced Homogenization Principles in Anisotropic Media

5.1 Anisotropy in Dielectric Materials

In this chapter, we will shift our focus from just the geometry of the mixture to the complexities of matter and medium. The phenomenon of dielectric anisotropy can be defined by the response of the material media which depends on the direction of the electric field.

The fundamentals of anisotropy and the need for tensors have been explained in Chapter 2. In this chapter, we will explain the math involved in computing the effective permittivity in such a medium. In most practical cases of anisotropic materials the parameters in the respective tensor is generally less than 9. The three principal directions of the material response of an anisotropic material is determined by the rectangular crystal lattice structure.

Crystallographic structures can be classified into seven classes\(^{35}\). Biaxial crystals have the least symmetry among these structures. Orthorhombic, monoclinic and triclinic crystallographic structures fall under this category. Biaxial crystals have three different permittivity components along the three different principal axes. More symmetry is
observed in uniaxial crystals which have the tetragonal, hexagonal and trigonal classes categorized under them. In uniaxial crystals the permittivity component along the axis of the crystal is different from the other two components which are equal to each other. The last class of crystallographic structures is the cubic crystal in which all the three permittivity components are equal. This means that all the permittivity components in all three principal directions are equal and the response to the external electric field is isotropic.

There are several assumptions made, specially the one of losslessness. In the case of isotropy for lossy materials, the permittivity becomes complex. Same will be the case of anisotropic materials except that the tensor permittivity will now have real and both imaginary components. We have developed the formalism for lossless materials, which can be extended in a similar manner to include imaginary components of the permittivities.

The anisotropy of materials makes it necessary to ask further questions in homogenization analysis that were not applicable to isotropic materials. It can be said that the character of the anisotropic medium is changed when it is rotated. This suggests that although a polycrystalline material is made up of many crystals of the same medium, having the same permittivity tensor, is a mixture of many different materials. This is because all the different material tensors are different in the global coordinate system even if they are related to each other by obvious rotational transformation. We will deal in depth the homogenization mysteries involving anisotropy.
5.2 Vector Effective Permittivity

In our previous derivation of the Maxwell Garnett Equation with depolarization factors for randomly oriented ellipsoids, we assumed the polarizability to be one third of the sum of all polarizability components. This was applicable for randomly oriented ellipsoids but in case of aligned ellipsoids as shown in Figure 5.1, this will not be the case. We will have to treat each polarizability component to calculate the respective effective permittivity component and hence the effective permittivity becomes a vector.

\[
\alpha_{x,y,z} = V \left[ \frac{\epsilon_h (\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{x,y,z} (\epsilon_1 - \epsilon_h)} \right]
\]

(5.1)

Figure 5.1 A Mixture with Aligned Ellipsoidal Inclusions

This case is very interesting as we start with all the elements being isotropic and end up with the effective permittivity being anisotropic or a vector.

From equation (4.27) we have
We are assuming in the previous equation that only one type of inclusion is embedded in the host medium.

Therefore the polarization can be now given as

\[
\vec{p}_{x,y,z} = n\vec{p}_{x,y,z} = n\alpha_{x,y,z}\vec{E}_{x,y,z}
\]

\[
= nV\left[\frac{\epsilon_h(\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{x,y,z}(\epsilon_1 - \epsilon_h)}\right]\vec{E}_{x,y,z}
\]  \(\text{(5.2)}\)

Let us apply the effective medium theory, which will take into account the effect of polarization caused by the medium as well as the geometry of the inclusions and their interactions with each other. Therefore the polarization in three principal direction becomes

\[
\vec{p}_{x,y,z} = nV\left[\frac{\epsilon_h(\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{x,y,z}(\epsilon_1 - \epsilon_h)}\right]\vec{E}_{loc(x,y,z)}
\]  \(\text{(5.3)}\)

Equation (4.30) becomes,

\[
\vec{E}_{loc(x,y,z)} = \vec{E}_{x,y,z} + \frac{N_{x,y,z}}{\epsilon_h} \vec{p}_{x,y,z}
\]  \(\text{(5.4)}\)

\[
\vec{E}_{loc} = \frac{\vec{E}}{1 - \frac{N_{x,y,z}}{\epsilon_h} f \left[\frac{\epsilon_h(\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{x,y,z}(\epsilon_1 - \epsilon_h)}\right]}
\]  \(\text{(5.5)}\)

The volume fraction \(f\) replaces \(nV\) in the above equation. Now again substituting the value of \(\vec{E}_{loc}\) from equation (5.5) in equation (5.3) to recompute the polarization,

\[
\vec{p}_{x,y,z} = \frac{f \left[\frac{\epsilon_h(\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{x,y,z}(\epsilon_1 - \epsilon_h)}\right]}{1 - f \left[\frac{N_{x,y,z}(\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{x,y,z}(\epsilon_1 - \epsilon_h)}\right]} \vec{E}
\]  \(\text{(5.6)}\)
Now applying the same formalism on equation (4.34) and writing the equation in terms of the three principal components.

\[
\epsilon_{\text{eff}(x,y,z)} = \epsilon_h + \frac{\vec{p}_{x,y,z}}{E} \quad (5.7)
\]

\[
\epsilon_{\text{eff}(x,y,z)} = \epsilon_h + \frac{f \left[ \frac{\epsilon_h(\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{x,y,z}(\epsilon_1 - \epsilon_h)} \right]}{1 - f \left[ \frac{N_{x,y,z}(\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{x,y,z}(\epsilon_1 - \epsilon_h)} \right]} \quad (5.8)
\]

We can write this in vector form as,

\[
\begin{bmatrix}
\epsilon_{\text{eff}x} \\
\epsilon_{\text{eff}y} \\
\epsilon_{\text{eff}z}
\end{bmatrix} = \epsilon_h + \frac{f \left[ \frac{\epsilon_h(\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{x}(\epsilon_1 - \epsilon_h)} \right]}{1 - f \left[ \frac{N_{x}(\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{x}(\epsilon_1 - \epsilon_h)} \right]} \begin{bmatrix}
\epsilon_h \\
\epsilon_h \\
\epsilon_h
\end{bmatrix} + \frac{f \left[ \frac{\epsilon_h(\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{y}(\epsilon_1 - \epsilon_h)} \right]}{1 - f \left[ \frac{N_{y}(\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{y}(\epsilon_1 - \epsilon_h)} \right]} \begin{bmatrix}
\epsilon_h \\
\epsilon_h \\
\epsilon_h
\end{bmatrix} + \frac{f \left[ \frac{\epsilon_h(\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{z}(\epsilon_1 - \epsilon_h)} \right]}{1 - f \left[ \frac{N_{z}(\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{z}(\epsilon_1 - \epsilon_h)} \right]} \begin{bmatrix}
\epsilon_h \\
\epsilon_h \\
\epsilon_h
\end{bmatrix} \quad (5.9)
\]

Therefore it is proven that the effective permittivity can be shown in vector form also and anisotropy is observed even when we started with isotropic materials. It is very easy to generalize the above formalism for multiple types of inclusions, as we did previously. Therefore after generalizing the above equation will appear as shown below
In the subsequent sections of this chapter we will begin with anisotropic tensor materials as input and achieve a tensor for the effective permittivity.

\[
\begin{bmatrix}
\varepsilon_{\text{effx}} \\ 
\varepsilon_{\text{effy}} \\ 
\varepsilon_{\text{effz}}
\end{bmatrix} = 
\begin{bmatrix}
\sum_{i=1}^{\text{types of inclusions}} \frac{f_i \varepsilon_h (\varepsilon_i - \varepsilon_h)}{\varepsilon_h + N_{xi}(\varepsilon_i - \varepsilon_h)} \\
\sum_{i=1}^{\text{types of inclusions}} \frac{f_i \varepsilon_h (\varepsilon_i - \varepsilon_h)}{\varepsilon_h + N_{yi}(\varepsilon_i - \varepsilon_h)} \\
\sum_{i=1}^{\text{types of inclusions}} \frac{f_i \varepsilon_h (\varepsilon_i - \varepsilon_h)}{\varepsilon_h + N_{zi}(\varepsilon_i - \varepsilon_h)} \\
1 - \sum_{i=1}^{\text{types of inclusions}} \frac{f_i \varepsilon_h (\varepsilon_i - \varepsilon_h)}{\varepsilon_h + N_{yi}(\varepsilon_i - \varepsilon_h)} \\
1 - \sum_{i=1}^{\text{types of inclusions}} \frac{f_i \varepsilon_h (\varepsilon_i - \varepsilon_h)}{\varepsilon_h + N_{zi}(\varepsilon_i - \varepsilon_h)}
\end{bmatrix}
\]

(5.10)

In the subsequent sections of this chapter we will begin with anisotropic tensor materials as input and achieve a tensor for the effective permittivity.

### 5.3 Polarizability Tensor for an Anisotropic Sphere

Three dimensional vectors can also be represented by dyadics. The origin of dyadic algebra can be traced as back as 1880’s and was introduced by J.W. Gibbs. Therefore, it is important to understand the fundamentals of dyadic algebra before trying to deal with tensors. A dyadic is a function that acts on a vector to reproduce another vector. The use of dyadics gives us an advantage of keeping the equations written in vector form for dielectric phenomenon for isotropic materials and extending the same treatment for anisotropic materials also. The only change in terms of writing the equation is that the parameters now have a double bar over them.
5.3.1 From Scalar Polarizability to Tensor Polarizability

If we recall the equation of dipole moment from chapter 3 i.e. equation (3.28)

\[
\vec{p} = \left[ \frac{\varepsilon_i - \varepsilon_h}{\varepsilon_i + 2\varepsilon_h} \right] r^3 \vec{E}
\]

Converting it into M.K.S. unit systems, we get

\[
\vec{p} = 3V\varepsilon_h \left[ \frac{\varepsilon_i - \varepsilon_h}{\varepsilon_i + 2\varepsilon_h} \right] \vec{E}
\]

Therefore we can write the polarizability as,

\[
\alpha = 3V\varepsilon_h \left[ \frac{\varepsilon_i - \varepsilon_h}{\varepsilon_i + 2\varepsilon_h} \right]
\]

Where, \(V\) = Volume of the Dielectric Sphere. In equation (5.13) the polarizability \(\alpha\) is a scalar. Hence, the dipole moment and the external field are in the same direction. This is not the case when the polarizability is anisotropic and the dipole moment is not in the same direction as the electric field as shown in the Figure 5.2 (a) and (b).

