Semester-VI

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(Core Course-14: Condensed Matter Physics)

Chapter name: Dielectric Properties of materials.

Class No.:-01

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Class No.:01 Polarization, Local electric field at an atom. Depolarization field.

Dielectrics are ordinarily the insulators which do not contain free charge carriers, as a result the electrical conduction could not take place in dielectrics. All the electrons in dielectrics are bound to their parent molecules and hence could be affected by any externally applied electric fields. Now, we will try to explain or understand few important properties of dielectrics.

Polarization:- The polarization $\vec{P}$ is defined as the dipole moment per unit volume, averaged over the volume of a cell. The total dipole moment is defined as - $\vec{p} = \sum_n q_n \vec{r}_n$ ——— (1)
where, $\vec{r}_n$ is the position vector of the $n^{th}$ charge $q_n$.

Let us consider, two plane parallel plates of area A and separation d are charged with a surface charge density $\sigma$, one plate being positive, the other negative. If the space between the plates is evacuated and if d is small compared with the dimensions of the plates, there will result a homogeneous electric field between the plates.

$$E_{vac} = 4\pi\sigma = D \quad \text{——— (2) in esu;}$$

D is called the electric displacement. The potential difference between the plates is equal to, $\phi_{vac} = E_{vac} d$ ——— (3)
and the capacitance of the system is defined as,

$$C_{vac} = \frac{Aq}{\phi_{vac}} = \frac{\sigma}{\phi_{vac}} \quad \text{——— (4)}$$

Suppose now that the space between the plates is filled with a dielectric material, the charge on the plates being kept constant. It is then observed that the new potential difference $\phi$ is lower than $\phi_{vac}$ and similarly, the capacitance C of the system is increased. The static dielectric constant $\epsilon_s$ is then defined by.

$$\epsilon_s = \frac{\phi_{vac}}{\phi} = \frac{C}{C_{vac}} \quad \text{——— (5)}$$

Thus, as a result of introducing the dielectric,

the field strength is reduced from the value $E_{vac}$ to the value $E$, where $E_{vac} = D = \epsilon_s E$ ——— (6)

In other words, the effective surface charge density on the plates is now $q' = E/4\pi$ rather than $q = E_{vac}/4\pi$, thus, introducing the dielectric is equivalent to reducing the surface charge density by an amount,

$$P = q - q' = E_{vac}/4\pi\,(1 - 1/\epsilon_s) = \frac{(\epsilon_s - 1)E}{4\pi} \quad —(7)$$

Thus, under influence of the external electric field, the dielectric facing the positive plate acquires a negative induced surface charge density P and vice-versa. From the atomic interpretation of the dielectric constant, it can be shown that P is equal to the electric dipole moment induced in the substance per unit volume by the external field, P is called the polarization of the substance.

Fig-1 Schematic illustration of charges induced at the surface of a dielectric.

From eqns (6) and (7) it follows that one may write,

$$D = E + 4\pi P = \epsilon_s E \quad ——— (8)$$

## # Macroscopic electric field :-

One contribution to the electric field inside a body is that of the applied electric field, defined as,

$E_0 \equiv$ field produced by fixed charges external to the body.

The other contribution to the electric field is the sum of the fields of all charges that constitute the body. If the body is neutral, the contribution to the average field may be expressed in terms of the sum of the fields of atomic dipoles.

We define the average electric field $\vec{E}(\vec{r}_0)$ as the average field over the volume of the crystal cell that contains the lattice point $\vec{r}_0$: $E(\vec{r}_0) = 1/V_c \int dV\, \vec{e}(\vec{r})$. ——— (9)

where, $\vec{e}(\vec{r})$ is the microscopic electric field at the point $\vec{r}$. The macroscopic field $\vec{E}$ is a much smoother quantity than the microscopic field $\vec{e}$.

To find the contribution of the polarization to the macroscopic field, we can simply the sum over all the dipoles in the specimen. From electrostatics, we have the macroscopic electric field caused by a uniform polarization is equal to the electric field in vacuum of a fictitious surface charge density $\sigma = \hat{n} \cdot \vec{P}$ on the surface of the body. Here $\hat{n}$ is the unit vector normal to the surface, drawn outward from the polarized matter.

