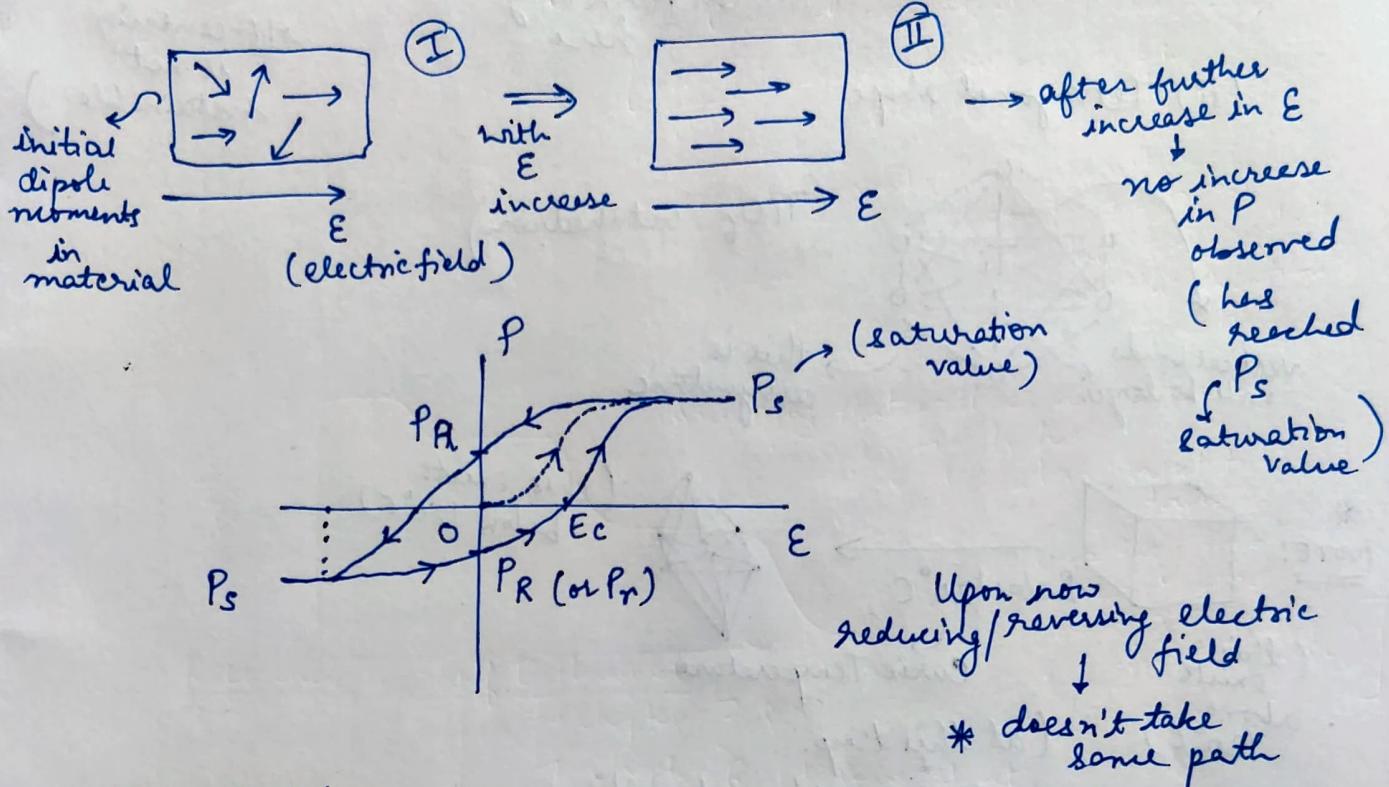


LECTURE-18

56] Ferroelectric Properties

they
are
solids → have permanent
dipole moment

e.g.: BaTiO_3



* The path taken the first time upon increase in E

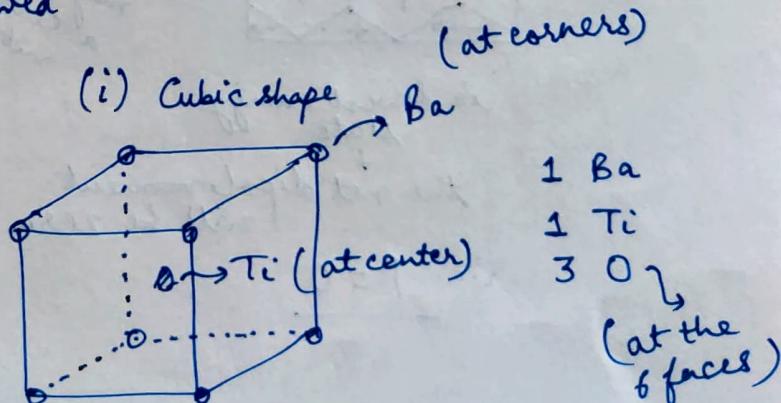
Is ONLY taken the first time

(shown by dotted line/curve in middle of Ist quadrant)

$P_s \rightarrow$ saturation
 $P_R \rightarrow$ Remnant
(or P_r)

$E_c \rightarrow$ Coercive field

57] Perovskite structure (e.g. in BaTiO_3)



* NOTE: Perovskite structure

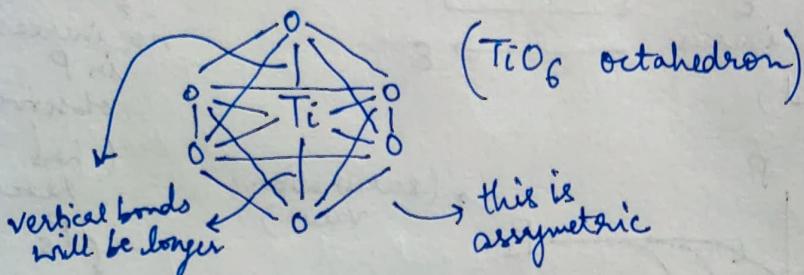
can exist in
two forms

Cubic Tetragonal

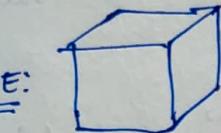
+
permanent
dipole moment
can form only
here

(* Not possible
in Cubic
bcz of its symmetry
off-centering
is not
sustainable)

(ii) Tetragonal shape



* NOTE:



Below 120°C

(this exists
above
 120°C)

(at this temp.)

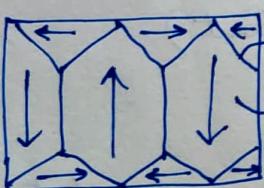
(this exists
below 120°C)

BaTiO₃ phase transitions
into the tetragonal
shape

can be thought of as grain boundaries

individual units (domains)