---

Figure 5.2 (a) The Dipole Moment \(\vec{p}\) in same direction as the Electric Field \(\vec{E}\), when the Inclusion is Isotropic

Figure 5.2 (b) The Dipole Moment \(\vec{p}\) in different direction as the Electric Field \(\vec{E}\), when the Inclusion is Anisotropic
The anisotropic polarizability is given by

\[ \overline{\alpha} = 3\epsilon_0 V \left( \overline{\varepsilon_1} - \epsilon_h \overline{I} \right) \left( \overline{\varepsilon_1} + 2\epsilon_h \overline{I} \right)^{-1} \] (5.14)

It is important to understand what these double overbars mean in practice and how they contribute and complicate the calculations. In most cases of anisotropies the inclusion permittivity tensor has only real components and is symmetric\(^3\). This does not complicate the calculations a lot. We can write the symmetric inclusion permittivity dyadic as

\[ \overline{\varepsilon_1} = \sum_{j=1}^{3} \epsilon_{1,j} \overline{u}_j \overline{u}_j^T \] (5.15)

Where, \( \epsilon_{1,j} \) are the three eigen values of the inclusion permittivity dyadic and \( \overline{u}_j \) is a \( 1 \times 3 \) matrix and \( \overline{u}_j^T \) is its transpose, which are the corresponding eigen vectors. Similarly we can write the polarizability tensor as,

\[ \overline{\alpha} = \sum_{j=1}^{3} \alpha_j \overline{u}_j \overline{u}_j^T \] (5.16)

### 5.3.2 Depolarization and Shape Effect

Let us imagine a situation where an anisotropic ellipsoidal inclusion is placed in an isotropic environment. When the ellipsoidal inclusion is not present, let there be a uniform electric field \( \overline{E}_e \). This comes into existence due to free charge distribution \( \varrho \) very far away. Therefore we have \( \nabla \cdot (\epsilon_0 \overline{E}_e) = \varrho \). But now when the inclusion is present the total electric is field is no longer \( \overline{E}_e \) but becomes perturbed by a scattered field \( \overline{E}_s \). This
scattered field is created by a polarization source with which the inclusion can be replaced. This is explained in the Figure 5.3.

\[\vec{E} = \vec{E}_e + \vec{E}_s\]

Figure 5.3 The External Field with and without the Anisotropic Inclusions

No more free charges are created due to the polarization source and hence

\[
\nabla \cdot \vec{D} = \nabla \cdot (\varepsilon_h \vec{E} + \vec{P}) = \nabla \cdot [\varepsilon_h (\vec{E}_e + \vec{E}_s) + \vec{P}] = \rho
\]

\[
\nabla \cdot (\varepsilon_h \vec{E}_s) = -\nabla \cdot \vec{P}
\]

(5.17)

Where, \(\vec{E}_s = \) Scattered Electric Field,

\(\vec{P} = \) Polarization Source.

It can be inferred from the above equation that polarization is the source of the scattered field. Let us assume that the volume of the anisotropic inclusion is \(V\). According to Coulomb’s Law the solution of the above equation can be written as the integral over the polarization source over the volume \(V\).

\[
\vec{E}_s(\vec{r}) = -\int_V \frac{\nabla \cdot \vec{P}(\vec{r}')} {4\pi \varepsilon_h R^2} \vec{u}_R dV'
\]

(5.18)
Where, \( \vec{r} \) = Position Vector of the field,

\[ \vec{r}' = \text{Position Vector of the source point}, \]

\[ R = |\vec{r} - \vec{r}'| = \text{Distance from the source point to the field point}, \]

\[ \vec{u}_R = (\vec{r} - \vec{r}')/R = \text{unit vector along the direction towards } R. \]

Let us make a very important assumption that the polarization density is constant, i.e. \( \vec{P}(\vec{r}') = \vec{P} \) inside the inclusion and outside it is zero. It means that the divergence vanishes immediately inside and outside the anisotropic inclusion. There is only a sudden drop in the amplitude of its divergence only when we move through the surface. Therefore the above integral reduces to an integral over the surface of the inclusion rather than an integral over the volume of the inclusion.

\[
\vec{E}_s(\vec{r}) = -\int_S \vec{P} \cdot \vec{n}' \frac{\vec{u}_R}{4\pi\varepsilon_0 R^2} dS' = -\vec{P} \cdot \int_S \frac{\vec{n}' \cdot \vec{u}_R}{4\pi\varepsilon_0 R^2} dS' \quad (5.19)
\]

Therefore we can write the scattered field as

\[
\vec{E}_s(\vec{r}) = -\frac{1}{\varepsilon_0} \vec{N} \cdot \vec{P} \quad \quad (5.20)
\]

Where,

\[
\vec{N} = \int_S \frac{\vec{n}' \cdot \vec{u}_R}{4\pi R^2} dS'
\]

\( \vec{N} \) is the “Depolarization Dyadic” and \( \vec{n}' \) is a normal vector to the the surface.

A very important property of the depolarization dyadic is that it is independent of the field vector \( \vec{r} \) for spheres and ellipsoids. Therefore also the scattered field is
independent of the field vector and hence the internal field will be uniform. Therefore our assumption of choosing the polarization to be uniform is a valid one.

5.3.3 Polarizability Tensor with Depolarization Dyadic

The depolarization dyadic for the geometry of an ellipsoid consists of three depolarization factors as before, but now in the form of eigen values with their eigen vectors $\vec{v}_{x,y,z}$ which is a $1 \times 3$ matrix and $\vec{v}_{x,y,z}^T$ is its transpose. The three depolarization factors can be calculated by the formula given by equations (4.17), (4.18) and (4.19), being the function of the semi-axes of the ellipsoidal inclusion.

\[
\vec{L} = N_x \vec{v}_x \vec{v}_x^T + N_y \vec{v}_y \vec{v}_y^T + N_z \vec{v}_z \vec{v}_z^T
\]  

(5.21)

With the symmetry of the sphere, $\vec{L}$ must be a multiple of the unit dyadic and because the trace of unit dyadic is 3, the depolarization dyadic is $\vec{I}/3$. We had the sum of the three depolarization factors to be one in the isotropic case. Similarly in the anisotropic case the trace of the depolarization dyadic is equal to one. We can therefore write the internal electric field of the ellipsoid to be,

\[
\vec{E}_i = \vec{E} - \frac{1}{\epsilon_h} \vec{L} \left( \vec{\epsilon}_1 - \epsilon_h \vec{I} \right) \cdot \vec{E}_i
\]  

(5.22)

Therefore we can write the polarizability dyadic to be

\[
\vec{\alpha} = V \left( \vec{\epsilon}_1 - \epsilon_h \vec{I} \right) \left[ \epsilon_h \vec{L} + \vec{L} \left( \vec{\epsilon}_1 - \epsilon_h \vec{I} \right) \right]^{-1} \epsilon_h
\]  

(5.23)
5.4 Anisotropic Background Medium

We have calculated the polarizability tensor assuming the inclusions to be anisotropic and the host background medium to be isotropic as before. Now the next question in line is what changes have to be made when the host background medium also becomes anisotropic.

5.4.1 Transformation of the Host Permittivity

All our previous analysis in Chapters 3 and 4 are based on the fundamentals that the inclusion is a dielectric in-homogeneity and also a point dipole radiating a static field in uniform space. Considering the isotropic case, the field produced by the dipole could be recognized and segregated from the solution of the total field of the inclusion in uniform external field. Now when we assume the host to be anisotropic the above mentioned solution will not remain the same and we have to apply a different formalism to calculate it.

The tactic to be used for solving the field of the dipole in an uniform anisotropic medium is to try to rewrite the field equations in such a manner that we could see the Laplace Equation \( \vec{\nabla}^2 \varphi(\vec{r}) = 0 \). Therefore in source free uniform anisotropic media

\[
\vec{\nabla} \left[ \vec{\epsilon}_h \cdot \vec{\nabla} \varphi(\vec{r}) \right] = 0
\]

The above equation suggests a new affine transformation \(^{31,38}\) where a new operator is defined,
\[ \vec{\nabla}_a = \frac{1}{\vec{\xi}_r^2} \vec{\nabla} \]  \hspace{1cm} (5.25)

Where, \( \vec{\xi}_r = \vec{\xi}_h / \epsilon_0 \) = dimensionless relative environment permittivity tensor.

The power of half, means that it is the square root of the tensor matrix. Various methods can be used to compute the square root of a matrix\(^{39,40}\). These methods are very intensive and profound. If we assume the host relative permittivity tensor to be just a diagonal matrix then the square root is simply,

\[ \sqrt{\vec{\xi}_r} = \sum_{j=1}^{3} \sqrt{\epsilon_{r,j}} \vec{w}_j \vec{w}_j^T \]  \hspace{1cm} (5.26)

Where, \( \epsilon_{r,j} = \) eigen values,

\[ \vec{w}_j = \text{is a } 1 \times 3 \text{ matrix and the corresponding eigen vectors in three orthogonal directions and } \vec{w}_j^T \text{is its transpose.} \]

Therefore we can write the Laplace equation as,

\[ \vec{\nabla}_a^2 \varphi(\vec{r}_a) = 0 \]  \hspace{1cm} (5.27)

The above equation is very similar to the laplace equation mentioned above. So in this new transformation \( \vec{r}_a = \vec{r} \vec{r}_r^{-2} \vec{r} \) is the solution to the usual isotropic one. This implies that the geometrical boundaries also change. It is fortunate for us that the ellipsoidal boundaries remain ellipsoidal but only the axial ratios change. For example, a sphere gets squeezed in different orthogonal directions in accordance with the host or environment permittivity tensor. A positive uniaxial environment means that the axial component is greater than the transversal component. To understand this we need to recall the concepts explained in sections 2.3.3 and 2.3.4. In such a positive uniaxial environment a sphere...
becomes an oblate spheroid and hence the depolarization factors have to be recalculated for the affinely transformed shape.

