AN ABSTRACT OF THE THESIS OF

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The dielectric constant is a property of matter, which describes the macroscopic response of an insulating material to an applied electric field. When the dielectric is placed in an electric field, molecular dipole moments are induced inside the dielectric and consequently the material becomes polarized.

In this thesis the macroscopic and microscopic phenomenon of polarization as well as the influence of electromagnetic waves on dielectrics are discussed. The relations among the microscopic polarizability, dielectric constant and index of refraction are also discussed. Finally, a theoretical model for the effect of an electric field on an interacting system of discrete dipoles is presented.

THEORY OF DIELECTRIC CONSTANT, POLARIZABILITY AND DISCRETE DIPOLES

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In the Name of God, the Compassionate, the Merciful

قل يستوى الذين يعلمون والذين لا يعلمون

Are those who possess knowledge equal to those who do not?
(Holy Qur'an, chapter 39, verse 9)

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I would like to dedicate this humble work to the living memory of my esteemed father, who from my youth upwards, until his premature and deeply lamented death, always encouraged and supported my academic endeavors.

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Chapter 1

Introduction

The response of matter to external electric fields is of interest in many areas of study. In astrophysics, for example, the existence of small interstellar dust grains has been inferred from astronomical observations. Understanding the response of these hypothetical dust grains to interstellar electromagnetic fields is critical to investigating their role in the universe. This response is described theoretically by modeling the grains as polarizable spheres. Such polarizable spheres are also used in theoretical descriptions of many other phenomena. For example, related models are also used in atmospheric physics.

Several references describe the interaction of small particles with electromagnetic fields. Van de Hulst[1] discusses general theoretical models of the interaction, with an emphasis on electromagnetic theory and mathematical solutions. This reference discusses the importance of polarizability and the dipole moment in the discussion of scattering and the efficiency factor for scattering. The first term of the efficiency factor is the radiation from an electric dipole. This book was originally published in 1957 so although the mathematical solutions have not changed, the applications and methods of calculation have changed.

Bohren and Huffman[2], published in 1983, updates much material from van de Hulst[1]. It also gives more practical information. This book discusses the importance of the dielectric constant and its use in optics. One topic, which is particularly important for the present work, is that it extends the discussion of dielectric constant to anisotropic materials where the use of the

dielectric tensor is essential. This book uses the dielectric tensor to relate the electric field $\vec{E}$ to the displacement $\vec{D}$. It indicates that the dielectric constant is often symmetric with the principal dielectric constant being the diagonal of the matrix. In this case the displacement $\vec{D}$ and the electric field $\vec{E}$ are parallel. In one example, it uses the dielectric constant to discuss the oscillations of the atoms in crystals.

Evans[3] discusses astrophysical applications. The specific part of this book that is related to this thesis is the employment of the dielectric constant and the polarizability to describe the electrical properties of the dust grains. It also relates the refractive index to the dielectric constant. It states that the absorption of electromagnetic radiation can be described by an absorption coefficient. This coefficient can be used to define a complex refractive index, which requires the knowledge of the dielectric constant

Stephens[4] uses the concept of electric dipole and the dielectric constant in an indirect way for remote sensing applications. An electric dipole is a particular charge distribution where two equal but oppositely charged particles are separated by a distance s. The oscillating dipole produces electromagnetic radiation, which scatters while interacting with particles. This phenomenon is the basis for remote sensing techniques. Another phenomenon in which scattering occurs is observed in variations of the refractive index in the atmosphere. The dielectric constant of materials is temperature dependent. Thus, as the dielectric constant changes with variation in temperature, so does the refractive index of that material since it is related to the dielectric constant. This change in dielectric constant and refractive index results in the scattering of electromagnetic radiation. In this application, one is interested in the effect of the atmosphere on

electromagnetic waves as they travel from source to detector. For example, UHF and VHF radars receive echoes caused by scattering from atmospheric regions with variable refractive index resulting from variations in temperature and humidity

Gueguen and Palciauskas[5] introduce electromagnetic measurements for geophysical exploration. By electromagnetic measurement techniques, it is possible to probe the earth over seventeen orders of magnitude in frequency, from 10^{-6} Hz to the highest microwave frequencies 10^{11} Hz. At high frequencies, where the wavelength is short, microwave radiometry can detect distances over fractions of a meter, while at low frequencies, where the wavelength is large, deep magnetic sounding can detect distances of more than a hundred kilometers. With low frequencies the conductivity of the rocks can be measured, while with high frequencies the dielectric properties are measured. This is why this book utilizes the measurement and the computation of the dielectric constant as a tool for probing the rocks or the other materials under the earth. It also states that the dielectric constant of rocks is dependent on the frequency of the time-varying electric field and the dielectric constant of water saturated rocks is higher than that of dry rocks.

The application of dielectric theory to interstellar dust grains has been significant in several Master's thesis or projects at Emporia State University (Shi[6], Ding[7], Robertson[8]). Shi calculated the photoelectric yield of small graphite and silicate grains. Ding extended these calculations to a larger range of sizes. Finally, Robertson incorporated the calculations of Shi and Ding into a model of the heating of the interstellar gas by the emission of photoelectrons.

The general aim of this study is to analyze the microscopic polarizability and its influence on the dielectric constant. This will begin with the discussion of the macroscopic dielectric properties of electrical insulators. It may appear that since insulators do not conduct electricity they are not responsive to electric fields. However, Faraday[11] discovered that this was not so. He found that the capacitance of a capacitor increased by a factor κ when an insulator is put between the plates. The factor κ is a property of the insulator called the dielectric constant. Therefore, insulators are often referred to as dielectrics.

Macroscopic dielectric phenomena can be understood more clearly by discussing what happens inside the individual atoms and molecules of the dielectric material. Consider an isolated atom in the absence of an electric field. The negative electronic charges are distributed symmetrically around the positively charged nucleus. In this case, the atom has a zero dipole moment. When the electric field is present, a force is exerted on the charges. The positive charges move in the direction of the field and the negative charges move to the opposite side. These charges are no longer in the previous spherically symmetric form and therefore, the center of charge of the negatively charged electrons and the positively charged nucleus don't coincide. This means that the atom has a nonzero dipole moment $\vec{p}$. Thus the atom has become polarized and this is referred to as induced polarization. In general, materials which are highly polarizable also have large dielectric constants.

Another possibility is that some molecules have their positive and negative charges distributed in such a way that they have dipole moments even in the absence of an electric field. These molecules are called polar molecules, and the dipole moment is referred to as a permanent dipole

moment. The total charge, which is also referred to as the monopole moment, is zero. An example of this type of dipole moment is the water molecule where the hydrogen's electronic charge moves away from the nucleus and clusters around the oxygen. When there are many water molecules in the liquid or gas state, these dipole moments are randomly oriented so that in the absence of an electric field they sum to zero. When an electric field is present, the field exerts forces on the dipoles and causes them to rotate until they are aligned with the direction of the field, thus polarizing the material. Ionic polarization is produced from the displacement and deformation of a charged ion with respect to another ion. The dipoles of some solid materials are aligned to some extent, even in the absence of an electric field. These materials are called electrets and are said to be permanently polarized.

Ferroelectric crystals are another possibility that exhibit dipole moments even in the absence of an electric field. Their polarization properties are highly temperature-dependent. In some crystals the ferroelectric dipole is not changed by a high intensity electric field but is very sensitive to changes in the temperature. These crystals are called pyroelectric. Lithium niobate, $LiNbO_3$, is a pyroelectric at room temperature. It can be polarized by an electric field applied, provided the temperature is over 1400 K. Above this transition temperature, ferroelectricity disappears and it is said to be in the paraelectric state and the dielectric constant drops rapidly.

Polarization is related to the relative capacitivity or relative permitivity, ε, which is a measure of the degree to which the electric field influences the material. Permitivity is defined by, $\varepsilon = \varepsilon_0(1+\chi)$, where χ is

the susceptibility of the material. The susceptibility is a measure of how easily the material can be polarized and relates the polarization to the applied electric field by the equation, $\vec{P} = \chi \varepsilon_0 \vec{E}$ where $\vec{P}$ is the polarizatoin and $\vec{E}$ represents the electric field. Polarization is also directly proportional to the molecular dipole moment $\vec{p}$. In some materials, rotation of the permanent molecular dipole moment may take place in such a way that it can contribute to the total polarization $\vec{P}$. However, in others, rotation is hindered so that the permanent molecular dipole does not contribute to $\vec{P}$. Examples of these materials are nitromethane, CH_3NO_2, and hydrogen chloride, HCl.

The moment of a molecule of nitromethane in the liquid state is large which causes the relative permitivity of this material to be large, about 11.1×10^{-30} Coulomb m. The relative permitivity of this material in the liquid state increases as the temperature decreases because the molecules can rotate easily in the liquid state. However, the permitivity of nitromethane drops sharply at the freezing point of the liquid, 244 K. In the solid state the molecules of nitromethane are not free to move thus they do not contribute to polarization. The low value of relative permitivity, ε, is due to only induced and ionic moments as ε in solids doesn't changed with temperature.

This phenomenon is not true for all solids, for instance, it does not work the same way with HCl. The permitivity of HCl in the liquid state is relatively high, and its temperature dependence indicates the occurrence of rotation. At the freezing point of HCl, 165 K, the permitivity slightly increases but the molecules in the solid keep orienting themselves in the direction of the field. The permitivity of HCl keeps increasing until the temperature reaches 100 K and then it starts decreasing sharply as the

molecules can no longer rotate and thus the polarization ceases. Below 100 K, the polarization is partly induced and partly ionic.

According to Kittel[12], in piezoelectric materials, stress as well as electric field changes the polarization. For small stress, the polarization is linearly proportional to the stress. The application of electric field causes strain in these materials. All ferroelectric materials are piezoelectric materials but the converse is not true. The best piezoelectric material is quartz, which is not ferroelectric.

Polarization is also frequency dependent. At low and moderate frequencies polarization occurs due to both electronic and molecular dipole. However, at high frequencies the molecular polarization ceases because the molecular moment of inertia is too large to allow the molecule to quickly switch directions and align itself to the alternating electric field. On the other hand, electrons, which are light and having a small moment of inertia, can align themselves with the alternating field and result in electronic polarization.

The purpose of this thesis is two-fold. First, we survey the general theoretical relationship between microscopic polarization and the macroscopic dielectric constant. Extensive use was made of readily available general references. Feynman's Lectures in Physics, Wangsness[10], and Bohren and Huffman[2] have been particularly useful. Other references are noted in the body of the thesis. Secondly the mutual interactions of systems of polarizable particles subjected to an applied external field are discussed. This topic is introduced in the form of solutions and extensions to problems from Feynman[9].

The organization of the thesis is as follows. Chapter 1 introduces the subject and describes polarization phenomena in general terms. Chapter 2

has three sections. In the first section the dielectric constant and polarization are discussed on a macroscopic scale. The next section discusses the polarization on a microscopic scale. In this section the dielectric constant of gases, liquids, and solids are discussed as well. The third section is about wave propagation in dielectrics. In this section, Maxwell's equations in a dielectric, the index of refraction, wave speed, and the frequency-dependent dielectric constant are discussed. The concept of the index of a mixture is also mentioned. Chapter 3 describes the problem of the effective polarizability of two dipoles, which is the principal focus of this thesis. This section focuses on different methods for the determination of the effective polarizability of two dipoles subjected to an external electric field. The methods considered are simultaneous equation, iteration method, and polarizability tensor. The conclusions of this study are the subject of Chapter 4.

Chapter 2

Dielectric Theory

1. Macroscopic Properties

The principal references for most of the concepts in this section are Feynman[9] and Wangsness[10]. This work elaborates on some details omitted in both references. We have solved some of the problems in Feynman[9] and Wangsness[10] and used them as the basis for some relevant discussions. When we reach to the solved problems we will point that out.

In conductors free charges move in response to applied electric fields. The free charges redistribute themselves until the total electric field inside the conductor vanishes. In dielectrics (also known as insulators) the case is different. One may think that since dielectrics don't conduct electricity electric fields should not have any effect. However, using a simple electroscope and parallel plate capacitor, Faraday[11] discovered that this was not true. He found that by inserting a dielectric between the two plates of a capacitor the capacitance of a capacitor increased by a factor κ. The factor κ is a property of the dielectric, and it is called the dielectric constant.

Now let's see what happens when a dielectric is placed between the plates of the capacitor. Given a charged capacitor with the positive charges on the top plate and the negative charges on the bottom plate, when a dielectric is placed between the two plates the potential difference across the capacitor falls, which results in an increase of capacitance for the same

charge. Suppose A is the area of the plates and d is the spacing between the plates, then

$$C = \varepsilon_0 \frac{A}{d}, \tag{1}$$

and

$$Q = CV, \tag{2}$$

where Q is the charge on the plates, V is the voltage between the plates and C is the capacitance of the capacitor. In order to show why the voltage drops another phenomenon, called polarization is introduced. In the absence of an applied electric field, the positively charged nucleus of each atom of the dielectric is surrounded by negatively charged electrons. In this case the positive and negative charge distributions have a common center of charge, analogous to the center of mass, which results in the absence of a dipole moment as in Figure 1. However, in the presence of a low or a moderate electric field the electrons move to one side and the nucleus to the other side, result in different centers of charge for the oppositely charged particles. This phenomenon induces a dipole moment as in Figure 2. If we assume $\vec{p}$ to be the dipole moment, q to be the charge, and $\vec{r}$ the separation distance between the opposite charges then we will have

$$\vec{p} = q\vec{r}. \tag{3}$$

If there are N atoms per unit volume, the dipole moments per unit volume are

$$\vec{P} = N\vec{p} = Nq\vec{r}, \tag{4}$$

where $\vec{P}$ is the polarization vector and it is linearly related to the electric field, provided the electric field is not very high. In this chapter the electric field is assumed to be low and that $\vec{P}$ is linearly proportional to $\vec{E}$.

The relationship between this model and the capacitor will be discussed shortly. Assume a sheet of material polarized. Considering the polarization of this material is uniform, which means the positively charged protons and negatively charged electrons are distributed in such away that the positive charges per volume and the negative charges per volume are equal. This implies that there is no net charge per volume, or in other words, the volume charge density is zero. Consider what happens to a dielectric being inserted between the two plates of a capacitor. Assuming the polarization of the capacitor is uniform. In this case, of course, the volume charge density is zero. However, at one surface the electrons will be moved in a distance d and at the other, they will be moved out, leaving some positive charges out a distance d which induces surface charge density or polarization charge as in Figure 3. If A is the area of the plate, N is the number of charges per unit volume and d the displacement then the total charge, Q, on the surface of the plates is

$$Q = NqAd . \qquad (5)$$

The surface charge density, σ_{pol}, is

$$\sigma_{pol} = Nqd . \qquad (6)$$

The surface charge density equals the magnitude of polarization inside the material because $P = Nqd$. Therefore,

$$\sigma_{pol} = P . \qquad (7)$$

The surface charge is positive on one surface and negative on the other. Not only does the dielectric but also the plates of the capacitor get polarized. If the capacitor is discharged, then the dielectric will no longer be polarized. The plates of the capacitor also have surface charge density, σ_{free}. The subscript, free, indicates the free electrons on the plates of conductor, where the electrons can move freely. Thus, the net electric field is the total surface charge density divided by ε_0. Note that the surface charge density of the dielectric and the plates oppose one another. It also should be noted that the electric field, E_0, in the absence of the dielectric is greater than the electric field, E, when dielectric is present. Then

$$E = \frac{\sigma_{free} - \sigma_{pol}}{\varepsilon_0} . \qquad (8)$$

This equation can also be written as follows

$$E = \frac{\sigma_{free} - P}{\varepsilon_0} . \qquad (9)$$

This equation does not reveal anything about the net electric field unless the polarization is known. As already mentioned, polarization is linearly related to electric field. Therefore,

$$\vec{P} = \chi \varepsilon_0 \vec{E}, \qquad (10)$$

where χ is a constant and is called the electric susceptibility. Now using Equation (10), Equation (9) becomes

$$E = \frac{\sigma_{free}}{\varepsilon_0} \frac{1}{(1+\chi)}. \qquad (11)$$

This formula implies that in the presence of dielectric, the electric field is decreased by a factor $1/(1+\chi)$. Equation (10) can't be applied to all materials, but it does apply to most materials.

Since the electric field between the plates is uniform, the voltage will be,

$$V = Ed = \frac{\sigma_{free} d}{\varepsilon_0 (1+\chi)}. \qquad (12)$$

Now using Equations (2), (12) and the fact that the total charge on the capacitor is $\sigma_{free} d$ the equation of capacitance defined in Equation (1) becomes,

$$C = \frac{\varepsilon_0 A(1+\chi)}{d} = \frac{\kappa \varepsilon_0 A}{d}. \qquad (13)$$

This equation shows that when a dielectric is inserted between the plates of a capacitor the capacitance increases by the factor

$$\kappa = 1+\chi, \qquad (14)$$

where κ is the dielectric constant which is a property of the material.

Next consider the case where polarization is not homogeneous on a material. In this case the existence of volume charge density is expected, because how much charge moves in one volume element may not be the same as how much charge leaves the other.

To calculate how much charge is gained or lost, it is necessary to find how much charge moves across the imaginary surface. The total charge moving across the imaginary surface is the product of the imaginary surface area, A, and the normal component of polarization, P. If the polarization is tangential then no charge moves across the imaginary surface. Let $\hat{n}$ be the normal unit vector, then Equation (7) should, in general, be written as

$$\sigma_{pol} = \vec{P} \cdot \hat{n} . \qquad (15)$$

Equation (15) represents the charge that moves across the imaginary surface but not the net charge on the dielectric. This is because the dielectric contributes equally and oppositely on the two sides of the surface. The charge displacement may result in volume charge density. The charges displaced out of a volume by polarization could be calculated by taking the integral of the normal component of polarization over the surface bounding the volume, see Figure 4.

$$\Delta Q_{poll} = -\int_S \vec{P} \cdot \hat{n} da . \qquad (16)$$

This charge displaced out by polarization can also be written in terms of volume charge density as

$$\Delta Q_{pol} = \int_V \rho_{pol} d\tau . \qquad (17)$$

Combining Equations (16) and (17) yields

$$\int_V \rho_{pol} d\tau = -\int_S \vec{P} \cdot \hat{n} da . \qquad (18)$$

Using Gauss' theorem yields

$$\int_S \vec{P} \cdot \hat{n} da = \int_V \nabla \cdot \vec{P} d\tau \qquad (19)$$

Therefore

$$\int_V \rho_{pol} d\tau = -\int_V \nabla \cdot \vec{P} d\tau . \qquad (20)$$

It is trivial that the integrands of both integrals are equal, therefore

$$\rho_{pol} = -\nabla \cdot \vec{P} . \qquad (21)$$

This result implies that if the polarization is nonuniform then the divergence of polarization induces the volume charge density in the material.

Relating the above results to electromagnetic theory will give useful results, which will be used in the subsequent sections.

$$\nabla \cdot \vec{E} = \frac{\rho}{\varepsilon_0} . \qquad (22)$$

Assume ρ is the total volume charge density, which is the summation of, ρ_{pol} and ρ_{free} then

$$\nabla \cdot \vec{E} = \frac{\rho_{free} + \rho_{pol}}{\varepsilon_o} = \frac{\rho_{free} - \nabla \cdot \vec{P}}{\varepsilon_0} , \qquad (23)$$

$$\nabla \cdot (\vec{E} + \frac{\vec{P}}{\varepsilon_0}) = \frac{\rho_{free}}{\varepsilon_0}, \tag{24}$$

and

$$\nabla \cdot (\varepsilon_0 \vec{E} + \vec{P}) = \rho_{free}. \tag{25}$$

Now another vector field $\vec{D}(r)$ is defined as

$$\vec{D} = \varepsilon_0 \vec{E} + \vec{P}, \tag{26}$$

with

$$\nabla \cdot \vec{D} = \rho_{free}. \tag{27}$$

The vector $\vec{D}$ is called the electric displacement or the displacement, or, the $\vec{D}$ field. The significance of the $\vec{D}$ field is that its divergence only depends on the free charge density. The unit of the $\vec{D}$ field is the same as the polarization. It is measured in Coulombs per square meter.

Now by using boundary conditions, and the divergence and curl of a general field $\vec{F}$, some of the properties of the field can be determined. Assume there are two different mediums with a boundary common between them. At a region close to the boundary the field changes continuously, maybe quickly but not abruptly. This region, where the field changes, is called transition layer. Assume the thickness of this region is *h*. When the transition layer shrinks to zero the field becomes discontinuous. In the beginning, the divergence and the curl of the field is used in a continuous region and then where $h \to 0$.

