

Theory and Applications of Dielectric Materials

– Introduction

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Outline

- **Historical perspective**
- **Introduction**
- **Electric dipole**
- **Waves in media**
- **Constitutive matrices**
- **Polarization and dielectric constant**

Historical Perspective

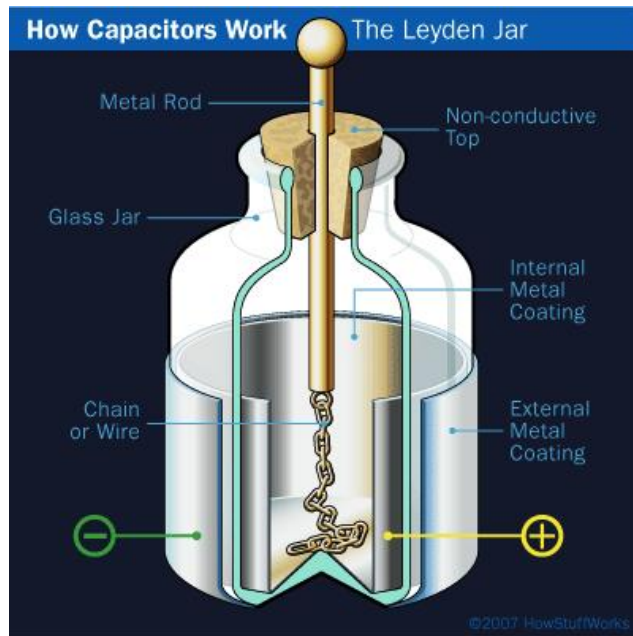
- 1745 – First condenser (capacitor) constructed by A. Cunnæus and P. van Musschenbroek and is known as the "Leyden jar". Similar device was invented by E.G. von Kleist. The jar was made of glass, partially filled with water and contained a brass wire projecting through its cork stopper. An experimenter produced static electricity by friction, and used the wire to store it inside the jar. Without the jar, the electrified material would lose its charge rapidly to the surrounding air, in particular if it was humid.

Historical Perspective



left Pieter Van Musschenbroek (1692-1761); (center) Ewald Georg von Kleist (1700-1748); (right) Leyden jar, the first electrical capacitor

Historical Perspective



The jar was made of glass, partially filled with water and contained a brass wire projecting through its cork stopper. An experimenter produced static electricity by friction, and used the wire to store it inside the jar. Without the jar, the electrified material would lose its charge rapidly to the surrounding air, in particular if it was humid.

Historical Perspective

- 1837 – M. Faraday studied the insulation materials, which he called the "dielectrics".
- 1847 – O-F. Mossotti explained how stationary electromagnetic waves propagate in dielectrics.
- 1865 – J.C. Maxwell proposed the unified theory of electromagnetism. → Maxwell's curl equations

Historical Perspective



(left) Michael Faraday (1791-1867); (center) Ottaviano-Fabrizio Mossotti (1791-1863); (right) James Clerk Maxwell (1831-1879)

Historical Perspective

- 1879 – R. Clausius formulated the relationship between the dielectric constants of two different materials. → The Clausius-Mossotti relation.

$$\boxed{\frac{\epsilon_r^* - 1}{\epsilon_r^* + 2} \cdot \frac{M}{d} = \frac{4\pi N_A \alpha}{3}} \quad (1)$$

where ϵ_r^* is the complex electric permittivity (F/m), M the molecular weight of the substance (kg), d the density (kg/m³), N_A the Avogadro number for a kg mole (6.022×10^{26}), and α the polarizability per molecule.

- 1887 – H.R. Hertz developed the Hertz antenna receiver (1886) and experimentally proved the existence of electromagnetic waves.

Historical Perspective



(left) Rudolf Julius Emanuel Clausius (1822-1888); (right) Heinrich Rudolf Hertz (1857-1894)

Historical Perspective

- 1897 – P. Drude integrated the optics with Maxwell's theories of electromagnetism. → Drude's model