5.4.2 Transformed Depolarization Factors and Polarizability

We have already discussed how the depolarization dyadic has to be computed in section 5.3.3. But now, as we have learnt about the transformation in the previous section we have to recompute the new transformed depolarization dyadic and the polarizability dyadic.

Remembering the equation (5.21) we can write,

\[
\bar{L} = \sum_{i=x,y,z} N_i \bar{v}_i \bar{v}_i^T
\]  \hspace{1cm} (5.28)

\[
= \frac{\det (\bar{A})}{2} \int_0^\infty ds \frac{(\bar{A}^2 + s\bar{I})^{-1}}{\sqrt{\det (\bar{A}^2 + s\bar{I})}}
\]  \hspace{1cm} (5.29)

Where,

\[
\bar{A} = \sum_{i=x,y,z} a_i \bar{v}_i \bar{v}_i^T
\]  \hspace{1cm} (5.30)

And

\[
\det (\bar{A}) = a_x a_y a_z
\]  \hspace{1cm} (5.31)

Now we have to consider the situation where an anisotropic ellipsoid or an inclusion is placed in an environment which is anisotropic having \( \bar{\epsilon}_h = \bar{\epsilon}_i \bar{\epsilon}_o \). Figure 5.4 helps in explaining the geometry a little better.
The semi-axes of the ellipsoid are the same as before. If this anisotropic ellipsoid or inclusion is now placed in an anisotropic environment with permittivity, $\bar{\epsilon}_h = \bar{\epsilon}_r \epsilon_0$, it is to be remembered that now we have to calculate the transformed depolarization tensor after it has been affinely transformed by the anisotropic environment. The new depolarization factor tensor is given by

$$\bar{L} = \frac{\det(\bar{A})}{2} \int_0^\infty d\bar{s}\bar{\epsilon}_r \left( \bar{A}^2 + s\bar{\epsilon}_r \right)^{-1} \sqrt{\det(\bar{A}^2 + s\bar{\epsilon}_r)}$$

Analyzing the equation for the depolarization tensor of an ordinary ellipsoid i.e. equation (5.29) and that for a transformed ellipsoid i.e. equation (5.30), we can note the difference that $s\bar{I}$ has been replaced by $s\bar{\epsilon}_r$. Hence the polarizability tensor will now be as shown below,

$$\bar{\chi} = V(\bar{\epsilon}_1 - \bar{\epsilon}_h).[\bar{\epsilon}_h + \bar{L}'.(\bar{\epsilon}_1 - \bar{\epsilon}_h)]^{-1}.\bar{\epsilon}_h$$

We will calculate the depolarization tensor in our program using the formula.
Where,

\[
\bar{L} = \frac{1}{\varepsilon_r^2} \cdot \bar{L}_a \cdot \varepsilon_r^{-\frac{1}{2}}
\]

(5.34)

Where,

\[
\bar{L}_a = \frac{\text{det} \bar{A}_a}{2} \int_0^\infty ds \frac{(\bar{A}_a^2 + s\bar{I})^{-1}}{\sqrt{\text{det} (\bar{A}_a^2 + s\bar{I})}}
\]

(5.35)

This depolarization tensor \(\bar{L}_a\) is the transformed depolarization tensor when the ellipsoid is transformed and the host environment becomes isotropic vacuum. Here

\[
\bar{A}_a^2 = \varepsilon_r^{-\frac{1}{2}} \cdot \bar{A}^2 \cdot \varepsilon_r^{-\frac{1}{2}}.
\]

5.5 Anisotropic Effective Permittivity

In this section we will derive effective permittivity tensor, when the inclusion is also anisotropic and the host environment is also anisotropic. The derivation involves understanding the concepts of linear algebra and matrix operations and manipulations. We will first derive the anisotropic Maxwell Garnett Equation for just one type of inclusion and then we will further generalize it for multiple types of inclusions.
5.5.1 Derivation of Effective Permittivity Tensor when Inclusion and Host Environment are Anisotropic

From previous derivations we have important constituent equations for deriving the effective permittivity given by equations (4.26), (4.30) and (4.34)

\[
\tilde{p}_{x,y,z} = \left[ \frac{V \epsilon_h (\epsilon_1 - \epsilon_h)}{\epsilon_h + N_{x,y,z} (\epsilon_1 - \epsilon_h)} \right] \tilde{E}
\]

\[
\tilde{E}_{loc} = \tilde{E} + \frac{N_{x,y,z}}{\epsilon_h} \tilde{p}
\]

\[
\epsilon_{eff} = \epsilon_h + \tilde{p} \cdot \tilde{E}^{-1}
\]

Now to calculate the effective permittivity which is going to be a tensor, we have to convert the above equations in tensorial and matrix form.

\[
\tilde{p} = V. (\bar{\epsilon}_1 - \bar{\epsilon}_h). \left[ \bar{\epsilon}_h + \bar{\varepsilon}'(\bar{\epsilon}_1 - \bar{\epsilon}_h) \right]^{-1} \bar{\epsilon}_h \cdot \tilde{E} \quad (5.36)
\]

\[
\tilde{E}_{loc} = \tilde{E} + \bar{\epsilon}_h^{-1} \bar{\varepsilon}' \cdot \tilde{p} \quad (5.37)
\]

\[
\bar{\epsilon}_{eff} \cdot \tilde{E} = \bar{\epsilon}_h \cdot \tilde{E} + \tilde{p} \quad (5.38)
\]

Now let us write the equation

\[
\tilde{p} = \bar{\alpha} \cdot \tilde{E} \quad (5.39)
\]

From equations (5.36) and (5.39) we can write the polarizability as given in equation (5.33)

\[
\bar{\alpha} = V (\bar{\epsilon}_1 - \bar{\epsilon}_h). \left[ \bar{\epsilon}_h + \bar{\varepsilon}'(\bar{\epsilon}_1 - \bar{\epsilon}_h) \right]^{-1} \bar{\epsilon}_h \quad (5.40)
\]

Now the polarization is given by,

\[
\tilde{p} = n \tilde{P} = n \bar{\alpha} \cdot \tilde{E} \quad (5.41)
\]
Now again we have to perform the same routine as we did for all the previous derivations. We have to apply the effective medium theory. Therefore the $\vec{E}$ in equation (5.41) has to be replaced by $\vec{E}_{loc}$. Equation (5.41) becomes,

$$\vec{p} = n \vec{\alpha}. \vec{E}_{loc}$$  

(5.42)

Let us replace the polarization in equation (5.37)

$$\vec{E}_{loc} = \vec{E} + \bar{\varepsilon}_{h}^{-1}. \vec{L}'. n \vec{\alpha}. \vec{E}_{loc}$$

$$[I - n\bar{\varepsilon}_{h}^{-1}. \vec{L}'. \vec{\alpha}]. \vec{E}_{loc} = \vec{E}$$  

(5.43)

Now let us substitute the value of $\vec{E}$ in equation (5.38)

$$\bar{\varepsilon}_{eff}. [I - n\bar{\varepsilon}_{h}^{-1}. \vec{L}'. \vec{\alpha}]. \vec{E}_{loc} = \bar{\varepsilon}_{h}. [I - n\bar{\varepsilon}_{h}^{-1}. \vec{L}'. \vec{\alpha}]. \vec{E}_{loc} + n \vec{\alpha}. \vec{E}_{loc}$$  

(5.44)

Now let us write $\vec{\alpha} = \vec{V}_{k}. \bar{\varepsilon}_{h}$, where $\vec{k} = (\bar{\varepsilon}_{1} - \bar{\varepsilon}_{h}). [\bar{\varepsilon}_{h} + \vec{L}'. (\bar{\varepsilon}_{1} - \bar{\varepsilon}_{h})]^{-1}$.

Equation (5.44) becomes,

$$\bar{\varepsilon}_{eff}. [I - n\bar{\varepsilon}_{h}^{-1}. \vec{L}'. \vec{\alpha}]. \vec{E}_{loc} = \bar{\varepsilon}_{h}. [I - n\bar{\varepsilon}_{h}^{-1}. \vec{L}'. \vec{\alpha}]. \vec{E}_{loc} + n \vec{\alpha}. \bar{\varepsilon}_{h}$$

$$= \bar{\varepsilon}_{eff}. [I - f\bar{\varepsilon}_{h}^{-1}. \vec{L}'. \vec{\alpha}]. \bar{\varepsilon}_{h}$$

$$= \bar{\varepsilon}_{h}. [I - f\bar{\varepsilon}_{h}^{-1}. \vec{L}'. \vec{\alpha}]. \bar{\varepsilon}_{h} + f \vec{k}. \bar{\varepsilon}_{h}$$  

(5.45)

Post-Multiplying both sides of equation (5.45) by $\bar{\varepsilon}_{h}^{-1}$,

$$\bar{\varepsilon}_{eff}. [\bar{\varepsilon}_{h}^{-1} - f\bar{\varepsilon}_{h}^{-1}. \vec{L}'. \vec{\alpha}]. \bar{\varepsilon}_{h}$$

$$= \bar{\varepsilon}_{h}. [\bar{\varepsilon}_{h}^{-1} - f\bar{\varepsilon}_{h}^{-1}. \vec{L}'. \vec{\alpha}]. \bar{\varepsilon}_{h} + f \vec{k}$$

$$= \bar{\varepsilon}_{eff}. \bar{\varepsilon}_{h}^{-1} [I - f\vec{L}'. \vec{\alpha}]. \bar{\varepsilon}_{h}$$

$$= [I - f\vec{L}'. \vec{\alpha}]. \bar{\varepsilon}_{h} + f \vec{k}$$

Post – Multiplying both sides of above equation by $[I - f\vec{L}'. \vec{\alpha}]^{-1}$,

$$\bar{\varepsilon}_{eff}. \bar{\varepsilon}_{h}^{-1}$$

$$= 1 + f \vec{k}. [I - f\vec{L}'. \vec{\alpha}]^{-1}$$
Now let us substitute the value of \( \bar{k} \) in above equation,

\[
\bar{\varepsilon}_{\text{eff}} = \bar{\varepsilon}_h + f \bar{k} \cdot [\bar{I} - f \bar{L} \cdot \bar{k}]^{-1} \cdot \bar{\varepsilon}_h
\]