Assume $d\tau$ is a volume element and use the divergence theorem to get

$$\oint_S \vec{F} \cdot d\vec{a} = \int_V \nabla \cdot \vec{F} d\tau \,. \qquad (28)$$

This could be applied to a small cylinder with height h and a cross sectional area Δa inside the transition layer. Assuming $\hat{n}$ is the normal unit vector to the cross sectional area, $\hat{n}_2 = \hat{n}$, $\hat{n}_1 = -\hat{n}$ and W is the field times the area of the wall of the cylinder, then

$$\oint_S \vec{F} \cdot d\vec{a} = \vec{F}_2 \cdot \Delta\vec{a} + \vec{F}_1 \cdot \Delta\vec{a} + W \,, \qquad (29)$$

and

$$\hat{n} \cdot (\vec{F}_2 - \vec{F}_1)\Delta a + W = \int_V \nabla \cdot \vec{F} d\tau = (h\nabla \cdot \vec{F})\Delta a \,. \qquad (30)$$

Assuming the transition layer shrinks to zero, W=0 since W is related to h. Therefore,

$$\vec{n} \cdot (\vec{F}_2 - \vec{F}_1) = \lim_{h \to 0} (h\nabla \cdot \vec{F}), \qquad (31)$$

and

$$\vec{F}_{2n} - \vec{F}_{1n} = \lim_{h \to 0} \left(h\nabla \cdot \vec{F}\right), \qquad (32)$$

where it is assumed that $\nabla \cdot \vec{F}$ increases as $h \to 0$, so that $h\nabla \cdot \vec{F}$ remains finite.

The curl of a general field can be used to find the tangential component of the field. Assume that $\hat{t}$ is the tangential unit vector to the

path C, $\hat{n}$ is the normal unit vector to the path C and $\hat{n}'$ is the normal unit vector to the area bounded by the path. These three unit vectors are perpendicular to one another. We can relate these unit vectors as follows:

$$\hat{n}' = \hat{n} \times \hat{t} \qquad \hat{t} = \hat{n}' \times \hat{n} \qquad \hat{n} = \hat{t} \times \hat{n}' \tag{33}$$

Also in this case consider a continuous region and then transfer to the discontinuous region where the transition layer shrinks to zero. Assume that $\hat{t}_2 = \hat{t}$ and $\hat{t}_1 = -\hat{t}$. In the following equations W is the contribution to the integral from the ends of the path.

$$\oint_C \vec{F} \cdot d\vec{s} = \oint_S (\nabla \times \vec{F}) \cdot d\vec{a}\,, \tag{34}$$

and

$$\oint_C \vec{F} \cdot d\vec{s} = \vec{F}_2 \cdot \hat{t}_2 \Delta s + \vec{F}_1 \cdot \hat{t}_1 \Delta s + W\,, \tag{35}$$

Strictly speaking $\vec{F}_2$, $\vec{F}_1$ and $\nabla \times \vec{F}$ are average values, and because h and Δs are very small, these vectors can be considered to be constant. Therefore,

$$\oint_C F \cdot d\vec{s} = (\nabla \times \vec{F}) \cdot \hat{n}' h \Delta s = \hat{t} \cdot (\vec{F}_2 - \vec{F}_1) \Delta s + W\,. \tag{36}$$

It is known that for vectors, $\vec{A}, \vec{B}, \vec{C}$

$$\vec{A} \cdot (\vec{B} \times \vec{C}) = (\vec{A} \times \vec{B}) \cdot \vec{C}\,. \tag{37}$$

Assume $h \to 0$ then W =0 as it is related to h. Now divide both sides of the Equation (36) by Δs. Next using the middle property of Equation (33) and Equation (37) then Equation (36) becomes

$$\hat{n}' \cdot [\hat{n} \times (\vec{F}_2 - \vec{F}_1) - \lim_{h \to 0} (h \nabla \times \vec{F})] = 0 . \qquad (38)$$

The only way for Equation (38) to always be true is for the term in the brackets to be zero. Therefore, Equation (38) becomes,

$$\hat{n} \times (\vec{F}_2 - \vec{F}_1) = \lim_{h \to 0} [(h \nabla \times \vec{F})] \qquad (39)$$

To make Equation (39) more easily interpretable define $\vec{F}$ in terms of its tangential and normal components

$$\vec{F} = \vec{F}_n + \vec{F}_t = F_n \hat{n} + \vec{F}_t . \qquad (40)$$

Consequently,

$$\hat{n} \times \vec{F} = F_n \hat{n} \times \hat{n} + \hat{n} \times \vec{F}_t = \hat{n} \times \vec{F}_t , \qquad (41)$$

This result indicates that only the tangential component of $\vec{F}$ is involved. Therefore, Equation (39) becomes,

$$\hat{n} \times (\vec{F}_{2t} - \vec{F}_{1t}) = \lim_{h \to 0} (h \nabla \times \vec{F}) . \qquad (42)$$

Other useful vector properties are

$$\begin{matrix} \vec{A}\times\vec{B} = -(\vec{B}\times\vec{A}) \\ \vec{A}\cdot\vec{A} = A^2 \end{matrix} , \qquad (43)$$

and

$$\vec{A}\times(\vec{B}\times\vec{C}) = \vec{B}(\vec{A}\cdot\vec{C}) - \vec{C}(\vec{A}\cdot\vec{B}) \qquad (44)$$

Using Equations (43), (44) and (40), yields

$$(\hat{n}\times\vec{F})\times\hat{n} = -\hat{n}\times(\hat{n}\times\vec{F}) = -[\hat{n}(\hat{n}\cdot\vec{F}) - \vec{F}(\hat{n}\cdot\hat{n})]. \quad (45)$$

Consequently,

$$(\hat{n}\times\vec{F})\times\hat{n} = -\vec{F}_n\hat{n} + \vec{F} = \vec{F} - \vec{F}_n\hat{n} = \vec{F}_t. \qquad (46)$$

Crossing Equation (42) into $\hat{n}$ and using Equation (46),

$$\vec{F}_{2t} - \vec{F}_{1t} = \lim_{h\to 0}[h(\nabla\times\vec{F})\times\hat{n}]. \qquad (47)$$

If this difference is not zero then the tangential component of the field is discontinuous. However, if this difference is zero then the tangential component of the field is unchanged and continuous.

When the transition layer is shrunk to zero, the total charge remains conserved and can be determined by the surface charge density, σ, as follows:

$$\Delta q = \sigma\Delta a = (\lim_{h\to 0} h\rho)\Delta a, \qquad (48)$$

and

$$\sigma = \lim_{h \to 0} (h\rho). \tag{49}$$

Using Equations (32), (22) and (49) some of the properties of the electric field can be shown, such as

$$\hat{n} \cdot (\vec{E}_2 - \vec{E}_1) = \vec{E}_{2n} - E_{1n} = \frac{\sigma}{\varepsilon_0}. \tag{50}$$

Using the vector property that the curl of the gradient of any function is zero and assuming V to be the potential difference, another property of electric field is

$$\nabla \times \vec{E} = \nabla \times \nabla V = 0. \tag{51}$$

Therefore, the tangential component of electric field is unchanged and continuous as it is related to the curl of the electric field. Therefore

$$\vec{E}_{2t} - \vec{E}_{1t} = 0. \tag{52}$$

Now some of the properties of the $\vec{D}$ field can be determined. Using Equations (27), (32) and (49)

$$\hat{n} \cdot (\vec{D}_2 - \vec{D}_1) = D_{2n} - D_{1n} = \sigma_{free}, \tag{53}$$

where σ_{free} is the surface density of free charge. This result indicates that the $\vec{D}$ field is discontinuous when free surface charge density is present, whereas the electric field is discontinuous when a surface charge density of any kind is present.

Now find the curl of the $\vec{D}$ field by taking the curl of Equation (26) and applying Equation (51),

$$\nabla \times \vec{D} = \nabla \times \vec{P}. \qquad (54)$$

This result shows that the $\vec{D}$ field can have sources in bound charges as well as free charges. The tangential component of the $\vec{D}$ field can be found by using Equations (26), and (52)

$$\vec{D}_{2t} - \vec{D}_{1t} = \vec{P}_{2t} - \vec{P}_{1t}. \qquad (55)$$

2. Microscopic Properties

Gases

In this section most of the discussion is based on Feynman[9] and Wangsness[10]. However, Kittel[12], Jackson[13], Hecht[14] and Wert and Thomson[15] were also used. The microscopic discussions are adapted from Feynman[9] and Hecht[14], and the macroscopic discussions are adapted from Wangsness[10], Jackson[13], Hecht[14], and Wert and Thomson[15].

In this section, the nature of dielectrics and why they are dielectric are discussed. In the last section it was mentioned that the properties of electrical systems with dielectrics could be understood by applying an electric field to a dielectric. When an electric field is applied to the dielectric it induces dipole moments in the atoms. If the electric field induces an average dipole moment per unit volume P, then the dielectric constant κ is given by

$$\kappa - 1 = \frac{P}{\varepsilon_0 E}. \tag{56}$$

The application of this equation has already been discussed; now the mechanism by which polarization occurs when an electric field is present in the material is discussed. Although complications can't be avoid completely, they can be reduced by beginning with gases. There are two types of gases. The molecules of some gases like oxygen have no inherent dipole moment. This is due to the symmetric pair of atoms in each molecule, which creates the same center of charge for both positive charges and negative charges as shown in Figure 5. Such a molecule is called a

nonpolar molecule. It does become a polar molecule when it is subject to an electric field. On the other hand, a molecule of water vapor has an average positive charge on hydrogen atoms and an average negative charge on oxygen atom. Since the center of charge of the positively charged atoms, hydrogen, and negatively charged atoms, oxygen, do not coincide the total charge distribution has a dipole moment as shown in Figure 6.

In the case of the simplest monatomic nonpolar gas like helium the electrons and the protons are displaced relative to each other when the electric field is present. Thus, the dipole moment is induced and consequently polarization is induced. This type of polarization is called electronic polarization.

When an atom is subject to an oscillating field the position of the electron obeys the equation

$$m\frac{d^2x}{dt^2} + m\omega_0^2 x = qE. \qquad (57)$$

The first term is the electron mass times its acceleration, the second is the restoring force, while the right hand side is the external force due to the electric field. For a frequency-varying field, Equation (57) has the solution

$$x = \frac{qE}{m(\omega_0^2 - \omega^2)}, \qquad (58)$$

where ω_0 is the natural frequency and ω is the optical frequency. It has a resonance at $\omega = \omega_0$. At this frequency the optical frequency is absorbed. However, in this section consider the case where the field is constant and

changing with neither time nor frequency. Thus, first term is cancelled and the solution will be

$$x = \frac{qE}{m\omega_0^2}. \tag{59}$$

Thus, the magnitude of the dipole moment of a single atom is

$$p = qx = \frac{q^2 E}{m\omega_0^2}. \tag{60}$$

From Equation (60) it is obvious that the dipole moment of an atom is linearly proportional to the applied electric field. Equation (60) can be written as follows

$$\vec{p} = \alpha\, \varepsilon_0 \vec{E}. \tag{61}$$

The constant α is called polarizability and it measures how easily the dipole of moment is induced in an atom by electric field. It is measured in m^3. Equations (60) and (61) indicate that

$$\alpha = \frac{q^2}{\varepsilon_0 m\omega_0^2} = \frac{4\pi e^2}{m\omega_0^2}, \tag{62}$$

where the middle expression of Equation (62) is in Gaussian units, the expression to the right is in SI units and e is the charge of the electron.

If there are N atoms in a unit volume then the polarization, the dipole moment per unit volume, is given by

$$\vec{P} = Np = N\alpha\,\varepsilon_0 \vec{E}\,. \qquad (63)$$

Combining Equations (56) and (63) yields,

$$\kappa - 1 = \frac{P}{\varepsilon_0 E} = N\alpha\,. \qquad (64)$$

From Equation (62),

$$\kappa - 1 = \frac{4\pi\ Ne^2}{m\,\omega_0^2}\,. \qquad (65)$$

Equation (64) indicates that the dielectric constant is dependent on the density of the gases.

Equation (65) is a rough approximation as it ignores complications due to quantum mechanics. This formula works quite accurately for a gas with one frequency. This classical formula gives a reasonable estimate for the dielectric constant.

Now consider the case where the molecule is a polar molecule, which carries a permanent dipole moment such as water molecule. When an electric field is not present the dipole moments are randomly oriented; thus, the net polarization is zero as in Figure 7. When an electric field is applied, two things may happen. First, the electric field pushes the negative and positive charges to opposite sides and a dipole moment per unit volume is induced exactly the same as the electronic polarization. Second, the electric field also induces an extra dipole moment per unit volume because the electric field lines up the permanent dipole moment of the polar molecules. However, at normal temperature and low electric field, the collision of

molecules due to thermal motion keeps them from lining up. Therefore, the electric field can not align all the permanent dipole moment. Yet, there is some net alignment and consequently some polarization, see Figure 8. The polarization can be calculated by the method of statistical mechanics.

Methods from statistical mechanics can be used to discuss the energy a dipole, p_0, in an electric field, E. Assume the energy of the positive charge is $qV(1)$ and that of the negative charge is $-qV(2)$. Thus, the energy of the dipole is

$$U = qV(1) - qV(2) = q\vec{d} \cdot \nabla V , \qquad (66)$$

or

$$U = -\vec{p}_0 \cdot \vec{E} = -p_0 E \cos(\theta), \qquad (67)$$

where θ is the angle between the permanent moment p_0 and E. The energy is lower when the dipoles are lined up with the electric field.

How many dipoles line up with the field is calculated by using statistical mechanics. From thermodynamics it is known that the relative number of molecules with a given potential energy is proportional to

$$e^{-U/kT}, \qquad (68)$$

where $U(x,y,z)$ is the potential energy as a function of position, T is the temperature and k is the Boltzmann constant. The same argument states that Equation (67) is the potential energy as a function of angle, θ. The number of molecules at θ per unit solid angle is proportional to $e^{-U/KT}$.

Assuming $N(\theta)$ is the number of molecule per unit solid angle at θ and using Equation (67) for potential energy one obtains

$$N(\theta) = N_0 e^{p_0 E\cos(\theta)/kT}. \qquad (69)$$

For ordinary temperatures and fields, the exponent is small which permits the approximation of Equation (69) by expanding the exponential. Thus,

$$N(\theta) = \left(1 + \frac{p_o E\cos\theta}{kT}\right). \qquad (70)$$

N_0 is found by integrating Equation (69) over all angles. The result should be the total number of molecules per unit volume, n. Therefore,

$$N = \int_0^{4\pi} N(\theta)d\Omega = \int_0^{4\pi} N_0\left(1 + \frac{p_0 E\cos\theta}{kT}\right)d\Omega, \qquad (71)$$

$$N = 4\pi N_0. \qquad (72)$$

Therefore,

$$N_0 = \frac{N}{4\pi}. \qquad (73)$$

It is obvious from Equation (70) that more molecules are accumulated along the field when $\cos(\theta) = 1$ than when $\cos(\theta) = -1$. This ensures the existence of a dipole moment per unit volume, a polarization P. To calculate the polarization $\vec{P}$, the vector sum of the polarization of the molecules is

required. Since the direction of the polarization $\vec{P}$ is in the same as the direction of the field, thus just sum the components in that direction. The components normal to this direction will sum to zero. Therefore,

$$P = \sum_{\substack{unit \\ volume}} p_0 \cos\theta_i . \qquad (74)$$

This can be evaluated by integrating over the angular distribution. The solid angle at θ is $2\pi \sin\theta d\theta$, thus

$$P = \int_0^{\pi} N(\theta) p_0 \cos(\theta) 2\pi \sin(\theta) d\theta . \qquad (75)$$

Substituting from Equation (70) yields,

$$P = -\frac{N}{2} \int_0^{\pi} (1 + \frac{p_0 E}{kT} \cos\theta) p_0 \cos(\theta) d(\cos\theta) . \qquad (76)$$

This integration could easily be solved to give,

$$P = \frac{N p_0^2 E}{3kT} . \qquad (77)$$

Equation (77) shows that the polarization is linearly proportional to the electric field, so there will be normal dielectric behavior. It also shows that polarization is inversely proportional to the temperature, because the higher the temperature the more misalignment by collisions. The inverse

proportionality of polarization to temperature ($P \propto 1/T$) is called Curie's law. The aligning force depends on the permanent moment p_0 and so does the mean moment produced by lining up. Therefore, the induced moment is proportional to p_0^2. This is why in Equation (77) the polarization is linearly proportional to the square of the permanent moment. However, polarization $\vec{P}$ can't be evaluated because p_0 is unknown.

Using the result of polarization from Equation (77) in Equation (56) yields,

$$\kappa - 1 = \frac{P}{\varepsilon_0 E} = \frac{N p_0^2}{3 \varepsilon_0 kT}. \qquad (78)$$

This equation indicates that $\kappa - 1$ is linearly proportional to the density, N and inversely proportional to the temperature T.

Liquids

Liquids are denser materials than gas which makes the subject more interesting and at the same time more complicated. Assume some nonpolar liquid like liquid helium or liquid argon. These liquids may not have a molecular polarization. However, they can still have electronic polarization since electrons are very light and can adjust themselves to optical frequencies. Polarization in dense materials is high, so that the polarization of atoms will influence the electric field on an individual atom. The question may arise as to what electric field acts on an atom.

Assume liquid is put between the plates of a capacitor. When the plates are charged there will be electric field in the liquid. Yet, there is electric field due to the charges of atoms as well. Consequently, the total

electric field is the sum of the external electric field and the electric field due to the charges of an individual atom. This electric field is no longer constant but changes very rapidly. It differs from one point to another. It is high inside the atom especially closer to the nucleus, and small between the atoms. The potential difference between the plates of the capacitor can be evaluated by taking the line integral of this field. Ignoring the small variation of the field then the field is just V/d. It should be considered that this is the average field over a space containing many atoms.

However, this is not that simple because different-shaped holes in a polarized dielectric produce different fields. For instance, if we cut a slot in a dielectric parallel to the field as shown in Figure 9, then $\nabla \times \vec{E} = 0$ which yields the line integral of $\vec{E}$ around the curve to be zero. This means that the field inside cancels the field outside. Therefore, the field inside at the center of the slot, $\vec{E}_i$ is the same as the average field found in the dielectric, $\vec{E}$.

Now assume that the slot is cut perpendicular to the field in a previously polarized dielectric as illustrated in Figure 10. In this case the field inside the slot, $\vec{E}_i$ is not the same as the average field, $\vec{E}$. The field inside the slot is the sum of the average field in dielectric and the field due to polarization. Therefore,

$$E_i = E + \frac{P}{\varepsilon_0}, \tag{79}$$

$$\varepsilon_0 E_i = \varepsilon_0 E + P. \tag{80}$$

From Equation (26) $D = \varepsilon_0 E + P$; thus, it can be inferred that $\varepsilon E_i = D_i$ which is equal to D in the dielectric. The average field $\vec{E}$ can be measured by measuring the electric field $\vec{E}_i$ inside the slot cut parallel to the field. Also the $\vec{D}$ field can be found by measuring the field $\vec{E}_i$ inside the slot cut normal to the field.