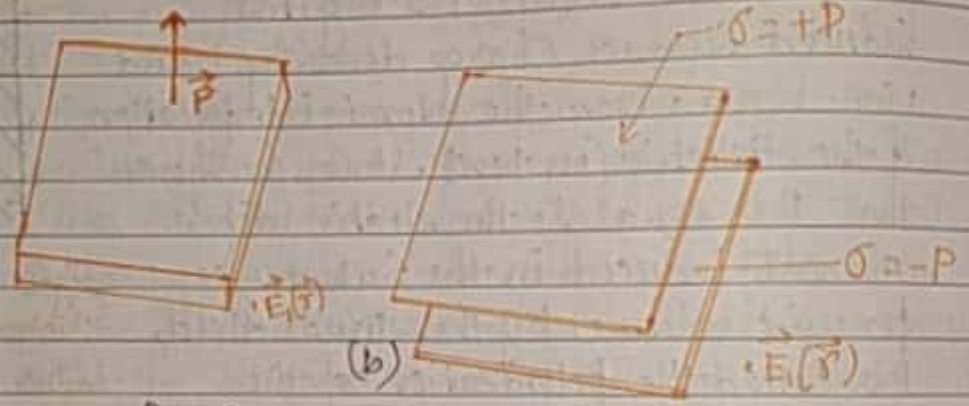


Fig:- (a) A uniformly polarized dielectric slab, with $\vec{P}$ normal to the slab. (b) A pair of uniformly charged parallel plates which give rise to the identical electric field $\vec{E}_1$ as in fig (a).

The electric field $\vec{E}_1(\vec{r})$ produced by the polarization is equal to the field produced by the fictitious surface charge density $\sigma = \hat{n} \cdot \vec{P}$ on the surface of the slab. The upper surface has the fictitious charge $\sigma = \hat{n} \cdot \vec{P} = P$ per unit area, and the lower boundary has $\sigma = -P$ per unit area.

The electric field $\vec{E}_1$ due to these charges has a simple form at any point between the plates, but ~~Compare~~ comfortably removed from their edges. By Gauss's law, $E_1 = -\sigma/\epsilon_0 = -P/\epsilon_0$ — 10(a) (In SI)

We add $\vec{E}_1$ to the applied field $\vec{E}_0$ to obtain the total macroscopic field inside the slab, with $\hat{z}$ the unit vector normal to the plane of the slab:

$$\vec{E} = \vec{E}_0 + \vec{E}_1 = \vec{E}_0 - P/\epsilon_0 \hat{z} \quad \text{——— (11)}$$

we define,

$\vec{E}_1$ = field of the surface charge density $\hat{n}\cdot\vec{P}$ on the boundary.

## Depolarization field, $\vec{E}_1$

For uniformly polarized body, the contributions of $\vec{E}_0$ and $\vec{E}_1$ to the macroscopic field $\vec{E}$ is such that,

$$\vec{E} = \vec{E}_0 + \vec{E}_1 \quad \text{——— (12)}$$

Here, $\vec{E}_0$ is the applied field and $\vec{E}_1$ is the field due to the uniform polarization.

The field $\vec{E}_1$ is called the depolarization field, for within the body it tends to oppose the applied field $\vec{E}_0$.

If $P_x, P_y, P_z$ are the components of the polarization $\vec{P}$ referred to the principal axes of an ellipsoid, then the components of the depolarization field are written,

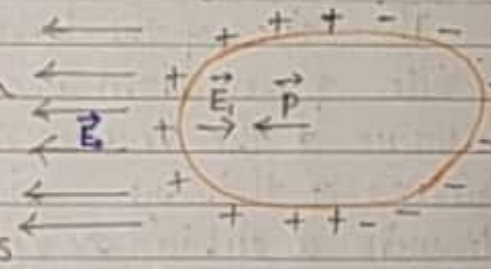


Fig:- The depolarization field $\vec{E}_1$ is opposite to $\vec{P}$.

$$E_{1x} = -\frac{N_x P_x}{\epsilon_0}\,;\; E_{1y} = -\frac{N_y P_y}{\epsilon_0}\,;\; E_{1z} = -\frac{N_z P_z}{\epsilon_0} \quad \text{-(12)}$$

Here, $N_x, N_y, N_z$ are the depolarization factors, their values depend on the ratios of the principal axes of the ellipsoid. The N's are positive and satisfy the sum rule $N_x + N_y + N_z = 1$

We can reduce the depolarization field to zero in two ways, either by working with a long fine specimen or by making an electrical connection between electrodes deposited on the opposite surfaces of a thin slab.