The above equation can be used to calculate the effective permittivity tensor, if all the other input parameters, such as the inclusion permittivity tensor, its volume fraction, its semi-axes values and the host permittivity tensor. The more popular form of the above expression can also be derived. The derivation is shown below,

Again replace the value of \( \bar{k} \) as shown before.

\[
\bar{\varepsilon}_{\text{eff}} = \bar{\varepsilon}_h + f \bar{\varepsilon}_h \cdot [\bar{I} - f \bar{L} \cdot \bar{k}]^{-1} \cdot \bar{\varepsilon}_h
\]

Post – Multiply the above equation with \( \bar{\varepsilon}_h^{-1} \) on both sides,

\[
\Rightarrow \quad \bar{\varepsilon}_{\text{eff}} \cdot \bar{\varepsilon}_h^{-1} = \bar{I} + f \bar{k} \cdot [\bar{I} - f \bar{L} \cdot \bar{k}]^{-1}
\]

Post – Multiply the above equation with \( [\bar{I} - f \bar{L} \cdot \bar{k}] \) on both sides,

\[
\Rightarrow \quad \bar{\varepsilon}_{\text{eff}} \cdot \bar{\varepsilon}_h^{-1} \cdot [\bar{I} - f \bar{L} \cdot \bar{k}] = \bar{I} - f \bar{L} \cdot \bar{k} + f \bar{k}
\]

\[
\Rightarrow \quad \bar{\varepsilon}_{\text{eff}} = \bar{\varepsilon}_h \cdot [\bar{I} - f \bar{L} \cdot \bar{k}]^{-1}
\]

Again replace the value of \( \bar{k} \) in above equation, we get

\[
\bar{\varepsilon}_{\text{eff}} \cdot \bar{\varepsilon}_h^{-1} \cdot [\bar{I} - f \bar{L} \cdot (\bar{\varepsilon}_h - \bar{\varepsilon}_h)] \cdot [\bar{\varepsilon}_h + \bar{\varepsilon}_h \cdot (\bar{\varepsilon}_l - \bar{\varepsilon}_h)]^{-1} = \bar{I} + f (\bar{I} - \bar{L}) \cdot (\bar{\varepsilon}_l - \bar{\varepsilon}_h) \cdot [\bar{\varepsilon}_h + \bar{\varepsilon}_h \cdot (\bar{\varepsilon}_l - \bar{\varepsilon}_h)]^{-1}
\]

Post – Multiplying the above equation with \( [\bar{\varepsilon}_h + \bar{\varepsilon}_h \cdot (\bar{\varepsilon}_l - \bar{\varepsilon}_h)] \) on both sides,
Post – Multiplying the above equation with $[\bar{\varepsilon}_h + (1 - f)\bar{L}'_1.(\bar{\varepsilon}_1 - \bar{\varepsilon}_h)]^{-1}$ on both sides,

$$\bar{\varepsilon}_{eff} \cdot \bar{\varepsilon}_h^{-1} = \bar{I} + f(\bar{\varepsilon}_1 - \bar{\varepsilon}_h).[\bar{\varepsilon}_h + (1 - f)\bar{L}'_1.(\bar{\varepsilon}_1 - \bar{\varepsilon}_h)]^{-1}$$

$$\Rightarrow \bar{\varepsilon}_{eff} = \bar{\varepsilon}_h + f(\bar{\varepsilon}_1 - \bar{\varepsilon}_h).[\bar{\varepsilon}_h + (1 - f)\bar{L}'_1.(\bar{\varepsilon}_1 - \bar{\varepsilon}_h)]^{-1} \cdot \bar{\varepsilon}_h$$

### 5.5.2 Generalization of the Anisotropic Maxwell Garnett Equation for Multiple Types of Inclusions

The equation (5.46) has been very carefully derived using sound matrix operations. A direct conclusion cannot be made, what the effective permittivity tensor could be for multiple types of ellipsoidal inclusions. Let us again start with constitutional relations to derive the effective permittivity tensor, but only with two types of inclusions and then generalize it for multiple types also.

$$\vec{E}_{loc} = \vec{E} + \bar{\varepsilon}_h^{-1} \cdot (\bar{L}_1 \vec{P}_1 + \bar{L}_2 \vec{P}_2) \quad (5.47)$$

$$\bar{\varepsilon}_{eff} \cdot \vec{E} = \bar{\varepsilon}_h \cdot \vec{E} + \vec{P} \quad (5.48)$$

Where,

$$\vec{P} = \vec{P}_1 + \vec{P}_2 \quad (5.49)$$

Where, $\bar{L}_1$ and $\bar{L}_2$ are the depolarization tensors of inclusion 1 and 2, $\vec{P}_1$ and $\vec{P}_2$ are the Polarizations caused by inclusion 1 and 2.
The dipole moment is given by,

\[ \mathbf{p} = V_1 \cdot (\bar{\varepsilon}_1 - \bar{\varepsilon}_h) \cdot (\bar{\varepsilon}_h + \bar{L}_1 \cdot (\bar{\varepsilon}_1 - \bar{\varepsilon}_h))^{-1} \cdot \bar{\varepsilon}_h \cdot \bar{E} \]
\[ + V_2 \cdot (\bar{\varepsilon}_2 - \bar{\varepsilon}_h) \cdot (\bar{\varepsilon}_h + \bar{L}_2 \cdot (\bar{\varepsilon}_2 - \bar{\varepsilon}_h))^{-1} \cdot \bar{\varepsilon}_h \cdot \bar{E} \]  
(5.50)

\[ \mathbf{p} = (\bar{\alpha}_1 + \bar{\alpha}_2) \cdot \bar{E} \]  
(5.51)

Where, \( \bar{\alpha}_1 \) = Polarizability of the inclusion 1,

\( \bar{\alpha}_2 \) = Polarizability of the inclusion 2.

The polarization can therefore be given as,

\[ \mathbf{p} = (n_1 \bar{\alpha}_1 + n_2 \bar{\alpha}_2) \cdot \bar{E} \]  
(5.52)

Let us now replace \( \bar{E} \) with \( \bar{E}_{loc} \) to apply the effective medium theory. Therefore the above equation (5.52) can be written as,

\[ \mathbf{p} = (n_1 \bar{\alpha}_1 + n_2 \bar{\alpha}_2) \cdot \bar{E}_{loc} \]  
(5.53)

Let us now consider equation (5.47) in order to replace the local field in equation (5.53),

\[ \bar{E}_{loc} = \bar{E} + \bar{\varepsilon}_h^{-1} \cdot (\bar{L}_1 n_1 \bar{\alpha}_1 + \bar{L}_2 n_2 \bar{\alpha}_2) \]

\[ [\bar{I} - \bar{\varepsilon}_h^{-1} \cdot (\bar{L}_1 n_1 \bar{\alpha}_1 + \bar{L}_2 n_2 \bar{\alpha}_2)] \cdot \bar{E}_{loc} = \bar{E} \]

\[ \bar{\varepsilon}_{eff} \cdot [\bar{I} - \bar{\varepsilon}_h^{-1} \cdot (\bar{L}_1 n_1 \bar{\alpha}_1 + \bar{L}_2 n_2 \bar{\alpha}_2)] \cdot \bar{E}_{loc} \]
\[ = \bar{\varepsilon}_h \cdot [\bar{I} - \bar{\varepsilon}_h^{-1} \cdot (\bar{L}_1 n_1 \bar{\alpha}_1 + \bar{L}_2 n_2 \bar{\alpha}_2)] \cdot \bar{E}_{loc} \]
\[ + (n_1 \bar{\alpha}_1 + n_2 \bar{\alpha}_2) \cdot \bar{E}_{loc} \]  
(5.54)

Let \( \bar{\alpha}_1 = V_1 \bar{k}_1 \bar{\varepsilon}_h \) and \( \bar{\alpha}_2 = V_2 \bar{k}_2 \bar{\varepsilon}_h \)

Where, \( \bar{k}_1 = (\bar{\varepsilon}_1 - \bar{\varepsilon}_h) \cdot (\bar{\varepsilon}_h + \bar{L}_1 \cdot (\bar{\varepsilon}_1 - \bar{\varepsilon}_h))^{-1} \),

\[ \bar{k}_2 = (\bar{\varepsilon}_2 - \bar{\varepsilon}_h) \cdot (\bar{\varepsilon}_h + \bar{L}_2 \cdot (\bar{\varepsilon}_2 - \bar{\varepsilon}_h))^{-1}. \]
Equation (5.54) with substitution of \( \tilde{k}_1 \) and \( \tilde{k}_2 \) becomes,

\[
\bar{\varepsilon}_{\text{eff}} \cdot \left[ \bar{I} - \bar{\varepsilon}_h^{-1} \cdot (\bar{L}_1 \cdot n_1 \cdot V_1 \cdot \tilde{k}_1 + \bar{L}_2 \cdot n_2 \cdot V_2 \cdot \tilde{k}_2, \bar{\varepsilon}_h) \right] = \bar{\varepsilon}_h \cdot \left[ \bar{I} - \bar{\varepsilon}_h^{-1} \cdot (\bar{L}_1 \cdot n_1 \cdot V_1 \cdot \tilde{k}_1 + \bar{L}_2 \cdot n_2 \cdot V_2 \cdot \tilde{k}_2, \bar{\varepsilon}_h) \right] + (n_1 \cdot V_1 \cdot \tilde{k}_1, \bar{\varepsilon}_h + n_2 \cdot V_2 \cdot \tilde{k}_2, \bar{\varepsilon}_h)
\]

\[
\Rightarrow \bar{\varepsilon}_{\text{eff}} \cdot \left[ \bar{I} - \bar{\varepsilon}_h^{-1} \cdot (\bar{L}_1 \cdot f_1 \cdot \tilde{k}_1, \bar{\varepsilon}_h + \bar{L}_2 \cdot f_2 \cdot \tilde{k}_2, \bar{\varepsilon}_h) \right] = \bar{\varepsilon}_h \cdot \left[ \bar{I} - \bar{\varepsilon}_h^{-1} \cdot (\bar{L}_1 \cdot f_1 \cdot \tilde{k}_1, \bar{\varepsilon}_h + \bar{L}_2 \cdot f_2 \cdot \tilde{k}_2, \bar{\varepsilon}_h) \right] + (f_1 \cdot \tilde{k}_1, \bar{\varepsilon}_h + f_2 \cdot \tilde{k}_2, \bar{\varepsilon}_h)
\]