For most non-complicated liquids it can be expected that an atom is surrounded by other atoms and is influenced by them. The electric field on an atom is due to its charges and the charges of other atoms surrounding this atom. Now imagine that the atom is spherical in shape, then when the sphere is cut from the polarized dielectric the hole will be spherical. Thus, the field in that in the dielectric is the sum of the field in the hole, local field, E_L and the field of the polarized sphere E_{pol}. Therefore,

$$E = E_L + E_{pol}. \tag{81}$$

From this equation the field inside the hole can be determined which is

$$E_L = E - E_{pol}. \tag{82}$$

Now the field in the polarized sphere E_{pol} can be found. Consider a sphere of radius a with constant polarization $\vec{P}$. Assume electric field $\vec{E}$ is in the z direction and the origin is at the center of the sphere; thus $\vec{E} = E\hat{z}$. The subscripts o and i are used for outside and inside respectively. A boundary condition is used to find the electric field outside the sphere and inside the sphere. At large distances, the field is uniform, so one boundary condition is

$$V(r,\theta) \xrightarrow[r\to\infty]{} -E_o z = -E_o r\cos\theta \,. \qquad (83)$$

The surface of the sphere is the surface of discontinuity between the dielectric and the vacuum. At this region the normal component of $\vec{D}$ and tangential components of $\vec{E}$ are continuous. Therefore,

$$\begin{aligned} &\hat{n}\cdot(\varepsilon_2\vec{E}_2 - \varepsilon_1\vec{E}_1) = \sigma_{free} = 0 \\ &\vec{E}_{2t} - \vec{E}_{1t} = 0 \end{aligned} \qquad (84)$$

Since E_r and E_θ are the normal and tangential components of $\vec{E}$, so write Equation (84) can be written in terms of the derivatives of V. Thus, have

$$\begin{aligned} &\left(-\varepsilon_0 \frac{\partial V_o}{\partial r}\right)_{r=a} = \left(-\varepsilon \frac{\partial V_i}{\partial r}\right)_{r=0} \\ &\left(-\frac{1}{r}\frac{\partial V_o}{\partial \theta}\right)_{r=0} = \left(-\frac{1}{r}\frac{\partial V_i}{\partial \theta}\right)_{r=0} \end{aligned} \qquad (85)$$

There is another boundary condition, which is at $r = 0$. At this point assume that there is no charge located there, as this is the only option which results in finite electric potential. Therefore,

$$V \text{ is finite for } r = 0. \qquad (86)$$

Now the solution to Laplace's equation is used to find the potential outside the dielectric. Thus, the potential becomes

$$V(r,\theta)=\sum_{l=0}^{\infty}\left(A_l r^l+\frac{B_l}{r^{l+r}}\right)P_l(\cos\theta), \qquad (87)$$

The first few Legendre polynomials are

$$P_0(\cos\theta)=1 \quad P_1(\cos\theta)=\cos\theta$$
$$P_2(\cos\theta)=\frac{1}{2}(3\cos^2\theta-1) \qquad (88)$$

From these Legendre polynomials we can infer that $l=1$. Therefore,

$$V_o=\left(-A_o r+\frac{B_o}{r^2}\right)\cos\theta. \qquad (89)$$

Where A_o and B_o are constants. We can also write the same equation for V_i assuming A_i and B_i are constants

$$V_i=\left(-A_i r+\frac{B_i}{r^2}\right)\cos\theta. \qquad (90)$$

Combining Equations (83) and (89) $A_o = E_o$ and Equation (89) becomes

$$V_o = \left(-E_0 r + \frac{B_o}{r^2}\right)\cos\theta . \qquad (91)$$

It is obvious from Equation (90) that $B_i = 0$, otherwise $\frac{1}{r} \to \infty$ as $r \to 0$ which is not allowable according to Equation (86). Therefore, Equation (90) reduces to the following equation

$$V_i = -A_i r\cos\theta . \qquad (92)$$

Substituting (91) and (92) into (85) and using $\varepsilon = \kappa\varepsilon_0$ we get the following two equations

$$E_o + \frac{2B_o}{a^3} = \kappa A_i \qquad -E_o a + \frac{B_o}{a^2} = -A_i a . \qquad (93)$$

Solving these two equations we get $A_i = 3E_o/(\kappa+2)$ and $B_o = \left[(\kappa-1)/(\kappa+2)\right]a^3 E_o$, so the outer and inner potentials become

$$V_o = -E_o r\cos\theta + \left(\frac{\kappa-1}{\kappa+2}\right)\frac{a^3 E_o\cos\theta}{r^2}, \qquad (94)$$

$$V_i = -\left(\frac{3E_o}{\kappa+2}\right)r\cos\theta . \qquad (95)$$

Before finding the field inside the sphere, introduce a useful vector property and the del operator (∇) in spherical coordinates,

$$\hat{z} = \hat{r}\cos\theta - \hat{\theta}\sin\theta\,, \tag{96}$$

and

$$\nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}. \tag{97}$$

The field inside the sphere is $\vec{E}_i = -\nabla V_i = \vec{E}_i\hat{z}$, and using Equations (97) and (96) and $\vec{E}_o = E_o\hat{z}$ yields

$$\vec{E}_i = -\nabla V_i = \left(\frac{3E_o}{\kappa+2}\right)\left(\hat{r}\cos\theta - \hat{\theta}\sin\theta\right), \tag{98}$$

$$\vec{E}_i = \left(\frac{3E_o\hat{z}}{\kappa+2}\right) = \left(\frac{3}{\kappa+2}\right)\vec{E}_o. \tag{99}$$

This equation indicates that $|\vec{E}_i| < |\vec{E}_o|$ since $\kappa > 1$. However, the field inside the sphere is parallel to the external field but smaller than it. Consequently polarization is constant and can be evaluated from Equations (10), (14) and (99) as,

$$\vec{P} = \left(\frac{\kappa-1}{\kappa+2}\right)3\varepsilon_0 E_o. \tag{100}$$

The magnitude of the dipole moment can be found by multiplying P by the volume of the sphere

$$p = 4\pi\left(\frac{\kappa-1}{\kappa+2}\right)a^3\varepsilon_0 E_0. \tag{101}$$

Thus Equation (94) can be written as follows

$$V_o = -E_o r\cos\theta + \frac{p\cos\theta}{4\pi r^3}. \qquad 0(102)$$

Now substituting Equation (100) in Equation (99) and subtracting E_o from both sides yields,

$$\vec{E}_i = \vec{E}_o - \frac{\vec{P}}{3\varepsilon_0}. \qquad (103)$$

This equation is the general equation for a spherical dielectric in a field. Assume that this sphere is a tiny part of the dielectric, which is cut and isolated from it and no longer experiences the external field. The field inside the sphere is just due to the superposition of the field produced by the polarized molecules within the sphere. Consequently the field inside this sphere reduces to

$$\vec{E}_i = -\frac{\vec{P}}{3\varepsilon_0}. \qquad (104)$$

It should be noted that for points inside a polarized dielectric sphere, the direction of the electric field due to the polarization of the molecules is opposite of the polarization vector, see Figure 11. This is why the negative sign appears in Equation (104). Now substituting Equation (104) in Equation (82) produces

$$E_L = E + \frac{P}{3\varepsilon_0}. \qquad (105)$$

This result may be used for a spherical cavity as a local, microscopic field experienced by an atom inside the liquid. Since in a liquid dielectric the atoms are randomly distributed. For crystals in which the atoms are arranged in an orderly pattern, this result is not generally true.

Using Equation (105) in Equation (63),

$$P = N\alpha\,\varepsilon_0\left(E + \frac{P}{3\varepsilon_0}\right), \tag{106}$$

or

$$P = \frac{N\alpha}{1-(N\alpha/3)}\varepsilon_0 E. \tag{107}$$

Using Equation (56) in Equation (107) yields,

$$\kappa - 1 = \frac{N\alpha}{1-(N\alpha/3)}. \tag{108}$$

This gives the dielectric constant in terms of α, the atomic polarizability, which is called the Clausius-Mossotti equation.

Due to the small density in a gas, $N\alpha$ is very small and the term $N\alpha/3$ in the denominator of Equation (108) is negligible compared to 1. In this way the previous result in Equation (64) is obtained, which is $\kappa - 1 = N\alpha$.

Solids

Many phenomena that were well understood from gases are more complicated in the liquid and especially the solid state. Since distances of

separation are in the atomic range, the interaction between atoms can not be neglected. These interactions can be evaluated only by approximation. Consequently, the study of polarization of atoms and molecules in solids are more complicated than the same study for gases.

Some solids like crystalline substances have permanent polarization. The unit cells of such crystals have identical permanent polarizations pointing in the same direction. Some complicated crystals have permanent dipoles but because their surfaces gain free charges from air they are discharged and seem to be nonpolarized.

Another class of dielectrics that is of interest is the ferroelectrics, which exhibit the phenomenon of self-polarization. They are so called because of they are electrically analogous to ferromagnetics, not because they are related to iron. In such crystals, the dipoles align themselves by mutual interaction. This aligning tendency transfers from one atom to another so that the whole crystal may show polarization in a given direction. However, the polarization of such crystals is temperature dependent. In such crystals the polarization exists at low temperature up to certain temperature called the Curie temperature, T_c. Above the Curie temperature, the polarization of a ferroelectric substance may break down.

To find the polarization of a solid, the local field in each unit cell must first be found. The contribution due to polarization must be included. Yet, the use of a spherical hole is not possible for the determination of the local field, because a crystal is not homogenous like a liquid. To determine the local field for a crystal the factor 1/3 in Equation (104) will be slightly different. For a simple cubic crystal it could be assumed to be just 1/3.

In Equation (108) if $N\alpha$ is greater than 3 then κ will be negative which is not correct. If α is increased the polarization gets larger and so

does the local field. If this feedback is taken to its logical conclusion, the polarization increases without limit. Of course the polarization actually remains finite as for high fields the proportionality between the field and the polarization breaks down and Equation (108) is no longer correct. Therefore, the polarization and the field increase until $n\alpha = 3$.

Let us now consider barium titanate, $BaTiO_3$ which can be assumed to be a simple cubic crystal and the unit cell of which is shown in Figure 12. In addition to electronic polarization, it has ionic polarization due to the titanium ions, which can move a little bit within the lattice. Consequently, the crystal is left with a permanent dipole. An interesting thing about barium titanate is that if $N\alpha$ is decreased slightly the aligned dipoles become unstuck. Since N decreases as the temperature increases due to thermal expansion we can vary $N\alpha$ by varying the temperature. Below the Curie temperature T_C the dipoles are barely stuck that the polarization can be shifted and be locked in a different direction by applying an external field.

This matter can be analyzed in more detail. The Curie temperature is called T_c the temperature at which $N\alpha$ is 3. As the temperature increases, N goes down slightly because of the expansion of the lattice. Since the expansion is small,

$$N\alpha = 3 - \beta(T - T_c), \qquad (109)$$

where β is a small constant about 10^{-5} or 10^{-6} per $^{\circ}C$. Substituting this result in Equation (108) yields,

$$\kappa - 1 = \frac{3 - \beta(T - T_C)}{\beta(T - T_C)/3}. \qquad (110)$$

Under the assumption that $T \to T_C$, $\beta(T - T_C)$ is very small compared with 3 and can be neglected in the numerator and Equation (110) can be approximated by

$$\kappa - 1 = \frac{9}{\beta(T - T_C)}. \qquad (111)$$

This result is true only if $T > T_C$, it indicates that for a temperature slightly larger than the Curie temperature the dielectric constant increases enormously because $N\alpha$ gets close to 3. The dielectric constant may reach to 50,000 or 100,000 which indicates the sensitivity of the system to the temperature. This law is called the Curie-Weiss law.

For a cubic crystal like barium titanate the field for each atom in the chain as shown in Figure 13 can be found. Then the field for the whole chain can be found. Between the oxygen and titanate ions there are other chains of oxygen or titanium or others. These are ignored since they are weak due to the large spacing between the ions. The separation between ions of oxygen and titanium is a, which is half of the lattice constant. For simplicity assume that all ions on the main chain are identical.

What will happen when $T \to T_C$? Assume the dipole moment of each atom is p. First the field at one of the atoms from the dipoles in only one vertical chain is evaluated. The field at the distance r from a point dipole can be found by taking the derivative of the potential difference. The potential difference in terms of dipole moment can be written as,

$$V = \frac{\vec{p} \cdot \hat{r}}{4\pi\,\varepsilon_0 r^2} = \frac{p\cos\theta}{4\pi\,\varepsilon_0 r^2}. \qquad (112)$$

The electric field is calculated from,

$$\vec{E} = -\nabla V = -\frac{dV}{dr}\hat{r} - \frac{1}{r}\frac{dV}{d\theta}\hat{\theta}. \qquad (113)$$

Therefore,

$$\vec{E} = \frac{p}{4\pi\,\varepsilon_0 r^3}\left(2\cos\theta\,\hat{r} + \sin\theta\hat{\theta}\right). \qquad (114)$$

and

$$\vec{E} = \frac{p}{4\pi\,\varepsilon_0 r^3}\left(3\cos\theta\,\hat{r} - \cos\theta\,\hat{r} + \sin\theta\,\hat{\theta}\right).. \qquad (115)$$

From vector analysis $\hat{z} = \cos\theta\,\hat{r} - \sin\theta\,\hat{\theta}$, therefore

$$\vec{E} = \frac{p}{4\pi\,\varepsilon_0 r^3}\left(3\cos\theta\,\hat{r} - \hat{z}\right), \qquad (116)$$

and

$$\vec{E} = \frac{1}{4\pi\,\varepsilon_0 r^3}\left(3p\hat{r} - p\hat{z}\right) = \frac{1}{4\pi\,\varepsilon_0 r^3}\left[3\left(\vec{p}\cdot\hat{r}\right)\hat{r} - p\hat{z}\right].. \qquad (117)$$

Assume that p is in the z direction then the electric field is,

$$\vec{E} = \frac{1}{4\pi\,\varepsilon_0 r^3}\left(3p\hat{r} - p\hat{z}\right) = \frac{1}{4\pi\,\varepsilon_0 r^3}\left[3\left(\vec{p}\cdot\hat{r}\right)\hat{r} - \vec{p}\right]. \qquad (118)$$

Assuming $\vec{p}$ and $\vec{r}$ are in the same direction then the field at the distance r from a dipole in a direction along its axis is

$$E \frac{1}{4\pi \varepsilon_0} \frac{2p}{r^3}. \qquad (119)$$

The result in equation (118) is the solution to Wangsness problem 13 in chapter 8.

For a particular atom, the field above and below that atom for the whole chain, see Figure 13, is given by

$$E_{chain} = \frac{2p}{4\pi \varepsilon_0} \frac{1}{r^3} \left(2 + \frac{2}{8} + \frac{2}{27} + \frac{2}{64} + ... \right), \qquad (120)$$

Using the Quattro Pro spreadsheet[16], it was found that the summation in parenthesis converges to 2.406, therefore

$$E_{chain} = \frac{0.383}{a^3} \frac{p}{\varepsilon_0}. \qquad (121)$$

Assuming that the induced moment $\vec{p}$ of each atom of the chain is proportional to the field on it as in Equation (61), and using Equations (61) and (121) yields

$$\alpha = \frac{a^3}{0.383}. \qquad (122)$$

This result is true for barium titanate when it reaches the Curie temperature. The spacing for barium titanate is $2\times10^{-8}cm$, thus $\alpha = 2.18\times10^{-24}cm^3$. For oxygen $\alpha = 30.2\times10^{-24}cm^3$ and for barium $\alpha = 2.4\times10^{-24}cm^3$. If the average taken, which is $\alpha_{av} = 16.3\times10^{-24}cm^3$, a reasonable value is obtained. This is the electronic polarizability, the ionic polarizability should also be found and added to this result.

Feynman[9] offers a good question, problem (11.4), where a line of oxygen atoms with polarizability α_O, regularly spaced with a distance a between each atom and a titanium atom with polarizability α_T halfway in between successive oxygen atoms is given as shown in Figure 14 such that the system is ferroelectric. The electric field for both oxygen and titanium can be found as follow

$$E_O = \frac{2p_O}{4\pi\varepsilon_0}\left(\frac{2}{(a)^3}+\frac{2}{(2a)^3}+\frac{2}{(3a)^3}+....+\frac{2}{(Na)^3}\right)+ \frac{2p_T}{4\pi\varepsilon_0}\left(\frac{2}{(a/2)^3}+\frac{2}{(3a/2)^3}+....+\frac{2}{((2N-1)a/2)^3}+\right). \quad (123)$$

The quantity inside the parenthesis is multiplied by 2 for the symmetry above and below the specific atom.

$$E_O = \frac{p_O}{\pi\varepsilon_0 a^3}\sum_{N=1}^{\infty}\frac{1}{N^3}+\frac{8p_T}{\pi\varepsilon_0 a^3}\sum_{N=1}^{\infty}\frac{1}{(2N-1)^3}. \quad (124)$$

By using the Quattro Pro spreadsheet[16] it was found that,

$$\sum_{N=1}^{\infty}\frac{1}{N^3}=1.202 \quad \text{and} \quad \sum_{N=1}^{\infty}\frac{1}{(2N-1)^3}=1.0518. \tag{125}$$

Therefore,

$$\begin{aligned} E_O &= \frac{0.383\,p_O}{\varepsilon_0 a^3}+\frac{2.678\,p_T}{\varepsilon_0 a^3} \\ E_T &= \frac{0.383\,p_T}{\varepsilon_0 a^3}+\frac{2.678\,p_O}{\varepsilon_0 a^3}. \end{aligned} \tag{126}$$

From Equation (61) the following identities can be obtained,

$$\begin{aligned} p_O &= \alpha_O \varepsilon_O E_O \\ p_T &= \alpha_T \varepsilon_O E_T \end{aligned}. \tag{127}$$

Substituting Equation (127) in Equations (126) and rearranging the following results are obtained,

$$E_O\left(1-\frac{0.38}{a^3}\alpha_O\right)=E_T\left(\frac{2.678}{a^3}\alpha_T\right), \tag{128}$$

and

$$E_O\left(\frac{2.678}{a^3}\alpha_O\right)=E_T\left(1-\frac{0.38}{a^3}\alpha_T\right). \tag{129}$$

Dividing Equation (128) by (139), assuming $x_O=\frac{\alpha_O}{a^3}$ and $x_T=\frac{\alpha_T}{a^3}$ and rearranging the equation yields

$$x_O = \frac{1 - 0.383 x_T}{0.383 + 7.03 x_T}$$
$$x_T = \frac{1 - 0.383 x_O}{0.383 + 7.03 x_O}. \qquad (130)$$

The graph of which is shown in Figure (15).

The effective polarizability for barium titanate is

$$\alpha_{eff} = a^3 (x_O + x_T). \qquad (131)$$

3. Wave Propagation

In this section the principal references are Wangsness[10], Jackson[13], Feynman[17], Bohren and Huffman[2], and Hecht[14]. Bohren and Huffman[2] offered two good questions that were solved and were used as the basis for a relevant discussion.

Unlike the mechanical waves, electromagnetic waves can travel through free space without the need of any medium. They are so called because they are electric and magnetic fields that can travel in space. The electric and the magnetic fields are perpendicular to one another and that is why they are transverse waves. The main sources of the electromagnetic waves are oscillating and accelerating charges. When a charge starts to accelerate the electric field in the vicinity of the charge is changed. The time-varying electric field induces a time dependent magnetic field. The time dependent magnetic field generates a time dependent electric field, and this field again induces a magnetic field. This process continues and the electromagnetic wave is propagated in space. This is why electromagnetic waves can travel great distances through space and be detected.

