Dielectrics
Polarization

- A perfect insulator or a dielectric is the material with no free charge carriers.
- If an electric field, \( \mathbf{E} \), is applied to the insulator no charge flow. However, in the presence of the electric field the dielectric polarizes: it produces electric dipole moment per unit volume which is referred to as the polarization, \( \mathbf{P} \).
- The electric dipole moment vector, \( \mathbf{m} \), produced by two equal but opposite charges, each of magnitude \( q \), and separated by a distance \( d \) is given in magnitude by \( qd \) and its direction is from the negative to the positive charge.
- If there are \( N \) such dipoles per unit volume then the polarization vector \( \mathbf{P} = N \mathbf{m} \). \( \mathbf{P} \) is expressed in units of charge per area, e.g. C m\(^{-2}\).
- Another vector quantity that is very important in the discussion of dielectric is the electric displacement vector, \( \mathbf{D} \), which may be written, in terms of the electric field and polarization, as

\[
\mathbf{D} = \mathbf{E} + \mathbf{P}
\]

- \( \varepsilon_i = \kappa_i \varepsilon_0 \) is the dielectric permittivity of the insulator or dielectric. \( \kappa \), which is unitless, is the dielectric constant of the insulator.
- \( \mathbf{D} \) is expressed in units of charge per unit area.
- It can be seen that

\[
\mathbf{D} = \mathbf{E} + \mathbf{P}
\]

where \( \chi \) is the dielectric susceptibility of the insulator which is also unitless.
Polarization Mechanisms: I) Electronic

- We consider dielectric materials with purely covalent bonds.
- In the absence of externally applied electrical fields, and in the core atoms of these dielectrics the negative charge from the electrons is symmetrically distributed about the positively charged nuclei.
- However when an electric field is applied to the dielectric, electrons in the core atom move to one side of the atom leaving the positive charge in the nuclei in the opposite side.
- The electric dipole moment in the core atom, \( \mu_a \),

\[
a = q \delta
\]

where the distance \( \delta \) is the separation between the centroids of the negative and positive charges in the atom. \( q \) is the magnitude of the positive and negative charges.
• For $N_m$ dipoles per unit volume of the dielectric, $P$ in the dielectric is given by the total electric dipole moment per unit volume

$$a = a E$$

• at low to moderate applied electric field it can be assumed that the atomic dipole moment is directly proportional to the field via an atom property $\alpha_a$ called the atomic polarizability.

$$P = N_m a$$

or

$$k_i = 1 + \frac{N_m a}{\varepsilon_0} = 1 + c$$

• From above the atomic polarizability $\alpha$ and, hence, the dielectric constant $k_i$, also increase with increasing atomic volume.

• This is indeed the case if we consider the covalent crystals diamond, silicon, and germanium where the dielectric constant takes the values 5.9, 11.8 and 16, respectively. Low dielectric constants are possible to obtain in materials with small atoms, e.g., carbon, hydrogen and oxygen. Such atoms make up several of the low dielectric constant polymers used in microelectronics and chip manufacturing nowadays.
To examine the dependence of the electronic polarization on the frequency of the applied electric field, and analyze the electron motion we will use the classical “forced and damped oscillator” model. The electron displacement $x$ is

$$m \frac{d^2 x}{dt^2} + \frac{dx}{dt} + k_s x = e E_0 e^{-i \omega t}$$

$E_0 e^{-i \omega t}$ is the applied electric field of amplitude $E_0$ and angular frequency $\omega$. $E_0 e^{i \omega t} x$ is the restoring spring force with the spring constant $k_s$. The second term in the LHS represents a velocity dependent damping force and $b$ is the damping constant.

The restoring force term $k_s x$ is very important in dielectrics since it represents the force by which the electron is bound to the atom.