A uniform applied field $\vec{E}_0$ will induce uniform polarization in an ellipsoid, we introduce the dielectric susceptibility $\chi$ such that the relation,

$$\vec{P} = \epsilon_0 \chi \vec{E} \quad \text{——— (13) (In SI)}$$

Connect the macroscopic field $\vec{E}$ inside the ellipsoid with the polarization $\vec{P}$.

If $\vec{E}_0$ is uniform and parallel to a principal axis of the ellipsoid then $\vec{E} = \vec{E}_0 - \frac{N\vec{P}}{\epsilon_0}$ ——— (14)

From eqⁿ (13),

$$\vec{P} = \epsilon_0 \chi (\vec{E}_0 - N\vec{P}/\epsilon_0)$$
$$\Rightarrow \vec{P} = \chi(\epsilon_0 \vec{E}_0 - N\vec{P})$$
$$\Rightarrow \vec{P} + \chi N \vec{P} = \chi \epsilon_0 \vec{E}_0$$
$$\Rightarrow \vec{P}(1+\chi N) = \chi \epsilon_0 \vec{E}_0$$
$$\Rightarrow \vec{P} = \frac{\chi \epsilon_0}{(1+\chi N)} \vec{E}_0 \quad \text{——— (15)}$$

The value of the polarization depends on the depolarization factor N.

Local electric field at an atom :-

The value of the local electric field that acts at the site of an atom is significantly different from the value of the macroscopic field. We can convince ourselves of this by consideration of the local field at a site with a cubic arrangement of neighbours in a crystal of spherical shape. The macroscopic electric field in a sphere is, $\vec{E} = \vec{E}_0 + \vec{E}_1 = \vec{E}_0 - 1/3\epsilon_0 \vec{P}$ ——— (16)

But, consider the field that acts on the atom at the center of the sphere (this atom is not unrepresentative). If all dipoles are parallel to the z-axis and have magnitude p, the z-component of the field at the center due to all other dipoles is,

$$E_{dipole} = \frac{p}{4\pi\epsilon_0} \sum_i \frac{2z_i^2 - x_i^2 - y_i^2}{r_i^5} \quad \text{——— (17)}$$

Due to symmetry of the lattice and of the sphere we have $\sum_i \frac{z_i^2}{r_i^5} = \sum_i \frac{x_i^2}{r_i^5} = \sum_i \frac{y_i^2}{r_i^5}$

Thus, $E_{dipole} = 0$

Therefore, the correct local field is just equal to the applied field $\vec{E}_{local} = \vec{E}_0$ for an atom site with a cubic

arrangement in a spherical crystal specimen. Thus, the local field is not the same as the macroscopic field $\vec{E}$. Let us now develop a generalized expression for the local field at any lattice site. The local field is the sum of the electric field $\vec{E}_0$ from external sources and of the field from the dipoles within the specimen. It is convenient to decompose the dipole field so that part of the summation over dipoles may be replaced by integration. We write,

$$\vec{E}_{local} = \vec{E}_0 + \vec{E}_1 + \vec{E}_2 + \vec{E}_3 \qquad \text{(18)}$$

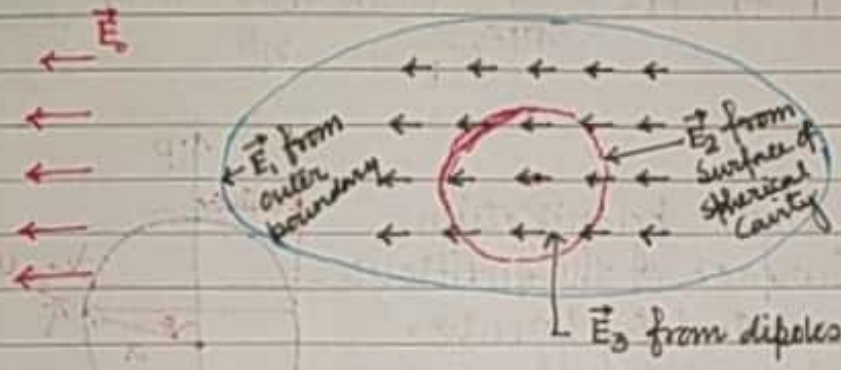


Figure:- The internal electric field on an atom in a crystal is the sum of the external applied field $\vec{E}_0$ and of the field due to the other atoms in the crystal. The standard method of summing the dipole fields of the other atoms is first to sum individually over a moderate number of neighboring atoms inside an imaginary sphere concentric with the reference atom: this defines the field $\vec{E}_3$, which vanishes at a reference site with cubic symmetry. The atoms outside the sphere can be treated as a uniformly polarized dielectric. Their contribution to the field at the reference point is $\vec{E}_1 + \vec{E}_2$, where, $\vec{E}_1$ is the depolarization field associated with the outer boundary and $\vec{E}_2$ is the field associated with the surface of the spherical cavity.