Let us post-multiply the above equation by \( \bar{\varepsilon}_h^{-1} \).

\[
\Rightarrow \bar{\varepsilon}_{\text{eff}} \cdot \bar{\varepsilon}_h^{-1} \cdot \left[ \bar{I} - (f_1 \cdot \tilde{k}_1 \cdot \bar{\varepsilon}_h + f_2 \cdot \tilde{k}_2 \cdot \bar{\varepsilon}_h) \right] = \bar{\varepsilon}_h \cdot \bar{\varepsilon}_h^{-1} \cdot \left[ \bar{I} - (f_1 \cdot \tilde{k}_1 \cdot \bar{\varepsilon}_h + f_2 \cdot \tilde{k}_2 \cdot \bar{\varepsilon}_h) \right] + (f_1 \cdot \tilde{k}_1 + f_2 \cdot \tilde{k}_2)
\]

Let us post multiply by \( \left[ \bar{I} - (f_1 \cdot \tilde{k}_1 \cdot \bar{\varepsilon}_h + f_2 \cdot \tilde{k}_2 \cdot \bar{\varepsilon}_h) \right]^{-1} \),

\[
\Rightarrow \bar{\varepsilon}_{\text{eff}} \cdot \bar{\varepsilon}_h^{-1} = \bar{I} + f_1 \cdot \tilde{k}_1 \cdot \left[ \bar{I} - (f_1 \cdot \tilde{k}_1 \cdot \bar{\varepsilon}_h + f_2 \cdot \tilde{k}_2 \cdot \bar{\varepsilon}_h) \right]^{-1} + f_2 \cdot \tilde{k}_2 \cdot \left[ \bar{I} - (f_1 \cdot \tilde{k}_1 \cdot \bar{\varepsilon}_h + f_2 \cdot \tilde{k}_2 \cdot \bar{\varepsilon}_h) \right]^{-1}
\]

Now again post multiplying by \( \bar{\varepsilon}_h \) we get,

\[
\Rightarrow \bar{\varepsilon}_{\text{eff}} = \bar{\varepsilon}_h + f_1 \cdot \tilde{k}_1 \cdot \left[ \bar{I} - (f_1 \cdot \tilde{k}_1 \cdot \bar{\varepsilon}_h + f_2 \cdot \tilde{k}_2 \cdot \bar{\varepsilon}_h) \right]^{-1} \cdot \bar{\varepsilon}_h + f_2 \cdot \tilde{k}_2 \cdot \left[ \bar{I} - (f_1 \cdot \tilde{k}_1 \cdot \bar{\varepsilon}_h + f_2 \cdot \tilde{k}_2 \cdot \bar{\varepsilon}_h) \right]^{-1} \cdot \bar{\varepsilon}_h
\]

\[
\Rightarrow \bar{\varepsilon}_{\text{eff}} = \bar{\varepsilon}_h + f_1 \cdot (\bar{\varepsilon}_1 - \bar{\varepsilon}_h) \cdot \left[ \bar{\varepsilon}_h + \bar{L}_1 \cdot (\bar{\varepsilon}_1 - \bar{\varepsilon}_h) \right]^{-1} \cdot \left[ \bar{I} - (f_1 \cdot \tilde{k}_1 \cdot (\bar{\varepsilon}_1 - \bar{\varepsilon}_h) \right] \cdot \left[ \bar{I} - (f_1 \cdot \tilde{k}_1 \cdot (\bar{\varepsilon}_1 - \bar{\varepsilon}_h) \right]^{-1} + f_2 \cdot \tilde{k}_2 \cdot (\bar{\varepsilon}_2 - \bar{\varepsilon}_h) \cdot \left[ \bar{I} - (f_1 \cdot \tilde{k}_1 \cdot (\bar{\varepsilon}_1 - \bar{\varepsilon}_h) \right] \cdot \left[ \bar{I} - (f_1 \cdot \tilde{k}_1 \cdot (\bar{\varepsilon}_1 - \bar{\varepsilon}_h) \right]^{-1} \cdot \bar{\varepsilon}_h + f_2 \cdot (\bar{\varepsilon}_2 - \bar{\varepsilon}_h) \cdot \left[ \bar{I} - (f_1 \cdot \tilde{k}_1 \cdot (\bar{\varepsilon}_1 - \bar{\varepsilon}_h) \right] \cdot \left[ \bar{I} - (f_1 \cdot \tilde{k}_1 \cdot (\bar{\varepsilon}_1 - \bar{\varepsilon}_h) \right]^{-1} \cdot \bar{\varepsilon}_h
The above equation can be used to calculate the effective permittivity tensor when two types of anisotropic inclusions are embedded in an anisotropic host medium. It is quite simple from this point to generalize the above equation. The generalized form is

\[ \bar{\varepsilon}_{\text{eff}} = \bar{\varepsilon}_h + \sum_{i=1}^{\text{types of inclusions}} f_i (\bar{\varepsilon}_i - \bar{\varepsilon}_h) \left[ \bar{\varepsilon}_h + \bar{L}_i : (\bar{\varepsilon}_i - \bar{\varepsilon}_h) \right]^{-1} \]

\[
\left\{ \bar{I} - \sum_{j=1}^{\text{types of inclusions}} f_j (\bar{\varepsilon}_j - \bar{\varepsilon}_h) \left[ \bar{\varepsilon}_h + \bar{L}_j : (\bar{\varepsilon}_j - \bar{\varepsilon}_h) \right]^{-1} \right\}^{-1} \cdot \bar{\varepsilon}_h \tag{5.57}
\]

Therefore we have been able to derive the generalized form for the anisotropic effective permittivity. In the code, we will input all the eigen values and eigen vectors required to reconstruct the inclusion tensor, the host tensor and the depolarization tensor.
Chapter 6

Results and Conclusions

In this chapter, we will discuss the results and some conclusions which will give a good idea about the isotropic and anisotropic mixture properties.

6.1 Isotropic Mixtures

Let us again consider the Maxwell Garnett Formula as derived in Chapter 3 for purely isotropic environment and inclusions.

\[
\varepsilon_{\text{eff}} = \varepsilon_h + \frac{3f \varepsilon_h \left( \frac{\varepsilon_1 - \varepsilon_h}{\varepsilon_1 + 2\varepsilon_h} \right)}{1 - f \left( \frac{\varepsilon_1 - \varepsilon_h}{\varepsilon_1 + 2\varepsilon_h} \right)}
\]  

(6.1)

It should be quite obvious to have effective permittivity equal to host permittivity when the volume fraction of the inclusions is equal to 0 and similarly, the effective permittivity equal to the inclusion permittivity when the volume fraction is equal to 1. This can also be determined from the above formula. However the case for volume fraction of the inclusions being 1 is debatable since practically, it will not be possible to fill up all the space using spheres. We can get close to the required result if the total volume is filled with very small spheres. We can write equation (6.1) as
For dilute mixtures we have $f \ll 1$. Equation (6.2) becomes

$$\epsilon_{eff} = \epsilon_h + \frac{3f\epsilon_h(\epsilon_1 - \epsilon_h)}{\epsilon_1 + 2\epsilon_h - f(\epsilon_1 - \epsilon_h)}$$  \hspace{1cm} (6.3)

The susceptibility ratio $\frac{\epsilon_{eff} - \epsilon_h}{\epsilon_1 - \epsilon_h}$ as seen from the equation (6.3) is equal to 0 for the volume fraction equal to 0 and approaches unity when volume fraction approaches unity. The Figure 6.1 depicts the effective permittivity or the susceptibility ratio as a function of the volume fraction for different dielectric contrasts $\epsilon_1/\epsilon_h$. It can be seen from the graph that the effective permittivity becomes quite a nonlinear function of the volume fraction for high dielectric constants.

There is one more case which further suggests that the dielectric contrasts between the environment phase and the inclusion phase can also be opposite. If the
permittivity of inclusions is less than the permittivity of the host the effective permittivity of the mixture comes out to be less than the permittivity of the host. This can be seen in figure 6.2 as shown below.

Figure 6.2 compares two mixtures in which the role of the inclusion and the environment phase have been interchanged.

Figure 6.2 Relative Effective Permittivity \( (\varepsilon_{\text{eff}}/\varepsilon_h) \) or \( (\varepsilon_{\text{eff}}/\varepsilon_i) \) using Equation 6.3 plotted as a function of the Volume Fraction \( f \) for dielectric contrast between the two phases as 20. The roles of the environment and inclusion phases have been interchanged. \( \varepsilon_i = 20\varepsilon_h \) for the rising curve and \( \varepsilon_h = 20\varepsilon_i \) for the falling curve.

Figure 6.2 compares two mixtures in which the role of the inclusion and the environment phase have been interchanged. The main message associated with figure 6.2 is that, it tells us that the Maxwell Garnett model is not symmetric. If the Maxwell Garnett model was symmetric then the above two curves should have intersected at volume fraction of 50%. This implies that the host and the inclusion phases do not contribute on an equal basis. This criterion is not required by the Maxwell Garnett model as the geometry of the mixture is non-symmetric to start with.
6.2 Isotropic Mixtures with Depolarization Factors

We have already explained in Chapter 4 about depolarization factors introduced in the Maxwell Garnett equation. Let us recall the equation for effective permittivity for randomly oriented ellipsoids or inclusions.