$$v_{th} = \sqrt{\frac{3k_B T}{m}} \quad (2)$$

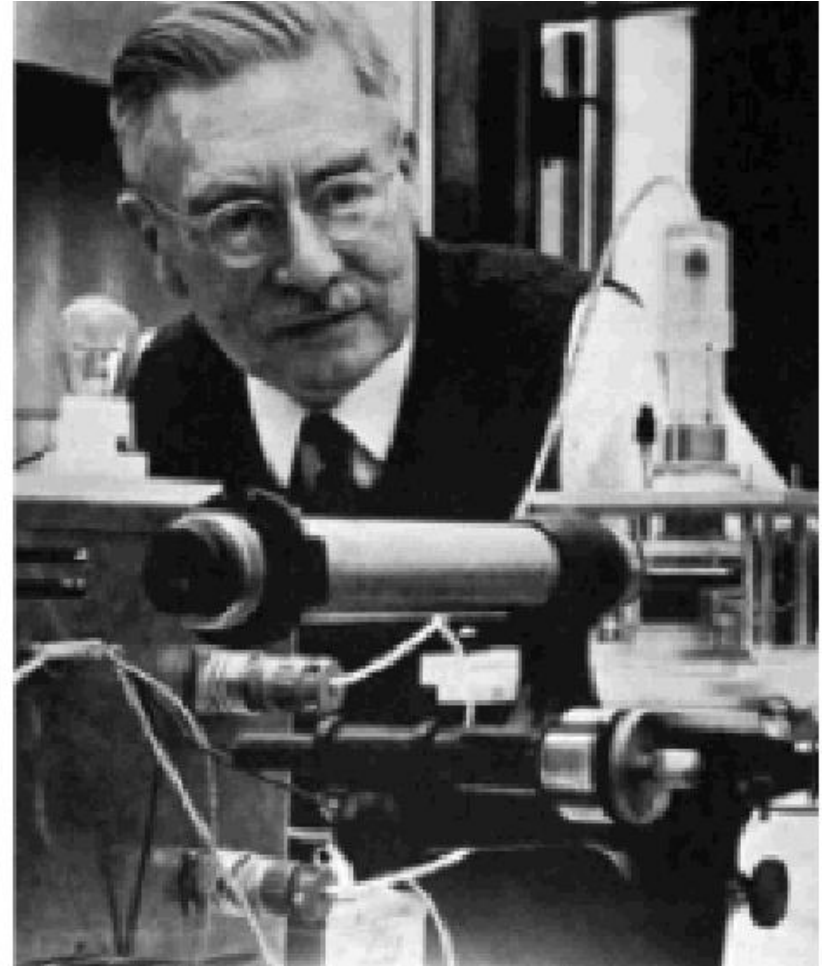
where v_{th} is average thermal velocity, k_B Boltzmann's constant, T the absolute temperature, and m the electron mass.

- 1919 – P. Debye funded the modern theory of dielectrics to explain dielectric dispersion and relaxation. → Debye's model

$$\epsilon^* = \frac{\epsilon_s}{1 - i\omega\tau} = \epsilon' + i\epsilon'' \quad (3)$$

where v_{th} is average thermal velocity, k_B Boltzmann's constant, T the absolute temperature, and m the electron mass.

Historical Perspective



(left) Paul Karl Ludwig Drude (1863-1906); (right) Peter J.W. Debye (1884-1966)