For the steady state solution of the differential equation, we try a solution of the form $x = A e^{-i \omega t}$ where $A$ is the amplitude of the oscillations to get

$$A = \frac{e E_0 \left[ \left( \frac{\omega}{\omega_0} \right)^2 + i \right]}{m \left[ \left( \frac{\omega}{\omega_0} \right)^2 + \frac{2}{2} \right]}$$

where $\omega_0^2 = \frac{k_s}{m}$

$\omega_0$ is called the “natural” frequency or the “resonant” frequency of oscillations and it represents the frequency of undamped oscillations in the absence of the electric field ($E_0 e^{-i \omega t} = 0$). The differential equation of motion for this case of natural oscillations takes the simple form

$$m \frac{d^2 x}{dt^2} + k_s x = 0$$
• $A$ is complex with the real, $A_r$, and imaginary, $A^{im}$, parts given by

\[ A_r = \frac{eE_o}{m} \left( \frac{\omega^2}{\omega_o^2} \right)^2 \left( \frac{\omega^2}{\omega_o^2} + \omega^2 \right) \]

and

\[ A^{im} = \frac{eE_o}{m} \left( \frac{\omega^2}{\omega_o^2} \right)^2 \left( \frac{\omega^2}{\omega_o^2} + \omega^2 \right) \]

• $\chi$ and $\kappa_i$ are both complex and depend in $\omega$ the same way $A_r$ and $A^{im}$ do (see figure).

• It can be seen that at low frequencies, $\omega << \omega_o$

\[ A^r \to \frac{eE_o}{m} \frac{\omega^2}{\omega_o^2} = \frac{eE_o}{k_s} \]

• As $\omega$ approaches $\omega_o$, or at $\omega = \omega_o$, $A^r \sim 0$, and for large $\omega$, i.e., $\omega >> \omega_o$, $A^r \to 0$

• $A^{im}$ vanishes for very low $\omega$ ($\omega << \omega_o$) as well as very high $\omega$ ($\omega >> \omega_o$). It is non-zero near $\omega = \omega_o$ and attains a maximum value at $\omega = \omega_o$. 
• At low $\omega$ electrons in the atom cores are able to follow the field; the resulting electronic polarization is in phase with the field and the dielectric constant is, therefore, real.

• If $\omega$ is very high, electrons are not able to follow and in this case the electronic polarization vanishes.

• At applied electric fields of frequencies near $\omega_o$ the electronic polarization is complex and so is the dielectric constant, $k_i$. In this case the electronic polarization is out of phase with the field.

• A typical value for $\omega_o$ is $10^6$ GHz, which is in the ultraviolet (UV) frequency range.

• A complex dielectric implies that the dielectric constant becomes lossy and energy is dissipated as heat.
Polarization Mechanisms: II) Ionic

- In response to an applied electric field, ions in ionic solids, e.g., NaCl crystals, tend to polarize: positive ions move in the direction of $\mathbf{E}$ and negative ions in the opposite direction.

- To describe ionic polarization one uses the same damped forced oscillations model employed for the electronic polarization.

- The same equations as before also describe the dependence of the ionic polarization on the frequency of the applied electric field: $m$ is the ion mass (heavier), and $\beta$ and $k_s$ are the damping and spring constants appropriate for ionic polarization.

- Also, the $A^r$ and $A^{im}$ are described by the same figure as before.

- Since the ion mass is large compared to the electron mass, the resonant frequency for ion oscillations, $\omega_0$, is in the infra-red (IR) range of $\sim 10^4$ GHz.
Some molecules making a solid or liquid have permanent dipole moments that are, in the absence of electric field, randomly oriented.

Upon the application of electric field, however, these dipoles orderly reorient and result in orientational polarization.

The reorientation of dipoles involves the rotation of molecules by the applied electric field which is, expectedly, a slower than the electronic and ionic polarizations.

This type of polarization is, therefore, insignificant at high frequencies and may dominate polarization at very low frequencies.

In most cases orientational polarization is unimportant in solids, except when the solid contains large concentrations of certain forms of molecules and defects with permanent dipole moments.
• According to Debey, the equilibrium orientational polarization, \( \tau \), in a given applied electric field, at any time \( t \) after the application of the field is

\[
P^{or}(t) = P^{or}_0 \left[ 1 - e^{-\frac{t}{\tau}} \right]
\]

\( \tau \) is the alignment time or “relaxation” time.

• At high frequencies, such that \( 1/\omega << \tau \) or \( \omega \tau >> 1 \), the orientation of molecules does not catch up with electric field oscillation and hence the contribution of the orientational polarization to the dielectric constant is insignificant.

• We will assign \( \varepsilon_i \) to the dielectric constant in the limit \( \omega \rightarrow \infty \), knowing that it is primarily determined by electronic and ionic polarizations and it includes no contribution from the orientational polarization.

• At low frequencies, i.e., \( \omega \tau << 1 \), the dielectric constant takes its static value \( \varepsilon_i^0 \), which would have a contribution from all of the three types of polarizations mentioned above.