![Graph showing the Susceptibility Ratio (ε\(_{eff}\) - ε\(_h\))/(ε\(_1\) - ε\(_h\)) vs f]

**Figure 6.3** The Susceptibility Ratio \((\epsilon_{eff} - \epsilon_h)/(\epsilon_1 - \epsilon_h)\) for the Maxwell Garnett Equation for randomly oriented ellipsoids (Equation 4.35) as a function of Volume Fraction \(f\) for Needles
We will examine the effect of shape on the effective permittivity using the figures 6.3 and 6.4. As we can see for figures 6.3 and 6.4 for needles the nonlinearity of the permittivity as a function of volume fraction curve is much more than that for discs, for the same dielectric contrast between the environment and the inclusion phase. This is strong evidence to the fact that the macroscopic permittivity is greatly affected by the form of the inclusions.

Figure 6.5 gives us more insight on the nonlinearity of the effective permittivity as a function of the volume fraction curve. We can conclude from figure 6.5 that inclusions shaped as needles can create larger effective permittivities and those shaped as spheres can create the lowest.

\[
\epsilon_{\text{eff}} = \epsilon_h + \frac{\epsilon_1}{3} \sum_{j=x,y,z} \frac{\epsilon_h (\epsilon_1 - \epsilon_h)}{\epsilon_h + N_j (\epsilon_1 - \epsilon_h)} P_j.
\]  

\[ (6.4) \]

We will examine the effect of shape on the effective permittivity using the figures 6.3 and 6.4. As we can see for figures 6.3 and 6.4 for needles the nonlinearity of the permittivity as a function of volume fraction curve is much more than that for discs, for the same dielectric contrast between the environment and the inclusion phase. This is strong evidence to the fact that the macroscopic permittivity is greatly affected by the form of the inclusions.

Figure 6.5 gives us more insight on the nonlinearity of the effective permittivity as a function of the volume fraction curve. We can conclude from figure 6.5 that inclusions shaped as needles can create larger effective permittivities and those shaped as spheres can create the lowest.
The vector effective permittivity is a special case as explained earlier. This is so because we get a vector effective permittivity from purely isotropic mixture. Since the effective permittivity is a vector, the permittivity vector has three components along each of the axes respectively. We will determine the results obtained for such a vector effective permittivity by evaluating and understanding the differences in behavior between these components.

Figure 6.5 The Effective Permittivity of a mixture as a function of the Volume Fraction \( f \) using Equation 4.35, for dielectric contrast between the inclusion and the environment as 50 i.e. \( \epsilon_i = 50\epsilon_h \). The three shapes covered are Spheres, Discs and Needles

6.3 Vector Effective Permittivity

The vector effective permittivity is a special case as explained earlier. This is so because we get a vector effective permittivity from purely isotropic mixture. Since the effective permittivity is a vector, the permittivity vector has three components along each of the axes respectively. We will determine the results obtained for such a vector effective permittivity by evaluating and understanding the differences in behavior between these components.
6.3.1 Inclusions of the form of Needles

We have chosen the ratios of the semiaxes of the ellipsoidal inclusions $a_x/a_y$ and $a_x/a_z$ to be equal to 10000, so that we can have a fine needle like structure. We observe the similarity of all the three components of the vector effective permittivity being equal to the permittivity of the host when the volume fraction of the inclusions is 0. Similarly when the volume fraction is equal to 1, then all the three components of the vector effective permittivity are equal to the permittivity of the inclusion.

Since we have a needle like structure we have chosen $a_y = a_z$. Therefore we always have the components of the effective permittivity vector in the y and z directions to be equal to each other. Hence we will only plot the relationships between the components in the x and y directions which will suffice for the component in the z direction as well.

As we can see from figure 6.6 the x component of the effective permittivity vector as a function of volume fraction follows a linear path for all dielectric contrasts between the environment and the inclusion phase. Whereas, the y(z) component of the effective permittivity tensor becomes more non linear as the dielectric contrast between the environment and the inclusion phases increases.

Figure 6.8 shows the difference between the x and y components as a function of the volume fraction. The plot tells us that the x component of the vector effective permittivity keeps on becoming greater than the y component, and this ratio keeps on increasing with increase in the dielectric contrast between the inclusion phase and the environment phase.
Figure 6.6 Susceptibility Ratio $(\epsilon_{effx} - \epsilon_h)/(\epsilon_1 - \epsilon_h)$ vs $f$, for Needles

Figure 6.7 Susceptibility Ratio $(\epsilon_{effy} - \epsilon_h)/(\epsilon_1 - \epsilon_h)$ vs $f$, for Needles

Figure 6.8 The ratio $\epsilon_{effx}/\epsilon_{effy}$ using Equation (5.8) plotted as function of the Volume Fraction $f$, for Needles
6.3.2 Inclusions of the form of Discs

For discs we have the semi axes ratio as $a_x/a_y$ as $1/1000000$. Again we have $a_y = a_z$. This helps us in defining well formed disc. We will only plot the relationship between the components in the x and y direction as the components in y and z directions are equal to each other. As seen in the case for needles, all the three components of the vector effective permittivity are equal to the permittivity of the host when the volume fraction is equal to 0, and equal to the permittivity of the inclusion when the volume fraction is equal to 1.

As can be seen from figure 6.9, we can see that for discs, the x component of the effective permittivity as a function of the volume fraction becomes more non linear as the dielectric contrast between the environment and the inclusion phases increases. Similarly, we can infer from figure 6.10 that the y and z components remain linear even if the dielectric contrasts increases or decreases. This is exactly the inverse of what we saw for needles.

Figure 6.11 shows that the difference between the y and x component goes on increasing as the dielectric contrast between the inclusion and environment phases goes on increasing, as a function of the volume fraction.
Figure 6.9 Susceptibility Ratio 
\( \frac{\varepsilon_{effx} - \varepsilon_h}{(\varepsilon_1 - \varepsilon_h)} \) as a function of the Volume Fraction \( f \), for Discs

Figure 6.10 Susceptibility Ratio 
\( \frac{\varepsilon_{effy} - \varepsilon_h}{(\varepsilon_1 - \varepsilon_h)} \) as a function of the Volume Fraction \( f \), for Discs

Figure 6.11 The ratio \( \varepsilon_{effx}/\varepsilon_{effy} \) using Equation (5.8) plotted as function of the Volume Fraction \( f \), for Discs
6.3.3 Inclusions of the form of Spheres

For spheres, we have all the three components of the effective permittivity vector equal to each other. Again, as it was seen for the case of spheres and discs, the vector effective permittivity components are equal to the permittivity of the host when the volume fraction is equal to 0 and is equal to the permittivity of the inclusion when the volume fraction is equal to 1.

As can be seen from the figure 6.12, for all components of the vector effective permittivity as a function of the volume fraction, the curve becomes more non linear when the dielectric contrast between the inclusion phase and the environment phase increases.

![Figure 6.12 The Susceptibility Ratio \((\epsilon_{eff x,y} - \epsilon_h)/(\epsilon_1 - \epsilon_h)\) vs \(f\) using Equation (5.8) as a function of the Volume Fraction \(f\), for Spheres](image-url)
6.4 Anisotropic Effective Permittivity

The effective permittivity becomes a tensor when the host environment and the inclusions are anisotropic. The basic fundamentals of anisotropy have been explained in Chapter 2 and 5. We have developed a code in C/C++ to calculate the anisotropic effective permittivity.

We have placed special stress on the orientation of the inclusions and the host to investigate the exhibited anisotropies. Due to the limitations of our code we have restricted the orientation of the host to have its optical axis parallel to the z axis. The inclusion orientation can be varied and various results can be obtained using the code. A solid attempt has been made to make the code as user friendly as possible. Also we have enhanced the capability of our code to accommodate the calculation of the tensor effective permittivity for any number of types of inclusions. But, for simplicity’s sake we use only one type of inclusion to interpret the results.

Since the effective permittivity is now a tensor, it has nine elements because it is a 3 x 3 matrix. As it is known to us from equation (2.16) and figure 2.2, that the displacement vector $\vec{D}$ is not in the same direction as the electric field vector $\vec{E}$. Hence we will measure the anisotropy using the equation

$$\vec{D} = \varepsilon \vec{E} \quad (6.5)$$

Therefore the effective permittivity tensor calculated using our code will be used to calculate the respective components of the displacement vector.
6.4.1 Anisotropic Inclusions of the form of Needles

For needles, we have the semiaxes ratio \( \frac{a_x}{a_y} \) equal to 10000. We also have \( a_y = a_z \). We have oriented the z axis of the host environment in such a way that it is parallel to the optical axis. The inclusion orientation can be set using the eigen vectors \( \hat{u}_i \) and the depolarization factor orientation can be set using the eigen vectors \( \hat{v}_i \). Again for simplicity we have the eigen vectors for the inclusion and the depolarization factors to be same, although various other combinations are possible. We have chosen the orientation of the z axis given by the eigen vector as \( \frac{[1,1,1]}{\sqrt{3}} \). We have two types of crystals, namely uniaxial and biaxial crystals which have been explained in earlier chapters.

6.4.1.1 Anisotropic Needle Shaped Inclusions as Uniaxial Crystals

As we already know, in uniaxial crystals, two diagonal elements of the permittivity tensor are equal. In our code we have \( xx \) and \( yy \) elements of the permittivity tensor to be equal. Since the host and the inclusion permittivities are both tensors, what we mean by dielectric contrasts is \( \epsilon_{hxx}/\epsilon_{ixx} \), \( \epsilon_{hyy}/\epsilon_{iyy} \) and \( \epsilon_{hzz}/\epsilon_{izz} \).