Historical Perspective

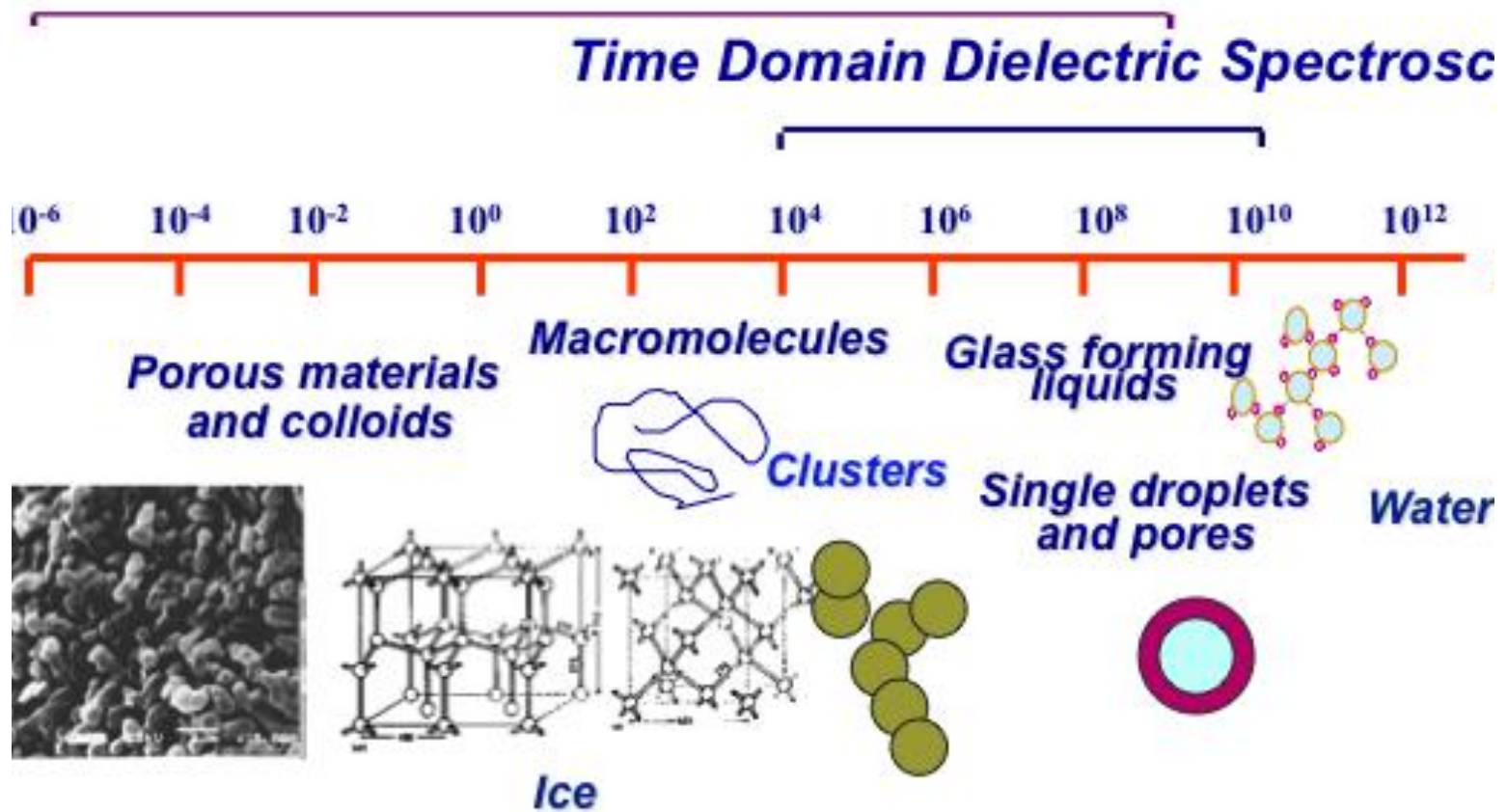
- Dielectrics are also called insulating materials, with low electric conductivities ranging from 10^{-18} S/m to 10^{-6} S/m. Metals have conductivities of the order of 10^8 S/m. Semiconductors have conductivities of the order of 10 S/m.
- Since the pioneering work done by early researchers, physical measurement and theoretical modelling of gaseous, liquid, and solid dielectrics have been reported in physics, chemistry, electrical engineering, mechanical engineering, and civil engineering.

Introduction

- When a dielectric is upon the application of an external electric field, very low electric conduction or an very slowly varying dielectric polarization is observed inside the dielectric. → Polarization means the orientation of dipoles.
- Dielectric spectroscopy – The study of frequency-dependent behaviors of dielectrics, sensitive to relaxation processes in an extremely wide range of characteristic times (frequencies).