The fundamental nature of different electromagnetic fields can be explained by Maxwell's equations. The electric and the magnetic properties of solids can also be described in detail by Maxwell's equations. Maxwell's equations are[10]

$$\nabla \cdot \vec{D} = \rho_{free}, \tag{132}$$

$$\nabla \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0, \tag{133}$$

$$\nabla \cdot \vec{B} = 0, \tag{134}$$

$$\nabla \times \vec{H} = \vec{J}_{free} + \frac{\partial \vec{D}}{\partial t}, \tag{135}$$

where $\vec{B}$, $\vec{H}$, and $\vec{J}_{free}$ are magnetic induction, magnetic field and displacement current density due to free charges respectively. Equation (132) is exactly the same as the Equation (27). The electric displacement or $\vec{D}$ field has already been defined in Equation (26), and the magnetic field $\vec{H}$ can be defined as,

$$\vec{H} = \frac{\vec{B}}{\mu_0} - \vec{M}, \tag{136}$$

where μ_0 is the permeability, and $\vec{M}$ is the magnetization, average magnetic dipole moment per unit volume. Equations (132)-(135) are not sufficient in themselves. It must be specified how $\vec{J}$, $\vec{B}$, $\vec{P}$, and $\vec{D}$ are related to $\vec{E}$ and $\vec{H}$. These "constitutive relations" are,

$$\vec{J}_{free} = \sigma \vec{E}, \tag{137}$$

$$\vec{B} = \mu \vec{H}, \tag{138}$$

$$\vec{P} = \varepsilon_0 \chi \vec{E}, \tag{139}$$

$$\vec{D} = \varepsilon \vec{E}, \tag{140}$$

where σ is the conductivity and μ is the permeability. The coefficients σ, χ and μ depend on the medium. Now assume that the fields are complex fields, hence,

$$\vec{F} = \vec{F}_c e^{-i\omega t}. \tag{141}$$

Then Equation (132) can be solved

$$\nabla \cdot \vec{D} = \rho_{free} \Rightarrow \nabla \cdot (\varepsilon' \vec{E}) = \rho_{free}. \tag{142}$$

$$\nabla \cdot (\varepsilon' \vec{E}_c e^{-i\omega t}) = \rho_{free}. \tag{143}$$

Differentiating both sides with respect to time and using the continuity relation gives,

$$\frac{\partial \rho_{free}}{\partial t} = -\nabla \cdot \vec{J}_{free}, \tag{144}$$

from which the following result can be obtained.

$$-i\omega \nabla \cdot (\varepsilon \vec{E}_c' e^{-i\omega t}) - \nabla \cdot \vec{J}_{free}. \tag{145}$$

Substituting Equation (137) in Equation (145) and rearranging yields,

$$\nabla \cdot \left(\varepsilon' + i\frac{\sigma}{\omega}\right)\vec{E}_c = 0. \tag{146}$$

Assume

$$\varepsilon = \varepsilon' + i\frac{\sigma}{\omega}, \tag{147}$$

then

$$\nabla \cdot (\varepsilon \vec{E}) = 0. \tag{148}$$

Maxwell's second equation, Equation (133), can be modified as,

$$\nabla \times \vec{E}_c e^{-i\omega t} + \frac{\partial}{\partial t} \vec{B}_c e^{-i\omega t} = 0, \tag{149}$$

and

$$\nabla \times \vec{E}_c - i\omega \vec{B}_c = 0. \tag{150}$$

Substituting Equation (138) into Equation (150), using Equation (141) and rearranging yields,

$$\nabla \times E_c = i\omega\mu H_c. \tag{151}$$

Maxwell's third equation, Equation (134), can easily be evaluated. Substituting Equation (138) in Equation (134) and using Equation (141) yields,

$$\nabla \cdot H_c = 0. \tag{152}$$

The fourth equation of Maxwell, Equation (135) becomes,

$$\nabla \times \vec{H}_c e^{-i\omega t} = \vec{J}_{free} e^{-i\omega t} - i\omega \vec{D}_c e^{-i\omega t}. \tag{153}$$

Substituting Equations (137), (10) and (26) in Equation (153) and rearranging yields,

$$\nabla \times \vec{H}_c = -i\omega\left(\varepsilon' + i\frac{\sigma}{\omega}\right)\vec{E}_c. \qquad (154)$$

The choice of $e^{-i\omega t}$ for the time-variation of the field is merely a convention. What will happen if the conjugate of the Equation (141) is used?

$$\vec{F} = \vec{F}_c e^{i\omega t}. \qquad (155)$$

Now the same procedure as before should be used to get the modified Maxwell's equations

$$\nabla \cdot \vec{D} = \rho_{free} \;\Rightarrow\; \nabla \cdot \left(\varepsilon' \vec{E}\right) = \rho_{free}. \qquad (156)$$

Substituting Equations (137), (155) and (144) in Equation (156) and differentiating it with respect to time yields,

$$\nabla \cdot \left(\varepsilon' - i\frac{\sigma}{\omega}\right)E_c. \qquad (157)$$

Define ε as

$$\varepsilon = \varepsilon' - i\frac{\sigma}{\omega}. \qquad (158)$$

Therefore,

$$\nabla \cdot \left(\varepsilon \vec{E}_c\right) = 0. \qquad (159)$$

This is the same result as Equation (148) except for the definition of ε. When negative complex function was used the complex part of ε was positive but for the conjugate of that field it was negative. Of course the second and the third equations remain the same because they are independent of ε. If Equation (155) is substituted into Equation (135), the fourth Maxwell's equation becomes,

$$\nabla \times \vec{H}_c e^{i\omega t} = \vec{J}_{free} e^{i\omega t} + i\omega \vec{D}_c e^{i\omega t}. \qquad (160)$$

Substituting Equation (137) into Equation (160) and rearranging gives,

$$\nabla \times \vec{H}_c = i\omega\left(\varepsilon' - i\frac{\sigma}{\omega}\right)\vec{E}_c. \qquad (161)$$

Defining ε as

$$\varepsilon = \varepsilon' - i\frac{\sigma}{\omega}, \qquad (162)$$

Equation (161) becomes,

$$\nabla \times \vec{H}_c = i\omega\varepsilon \vec{E}_c. \qquad (163)$$

Equations (158), (159), (162) and (163) are discussed in Bohren and Huffman[2].

This result indicates that if either a complex wave function is used for the fields in Maxwell's equations or its conjugate, the result is the same. However, the definition of the dielectric constant ε changes. In the first case, the complex part of the dielectric constant is positive while in the second case it is negative.

A wave equation can also be found by Maxwell's equations. The following useful vector identity will be introduced as a key to the derivation of the wave equation,

$$\nabla \times (\nabla \times \vec{A}) = \nabla(\nabla \cdot \vec{A}) - \nabla^2 \vec{A}. \qquad (164)$$

Substituting Equations (137), (138) and (140) in Equation (135) the following equation is obtained

$$\nabla \times \vec{B} = \mu\sigma\vec{E} + \mu\varepsilon \frac{\partial \vec{E}}{\partial t}. \qquad (165)$$

Taking the curl of Equation (133), and using Equations (164), (132) and (165) yields,

$$\nabla^2 \vec{E} = \mu\sigma \frac{\partial \vec{E}}{\partial t} + \mu\varepsilon \frac{\partial^2 \vec{E}}{\partial t}. \qquad (166)$$

Taking the wave function for any of the six fields results in

$$\nabla^2 \psi = \mu\sigma \frac{\partial \psi}{\partial t} + \mu\varepsilon \frac{\partial^2 \psi}{\partial t}. \qquad (167)$$

This is the wave equation in general. Now what will be the wave equation in dielectrics? In the dielectrics, the conductivity $\sigma = 0$, thus,

$$\nabla^2 \psi = \mu\varepsilon \frac{\partial^2 \psi}{\partial t}, \qquad (168)$$

where

$$\mu\varepsilon = \frac{1}{v^2}. \tag{169}$$

It is important to note that $\nabla \times \left(\nabla \times \vec{B}\right)$ gives the same result as Equation (168). The general solution for Equation (168) is

$$\psi(z,t) = f(z - vt) + g(z + vt). \tag{170}$$

Assume that the $\xi = z + vt$ and $\eta = z - vt$, then it can be shown that the resulting equation has the solution of the form $= f(\xi) + g(\eta)$. Using operators yields,

$$\frac{\partial}{\partial z} = \frac{\partial}{\partial \xi}\frac{\partial \xi}{\partial z} + \frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial z} = \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta}, \tag{171}$$

$$\frac{\partial^2}{\partial z^2} = \frac{\partial}{\partial \xi}\left(\frac{\partial}{\partial z} + \frac{\partial}{\partial z}\right) + \frac{\partial}{\partial \eta}\left(\frac{\partial}{\partial z} + \frac{\partial}{\partial z}\right), \tag{172}$$

$$\frac{\partial^2}{\partial z^2} = \frac{\partial^2}{\partial \xi^2} + 2\frac{\partial^2}{\partial \xi \partial \eta} + \frac{\partial^2}{\partial \eta^2}, \tag{173}$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \xi}\frac{\partial \xi}{\partial t} + \frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial t} = v\left(\frac{\partial}{\partial \xi} - \frac{\partial}{\partial \eta}\right), \tag{174}$$

$$\frac{\partial^2}{\partial t^2} = v^2\left(\frac{\partial^2}{\partial \xi^2} - 2\frac{\partial^2}{\partial \xi \partial \eta} + \frac{\partial^2}{\partial \eta^2}\right). \tag{175}$$

Using Equations (168), (169), (173) and (175) gives,

$$4\frac{\partial^2\psi}{\partial\xi\partial\eta}=0 \;\Rightarrow\; \frac{\partial^2\psi}{\partial\xi\partial\eta}=0. \qquad (176)$$

This result indicates that $f(\xi)$ is independent of η and that $g(\eta)$ is independent of ξ. Equation (176) is the solution to problem 1 of Chapter 24 in Wangsness[10].

Index of refraction

It is obvious that the speed of light in a denser medium is less than in lighter ones. The speed of light in solids is less than in liquids and it is less in liquids than in gases. This is because of the index of refraction. The index of refraction n is the ratio of the speed of light in a vacuum c to the speed of light in a medium v, $n=c/v$. From this, it can be inferred that the refractive index of solids is greater than the refractive index of liquids, and the refractive index of liquids is greater than that of gases. The index of refraction of vacuum is unity. When light travels in a medium its frequency remains constant but its wavelength changes. The speed of light in a medium is given by $v=c/n$. The wavelength of light in a vacuum is $\lambda_0 = c/f$ and the wavelength of light in a medium is $\lambda = v/f = c/(fn)$. λ_0 and λ are the wavelengths in a vacuum and a medium respectively, and f is the frequency. Light enters the medium from a vacuum and leaves the medium to the vacuum with the same speed. This means that the waves at both surfaces of the medium move together regardless of the time delay while traveling through the medium. The only factor that causes them to get

together is the bending of light in the medium as shown in Figure 16. The geometry of this figure shows that $\sin\theta_i / \sin\theta_r = c/v = \lambda_0/\lambda = n$, where the subscripts i and r stand for the incident and the refracted. This relation is called Snell's law.

The basis of this part of the section is mostly from Feynman[17]. It is true apparently that light travels at c/n through a material with index of refraction n, but the fields are still produced because of the oscillating charges. It is of interest to understand what causes the slowing down of light while travelling through a material. Suppose a source of light is placed at s, a large distance from a transparent material, glass plate. It is possible to find the field due to this source at point P, a large distance from the glass but at the opposite side. However, we can't find the field near the glass because we don't have a relevant formula to find the field near the source. In this case even the plate could be assumed as a source because of the oscillating charges. When light travels through the plate it oscillates the electron inside the atoms up and down, because it exerts a force on them. The oscillating electrons also produce an electric field. The field at point P is the summation of the field due to the source and the induced field due to the moving charges of the plate.

$$E = E_s + \sum_{all\ charges} E_{each\ charge}, \qquad (177)$$

where E_s is the field due to the source and the other term is due to the accelerating charges. If the thin plate were not present the field at P would exactly be the same as the source field which is

$$E_s = E_0 e^{i\omega(t-z/c)}. \qquad (178)$$

In the presence of the thin plate the field at P is different. What is the field due to the moving charges, E_a, that slows down the electromagnetic field or the wave? Assume Δz is the thickness of the plate. If the plate were not there, the light would move a distance Δz in time $\Delta z/c$. In the presence of the plate the wave moves a distance Δz in time $n\Delta z/c$, which takes a longer time. The additional time is, thus, $\Delta t = (n-1)\Delta z/c$. After the wave passes the plate it continues to travel with the speed c. The extra delay in time t due to the oscillating charges in Equation (178) should be replaced by $t-\Delta t$ or by $[t-(n-1)\Delta z/c]$. So the wave after placing the plate becomes,

$$E_{after\ plate} = E_0 e^{i\omega[t-(n-1)\Delta z/c - z/c]}. \qquad (179)$$

This equation can also be written as,

$$E_{after\ plate} = e^{-i\omega(n-1)\Delta z/c} E_0 e^{i\omega(t-z/c)} = e^{i\omega(n-1)\Delta z/c} E_s. \qquad (180)$$

The factor $i\omega(n-1)\Delta z/c$ is the phase shift that retards the wave because of the negative sign in the exponent. So the field is multiplied by a factor that shifts its phase. Using $e^x = 1+x$ for very small x results in,

$$E_{after\ plate} = E_0 e^{i\omega(t-z/c)} - \frac{i\omega(n-1)\Delta z}{c} E_0 e^{i\omega(t-z/c)}. \qquad (181)$$

The first term is the field due to the source and the second term is the field due to the oscillating charges, E_a, expressed in terms of index of refraction and dependent on the source field. The factor $-i$ indicates that if E_s is real then E_a is negative imaginary or in other words E_s and E_a make a right angle as shown in Figure 17.

Now the field due to the moving charges of dielectrics can be found. When light travels through a dielectric it exerts forces on the electrons inside the atoms and causes the electrons to oscillate. These oscillating charges also produce another field as well. In gases at the standard pressure and temperature the interatomic distances are large on the atomic scale, so the index of refraction is close to unity. In this case the damping factor due the frictional force is very small. Therefore,

$$m\frac{d^2x}{dt^2} - m\gamma\frac{dx}{dt} - m\omega_0^2 x = qE\,. \qquad (182)$$

The first term on the left is the mass of the electron times its acceleration, the middle term is the damping force, which is directly proportional to the velocity and the third term is the restoring force with natural frequency ω_0, and the term on the right is the driving force. If the displacement and the electric field are assumed to be as,

$$\begin{aligned} x &= x_0 e^{i\omega t} \\ E &= E_0 e^{i\omega t}\,. \end{aligned} \qquad (183)$$

Then the solution to Equation (182) becomes,

$$x(t) = \frac{q/m}{(\omega_0^2 - \omega^2 + i\gamma\omega)} E_0 e^{i\omega t} = \frac{q/m}{(\omega_0^2 - \omega^2 + i\gamma\omega)} E . \quad (184)$$

For gases at high pressure where the interatomic distances are small the factor γ is high because of the frictional force between the atoms. For the gases at standard pressure and temperature the factor γ is very small because of the small frictional force due to the large interatomic distances. Therefore, for gases at standard pressure and temperature the factor γ can be neglected. When $\omega_0 > \omega$ then $E(t)$ and $x(t)$ have the same signs, which means that the displacement and the field from the source are in phase. When $\omega_0 < \omega$, then $E(t)$ and $x(t)$ have opposite signs, which means that the field due to the source and the displacement are 180° out of phase.

From Equation (4), $\vec{P} = Nq\vec{r}$, so by substituting Equation (184) in Equation (4) yields,

$$\vec{P} = \frac{q^2 NE/m}{(\omega_0^2 - \omega^2 + i\gamma\omega)} . \quad (185)$$

Rearranging Equation (14), substituting it in Equation (10) and using Equation (185) and the fact that $\varepsilon = \kappa\varepsilon_0$ the following result is obtained,

$$\varepsilon = \varepsilon_0 + \frac{q^2 N/m}{(\omega_0^2 - \omega^2 + i\gamma\omega)} . \quad (186)$$

Now setting $v = 1/\sqrt{\varepsilon\mu}$, $c = 1/\sqrt{\varepsilon_0\mu_0}$ and $n = c/v$ gives,

$$n^2 = \kappa_e \kappa_m . \qquad (187)$$

For those materials with relative permeability equal to unity the following relationship is obtained

$$n^2 = \kappa_e = \varepsilon / \varepsilon_0 . \qquad (188)$$

Therefore,

$$n^2(\omega) = 1 + \frac{Nq^2}{\varepsilon_0 m} \frac{1}{(\omega_0^2 - \omega^2 + i\gamma\omega)} . \qquad (189)$$

This expression, index of refraction as a function of frequency, is called the dispersion equation. This equation indicates that at frequencies above the natural resonance frequency, the displacement is out of phase with the driving force and so is the polarization out of phase with the field of the source. Thus, the dielectric constant and the index of refraction are less than unity. At frequencies below the resonance, the displacement, the polarization and the applied field are all in phase. Therefore, the dielectric constant and as a result the index of refraction both are greater than unity. For gases at high pressure ($\sim 10^3$ atm) the interatomic distances are very small and consequently, the interaction between the atoms produces frictional forces that cause energy dissipation. Hence, the factor γ is large.

Equation (189) can be generalized as

$$n^2(\omega) = 1 + \frac{Nq^2}{\varepsilon_0 m} \sum_j \frac{f_j}{(\omega_{0j}^2 - \omega^2 + i\gamma\omega)} . \qquad (190)$$

The term f_j, where $\sum_j f_j = 1$, is called oscillator strength. The atoms in dielectrics have several natural frequencies. Also the strength of each mode is different, that is why the polarizability of each mode is multiplied by the term f_j. It is also called the transition probability because of the occurrence of atomic transition.

In denser materials like liquids and solids the atoms interact with one another and with the local field as well. Therefore, the atoms in addition to applied fields experience another field, $\vec{P}/3\varepsilon_0$. Using Equations (107), (56) and (14) yields,

$$\chi = \frac{N\alpha}{1-(N\alpha/3)}, \tag{191}$$

$$\frac{\chi}{\chi+3} = \frac{\kappa-1}{\kappa+2} = \frac{1}{3}N\alpha . \tag{192}$$

Now comparing Equations (63) and (185) the following result is obtained,

$$\alpha = \frac{q^2/\varepsilon_0 m}{(\omega_0^2 - \omega^2 + i\gamma\omega)}. \tag{193}$$

Substituting Equation (193) in Equation (192) and using Equation (188) yields,

$$\frac{n^2-1}{n^2+2} = \frac{Nq^2}{3\varepsilon_0 m}\frac{1}{(\omega_0^2 - \omega^2 + i\gamma\omega)}. \tag{194}$$

Equation (194) can be generalized for all natural frequencies

$$\frac{n^2-1}{n^2+2}=\frac{Nq^2}{3\varepsilon_0 m}\sum_j \frac{f_j}{\left(\omega_{0j}^2-\omega^2+i\gamma\omega\right)}. \qquad (195)$$

This equation is for the electron oscillator but it can work for the ion oscillator as well. To utilize it for ion oscillations the mass of the electron should be replaced by the mass of the ion. The electronic polarization contributes to n at all regions of the optical spectrum, whereas the ionic polarization affects n only in regions of resonance where $\omega=\omega_0$.

Transparent materials like glass have natural frequencies above the optical region, that is why they are colorless. They have natural frequencies in the ultraviolet region at wavelengths of about 100nm, where they are opaque. As the frequency gets close to the natural frequency of glass the index of refraction increases, which is called normal dispersion. At the ultraviolet regions where $\omega=\omega_0$, the oscillators will begin to resonate and the amplitudes increase. The damping due to the absorption of energy of the incident wave starts to increase and the damping term will be dominant. The regions in the vicinity of different natural frequencies ω_{0j}, as in Figure 18, are called absorption bands.

The index of refraction of a mixture is not just the average of the indexes. It should be evaluated by the summation of the polarizabilities of the individual elements. For example, to find the index of refraction of a sugar solution, the determination of the refractive index of water and sugar individually is required. Then they are added together as shown below.

$$3\left(\frac{n^2-1}{n^2+2}\right) = N_S \alpha_S + N_W \alpha_W . \qquad (196)$$

This equation gives a reasonable result, which agrees with the experimental results.

Chapter 3
Effective Polarizability

This chapter focuses on some modeling for the dipoles in an applied electric field. Bulk matter is made up of many atoms. First consider the effect of an applied electric field on a single atom. For weak electric fields the atom will acquire a dipole moment given by $p = \alpha \varepsilon_0 E$, where α is the polarizability. For a particular atom α can be calculated using quantum mechanical methods. In practice, it appears that the calculation is difficult. The approximate calculation of α for a hydrogen atom in its ground state is discussed by Park[18]. The result of this calculation is $\alpha_H = 0.6668 \times 10^{-30} m^3$. In this model, the calculation of the polarizabilities from quantum mechanics is not performed. Rather, α is assumed to be given. The polarizabilities of isolated atoms are given in the CRC Handbook[19]. The order of magnitude is $\sim 10^{-30}$ m^3 for all of them. For strong electric fields the dipole moment becomes a nonlinear function of the field.

In a crystal, atoms are arranged in a regular lattice. The dipole moment of each atom is determined by the total electric field acting on the atom. However, this field is a superposition of the externally applied field and the field due to other dipoles. Assume that the atoms are identical and their dipoles point along the direction of the local electric field. The situation is modeled with two atoms. It is assumed that the two atoms are located on the x-axis and are separated by a distance a. Initially, assume that the dipoles point along the same direction as the external electric field. The dipoles are subjected to an externally applied uniform electric field that is pointing along the x direction. Therefore, the dipoles also point along the x direction

as shown in Figure 19. It is important to note that when the atoms are placed in an external electric field their induced dipoles interact with one another continuously. Consequently, the electric field in the vicinity of the dipoles is altered. In the beginning the dipole moments are calculated for the case where the interaction between them is very weak. After this first approximation, higher order terms will be obtained.