Figures 6.13, 6.14 and 6.15 show the displacement vector as a function of the volume fraction with the electric field vector as \([1\ 0\ 0]\), \([0\ 1\ 0]\) and \([0\ 0\ 1]\) respectively. We observe that when the volume fraction of the inclusions is equal to 0, the displacement vector is in the same direction as that of the electric field vector. This means that there is no anisotropy even when the host permittivity is a tensor. The only reason for this case to arise is because we have chosen the orientation of the host permit-
Figure 6.13 The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [1 \ 0 \ 0]$ using Equation (5.46), for Needles (Uniaxial Crystals)

Figure 6.14 The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [0 \ 1 \ 0]$ using Equation (5.46), for Needles (Uniaxial Crystals)
activity to be in the same direction as that of the conventional x, y and z axes. Now, when the volume fraction of the inclusions is equal to 1, the displacement vector is in the direction governed by the orientation of the inclusions. As we can see when the effective permittivity is a tensor, for all volume fractions, the displacement vector is in a direction different to that of the electric field vector.

6.4.1.2 Anisotropic Needle Shaped Inclusions as Biaxial Crystals

For biaxial crystals we have all the three elements of the permittivity tensor are different. Similar results are observed for biaxial crystals as that for uniaxial crystals. The
**Figure 6.16** The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [1 0 0]$ using Equation (5.46), for Needles (Biaxial Crystals)

**Figure 6.17** The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [0 1 0]$ using Equation (5.46), for Needles (Biaxial Crystals)
important results to be noticed are that for higher dielectric contrasts, the displacement vector spreads more over the space and has much larger magnitude for larger dielectric contrasts and hence we can see more anisotropy. Also that, for biaxial crystals the displacement vector is much more stretched out further in space as compared to that of the uniaxial crystals.

6.4.2 Anisotropic Inclusions of the form of Discs

For discs, we have the semiaxes ratio $a_x/a_y$ equal to $1/10000$. We also have $a_y = a_z$. We have oriented the $z$ axis of the host environment in such a way that it is parallel to the optical axis. The inclusion orientation can be set as specified above. Again
we have the eigen vectors for the inclusion and the depolarization factors to be same. We have chosen the orientation of the z axis given by the eigen vector as $[1,1,1]/\sqrt{3}$.

6.4.2.1 Anisotropic Disc Shaped Inclusions as Uniaxial Crystals

We have the xx and yy elements of the permittivity tensor to be equal. Figures 6.19, 6.20 and 6.21 show the displacement vector as a function of the volume fraction with the electric field vector as $[1 \ 0 \ 0]$, $[0 \ 1 \ 0]$ and $[0 \ 0 \ 1]$ respectively. Again it is observed that when the volume fraction of the inclusions is equal to 0, the displacement vector is in the same direction as that of the electric field vector. This case is explained for the needles.

Figure 6.19 The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [1 \ 0 \ 0]$ using Equation (5.46), for Discs (Uniaxial Crystals)
Figure 6.20 The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [0 \ 1 \ 0]$ using Equation (5.46), for Discs (Uniaxial Crystals).

Figure 6.21 The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [0 \ 0 \ 1]$ using Equation (5.46), for Discs (Uniaxial Crystals).
6.4.2.2 Anisotropic Disc Shaped Inclusions as Biaxial Crystals

For biaxial crystals we have all the three elements of the permittivity tensor are different. Figures 6.22, 6.23, 6.24 show the displacement vector as a function of the volume fraction with the electric field vector as $[1\ 0\ 0]$, $[0\ 1\ 0]$ and $[0\ 0\ 1]$ respectively for biaxial crystals. The important results to be noticed are that for higher dielectric contrasts, the displacement vector spreads more over the space in the sense that the magnitude of the displacement vector is larger for larger dielectric contrasts and hence we can witness more anisotropy. Also that, for biaxial crystals the displacement vector is much more stretched out further as compared to the uniaxial crystals.

Figure 6.22 The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [1\ 0\ 0]$ using Equation (5.46), for Discs (Biaxial Crystals)
Figure 6.23 The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [0 \ 1 \ 0]$ using Equation (5.46), for Discs (Biaxial Crystals)

Figure 6.24 The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [0 \ 0 \ 1]$ using Equation (5.46), for Discs (Biaxial Crystals)
6.4.3 Anisotropic Inclusions of the form of Spheres

For spheres, we have the semiaxes ratio $a_x/a_y$ equal to i.e. we have $a_x = a_y = a_z$. We have oriented the z axis of the host environment in such a way that it is parallel to the optical axis. The inclusion orientation can be set as specified above. Again we have the eigen vectors for the inclusion and the depolarization factors to be same. We have chosen the orientation of the z axis given by the eigen vector as $[1,1,1]/\sqrt{3}$.

6.4.3.1 Anisotropic Sphere Shaped Inclusions as Uniaxial Crystals

We have the xx and yy elements of the permittivity tensor to be equal. Figures 6.25, 6.26 and 6.27 show the displacement vector as a function of the volume fraction with the electric field vector as $[1 0 0]$, $[0 1 0]$ and $[0 0 1]$ respectively. Again as it was observed for needles and discs, for spheres also when the volume fraction of the inclusions is equal to 0, the displacement vector is in the same direction as that of the electric field vector.
Figure 6.25 The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [1 0 0]$ using Equation (5.46), for Spheres (Uniaxial Crystals)

Figure 6.26 The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [0 1 0]$ using Equation (5.46), for Spheres (Uniaxial Crystals)
6.4.3.2 Anisotropic Sphere Shaped Inclusions as Biaxial Crystals

For biaxial crystals we have all the three elements of the permittivity tensor are different. Figures 6.28, 6.29, 6.30 show the displacement vector as a function of the volume fraction with the electric field vector as [1 0 0], [0 1 0] and [0 0 1] respectively for biaxial crystals. The important results to be noticed are that for higher dielectric contrasts, the displacement vector spreads more over the space in the sense that the magnitude of the displacement vector is larger for larger dielectric contrasts and hence we can witness more anisotropy with increasing dielectric contrasts. Also that, for biaxial crystals the displacement vector stretches out much further as compared to the uniaxial crystals.
Figure 6.28 The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [1 0 0]$ using Equation (5.46), for Spheres (Biaxial Crystals)

Figure 6.29 The Displacement Vector $\vec{D}$ plotted as a function of the Volume Fraction $f$, when the Electric Field Vector $\vec{E} = [0 1 0]$ using Equation (5.46), for Spheres (Biaxial Crystals)
6.5 Controlling Shape of Inclusions

Figure 6.31 shows the how the semiaxes of an ellipsoid can be chosen to attain different shapes. From a sphere we can range from needles to discs and approximate various other shapes for selecting the shape of the inclusions. For spheres we have the all the three semiaxes of the ellipsoid to be equal i.e. \(a_x = a_y = a_z\). For needles we would have one of the semiaxes to be much greater than the other two semiaxes so that we can approximate it as a needle shaped structure. For our simulations we have \(a_x \gg a_y = a_z\).
Similarly for discs we have two of the semiaxes of the ellipsoid to be much greater than the third semiaxes, to approximate it as a disc shaped structure. For our purposes we have $a_x \ll a_y = a_z$. 

Figure 6.31 Variation of Semi-Axes to achieve different shapes of Inclusions
References


Appendix

1. Derivation of the Depolarization Dyadic ($\bar{L}$)

Let us recall the equation for depolarization factors for a general ellipsoid given

by equation (4.17), (4.18) and (4.19)

\[
N_x = \frac{a_x a_y a_z}{2} \int_0^\infty \frac{ds}{(s + a_x^2)(s + a_y^2)(s + a_z^2)} \tag{A.1}
\]

\[
N_y = \frac{a_x a_y a_z}{2} \int_0^\infty \frac{ds}{(s + a_y^2)(s + a_z^2)(s + a_x^2)} \tag{A.2}
\]

\[
N_z = \frac{a_x a_y a_z}{2} \int_0^\infty \frac{ds}{(s + a_z^2)(s + a_x^2)(s + a_y^2)} \tag{A.3}
\]

Also we can recall from equation (5.21) that

\[
\bar{L} = N_x \tilde{v}_x \tilde{v}_x^T + N_y \tilde{v}_y \tilde{v}_y^T + N_z \tilde{v}_z \tilde{v}_z^T \tag{A.4}
\]

With this information and more let us go ahead and derive equation (5.29)

\[
\bar{L} = \frac{\det (\bar{A})}{2} \int_0^\infty ds \frac{(A^2 + sI)^{-1}}{\sqrt{\det (A^2 + sI)}} \tag{A.5}
\]

Where,

\[
\bar{A} = \sum_{i=x,y,z} a_i \tilde{v}_i \tilde{v}_i^T \tag{A.6}
\]

And

\[
\det (\bar{A}) = a_x a_y a_z \tag{A.7}
\]
From above equations we can write

\[
\bar{A} = \begin{bmatrix}
a_x & 0 & 0 \\
0 & a_y & 0 \\
0 & 0 & a_z
\end{bmatrix}
\]  
(A.8)

Also we know that the identity matrix

\[
\bar{I} = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}
\]  
(A.9)

Let us evaluate certain matrix equation and slowly get to the point where we can put them together to get to our equation that needs to be derived.