Introduction

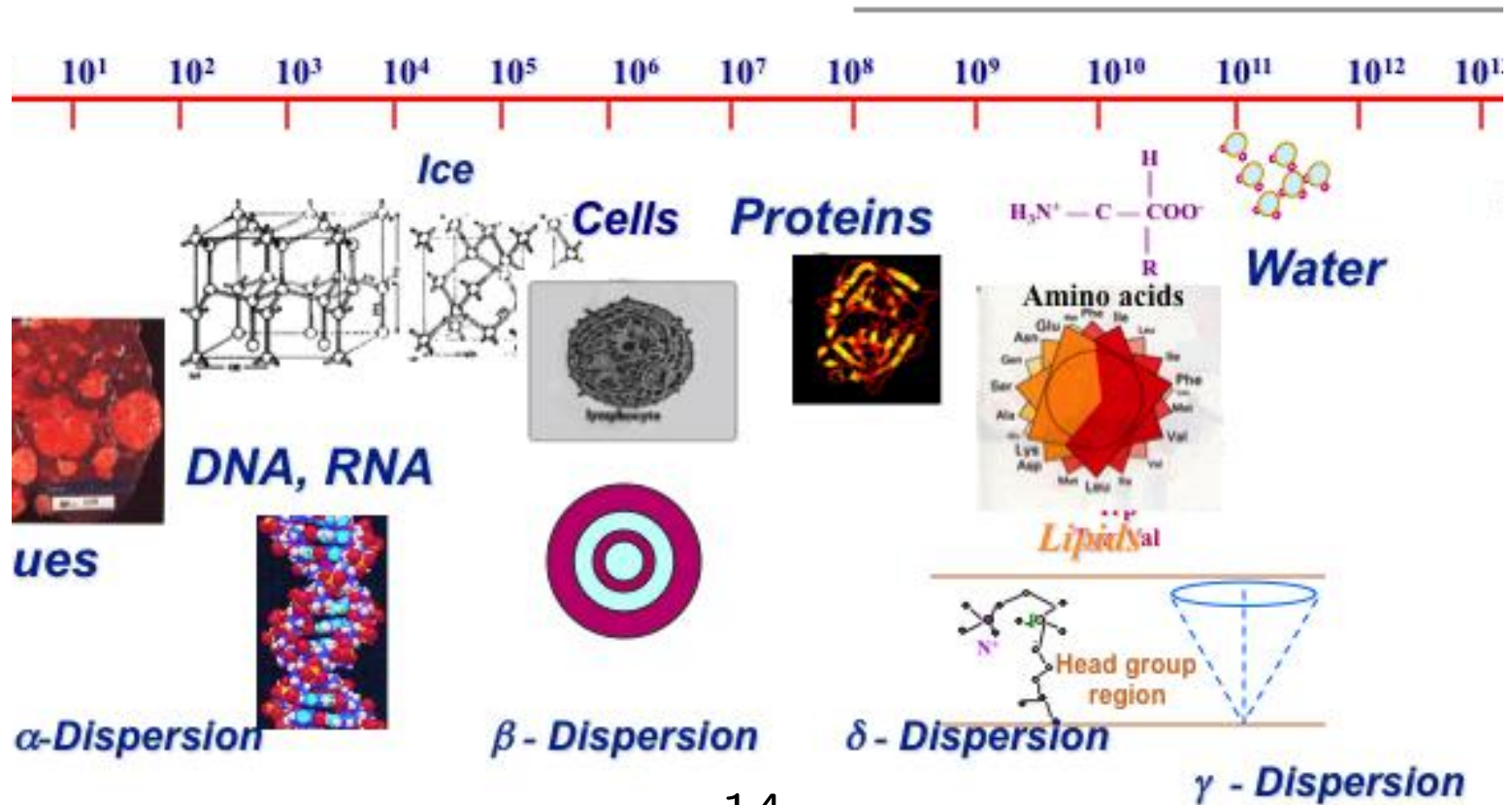
Broadband Dielectric Spectroscopy



Introduction

Broadband Dielectric Spectroscopy

Time Domain Dielectric Spectroscopy



Electric Dipole

- The electric moment of a point charge q relative to a fixed point is defined as qr , where r is the radius vector from the fixed point to the charge. The total dipole moment of a whole system of a charge q_i relative to a fixed origin is defined as

$$m = \sum_i q_i r_i \quad (4)$$

A dielectric can be considered as consisting of elementary charges q_i . Without the application of an external electric field and any net charge inside the dielectric,

$$\sum_i q_i = 0 \quad (5)$$

As long as the net charge of the dielectric diminishes, the electric moment is independent of the choice of the

Electric Dipole

origin. When the origin is displaced at a distance r_0 , the increase of the total dipole moment is

$$\Delta m = - \sum_i q_i r_0 = -r_0 \sum_i q_i \quad (6)$$

It becomes zero when the net charge is zero. This way, we can determine the electric centers of the positive and the negative charges by

$$\sum_{\text{positive}} q_i r_i = r_p \sum_{\text{positive}} q_i = r_p Q \quad (7)$$

$$\sum_{\text{negative}} q_i r_i = r_n \sum_{\text{negative}} q_i = r_n Q \quad (8)$$

$$(9)$$

in which the radius vectors from the origin to the electric centers are denoted by r_p and r_n . The total charge is

Electric Dipole

denoted by Q . When the net charge is zero, Eq.(4) can be rewritten by

$$m = (r_p - r_n)Q \quad (10)$$

The difference $(r_p - r_n)$ equals to the vector distance between the electric centers, pointing from the negative to the positive center. In the vector form, we have

$$\bar{m} = (\bar{r}_p - \bar{r}_n) Q = \bar{a}Q \quad (11)$$

which is the expression of the electric moment of a system of charges with zero net charge, called the electric dipole moment of the system.

- Ideal dipole – An ideal or point dipole has a distance a/n

Electric Dipole

between two point charges q^+ and q^- by replacing the charge by qn .

- Permanent dipole moment – In the molecular systems where the electric centers of the positive and the negative charge distributions do not coincide/overlap, a finite electric (permanent, intrinsic) dipole moment can be determined.
- Polar molecules – The molecules which have a permanent dipole moment (e.g., water).