Here, $\vec{E}_0$ = field produced by fixed charges external to the body.

$\vec{E}_1$ = depolarization field, from a surface charge density $\hat{n}\cdot\vec{P}$ on the outer surface of the specimen.

$\vec{E}_2$ = Lorentz cavity field: field from polarization charges on inside of a spherical cavity cut (as a mathematical

fiction) out of the specimen with the reference atom as center as shown in figure, $\vec{E}_1+\vec{E}_2$ is the field due to uniform polarization of the body in which a hole has been created.

$\vec{E}_3$ = field of atoms inside cavity.

The contribution $\vec{E}_1+\vec{E}_2+\vec{E}_3$ to the local field is the total field at one atom caused by the dipole moments of all the other atoms in the specimen:

$$\vec{E}_1+\vec{E}_2+\vec{E}_3 = \frac{1}{4\pi\epsilon_0}\sum_i \frac{3(\vec{p}_i\cdot\vec{r}_i)\vec{r}_i - r_i^2\vec{p}_i}{r_i^5} \qquad \text{——— (19)}$$

# Lorentz field, $\vec{E}_2$

The field $\vec{E}_2$ due to the polarization charges on the surface of the fictitious cavity was calculated by Lorentz. If $\theta$ is the polar angle referred to the polarization direction, the surface charge density on the surface of the cavity is $-P\cos\theta$.

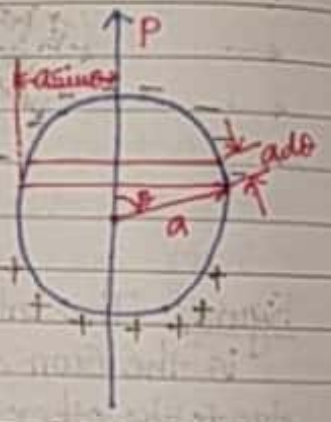


Fig:- Calculation of the field in a spherical cavity in a uniformly polarized medium.

Charge on the ring,

$$(P\cos\theta)\cdot(2\pi a\sin\theta)\cdot(a\,d\theta)$$
$$= P(2\pi a^2\sin\theta\cos\theta\,d\theta)$$

The electric field at the center of the spherical cavity of radius a is,

$$\vec{E}_2 = \frac{1}{4\pi\epsilon_0}\int_0^{\pi}\frac{P\cdot(2\pi a^2\sin\theta\cos\theta\,d\theta)\cdot\cos\theta}{a^2}$$
$$= \frac{1}{2\epsilon_0}P\int_0^{\pi}\cos^2\theta\sin\theta\,d\theta$$
$$= P/2\epsilon_0\int_0^{\pi}\cos^2\theta\,d(-\cos\theta) = -P/2\epsilon_0\int_0^{\pi}\cos^2\theta\,d(\cos\theta)$$

$$E_2 = -P/2\epsilon_0 \left[\frac{\cos^3\theta}{3}\right]_0^{\pi} = -\frac{P}{6\epsilon_0}[-1-1] = +P/3\epsilon_0$$

$$\therefore \vec{E}_2 = +\vec{P}/3\epsilon_0$$

This is the negative of the depolarization field $\vec{E}_1$ in a polarized sphere, so that $\vec{E}_1 + \vec{E}_2 = 0$ for a sphere.

## Field of dipoles inside Cavity, $\vec{E}_3$:-

The field $\vec{E}_3$ due to the dipoles within the spherical cavity is the only term that depends on the crystal structure. We showed for a reference site with cubic surroundings in a sphere that $\vec{E}_3 = 0$ if all the atoms may be replaced by point dipoles parallel to each other

The total local field at a cubic site is,

$$\boxed{\vec{E}_{local} = \vec{E} + \vec{P}/3\epsilon_0} \quad \text{——— (20)}$$

This is the Lorentz relation: the field acting at an atom in a cubic site, which is always larger than the applied field $\vec{E}$.

## Reference:-


1. Introduction to Solid State Physics, Charles Kittel.

2. Solid State Physics : A J Dekker.