Now,

\[
\bar{A}^2 + s\bar{I} = \begin{bmatrix}
a_x^2 & 0 & 0 \\
0 & a_y^2 & 0 \\
0 & 0 & a_z^2
\end{bmatrix} + \begin{bmatrix}
s & 0 & 0 \\
0 & s & 0 \\
0 & 0 & s
\end{bmatrix} = \begin{bmatrix}
a_x^2 + s & 0 & 0 \\
0 & a_y^2 + s & 0 \\
0 & 0 & a_z^2 + s
\end{bmatrix}
\]  
(A.10)

And,

\[
[\bar{A}^2 + s\bar{I}]^{-1} = \begin{bmatrix}
\frac{1}{a_x^2 + s} & 0 & 0 \\
0 & \frac{1}{a_y^2 + s} & 0 \\
0 & 0 & \frac{1}{a_z^2 + s}
\end{bmatrix}
\]  
(A.11)

And,

\[
\text{det}(\bar{A}^2 + s\bar{I}) = (a_x^2 + s) \cdot (a_y^2 + s) \cdot (a_z^2 + s)
\]

\[
\Rightarrow \sqrt{\text{det}(\bar{A}^2 + s\bar{I})} = \sqrt{(a_x^2 + s) \cdot (a_y^2 + s) \cdot (a_z^2 + s)}
\]  
(A.12)

We also have,
\[ \det(\bar{\mathbf{A}}) = a_x a_y a_z \]  

(A.13)

Now let us expand equation (A.4) considering that the respective eigen vectors are parallel to the x, y and z axes.

\[ \bar{\mathbf{L}} = N_x \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + N_y \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} + N_z \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \]

(A.14)

\[ \begin{bmatrix} N_x & 0 & 0 \\ 0 & N_y & 0 \\ 0 & 0 & N_z \end{bmatrix} \]

If we replace \( N_x, N_y, N_z \) from equations (A.1), (A.2) and (A.3) we get,

\[ \bar{\mathbf{L}} = \frac{a_x a_y a_z}{2} \int_0^\infty ds \frac{1}{\sqrt{(s + a_x^2)(s + a_y^2)(s + a_z^2)}} \begin{bmatrix} 1 \\ s + a_x^2 \\ s + a_y^2 \\ s + a_z^2 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \]

(A.15)

From equation (A.7), (A.8), (A.9), (A.10) (A.11), (A.12), (A.13) we get,

\[ \bar{\mathbf{L}} = \frac{\det(\bar{\mathbf{A}})}{2} \int_0^\infty ds \frac{[\bar{\mathbf{A}}^2 + s\bar{\mathbf{I}}]^{-1}}{\sqrt{\det[\bar{\mathbf{A}}^2 + s\bar{\mathbf{I}}]}} \]

(A.16)

The equation (A.16) is the derived equation of the depolarization tensor.

\[ \bar{\mathbf{L}} \]

2. Derivation of the Internal Electric Field when Host and Inclusions are Anisotropic

Let us rewrite the equation for internal electric field as derived in Chapter 3 and equation (3.27).
\[ E_{in} = \left[ \frac{3}{\epsilon_r + 2} \right] \vec{E} \]  \hspace{2cm} (A.17)

\( \epsilon_r \) is the relative permittivity which can also be written as

\[ \epsilon_r = \frac{\epsilon_1}{\epsilon_0} = \frac{\epsilon_1}{\epsilon_h} \]

Since, in our case the permittivity of free space is replaced by the permittivity of the host. Replacing these conversions in equation (A.17) we get

\[ E_{in} = \left[ \frac{3\epsilon_h}{\epsilon_1 + 2\epsilon_h} \right] \vec{E} \]  \hspace{2cm} (A.18)

The above equation is written for spheres. If we want to consider the shapes we will have to introduce the depolarization factors in \( x \), \( y \) and \( z \) directions.

\[ E_{in(x,y,z)} = \left[ \frac{\epsilon_h}{\epsilon_h + N_{(x,y,z)}(\epsilon_1 - \epsilon_h)} \right] \vec{E}_{(x,y,z)} \]  \hspace{2cm} (A.19)

Pre-multiplying the above equation by \( [\epsilon_h + N_{(x,y,z)}(\epsilon_1 - \epsilon_h)] \) we get

\[ [\epsilon_h + N_{(x,y,z)}(\epsilon_1 - \epsilon_h)] E_{in(x,y,z)} = \epsilon_h \vec{E}_{(x,y,z)} \]  \hspace{2cm} (A.20)

Now if we consider the inclusions \( \epsilon_1 \) to be anisotropic, the permittivity of the inclusions will become a tensor. Also the depolarization factors will be a tensor. Hence we have

\[ [\epsilon_h \vec{l} + \vec{l}. (\vec{\epsilon}_1 - \epsilon_h \vec{l})]. \vec{E}_{in} = \epsilon_h \vec{E} \]

\[ \Rightarrow \quad \epsilon_h \vec{E}_{in} + \vec{l}. (\vec{\epsilon}_1 - \epsilon_h \vec{l}). \vec{E}_{in} = \epsilon_h \vec{E} \]

\[ \Rightarrow \quad \vec{E}_{in} = \vec{E} - \frac{1}{\epsilon_h} \vec{l}. (\vec{\epsilon}_1 - \epsilon_h \vec{l}). \vec{E}_{in} \]  \hspace{2cm} (A.21)

Now when the host environment is also anisotropic the above equation becomes
\[ \mathbf{E}_{\text{in}} = \mathbf{E} - \tilde{\varepsilon}_h^{-1} \mathbf{L} (\tilde{\varepsilon}_1 - \tilde{\varepsilon}_h) \mathbf{E}_{\text{in}} \]  \hspace{1cm} (A.22)

The above equation is the equation for internal electric field when both the host and inclusions are anisotropic.

3. Derivation of the Polarizability Dyadic

Let us rewrite the equation for dipole moment as derived in Chapter 3 and equation (3.28)

\[ \mathbf{p} = \left[ \frac{\varepsilon_r - 1}{\varepsilon_r + 2} \right] r^3 \mathbf{E} \]  \hspace{1cm} (A.23)

Replacing the relative permittivity \( \varepsilon_r \) with \( \varepsilon_1/\varepsilon_h \) the above equation becomes

\[ \mathbf{p} = \left[ \frac{\varepsilon_1 - \varepsilon_h}{\varepsilon_1 + \varepsilon_h} \right] r^3 \mathbf{E} \]  \hspace{1cm} (A.24)

Now like the previous derivation we will include the depolarization factors to incorporate for shape effects. The above equation then becomes

\[ \mathbf{p}_{x,y,z} = \left[ \frac{\varepsilon_1 - \varepsilon_h}{\varepsilon_h + N_{x,y,z}(\varepsilon_1 - \varepsilon_h)} \right] \frac{a_x a_y a_z}{3} \mathbf{E}_{x,y,z} \]  \hspace{1cm} (A.25)

Post-multiplying the above equation with \( 4\pi \) on both sides we get,

\[ \mathbf{p}_{x,y,z} 4\pi = \left[ \frac{\varepsilon_1 - \varepsilon_h}{\varepsilon_h + N_{x,y,z}(\varepsilon_1 - \varepsilon_h)} \right] \frac{a_x a_y a_z}{3} \mathbf{E}_{x,y,z} 4\pi \]

\[ \Rightarrow \mathbf{p}_{x,y,z} 4\pi = \left[ \frac{\varepsilon_1 - \varepsilon_h}{\varepsilon_h + N_{x,y,z}(\varepsilon_1 - \varepsilon_h)} \right] V \mathbf{E}_{x,y,z} \]  \hspace{1cm} (A.26)

Since \( V = 4\pi a_x a_y a_z / 3 \), i.e. Volume of the ellipsoid.
Post-multiplying the equation (A.26) with \([\epsilon_h + N_{x,y,z}(\epsilon_1 - \epsilon_h)]\) on both sides we get

\[ \tilde{p}_{x,y,z} \cdot 4\pi \cdot [\epsilon_h + N_{x,y,z}(\epsilon_1 - \epsilon_h)] = (\epsilon_1 - \epsilon_h)V\vec{E}_{x,y,z} \]  
\[ (A.27) \]

The next step would be to consider the inclusions to be anisotropic and hence modify the above equation.

\[ \tilde{p} \cdot 4\pi \cdot [\epsilon_h \bar{I} + \bar{L}(\bar{\epsilon}_1 - \epsilon_h \bar{I})] = (\bar{\epsilon}_1 - \epsilon_h \bar{I})V\vec{E} \]  
\[ (A.28) \]

Let us convert the above equation into MKS form

\[ \tilde{p} \cdot \epsilon_h^{-1} \cdot [\epsilon_h \bar{I} + \bar{L}(\bar{\epsilon}_1 - \epsilon_h \bar{I})] = (\bar{\epsilon}_1 - \epsilon_h \bar{I})V\vec{E} \]  
\[ (A.29) \]

Post-multiplying the above equation with \([\epsilon_h \bar{I} + \bar{L}(\bar{\epsilon}_1 - \epsilon_h \bar{I})]^{-1}\) on both sides of the above equation we get

\[ \tilde{p} \cdot \epsilon_h^{-1} = V(\bar{\epsilon}_1 - \epsilon_h \bar{I}) \cdot [\epsilon_h \bar{I} + \bar{L}(\bar{\epsilon}_1 - \epsilon_h \bar{I})]^{-1} \vec{E} \]  
\[ (A.30) \]

Post-multiplying the above equation with \(\epsilon_h\) on both sides of the above equation we get

\[ \tilde{p} = V(\bar{\epsilon}_1 - \epsilon_h \bar{I}) \cdot [\epsilon_h \bar{I} + \bar{L}(\bar{\epsilon}_1 - \epsilon_h \bar{I})]^{-1} \epsilon_h \vec{E} \]  
\[ (A.31) \]

We can write the polarizability as

\[ \tilde{p} = \bar{\alpha} \cdot \vec{E} \]  
\[ (A.32) \]

From equations (A.31) and (A.32) we can infer that

\[ \bar{\alpha} = V(\bar{\epsilon}_1 - \epsilon_h \bar{I}) \cdot [\epsilon_h \bar{I} + \bar{L}(\bar{\epsilon}_1 - \epsilon_h \bar{I})]^{-1} \epsilon_h \]  
\[ (A.33) \]

When the host environment is also anisotropic, the polarizability tensor becomes
\[
\bar{\sigma} = V(\bar{\varepsilon}_1 - \bar{\varepsilon}_h) \cdot \left[ \bar{\varepsilon}_h + L(\bar{\varepsilon}_1 - \bar{\varepsilon}_h) \right]^{-1} \cdot \bar{\varepsilon}_h
\]  
(A.34)

The above equation is the equation for the polarizability tensor when the inclusions and host are anisotropic and the inclusions are of random shapes.