Electric Dipole

- Induced dipole moment – When a particle is upon the application of an external electric field, a temporary induced dipole moment can arise and will diminish when the field is removed.
- Polarized particles – A particle is polarized under the application of an external electric field. Upon the application of this field, the positive and negative charges are moved apart.
- Molecular dipole moments – The values of permanent or induced dipole moments in a molecule are expressed in Debye units (D , $1D = 10^{-18}$ electrostatic units or e.s.u).

Electric Dipole

- Non-symmetric molecules – The permanent dipole moments of non-symmetric molecules are in the range of $0.5 D$ to $5 D$. The value of the elementary charge e_0 is 4.4×10^{-10} e.s.u. The distance of the electric charge centers in these molecules is in the range of 10^{-11} m to 10^{-10} m.

Waves in Media

- Potentials and fields due to electric charges – From Coulomb's law, the force between two charges q and q' with a distance vector \vec{r} is

$$\vec{F} = \frac{qq'}{r^2} \cdot \frac{\vec{r}}{r} \quad (12)$$

producing an electric field strength (or intensity) \vec{E} to be

$$\vec{E} = \lim_{q' \rightarrow 0} \frac{\vec{F}}{q'} \quad (13)$$

Then the field strength due to an electric charge at a distance r is given by

$$\vec{E} = \frac{q}{r^2} \cdot \frac{\vec{r}}{r} \quad (14)$$

If we integrate field strength over any closed surface

Waves in Media

around the charge e , we have

$$\oint \vec{E} \cdot d\vec{S} = 4\pi q \quad (15)$$

where $d\vec{S}$ is the unit vector on the closed surface. The charge q can be expressed by the integration of a volume charge density ρ (or a surface charge density) by

$$\oint \vec{E} \cdot d\vec{S} = 4\pi \int \int \int_V \rho dv \quad (16)$$

With Gauss or divergence theorem,

$$\nabla \cdot \vec{E} = 4\pi\rho \quad (17)$$

and it leads to one of the Maxwell's curl equations; called the source equation.

Waves in Media

- Consider the curl of \bar{E} to be zero.

$$\nabla \times \bar{E} = 0 \quad (18)$$

With Stoke's theorem,

$$\int \int_S \nabla \times \bar{E} \cdot d\bar{S} = \oint_C \bar{E} d\bar{l} \quad (19)$$

(where C is the external contour bounding the open surface S , and $d\bar{l}$ a vector differential length), we have

$$\oint \bar{E} \cdot d\bar{l} = 0 \quad (20)$$

- When there is no time variation,

$$\bar{E} = -\nabla\Phi \quad (21)$$

Waves in Media

where Φ is a potential function. By virtue of the vector identity:

$$\nabla \times (\nabla\Phi) = 0 \quad (22)$$

we have

$$\nabla \times \bar{E} = 0 \quad (23)$$

and it is only true when there is no time variation in \bar{E} (static electric field), suggesting the term $\partial\bar{B}/\partial t$ in Faraday's law can be neglected (\bar{B} is the magnetic flux density (webers/m²)). In free space (vacuum), the Coulomb law (or Gauss' law for electricity) is

$$\nabla \cdot \bar{E} = \frac{\rho}{\epsilon_0} \quad (24)$$

Waves in Media

where ϵ_0 is the electric permittivity of vacuum ($=8.854 \times 10^{-12}$ F/m).

- Derivation of the value of ϵ_0 (Homework #1)

- With $\bar{E} = -\nabla\Phi$, we have

$$\nabla^2\Phi = \frac{\rho}{\epsilon_0} \quad (25)$$

which is known as the Poisson equation. When net charge is zero, it becomes

$$\nabla^2\Phi = 0 \quad (26)$$

Waves in Media

which is known as the Laplace equation.