Let one of the dipoles be p_1 and the other p_2, the polarizabilities be α_1 and α_2 respectively and the external electric field be E_0. Thus,

$$\vec{p}_1 = \alpha_1 \varepsilon_0 \left(\vec{E}_0 + \frac{1}{4\pi \varepsilon_0} \frac{2\vec{p}_2}{a^3} \right), \tag{197}$$

$$\vec{p}_2 = \alpha_2 \varepsilon_0 \left(\vec{E}_0 + \frac{1}{4\pi \varepsilon_0} \frac{2\vec{p}_1}{a^3} \right). \tag{198}$$

Assume the dipoles are identical, so $\alpha_1 = \alpha_2 = \alpha$ and $\vec{p}_1 = \vec{p}_2 = \vec{p}$. Therefore,

$$p = \alpha \varepsilon_0 \left(E_0 + \frac{1}{4\pi \varepsilon_0} \frac{2p}{a^3} \right), \tag{199}$$

$$\vec{p} = \left(\frac{2\pi a^3 \alpha \varepsilon_0}{2\pi a^3 - \alpha} \right) \vec{E}_0 = \frac{\alpha \varepsilon_0}{1 - \alpha / 2\pi a^3} \vec{E}_0 . \tag{200}$$

From Equation (200) the polarizability for this system can be found,

$$\alpha_{eff} = \frac{2\alpha}{1 - \alpha / 2\pi a^3}. \tag{201}$$

Referring to Equations (197) and (198) and solving them simultaneously yields,

$$\frac{\vec{p}_1}{\alpha_1 \varepsilon_0} - \frac{\vec{p}_2}{2\pi \varepsilon_0 a^3} = E_0, \tag{202}$$

$$\frac{\vec{p}_2}{\alpha_2 \varepsilon_0} - \frac{\vec{p}_1}{2\pi \varepsilon_0 a^3} = E_0. \tag{203}$$

Multiplying Equation (202) by $\alpha_1 \varepsilon_0$ and Equation (203) by $2\pi \varepsilon_0 a^3$ yields,

$$\frac{2\pi a^3}{\alpha_2} \vec{p}_2 - \frac{\alpha_1}{2\pi a^3} \vec{p}_2 = (\alpha_1 \varepsilon_0 + 2\pi a^3 \varepsilon_0) E_0. \tag{204}$$

Rearranging equation (204) the following result is obtained,

$$\vec{p}_2 = \left(\frac{2\pi a^3 \alpha_1 \alpha_2 \varepsilon_0 + (2\pi a^3)^2 \alpha_2 \varepsilon_0}{(2\pi a^3)^2 - \alpha_1 \alpha_2} \right). \tag{205}$$

Using the same procedure to solve for $\vec{p}_1$ yields,

$$\vec{p}_1 = \left(\frac{2\pi a^3 \alpha_1 \alpha_2 \varepsilon_0 + (2\pi a^3)^2 \alpha_1 \varepsilon_0}{(2\pi a^3)^2 - \alpha_1 \alpha_2} \right). \tag{206}$$

Since the dipoles are identical, then $\alpha_1 = \alpha_2 = \alpha$; consequently, $\vec{p}_1 = \vec{p}_2 = \vec{p}$, hence,

$$\vec{p} = \left(\frac{2\pi a^3 \alpha^2 \varepsilon_0 + (2\pi a^3)^2 \alpha \varepsilon_0}{(2\pi a^3)^2 - \alpha^2} \right). \qquad (207)$$

Solving for the polarizability of the system yields,

$$\alpha_{eff} = \frac{2\alpha}{1 - \alpha / 2\pi a^3}. \qquad (208)$$

This equation indicates that as $\alpha \to 2\pi a^3$, then $\alpha_{eff} \to \infty$. Now the question arises whether or not this phenomenon is physically acceptable. Of course, the answer to this question is no because the relation $p = \alpha \varepsilon_0 E$ holds only for low electric fields but for high electric field this relation is no longer true. If the effective polarizability increases the dipole moment and as a result the total electric field on each atom increases as well. As the field increases the linear relationship between the field and the induced dipole gradually breaks down.

Equations (201) and (208) also imply that for a given α there is a critical separation distance $a = (\alpha / 2\pi)^{1/3}$. It could be concluded that the effective polarizability of such a system is dependent on the separation distance.

Now the net electric field half way between the two dipoles is,

$$\vec{E}(0) = \vec{E}_0 + \frac{1}{4\pi\,\varepsilon_0}\left(\frac{2\,\vec{p}_1}{(a/2)^3} + \frac{2\,\vec{p}_2}{(a/2)^3}\right) = E_0 + \frac{4\,\vec{p}}{\pi\,\varepsilon_0 a^3}. \qquad (209)$$

Substituting the value of $\vec{p}$ from equation (200) in equation (209) yields,

$$\vec{E}(0) = \vec{E}_0 + \left(\frac{8\alpha}{2\pi a^3 - \alpha}\right)\vec{E}_0. \qquad (210)$$

Now it is possible to find the electric field at some distance r from the origin, which is half way in the middle between the two charges. Assume that r is much larger than a. Thus,

$$\vec{E}(0) = \vec{E}_0 + \frac{1}{4\pi\,\varepsilon_0}\left(\frac{2\,\vec{p}_1}{(r+a/2)^3} + \frac{2\,\vec{p}_2}{(r-a/2)^3}\right), \qquad (211)$$

therefore,

$$\vec{E}(r) = \vec{E}_0 + \frac{1}{4\pi\,\varepsilon_0 r^3}\left(\frac{2\,\vec{p}_1}{(1+a/2r)^3} + \frac{2\,\vec{p}_2}{(1-a/2r)^3}\right). \qquad (212)$$

Since $r>>a$, the term $a/2r \to 0$, and since $p_1 = p_2 = p$, then

$$\vec{E}(r) = \vec{E}_0 + \frac{\vec{p}}{4\pi\,\varepsilon_0 r^3}. \qquad (213)$$

Substituting equation (200) in equation (213) yields,

$$\vec{E}(r) = \vec{E}_0 + \frac{2a^3\alpha}{(2\pi a^3 - \alpha)^3}\vec{E}_0. \qquad (214)$$

Now the determination of the dipole moment of the higher terms is attempted, where the two dipoles interact strongly. Substituting the value of p_2 from Equation (198) into Equation (197) yields

$$\vec{p}_1 = \alpha_1 \varepsilon_0 \left(\vec{E}_0 + \frac{1}{4\pi \varepsilon_0} \frac{2}{a^3} \left(\alpha_2 \varepsilon_0 \left(\vec{E}_0 + \frac{1}{4\pi \varepsilon_0} \frac{2\vec{p}_1}{a^3} \right) \right) \right). \quad (215)$$

Assuming $\alpha_1 = \alpha_2 = \alpha$ and $\vec{p}_1 = \vec{p}_2 = \vec{p}$ and rearranging equation (215) yields,

$$\vec{p} = \alpha \varepsilon_0 \left(1 + \frac{\alpha}{2\pi a^3} \right) \vec{E}_0 + \left(\frac{\alpha}{2\pi a^3} \right)^2 \vec{p}. \quad (216)$$

Now substituting the value of $\vec{p}$ from equation (199) in equation (216) the following result is obtained,

$$\vec{p} = \alpha \varepsilon_0 \left(1 + \frac{\alpha}{2\pi a^3} \right) \vec{E}_0 + \left(\frac{\alpha}{2\pi a^3} \right)^2 \left(\alpha \varepsilon_0 \left(\vec{E}_0 + \frac{1}{4\pi \varepsilon_0} \frac{2\vec{p}}{a^3} \right) \right). \quad (217)$$

Rearranging equation (217) yields,

$$\vec{p} = \alpha \varepsilon_0 \left(1 + \frac{\alpha}{2\pi a^3} + \left(\frac{\alpha}{2\pi a^3} \right)^2 \right) \vec{E}_0 + \left(\frac{\alpha}{2\pi a^3} \right)^3 \vec{p}. \quad (218)$$

Continuing this process the following result is obtained,

$$\vec{p} = \alpha\,\varepsilon_0 \sum_{n=1}^{N} \left(\frac{\alpha}{2\pi a^3}\right)^{n-1} \vec{E}_0 + \left(\frac{\alpha}{2\pi a^3}\right)^{N} \vec{p}. \qquad (219)$$

Therefore,

$$\vec{p} = \frac{\alpha\ \varepsilon_0 \sum_{n=1}^{N} \left(\alpha/2\pi a^3\right)^{n-1} \vec{E}_0}{1-\left(\alpha/2\pi a^3\right)^{N}}. \qquad (220)$$

The effective polarizability in this case is

$$\alpha_{eff} = \frac{\alpha \sum_{n=1}^{N} \left(\alpha/2\pi a^3\right)^{n-1}}{1-\left(\alpha/2\pi a^3\right)^{N}}. \qquad (221)$$

Again the effective polarizability is dependent on the separation distance and the critical distance is $a = (\alpha/2\pi)^{1/3}$. Thus, $a > (\alpha/2\pi)^{1/3}$ because if $a = (\alpha/2\pi)^{1/3}$ the effective polarizability is infinite, which physically doesn't make sense. Likewise, when $a < (\alpha/2\pi)^{1/3}$ the effective polarizability is negative, which is also unphysical. For $a > (\alpha/2\pi)^{1/3}$, $\alpha/2\pi a^3 < 1$ and therefore $(\alpha/2\pi a^3)^N \to 0$ as $N \to \infty$. Using geometric infinite series the numerator, $\sum_{n=1}^{N} (\alpha/2\pi a^3)^{n-1}$, converges to $1/(1-(\alpha/2\pi a^3))$. Therefore,

$$\alpha_{eff} = \frac{\alpha}{1-\left(\alpha/2\pi a^3\right)}. \qquad (222)$$

It is noted that Equation (221) is the same as Equation (200). This indicates that the dipoles initially affect one another and after some point where the electric field exceeds some limit the linear relation between the dipole and the electric field breaks down and that the polarizability does not go beyond some limit.

Figure 20 shows the graphic relationship between α_{eff}/α and a for this orientation. The graph indicates that as $a \to (\alpha / 2\pi)^{1/3}$, $\alpha_{eff} \to \infty$ and that for $2\pi a^3 >> \alpha$ then $\alpha_{eff} \to \alpha$.

Up to this point the dipoles were assumed to be pointing along the preferred direction which is the direction of the externally applied electric field. Now the use of the general case and polarizability tensor is applied. Assume the dipoles are on the x-axis a distance a from each other as in Figure 19. Therefore,

$$\vec{E}_1 = \vec{E}_0 \hat{i} + \frac{3\left[\left(\vec{p}_{2x}\hat{i} + \vec{p}_{2y}\hat{j} + \vec{p}_{2z}\hat{k}\right)\cdot a\hat{i}\right] a\hat{i}}{4\pi\,\varepsilon_0 a^5} - \frac{a^2\left(\vec{p}_{2x}\hat{i} + \vec{p}_{2y}\hat{j} + \vec{p}_{2z}\hat{k}\right)}{4\pi\,\varepsilon_0 a^5} . \tag{223}$$

$$\vec{E}_1 = \vec{E}_0 \hat{i} + \frac{2\vec{p}_{2x}\hat{i} - \vec{p}_{2y}\hat{j} - \vec{p}_{2z}\hat{k}}{4\pi\,\varepsilon_0 a^3} = \frac{1}{\alpha_1 \varepsilon_0}\left(\vec{p}_{1x}\hat{i} + \vec{p}_{1y}\hat{j} + \vec{p}_{1z}\hat{k}\right) . \tag{224}$$

From Equation (224) the following result is obtained.

$$p_{1x} = \alpha_1 \varepsilon_0 E_0 + \frac{2\alpha_1}{4\pi a^3} p_{2x}, \tag{225}$$

and

$$p_{1y} = \frac{-\alpha_1}{4\pi a^3} p_{2y}. \qquad p_{1z} = \frac{-\alpha_1}{4\pi a^3} p_{2z}\ . \tag{226}$$

Similarly, it can be found that

$$p_{2x} = \alpha_0 \varepsilon_0 E_0 + \frac{2\alpha_1}{4\pi a^3} p_{1x}, \tag{227}$$

and

$$p_{2y} = \frac{-\alpha_1}{4\pi a^3} p_{1y} \qquad p_{2z} = \frac{-\alpha_1}{4\pi a^3} p_{1z}\ . \tag{228}$$

Solving this linear system by Maple[20] yields,

$$p_{1y} = p_{1z} = p_{2y} = p_{2z} = 0\,, \tag{229}$$

$$p_{1x} = 2\frac{\alpha_1 \varepsilon_0 E_0 \pi a^3 (2\pi a^3 + \alpha_2)}{-\alpha_1 \alpha_2 + 4\pi^2 a^6}, \tag{230}$$

and

$$p_{2x} = 2\frac{\alpha_2 \varepsilon_0 E_0 \pi a^3 (2\pi a^3 + \alpha_1)}{-\alpha_1 \alpha_2 + 4\pi^2 a^6}, \tag{231}$$

Therefore,

$$(\alpha_{eff})_1 = \frac{2\pi a^3 \alpha_1 (2\pi a^3 + \alpha_2)}{4\pi^2 a^6 - \alpha_1 \alpha_2}, \tag{232}$$

$$(\alpha_{eff})_1 = \frac{2\pi a^3 \alpha_2 (2\pi a^3 + \alpha_1)}{4\pi^2 a^6 - \alpha_1 \alpha_2}, \tag{233}$$

and,

$$\alpha_{eff} = \frac{4\pi a^3}{4\pi^2 a^6 - \alpha_1 \alpha_2}(\alpha_1 \alpha_2 + \pi a^3 (\alpha_1 + \alpha_2))\,. \tag{234}$$

Assume that $\alpha_1 = \alpha_2 = \alpha$, then,

$$\alpha_{eff} = \frac{4\pi a^3}{4\pi^2 a^6 - \alpha^2}\left(\alpha^2 + 2\pi a^3 \alpha\right). \tag{235}$$

Equation (235) can be reduced to

$$\alpha_{eff} = \frac{2\alpha}{1-\left(\alpha/2\pi a^3\right)}. \tag{236}$$

Equation (236) holds provided that $\alpha < 2\pi a^3$, so the critical distance is $r_c = (\alpha/2\pi)^{1/3}$.

Now assume that the dipoles are on the x-axis but the electric field is pointing along the y direction as shown in figure 21. Thus,

$$\vec{E}_1 = \vec{E}_0 \hat{j} + \frac{3\left[\left(\vec{p}_{2x}\hat{i} + \vec{p}_{2y}\hat{j} + \vec{p}_{2z}\hat{k}\right)\cdot a\hat{i}\right] a\hat{i}}{4\pi\,\varepsilon_0 a^5} - \frac{a^2\left(\vec{p}_{2x}\hat{i} + \vec{p}_{2y}\hat{j} + \vec{p}_{2z}\hat{k}\right)}{4\pi\,\varepsilon_0 a^5}, \tag{237}$$

and

$$\vec{E}_1 = \vec{E}_0 \hat{j} + \frac{2\vec{p}_{2x}\hat{i} - \vec{p}_{2y}\hat{j} - \vec{p}_{2z}\hat{k}}{4\pi\,\varepsilon_0 a^3} = \frac{1}{\alpha_1 \varepsilon_0}\left(\vec{p}_{1x}\hat{i} + \vec{p}_{1y}\hat{j} + \vec{p}_{1z}\hat{k}\right). \tag{238}$$

Therefore,

$$p_{1y} = \alpha_0 \varepsilon_0 E_0 + \frac{2\alpha_1}{4\pi a^3} p_{2y}, \tag{239}$$

and

$$p_{1x} = \frac{-\alpha_1}{4\pi a^3} p_{2x} \qquad p_{1z} = \frac{-\alpha_1}{4\pi a^3} p_{2z} \,. \tag{240}$$

Similarly, it is found that

$$p_{2y} = \alpha_0 \varepsilon_0 E_0 + \frac{2\alpha_1}{4\pi a^3} p_{1y}, \tag{241}$$

and

$$p_{2x} = \frac{-\alpha_1}{4\pi a^3} p_{1x} \qquad p_{2z} = \frac{-\alpha_1}{4\pi a^3} p_{1Z} \,. \tag{242}$$

Solving the linear system by Maple[20] yields,

$$p_{1x} = p_{1z} = p_{2x} = p_{2z} = 0, \tag{243}$$

$$p_{1y} = 4\frac{\alpha_1 \varepsilon_0 E_0 \pi a^3 (4\pi a^3 - \alpha_2)}{16\pi^2 a^6 - \alpha_1 \alpha_2}, \tag{244}$$

and

$$p_{2y} = 4\frac{\alpha_2 \varepsilon_0 E_0 \pi a^3 (4\pi a^3 - \alpha_1)}{16\pi^2 a^6 - \alpha_1 \alpha_2}. \tag{245}$$

Therefore,

$$(\alpha_{eff})_1 = \frac{4\pi a^3 \alpha_1 (2\pi a^3 + \alpha_2)}{16\pi^2 a^6 - \alpha_1 \alpha_2}, \tag{246}$$

$$(\alpha_{eff})_2 = \frac{4\pi a^3 \alpha_2 (2\pi a^3 + \alpha_1)}{16\pi^2 a^6 - \alpha_1 \alpha_2}, \tag{247}$$

and

$$\alpha_{eff} = \frac{4\pi a^3}{16\pi^2 a^6 - \alpha_1 \alpha_2}\left(4\pi a^3(\alpha_1+\alpha_2) - 2\alpha_1\alpha_2\right). \quad (248)$$

Now assume that $\alpha_1 = \alpha_2 = \alpha$, then

$$\alpha_{eff} = \frac{8\pi a^3}{16\pi^2 a^6 - \alpha^2}\left(4\pi a^3\alpha - \alpha^2\right). \quad (249)$$

Equation (249) reduces to

$$\alpha_{eff} = \frac{2\alpha}{1+\left(\alpha/4\pi a^3\right)}. \quad (250)$$

From Equation (250) it can be concluded that the critical distance is negative, $r_c = \left(-\alpha/4\pi\right)^{1/3}$, which physically does not make sense. Also the separation distance $a \neq 0$. Figure 22 shows the graphic relationship between α_{eff}/α and a for this orientation. The graph indicates that as the separation distance decreases the effective polarizability decreases too. When the separation distance gets larger and larger the effective polarizability approaches the summation of the individual polarizabilities.