• To obtain the overall dependence of the dielectric constant on the frequency of the applied electric field we need to find \( f(\omega) \) in the equation

\[
i(\ ) = \varepsilon_i + f(\ ) \quad \text{Such that} \quad f(0) = \varepsilon_i^0 \quad \text{as} \quad \omega \rightarrow 0
\]
• Using Fourier transforms of $P^{or}(t)$ and according to Debey’s analysis $f(\omega)$ is found to be

$$f(\omega) = C P^{or}_o e^{\frac{t}{r}} e^{i \omega t} dt = \frac{CP^{or}_o}{1 + \frac{\omega^2}{\omega}}$$

$C$ is a constant.

• In the limit $\omega = 0$, one gets

$$f(0) = CP^{or}_o = \frac{o}{i} i$$

• For the dependence of $k_i$ on $\omega$, one gets

$$i(\omega) = i + \frac{i}{i} = \frac{1}{1 + \frac{\omega^2}{\omega}}$$

• The contribution of the orientational polarization, or, to $k_i$ can be obtained by subtracting from $k_i$ the contributions of electronic and ionic polarizations, $i$.

$$or(\omega) = i(\omega) - \frac{1}{1 + \frac{\omega^2}{\omega}}$$

where

$$r_{or} = \frac{or(\omega = 0)}{1 + \frac{\omega^2}{\omega}}$$

and

$$im = \frac{or(\omega = 0)}{1 + \frac{\omega^2}{\omega}}$$
• The real and imaginary parts of the orientational-polarization dielectric constant as functions of frequency.
• It can be seen that the imaginary part goes through a maximum at $\omega t_r = 1$ where the dielectric is no longer lossless and energy is dissipated.
• This region corresponds to the microwave region of $\omega \sim 1$ GHz.
The Dielectric Constant and Loss Factor

- The dielectric constant dependence on the frequency of the applied electric field may be obtained by adding up all contributions from the different polarization mechanisms.
- From among these three polarization mechanisms the electronic mechanism comes with the lowest real dielectric constant, which is also associated with the weakest dependence on frequency from among the three mechanisms.
- Electronic polarization (e.g., in polymers) gives the lowest real dielectric constant followed by ionic and then orientational.
- For substantially large dielectric constants one uses ferroelectrics, which bring in polarization mechanisms other than the three discussed here.
The loss factor in a dielectric is defined as
\[ \tan \delta = \frac{im}{r} \]

The loss factor is sometimes referred to as the loss tangent and \( \delta \) is the loss angle which represents the phase difference between the applied electric field and the induced polarization.

Looking back to our analysis which relates the atomic dipole moment to the electric field it is assumed that the local electric field at the atom location is the same as the external electric field.

But we know this would not be the case since the presence of dipoles surrounding the location will contribute to the local field at the atom.

More elaborate analysis incorporating the true local field gives the "Clausius-Mosotti" equation for the atomic polarizability.

\[ a = \frac{i}{i + 2 \frac{3o}{N_m}} \]
Ferroelectric Response

• **Materials with high-$\kappa$ behavior due to ionic polarization can exhibit spontaneous polarization.**

• **This means they can polarize without the disturbance of an external electric field. This is termed “ferroelectric” behavior.**

• **When this spontaneous polarization is present, sub-regions of a crystal called domains each will be polarized in the same sense; i.e., all the dipoles in a domain will be aligned in the same manner.**

• **Generally the polarization of all the domains in a crystal will average to zero due the randomness of the orientations.**
• However, if such a material in the ferroelectric state is subjected to an external electric field, the domains can be forced to all align.

• When the external field is removed, this alignment can remain.

• An oppositely oriented external electric field can remove the polarization and then eventually oppositely direct it.

• Obviously this ability to “write” and “erase” in ferroelectric materials makes them useful for memory applications.
Piezoelectric Response

- All ferroelectric materials and some other ionic materials also display what is termed the “piezoelectric” effect.
- The prefix piezo is Greek for pressure and these materials are pressure electrics: the behavior is reversible too.
- Under stress they polarize and under an external field they contract or expand.
- The former will cause currents to flow if such a material is placed between two electrodes because positive charge will show up on one electrode and negative on the other due to polarization with stress.
- This can be used, for example for sound, vibration, and pressure wave detection.
- The reverse phenomenon can be used for variable extension probes such as are used in advanced microscopy and as transducers for converting electrical signals into sound.