- In three-dimensional vector notation, Maxwell's curl equations are

$$\nabla \times \bar{H} = \frac{\partial}{\partial t} \bar{D} + \bar{J} \quad (27)$$

$$\nabla \times \bar{E} = -\frac{\partial}{\partial t} \bar{B} \quad (28)$$

$$\nabla \cdot \bar{D} = \rho \quad (29)$$

$$\nabla \cdot \bar{B} = 0 \quad (30)$$

where \bar{H} is the magnetic field strength (A/m), D the electric displacement (C/m²), \bar{J} the electric current density

Waves in Media

(A/m²), and \bar{B} the magnetic flux density (webers/m²). The constitutive relations for materials are

$$\bar{D} = \epsilon \bar{E} \quad (31)$$

$$\bar{B} = \mu \bar{H} \quad (32)$$

where ϵ is the electric permittivity and ν the magnetic permeability. In source-free and homogeneous regions, the Maxwell curl equations become

$$\nabla \times \bar{H} = \epsilon \frac{\partial}{\partial t} \bar{E} \quad (33)$$

$$\nabla \times \bar{E} = -\mu \frac{\partial}{\partial t} \bar{H} \quad (34)$$

$$\nabla \cdot \bar{E} = 0 \quad (35)$$

$$\nabla \cdot \bar{H} = 0 \quad (36)$$

Waves in Media

A wave equation can be obtained by taking the curl of Eq.(34) and using Eqs.(35) and (36), leading to

$$\left(\nabla^2 - \mu\epsilon \frac{\partial^2}{\partial t^2} \right) \bar{E}(\bar{r}, t) = 0 \quad (37)$$

which is known as the homogeneous Helmholtz wave equation in source-free media. $\bar{E}(\bar{r}, t)$ is a time-space function. Consider the solution in the following form.

$$\bar{E}(\bar{r}, t) = \bar{E} \cos(k_x x + k_y y + k_z z - \omega t) \quad (38)$$

where \bar{E} is a constant vector, (k_x, k_y, k_z) are the wave number components of the wave (or propagation) vector \bar{k} .

$$\bar{k} = k_x \hat{x} + k_y \hat{y} + k_z \hat{z} \quad (39)$$

Waves in Media

Substituting the solution into the Helmholtz wave equation provides

$$k_x^2 + k_y^2 + k_z^2 = \omega^2 \mu \epsilon = k^2 \quad (40)$$

Use the wave vector, the electric field solution can be expressed by

$$\bar{E}(\bar{r}, t) = \bar{E} \cos(\bar{k} \cdot \bar{r} - \omega t) \quad (41)$$

where $\bar{r} = x\bar{x} + y\bar{y} + z\bar{z}$ is the position vector. Similarly, for the magnetic field vector \bar{H} ,

$$\bar{H}(\bar{r}, t) = \bar{H} \cos(\bar{k} \cdot \bar{r} - \omega t) \quad (42)$$

When $\bar{k} \cdot \bar{r} = \text{constant}$, a constant phase front is defined, suggesting a plane wave.

Waves in Media

- Waves in conducting media – Consider a conducting medium in which a conduction current source \bar{J}_c is modeled. With Ohm's law, source \bar{J}_c is related to \bar{E} .

$$\bar{J}_c = \sigma \bar{E} \quad (43)$$

The Helmholtz wave equation in a homogeneous, isotropic, conducting medium becomes

$$\left(\nabla^2 - \mu\epsilon \frac{\partial^2}{\partial t^2} - \mu\sigma \frac{\partial}{\partial t} \right) \bar{E}(\bar{r}, t) = 0 \quad (44)$$

One solution is

$$\bar{E}(\bar{r}, t) = E_0 e^{-k_I z} \cos(k_R z - \omega t) \hat{x} \quad (45)$$

where (k_R, k_I) are the real and imaginary components of the wave vector. Substituting this solution into Eq.(44)

Waves in Media

leads to

$$e^{-k_I z} [(k_I^2 - k_R^2 + \omega^2 \epsilon \mu) \cos(k_R z - \omega t) + (2k_R k_I - \omega \mu \sigma) \sin(k_R z - \omega t)] = 0 \quad (46)$$

with

$$k_R = \omega \sqrt{\mu \epsilon} \sqrt{\frac{1}{2} \left(\sqrt{1 + \frac{\sigma^2}{\epsilon^2 \omega^2}} + 1 \right)} \quad (47)$$

$$k_I = \omega \sqrt{\mu \epsilon} \sqrt{\frac{1}{2} \left(\sqrt{1 + \frac{\sigma^2}{\epsilon^2 \omega^2}} - 1 \right)} \quad (48)$$

satisfying the following dispersion relation:

$$k_R^2 - k_I^2 = \omega^2 \mu \epsilon \quad (49)$$

$$2k_R k_I = \omega \mu \sigma \quad (50)$$

Waves in Media

- Derivation of the unit of electric permittivity from Coulomb's Law (Homework #2)
- Penetration depth – When electromagnetic waves propagate in a conducting medium, the energy dissipates and attenuates in the direction of propagation. The attenuation depth is defined as

$$d_p = \frac{1}{k_I} \quad (51)$$

indicating that the electromagnetic wave amplitude attenuates by a factor of e^{-1} in a distance d_p .