Now assume that the applied electric field points along the z direction and the dipoles are still on x-axis as in Figure 23. Thus,

$$\vec{E}_1 = \vec{E}_0\hat{k} + \frac{3\left[\left(\vec{p}_{2x}\hat{i} + \vec{p}_{2y}\hat{j} + \vec{p}_{2z}\hat{k}\right)\cdot a\hat{i}\right]a\hat{i}}{4\pi\,\varepsilon_0 a^5} - \frac{a^2\left(\vec{p}_{2x}\hat{i} + \vec{p}_{2y}\hat{j} + \vec{p}_{2z}\hat{k}\right)}{4\pi\,\varepsilon_0 a^5}, \tag{251}$$

and

$$\vec{E}_1 = \vec{E}_0\hat{k} + \frac{2\vec{p}_{2x}\hat{i} - \vec{p}_{2y}\hat{j} - \vec{p}_{2z}\hat{k}}{4\pi\,\varepsilon_0 a^3} = \frac{1}{\alpha_1\varepsilon_0}\left(\vec{p}_{1x}\hat{i} + \vec{p}_{1y}\hat{j} + \vec{p}_{1z}\hat{k}\right). \tag{252}$$

Therefore,

$$p_{1z} = \alpha_0\varepsilon_0 E_0 + \frac{2\alpha_1}{4\pi a^3}p_{2z}, \tag{253}$$

and

$$p_{1x} = \frac{-\alpha_1}{4\pi a^3}p_{2x} \qquad p_{1y} = \frac{-\alpha_1}{4\pi a^3}p_{2y}. \tag{254}$$

Similarly, it is found that

$$p_{2z} = \alpha_0\varepsilon_0 E_0 + \frac{2\alpha_1}{4\pi a^3}p_{1z}, \tag{255}$$

and

$$p_{2x} = \frac{-\alpha_1}{4\pi a^3}p_{1x} \qquad p_{2y} = \frac{-\alpha_1}{4\pi a^3}p_{1y}. \tag{256}$$

Solving this linear equation by Maple[20] yields

$$p_{1x} = p_{1z} = p_{2x} = p_{2z} = 0, \tag{257}$$

$$p_{1z} = 4\frac{\alpha_1 \varepsilon_0 E_0 \pi a^3 (4\pi a^3 - \alpha_2)}{16\pi^2 a^6 - \alpha_1 \alpha_2}, \tag{258}$$

and

$$p_{2z} = 4\frac{\alpha_2 \varepsilon_0 E_0 \pi a^3 (4\pi a^3 - \alpha_1)}{16\pi^2 a^6 - \alpha_1 \alpha_2}. \tag{259}$$

The polarizability of this system is the same as the previous one except for the direction of the dipole that is along the z-axis. This indicates that the dipole points along the direction of the externally applied electric field. Thus, the polarizability of this system is

$$\alpha_{eff} = \frac{2\alpha}{1 + (\alpha / 4\pi a^3)}. \tag{260}$$

Now assume that the dipoles are on the y-axis and separated from one another by a distance a and the applied electric field is along the x direction as in Figure 24. Therefore,

$$\begin{aligned} \vec{E}_1 = \vec{E}_0 \hat{i} + & \frac{3\left[\left(\vec{p}_{2x}\hat{i} + \vec{p}_{2y}\hat{j} + \vec{p}_{2z}\hat{k}\right)\cdot a\hat{j}\right] a\hat{j}}{4\pi \varepsilon_0 a^5} \\ & - \frac{a^2\left(\vec{p}_{2x}\hat{i} + \vec{p}_{2y}\hat{j} + \vec{p}_{2z}\hat{k}\right)}{4\pi \varepsilon_0 a^5}, \end{aligned} \tag{261}$$

$$\vec{E}_1 = \vec{E}_0 \hat{i}\,\frac{2\vec{p}_{2y}\hat{j} - \vec{p}_{2x}\hat{i} - \vec{p}_{2z}\hat{k}}{4\pi\,\varepsilon_0 a^3} = \frac{1}{\alpha_1 \varepsilon_0}\left(\,\vec{p}_{1x}\hat{i} + \vec{p}_{1y}\hat{j} + \vec{p}_{1z}\hat{k}\right) \quad . \tag{262}$$

$$p_{1x} = \alpha_1 \varepsilon_0 E_0 - \frac{2\alpha_1}{4\pi a^3} p_{2x}, \tag{263}$$

$$p_{1y} = \frac{2\alpha_1}{4\pi a^3} p_{2y} \qquad p_{1z} = \frac{-\alpha_1}{4\pi a^3} p_{2z} \quad . \tag{264}$$

Similarly,

$$p_{2x} = \alpha_2 \varepsilon_0 E_0 - \frac{2\alpha_2}{4\pi a^3} p_{1x}, \tag{265}$$

$$p_{2y} = \frac{2\alpha_2}{4\pi a^3} p_{1y} \qquad p_{2z} = \frac{-\alpha_2}{4\pi a^3} p_{1z} \quad . \tag{266}$$

Solving this linear system by Maple[20] yields,

$$p_{1y} = p_{1z} = p_{2y} = p_{2z} = 0, \tag{267}$$

$$p_{1x} = 4\frac{\alpha_1 \varepsilon_0 E_0 \pi a^3 \left(4\pi a^3 - \alpha_2\right)}{16\pi^2 a^6 - \alpha_1 \alpha_2}, \tag{268}$$

$$p_{2x} = 4\frac{\alpha_2 \varepsilon_0 E_0 \pi a^3 \left(4\pi a^3 - \alpha_1\right)}{16\pi^2 a^6 - \alpha_1 \alpha_2}. \tag{269}$$

This is exactly the same as the second part where the dipoles were on the x-axis and the electric field pointed along the *y*-axis. However, the only difference is that in this system the dipole points along the x direction where in the second case it pointed along the *y* direction. This indicates that the direction of the dipole moment for this particular system is determined by the externally electric field. Therefore,

$$\alpha_{eff} = \frac{2\alpha}{1+(\alpha/4\pi a^3)}. \tag{270}$$

Now assume that the dipoles are on z-axis and the electric field points along the *x* direction as in Figure 25. Thus,

$$\vec{E}_1 = \vec{E}_0\hat{i} + \frac{3\left[\left(\vec{p}_{2x}\hat{i} + \vec{p}_{2y}\hat{j} + \vec{p}_{2z}\hat{k}\right)\cdot a\hat{k}\right]a\hat{k}}{4\pi\varepsilon_0 a^5} - \frac{a^2\left(\vec{p}_{2x}\hat{i} + \vec{p}_{2y}\hat{j} + \vec{p}_{2z}\hat{k}\right)}{4\pi\varepsilon_0 a^5}, \tag{271}$$

and

$$\vec{E}_1 = \vec{E}_0\hat{i}\,\frac{2\vec{p}_{2z}\hat{k} - \vec{p}_{2x}\hat{i} - \vec{p}_{2y}\hat{j}}{4\pi\varepsilon_0 a^3} = \frac{1}{\alpha_1\varepsilon_0}\left(\vec{p}_{1x}\hat{i} + \vec{p}_{1y}\hat{j} + \vec{p}_{1z}\hat{k}\right). \tag{272}$$

Solving

$$p_{1x} = \alpha_1\varepsilon_0 E_0 - \frac{\alpha_1}{4\pi a^3}p_{2x}, \tag{273}$$

$$p_{1y} = \frac{-\alpha_1}{4\pi a^3} p_{2y} \qquad p_{1z} = \frac{2\alpha_1}{4\pi a^3} p_{2z}\,, \tag{274}$$

$$p_{2x} = \alpha_2 \varepsilon_0 E_0 - \frac{\alpha_2}{4\pi a^3} p_{1x}\,, \tag{275}$$

and

$$p_{2y} = \frac{-\alpha_2}{4\pi a^3} p_{1y} \qquad p_{2z} = \frac{2\alpha_2}{4\pi a^3} p_{1z}\,. \tag{276}$$

Solving this linear system by Maple[20] yields,

$$p_{1y} = p_{1z} = p_{2y} = p_{2z} = 0\,, \tag{277}$$

$$p_{1x} = 4\frac{\alpha_1 \varepsilon_0 E_0 \pi a^3 (4\pi a^3 - \alpha_2)}{16\pi^2 a^6 - \alpha_1 \alpha_2}\,, \tag{278}$$

and

$$p_{2x} = 4\frac{\alpha_2 \varepsilon_0 E_0 \pi a^3 (4\pi a^3 - \alpha_1)}{16\pi^2 a^6 - \alpha_1 \alpha_2}\,. \tag{279}$$

Therefore,

$$\alpha_{eff} = \frac{2\alpha}{1 + (\alpha / 4\pi a^3)}\,. \tag{280}$$

This is the same as the case where the dipoles were on the x-axis and the applied electric field pointed along the z direction. The only difference is in the direction of the dipole, which in the former case pointed in the z direction while in the latter case it pointed along the x direction. This

indicates that the electric field determines the direction of the dipole for this particular system.

The whole work of this chapter can be summarized as a polarizability tensor. The mathematical expression of the polarizability tensor for this system is,

$$(\alpha_t)_{eff}=\begin{bmatrix} \dfrac{2\alpha}{1-\alpha/4\pi a^3} & 0 & 0 \\ 0 & \dfrac{2\alpha}{1+\alpha/4\pi a^3} & 0 \\ 0 & 0 & \dfrac{2\alpha}{1+\alpha/4\pi a^3} \end{bmatrix} . \qquad (281)$$

The first row elements are identified as α_{xx}, α_{xy}, α_{xz}, and similarly for the second and third rows. The term α_{xx} is the effective polarizability for the case where the externally applied electric field is parallel to the line connecting the dipoles. The other two polarizabilities on the diagonal of the matrix are the effective polarizabilities for the case where the externally applied electric field is perpendicular to the line connecting the dipoles. The fact that the off-diagonal elements are zero is related to the fact that the total dipole moment for this system always points in the direction of the applied external field.

The evaluation of the polarizability tensor for the general case of a larger system can be performed by the following procedure. First, the local electric field at each dipole location due to all the other dipoles is written as,

$$\vec{E}_{ij} = \frac{1}{4\pi\ \varepsilon_0 \left|\vec{r}_i-\vec{r}_j\right|^5}\{3[\vec{p}_j\cdot(\vec{r}_i-\vec{r}_j)](\vec{r}_i-\vec{r}_j)-\vec{p}_j\left|\vec{r}_i-\vec{r}_j\right|^2\} . \qquad (282)$$

Then the dipole moment at each site is expressed in terms of the local total electric field as,

$$\vec{p}_i = \alpha \varepsilon_0 \left(\vec{E}_0 + \sum_{\substack{j=1 \\ j \neq i}}^{N} \vec{E}_{ij} \right). \qquad (283)$$

In general, Equations (282) and (283) are a system of linear equations that can be solved for the dipole moments.

Chapter 4
Conclusions

In this thesis the general theory of the dielectric constant and polarizability, and the relationship between them were reviewed. Equation (64) is particularly important in that it shows the linear relationship between the dielectric constant and the polarizability. The dielectric constant is measured at a macroscopic scale while polarizability is measured at a microscopic scale. A couple of model problems for the effective polarizability of barium titanate were solved. Equations (122) and (131) are the polarizabilities for a chain of barium and titanium atoms (barium titanate) for two different structures. Maxwell's equations were discussed in detail as well. Equations (147) and (162) show the complex dielectric constant for a time varying complex wave and its conjugate, respectively, when applied to Maxwell's equations. When a complex exponential with a negative exponent was used, the imaginary part of the dielectric constant was positive, while for a positive exponent the imaginary part was negative.

Several model problems for the effective polarizability of small systems of discrete dipoles in the presence of an external electric field were solved in detail. These results are original in that they were not found in the published literature. For instance, Equation (201) indicates that when two dipoles are situated on an axis that is parallel to an externally applied electric field, the effective polarizability is larger than the summation of the individual polarizabilities of the dipoles. This is because near the second dipole the first dipole induces an electric field parallel to the external electric field. Likewise, near the first dipole the second dipole induces an electric

field parallel to the external electric field. The net electric field on one dipole is the summation of the external electric field and the induced electric field due to the other dipole. Therefore, the total dipole moment of the system is more than it would be if the dipoles did not interact. It also shows that the polarizability of the system increases as the distance between the dipoles decreases. When the distance shortens to a critical value the polarizability approaches infinity. This is not physically allowable for two reasons. First, there should be a certain limit beyond which the dipoles can't get closer, e.g., atomic dimensions. The second reason is that the polarizability expresses a linear relationship between the dipole moment and the electric field for a sufficiently weak field. For strong electric fields the linear relationship breaks down. When the dipoles are very close together the field acting on each dipole can be large enough to necessitate a nonlinear description.

Equation (250) shows that when the two dipoles are situated on an axis that is perpendicular to the electric field the effective polarizability of this system is smaller than the summation of the polarizabilities of the two individual dipoles. This is because each dipole induces an electric field opposite to the direction of the external electric field in the neighborhood of the other dipole. Thus, the net electric field is the difference of the external electric field and the induced electric field. The result of this calculation also indicates that the polarizability of the system decreases as the distance between the dipole decreases. In both cases, each induced dipole still points along the direction of the externally applied electric field. This last result may not apply to other more general discrete dipole configurations.

There are several opportunities for future work in this area. In this work, the discussion of the polarizability tensor was focused on the simple

two-dipole system. However, the general mathematical method was developed for larger configurations of dipoles. This makes it possible to determine the effective polarizability tensor for any finite number of discrete dipoles. In general, the systems of equations will be linear, but might require special mathematical and computational techniques. The connection between the microscopic polarizability tensor for a large collection of dipoles and the macroscopic dielectric constant should also be investigated. Future research should also focus on applying these methods to the theoretical description of interstellar dust grains.

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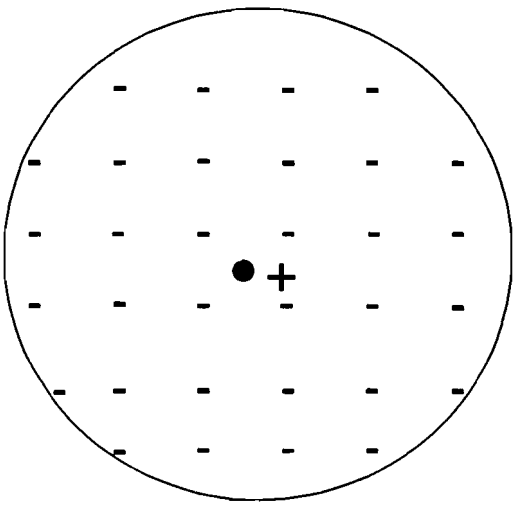


Figure 1. Electron distribution.

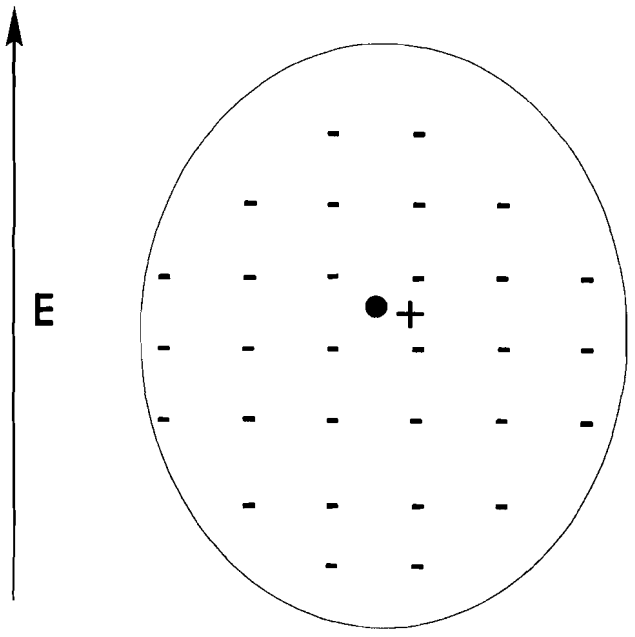


Figure 2. An atom in an electric field has its distribution of electrons displaced with respect to this nucleus.

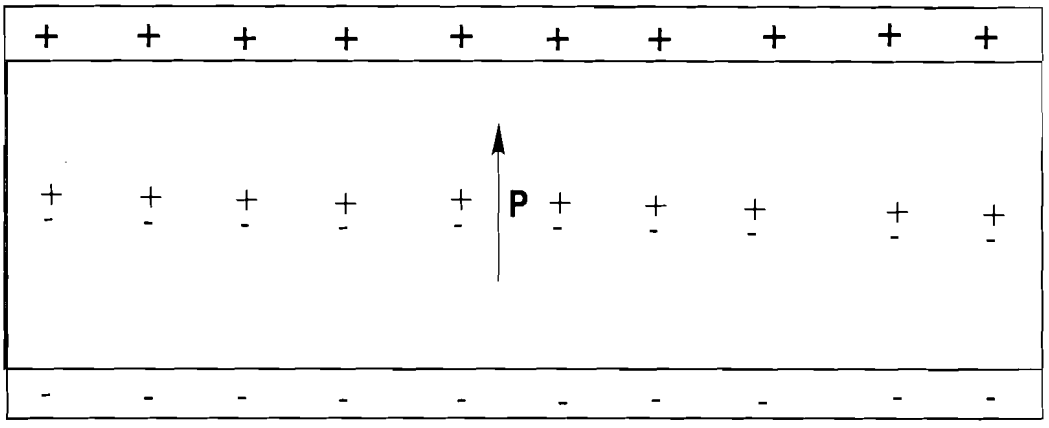


Figure 3. A dielectric slab in a uniform field. The positive charges displaced the distance δ with respect to the negatives.

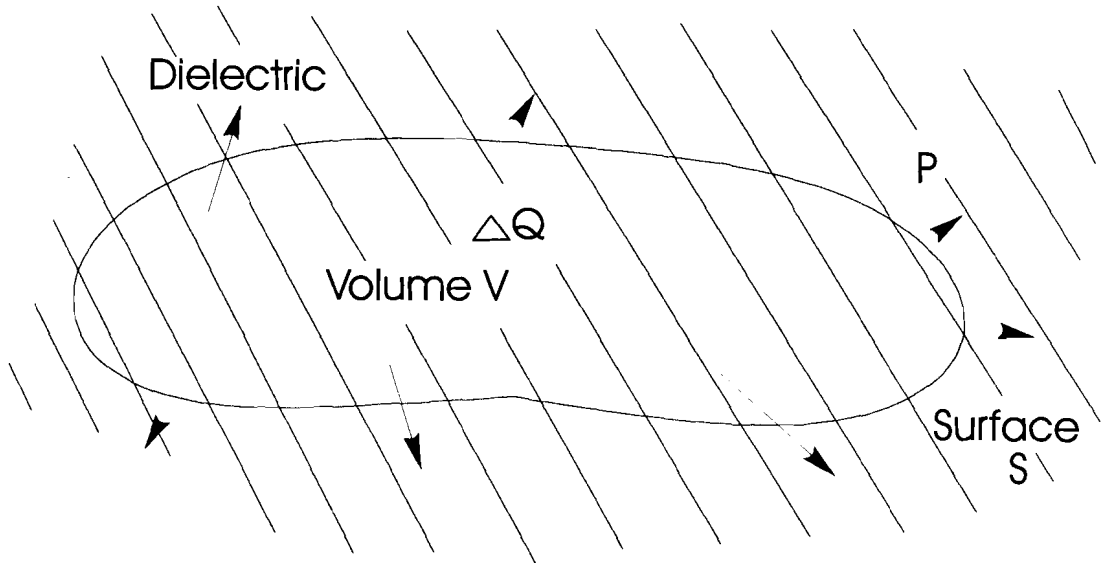


Figure 4. A nonuniform polarization $\vec{P}$ can result in a net charge in the body of a dielectric.

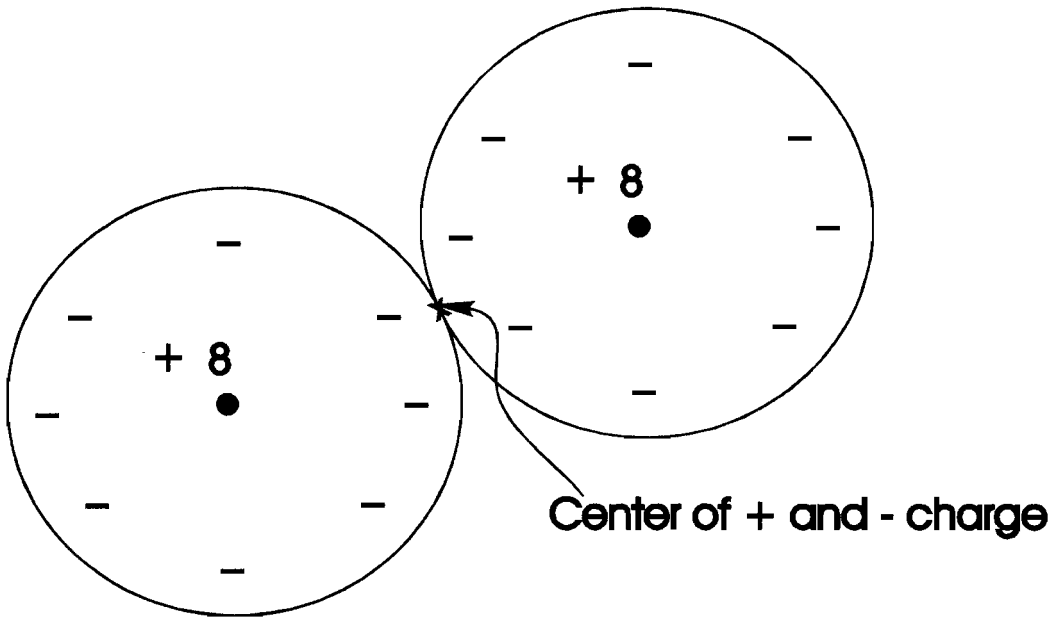


Figure 5. An oxygen molecule with zero dipole moment.

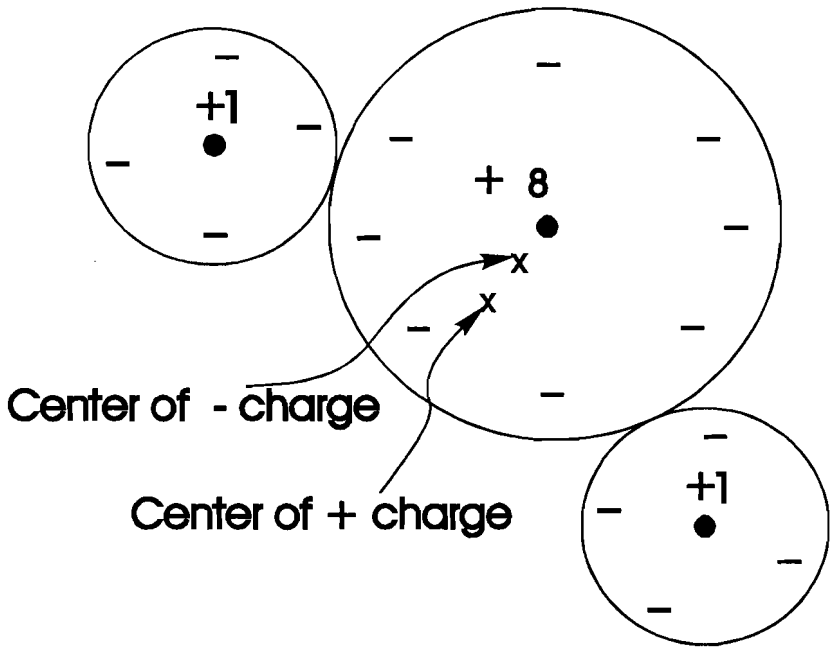


Figure 6. The water molecule has a permanent dipole moment.