Waves in Media

- For a highly conducting medium ($1 \ll \frac{\sigma}{\omega\epsilon}$) –

$$k_I \approx \sqrt{\frac{\omega\mu\epsilon}{2}} \quad (52)$$

The penetration depth is

$$d_p = \sqrt{\frac{2}{\omega\mu\epsilon}} \quad (53)$$

which is frequency-dependent.

- For a slightly conducting medium ($\frac{\sigma}{\omega\epsilon} \ll 1$) –

$$k_I \approx \frac{\sigma}{2} \sqrt{\frac{\mu}{\epsilon}} \quad (54)$$

Waves in Media

The penetration depth is

$$d_p = \frac{2}{\sigma} \sqrt{\frac{\epsilon}{\mu}} \quad (55)$$

which is frequency-independent.

Constitution Matrices

- Isotropic media – In an isotropic dielectric medium,

$$\bar{D} = \epsilon \bar{E} = \epsilon_0 \bar{E} + \bar{P} \quad (56)$$

where \bar{P} denotes the electric dipole moment per unit volume of the dielectric material. In an isotropic magnetic medium,

$$\bar{B} = \mu \bar{H} = \mu_0 \bar{H} + \mu_0 \bar{M} \quad (57)$$

where \bar{M} is the magnetization vector. When an isotropic or anisotropic medium is placed in an electric field, it is polarized. When placed in a magnetic field, it is magnetized.

- Anisotropic media – In anisotropic media,

$$\bar{D} = \bar{\epsilon} \cdot \bar{E} \quad (58)$$

Constitution Matrices

$$\bar{B} = \bar{\mu} \cdot \bar{H} \quad (59)$$

where

$$\bar{\epsilon} = \begin{bmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{bmatrix} \quad (60)$$

A medium is electrically anisotropic when it is described by an electric permittivity tensor $\bar{\epsilon}$ and a magnetic permeability scalar μ . A medium is magnetically anisotropic when it is described by a magnetic permeability tensor $\bar{\mu}$ and an electric permittivity scalar ϵ .

- Bianisotropic media – In a bianisotropic medium, electric and magnetic fields are coupled. The constitutive

Constitution Matrices

relations are

$$\bar{D} = \bar{\epsilon} \cdot \bar{E} + \bar{\xi} \cdot \bar{H} \quad (61)$$

$$\bar{B} = \bar{\zeta} \cdot \bar{E} + \bar{\mu} \cdot \bar{H} \quad (62)$$

Polarization and Dielectric Constant

- Polarization – When an external electric field F acting on a charge q exerts on it a force Fq , which displaces it in the direction of the field until the restoring force fr is equal to it, suggesting that

$$Fq = fr \quad (63)$$

where f is a proportionality constant. An electric moment $m = qr$ is created by this displacement r . With $r = m/q$, we have

$$m = \frac{Fq^2}{f} \quad (64)$$

In the case of a molecule containing several electrons, each of charge q , the total moment induced in the molecule

Polarization and Dielectric Constant

in the direction of the field is

$$\Sigma m = F \Sigma \frac{q^2}{f} \quad (65)$$

Molecular polarizability is defined by Eq.(65) as the dipole moment induced in a molecule by unit electric field E , which means

$$\alpha_0 = \Sigma \frac{q^2}{f} \quad (66)$$

and $F = 1$ e.s.u. = 300 volts per cm. It also suggests that f is the force constant for the binding of the electrons. The product of qr is called the dipole moment.

- Electric moment – Consider a condenser consist of two

Polarization and Dielectric Constant

parallel plates in vacuum whose distance apart is small in comparison with their dimensions. Inside the condenser the intensity of the electric field perpendicular to the plates is

$$E_0 = 4\pi\sigma \quad (67)$$

where σ is the surface density of charge. When the condenser is filled with a homogeneous dielectric material of dielectric constant ϵ'_r (This will be explained later in further detail), the field strength decreases to

$$E = \frac{4\pi\sigma}{\epsilon'_r} \quad (68)$$

The decrease in field strength is

$$E_0 - E = 4\pi\sigma \left(1 - \frac{1}{\epsilon'_r}\right) = 4\pi\sigma \frac{\epsilon'_r - 1}{\epsilon'_r} \quad (69)$$

Polarization and Dielectric Constant

The same decrease in field strength can be achieved by reducing σ by an amount

$$\frac{\sigma (\epsilon_r' - 1)}{\epsilon_r'} = P \quad (70)$$

where P is the equivalent surface density of this charge. It is produced by an induced charge shift throughout the dielectric material, which produces an electric moment per unit volume. Therefore, P is called the polarization which indicates the amount of surface charge inside the polarized dielectric condenser.