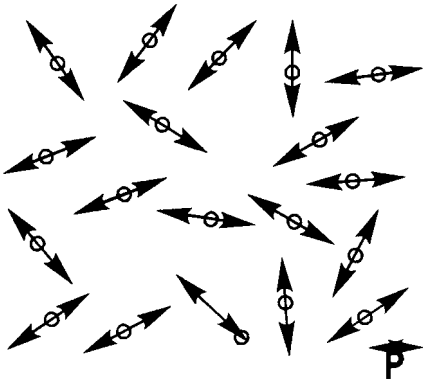


Figure 7. In a gas of polar molecules, the individual moments are oriented at random. The average moment in a small volume is zero.

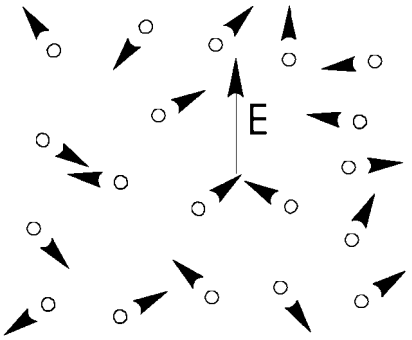


Figure 8. When there is an electric field, there is some average alignment of the molecules.

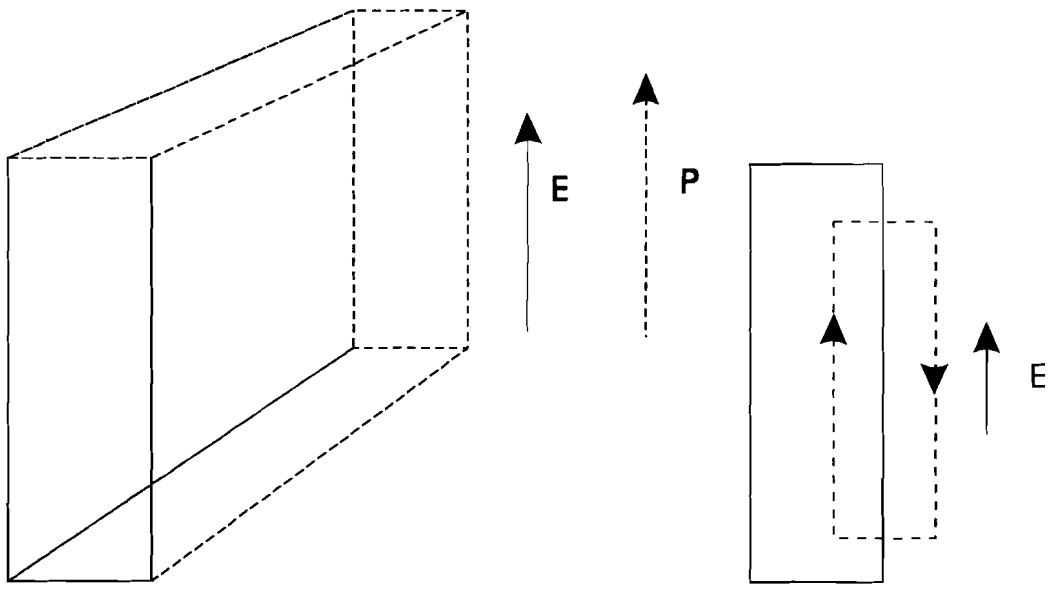


Figure 9. The field in a slot cut in a dielectric depends on the shape and the orientation of the slot.

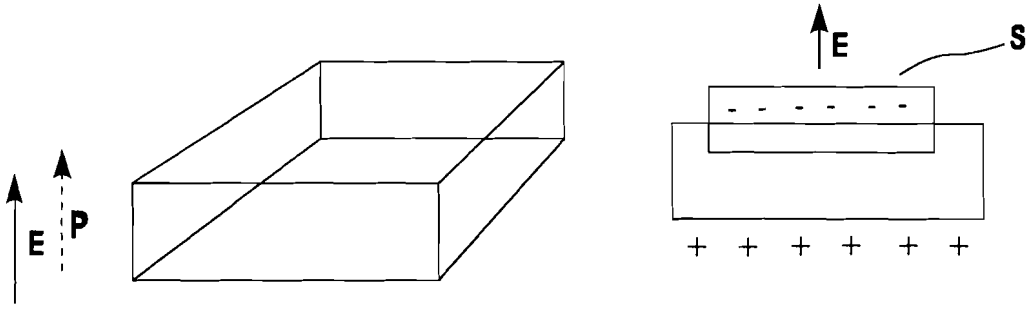


Figure 10. The field in a slot cut in a dielectric depends on the shape and the orientation of the slot.

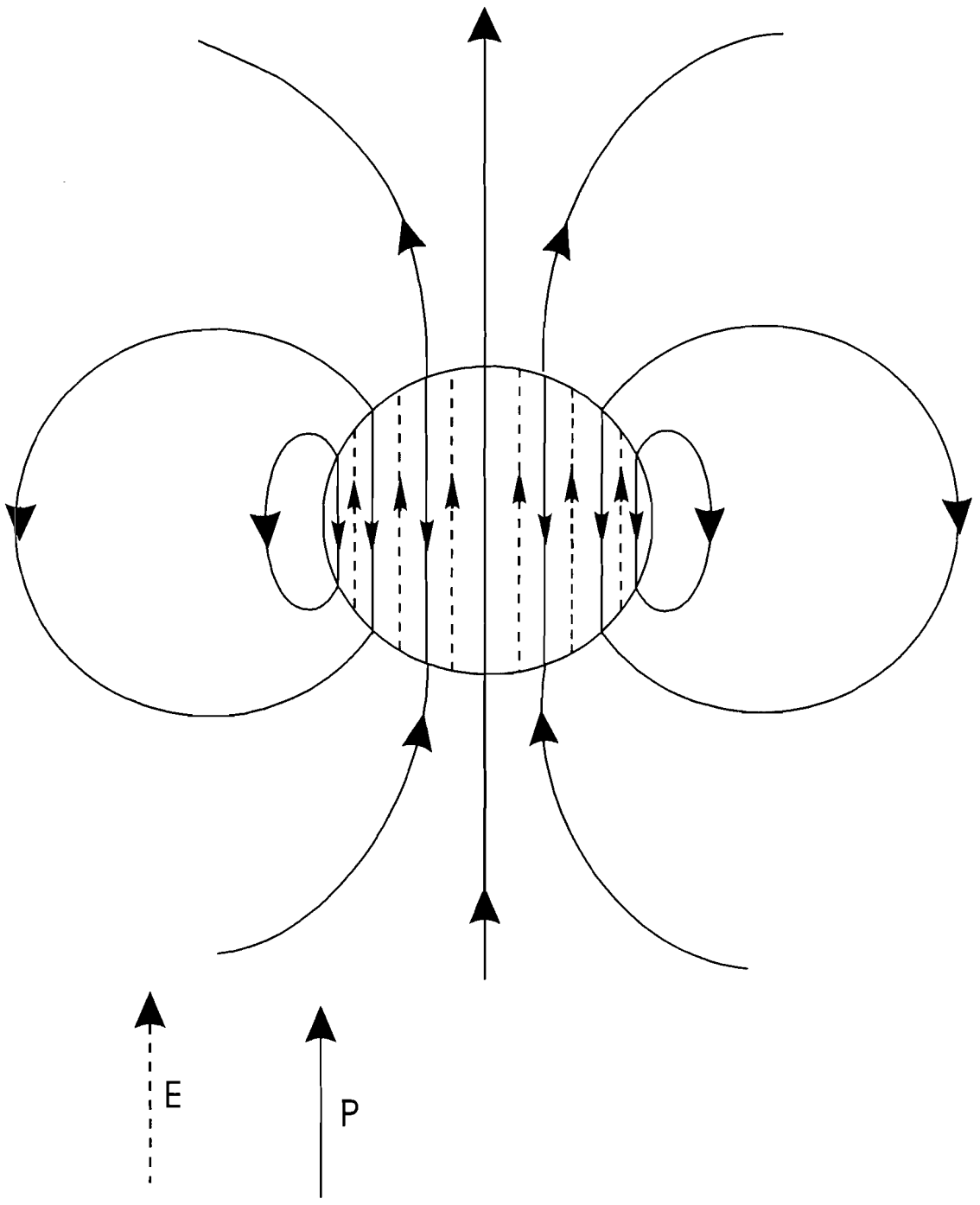


Figure 11. The electric field of a uniformly polarized sphere.

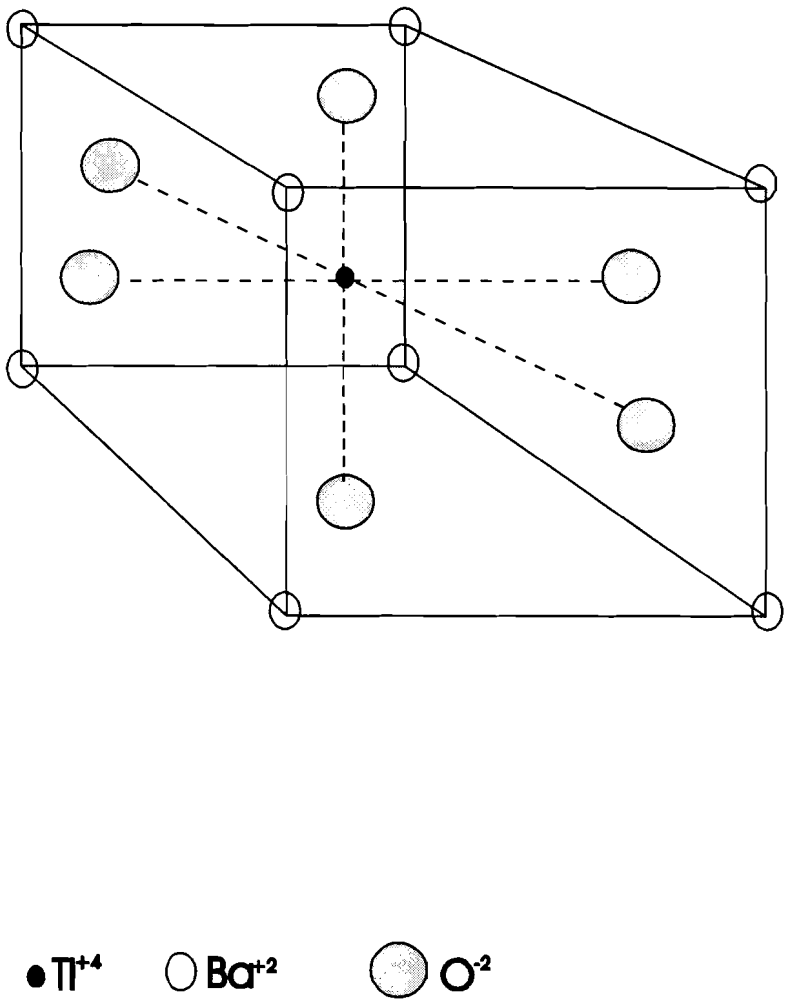


Figure 12. The unit cell of $BaTiO_3$. The atoms fill up most of the space; for clarity, only the positions of their centers are shown.

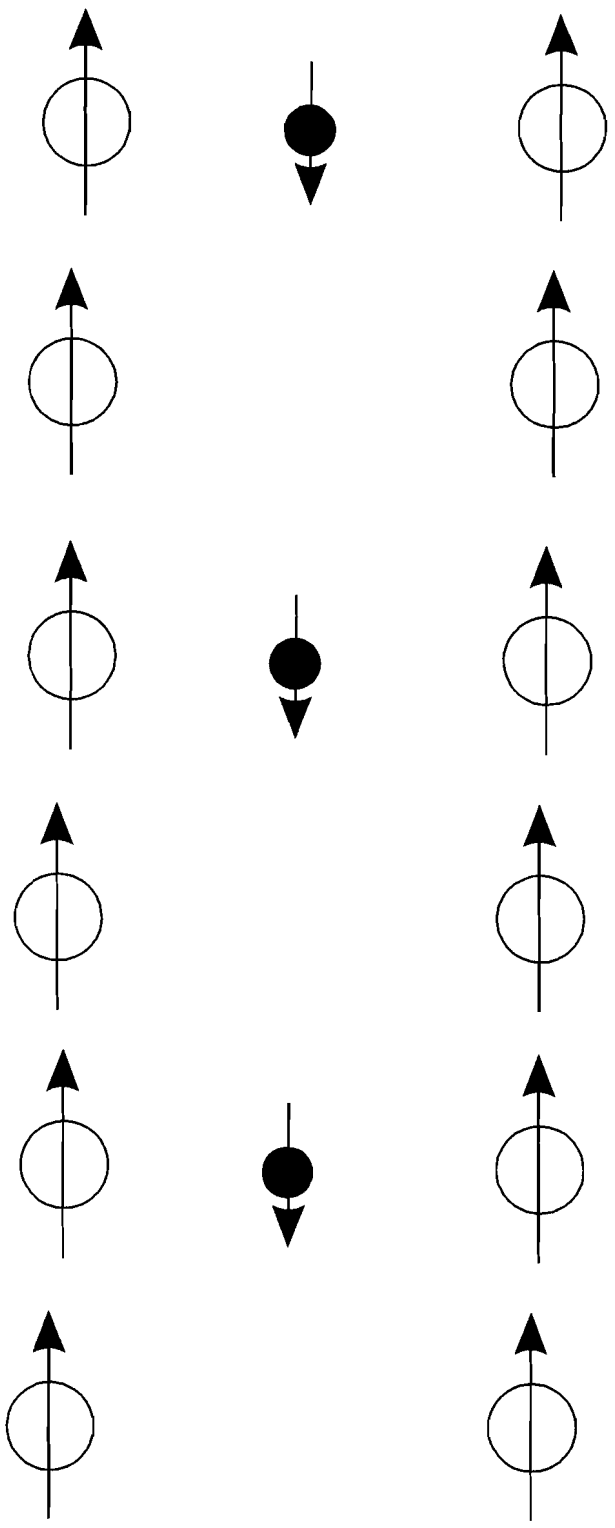


Figure 13. Models of a normal ferroelectric.

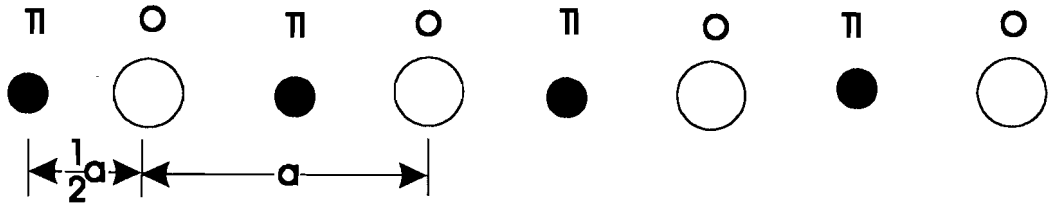


Figure 14. Another model of ferroelectric.

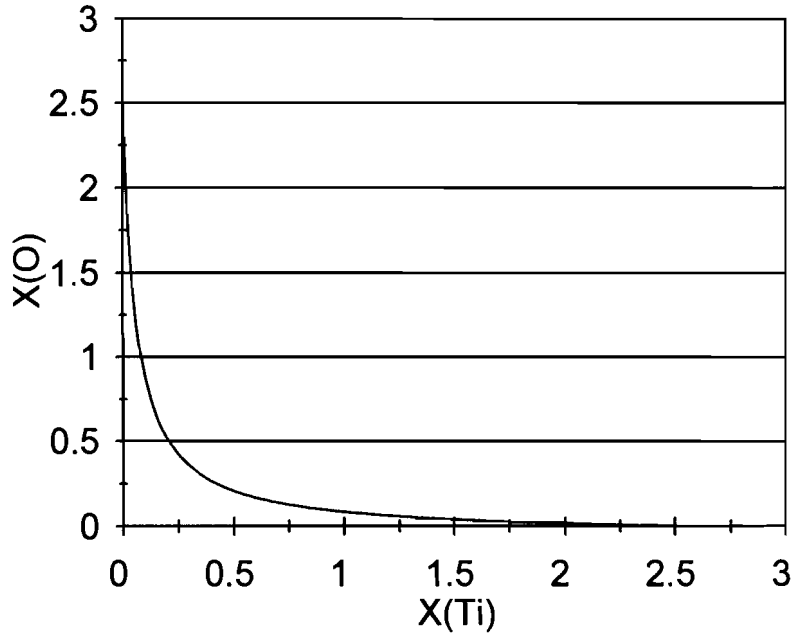
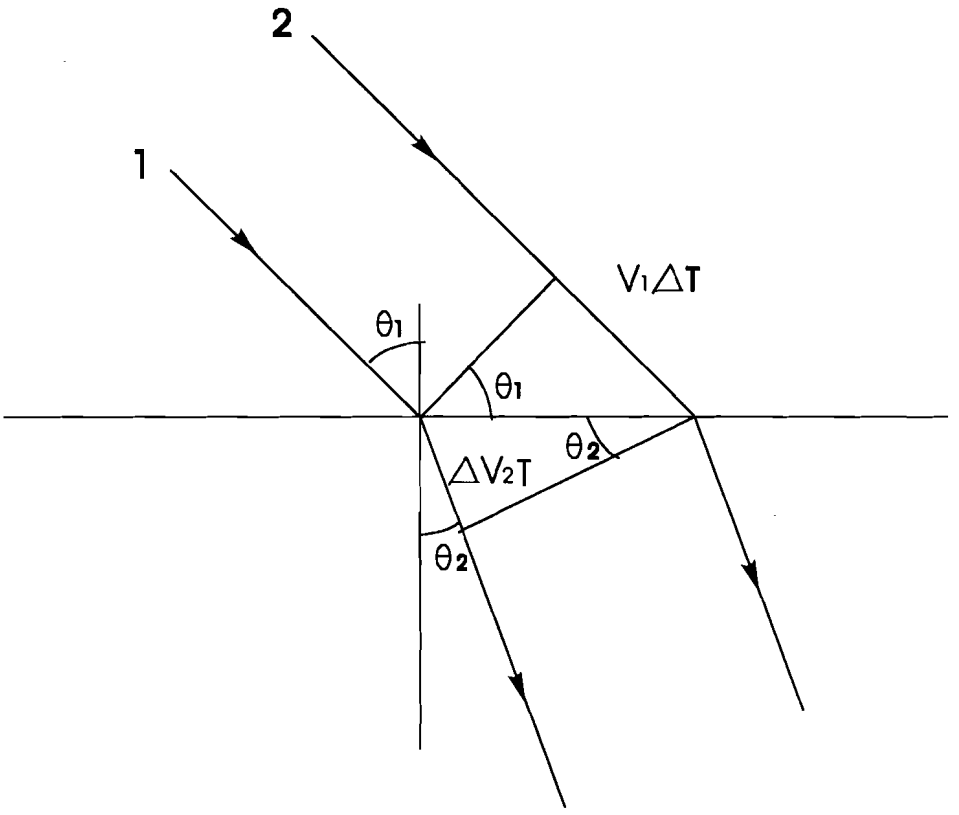


Figure 15. Polarizability of oxygen versus titanium.



Fifgure 16. Huygens construction for proving the law of refraction

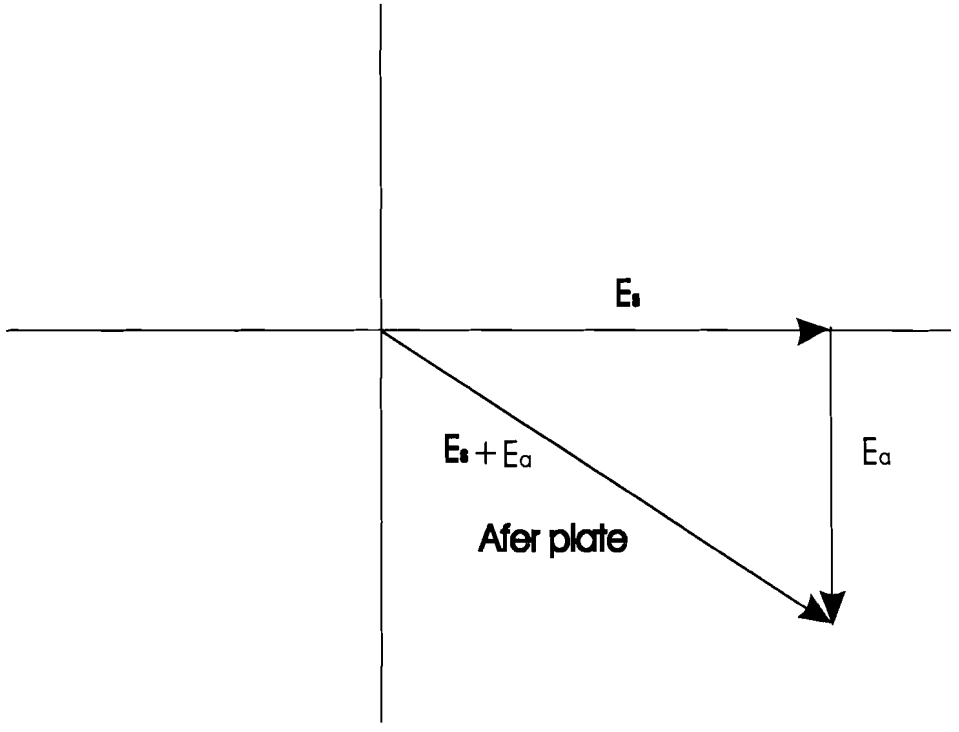


Figure 17. Diagram for the transmitted wave at a particular time and axis.

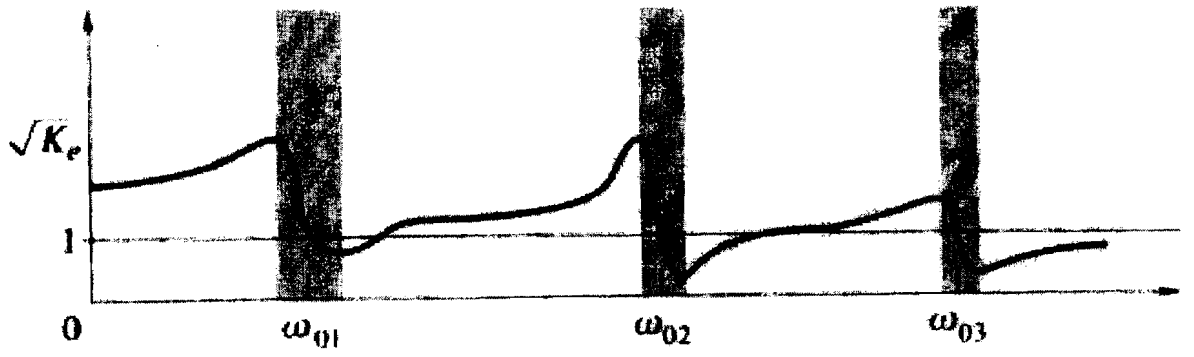


Figure 18. The index of refraction as a function of frequency.

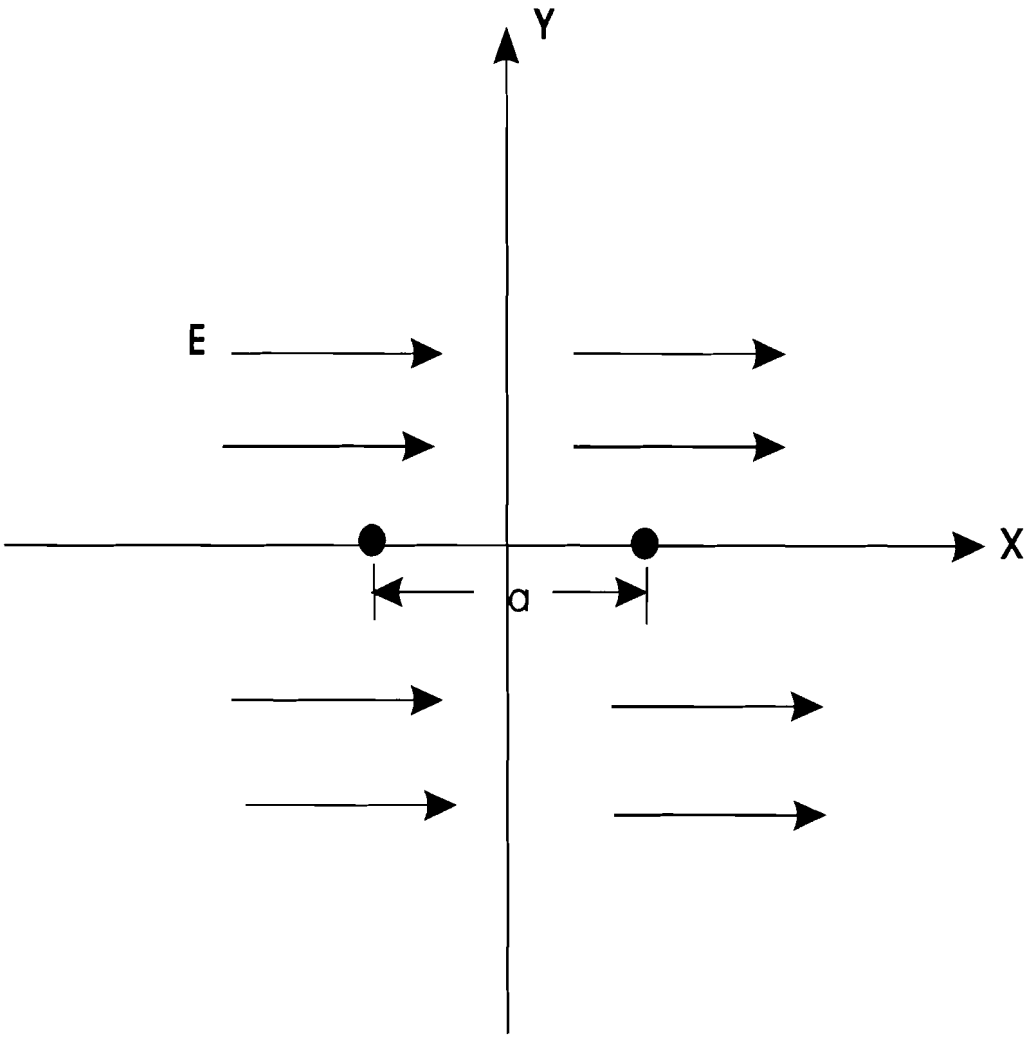


Figure 19. Discrete dipoles are parallel to the external electric field. Both the electric field and the discrete dipoles point on x direction.

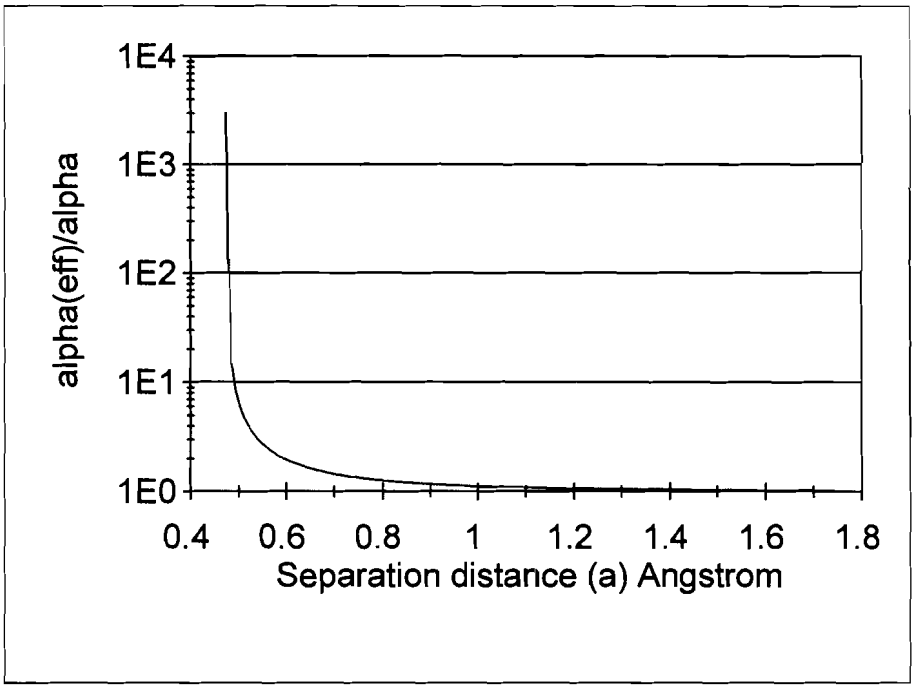


Figure 20. The ratio of effective polarizability to the original polarizability versus separation distance when the dipoles are parallel to the electric field.

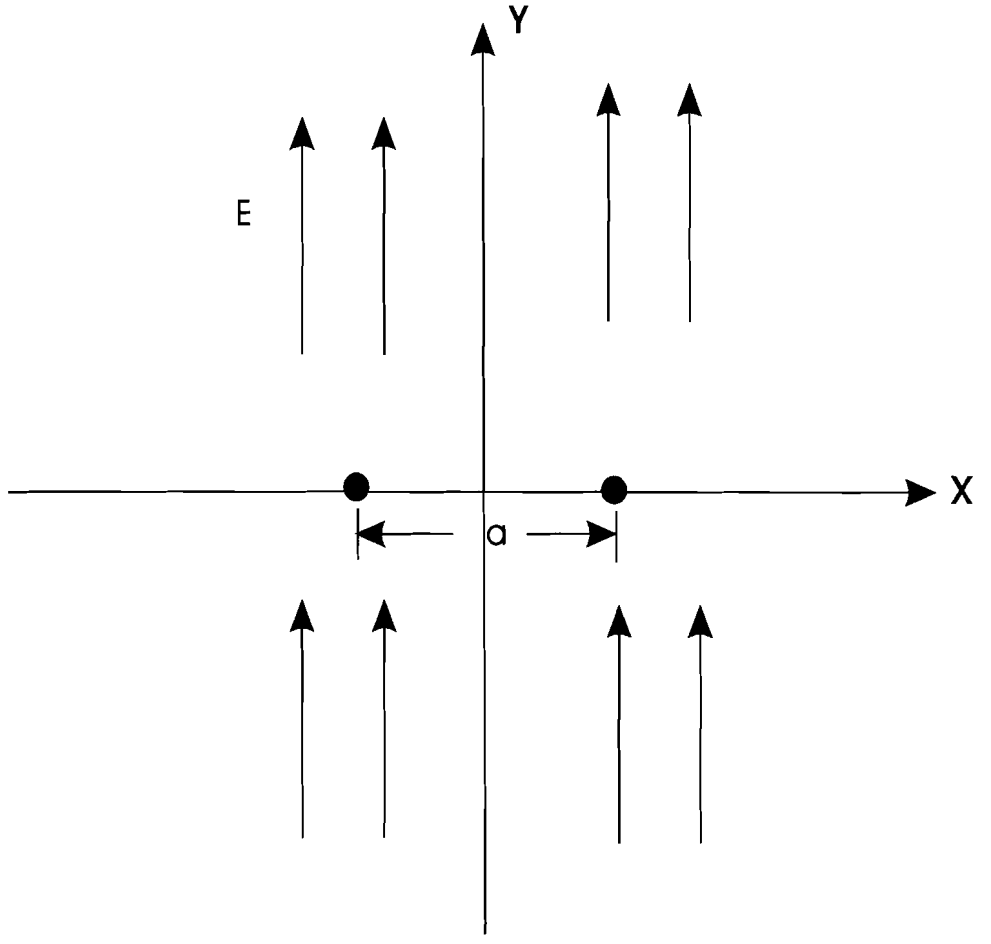


Figure 21. Discrete dipoles perpendicular to the external electric field. The dipoles are situated on x-axis and the electric field points in *y* direction.

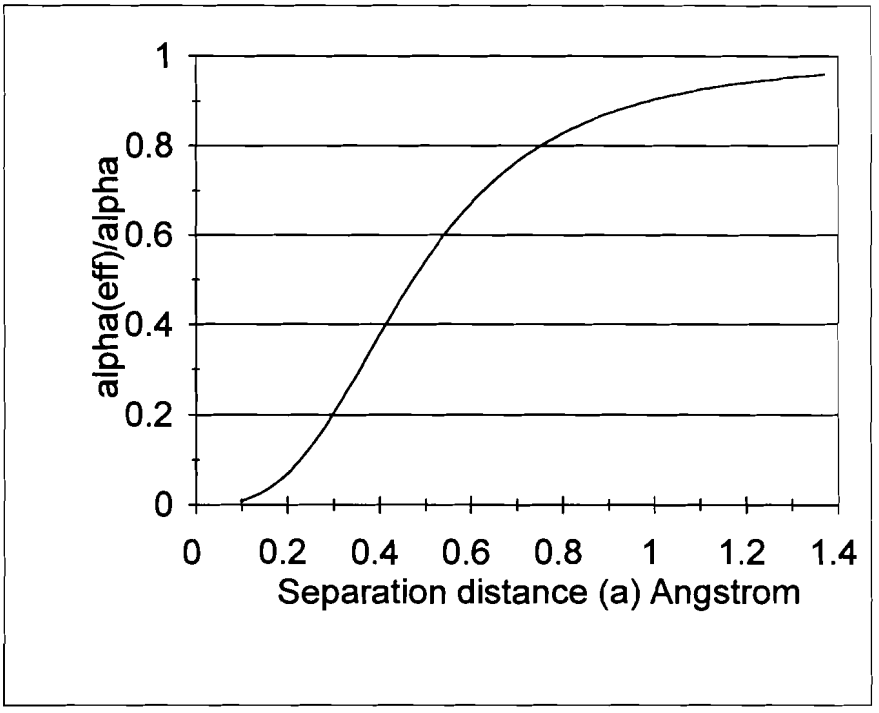


Figure 22. The ratio of effective polarizability to the original polarizability versus separation distance when the dipoles are parallel to the electric field.

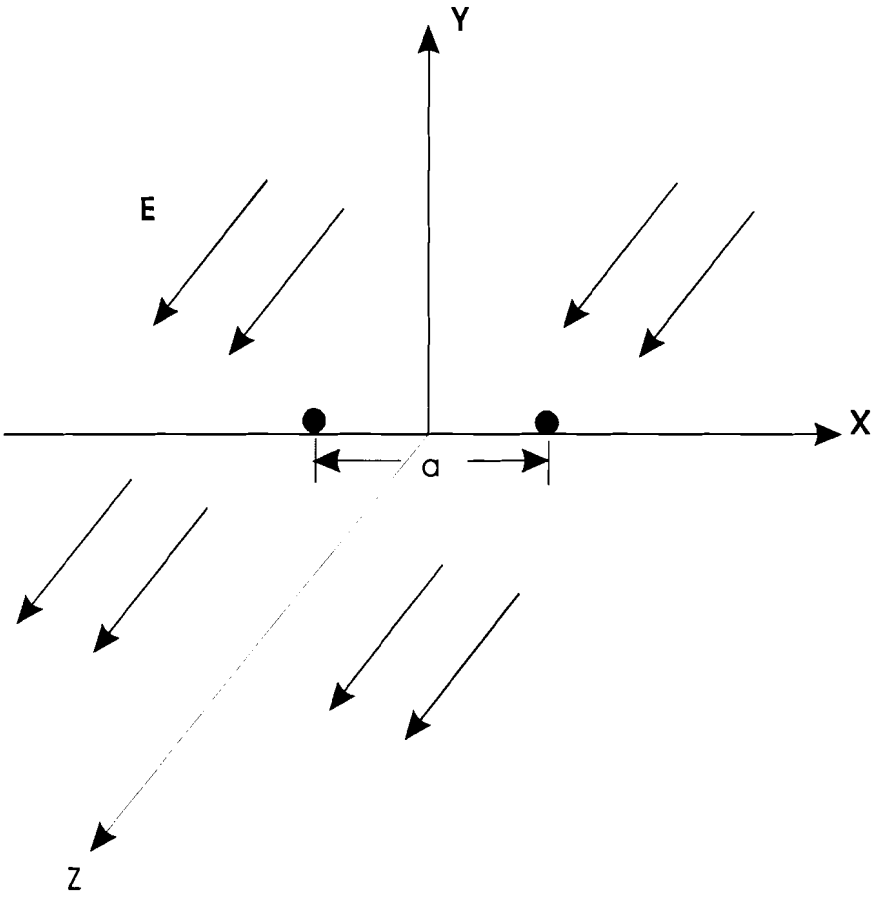


Figure 23. Discrete dipoles perpendicular to the external electric field. The dipoles are situated on x-axis and the electric field points in *z* direction.

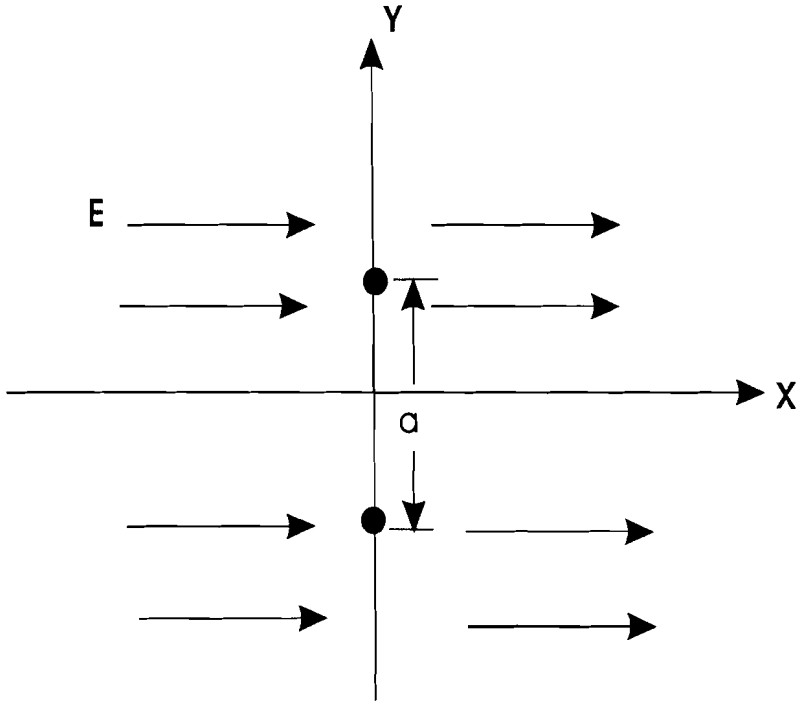


Figure 24. Discrete dipoles perpendicular to the external electric field. The dipoles are situated on y-axis and the electric field points in x direction.

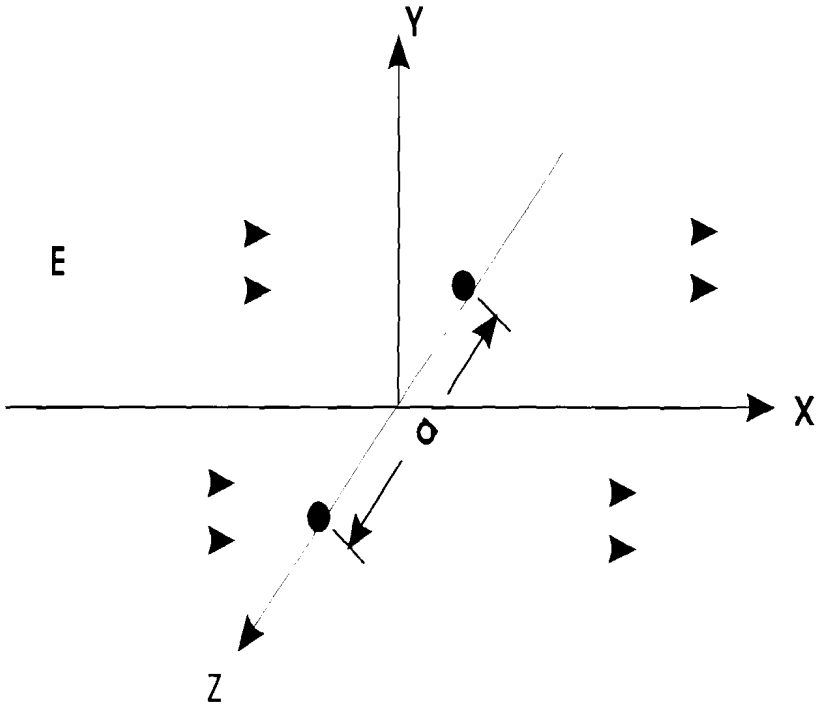


Figure 25. Discrete dipoles perpendicular to the external electric field. The dipoles are situated on z-axis and the electric field points in x direction.

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Majeed

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Date

Theory of Dielectric Constant,
Polarizability and Discrete Dipoles

Title of Thesis

Signature of Graduate Office Staff

May 12, 1999

Date Received