The dielectric displacement inside the dielectric condenser is defined as

$$D = 4\pi\sigma \quad (71)$$

Polarization and Dielectric Constant

From Eq.(68), it is clear that

$$D = \epsilon'_r E \quad (72)$$

With Eq.(70), we have

$$D = E + 4\pi P \quad (73)$$

Or

$$\epsilon'_r - 1 = \frac{4\pi P}{E} \quad (74)$$

- Clausius-Mossotti Equation – Consider a constant electric field E be applied to a sphere of a continuous isotropic

Polarization and Dielectric Constant

dielectric. The field produced inside the sphere is given by

$$E = \frac{3}{\epsilon + 2} F \quad (75)$$

The electric moment induced in the sphere is

$$m_s = \alpha_s F \quad (76)$$

where α_s is the polarizability of the sphere and is a macroscopic quantity. Since

$$P = \frac{(\epsilon_r' - 1) E}{4\pi} \quad (77)$$

and the volume of the sphere is

$$V = \frac{4\pi a_s^3}{3} \quad (78)$$

Polarization and Dielectric Constant

a_s is the radius of the sphere. The induced electric moment becomes

$$m_s = PV = \frac{(\epsilon'_r - 1) a_s^3}{3} E = \alpha_s F \quad (79)$$

With Eq.(75), we have

$$\frac{\epsilon'_r - 1}{\epsilon'_r + 2} = \frac{\alpha_s}{a_s^3} \quad (80)$$

which leads to the macroscopic expression of the Clausius-Mossotti equation for a sphere of dielectric. For a conducting sphere, ϵ'_r is infinite and

$$\alpha_s = a_s^3 \quad (81)$$

which is sometimes used for estimating molecular radius. Note that the volume of the sphere is taken as that of

Polarization and Dielectric Constant

a sphere. If the polarizability of a sphere α_s with N_s molecules equals the summation of individual molecular polarization α_0 .

$$\alpha_s = N_s \alpha_0 \quad (82)$$

then

$$\frac{4\pi a^3}{3} = \frac{V}{N_s} = \frac{4\pi a_s^3}{N_s} \quad (83)$$

where a is the radius of a sphere equal in volume to that occupied per molecule by the dielectric material. We then obtain

$$\frac{\epsilon_r' - 1}{\epsilon_r' + 2} = \frac{\alpha_0}{a^3} \quad (84)$$

Polarization and Dielectric Constant

Another expression of Eq.(84) is

$$\frac{\epsilon'_r - 1}{\epsilon'_r + 2} = \frac{M}{\rho N} \quad (85)$$

where M is the molecular weight of the dielectric, ρ the density, and N the number molecules per mole of the dielectric. With Eq.(85), we have

$$\frac{\epsilon'_r - 1}{\epsilon'_r + 2} \frac{M}{\rho} = \frac{4\pi N}{3} \alpha_0 \quad (86)$$

Since the refraction index n is related to ϵ'_r by

$$n^2 = \epsilon'_r, \quad (87)$$

it lead to

$$\boxed{\frac{n^2 - 1}{n^2 + 2} \frac{M}{\rho} = \frac{4\pi N}{3} \alpha_0} \quad (88)$$

Polarization and Dielectric Constant

which is the Lorentz-Lorenz expression for the molar refraction.

- Dielectric constant and loss factor – The electric property of dielectrics is defined by the complex electric permittivity (F/m).

$$\epsilon^* = \epsilon' - i\epsilon'' \quad (89)$$

where i is the imaginary number. In engineering, a relative expression is usually used, which is taking the ratio between the complex electric permittivity and the real part of the one of vacuum ϵ_0 .

$$\epsilon_r^* = \frac{\epsilon' - i\epsilon''}{\epsilon_0} = \epsilon_r' - i\epsilon_r'' \quad (90)$$

Polarization and Dielectric Constant

where ϵ'_r is called the dielectric constant and ϵ''_r the loss factor. A ratio between the imaginary part and the real part leads to another defined parameter.

$$\tan \delta = \frac{\epsilon''_r}{\epsilon'_r} = \frac{\epsilon''}{\epsilon'} \quad (91)$$

which is called the loss tangent. Note that, while the dielectric constant and loss factor are dimensionless, they are not "constants" at all. They are usually dependent on frequency and temperature. For dielectric mixtures, the effective dielectric constant and effective loss factor also depend on the composition.