may have
a certain
net dipole

58]



in lowest energy
state

the net dipole moment
will be zero

i.e. $\mathbf{P} = 0$

* NOTE:

For Ferroelectric
material

It MUST have
a permanent
dipole moment
in the absence
of an E

59] Piezoelectric materials

when \rightarrow mechanical strain applied \leadsto polarization occurs

thus it converts

\Rightarrow mechanical energy $\xrightarrow{\text{to}}$ electrical energy

} called:
transducers

* NOTE:

Dielectric
↓
Ferroelectric
↓
Piezoelectric

(* i.e. All dielectrics are ferroelectrics and all ferroelectrics are piezoelectrics)

60] Optical properties

generally:
earlier only these two were considered under optical properties
{ color Luster } \leadsto however this is NOT intrinsic to material (i.e. color)

Under optical properties we will generally study

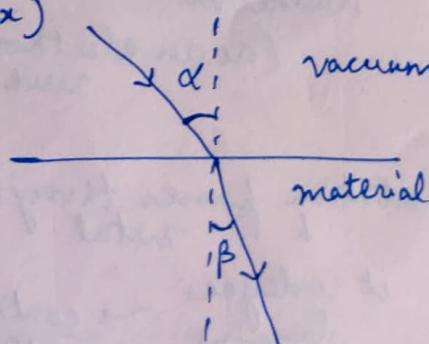
- index of refraction
- Reflectivity (spectral variations)

actually this should be:

$$n = \frac{\sin \alpha}{\sin \beta}$$

61] Index of Refraction

(or Refractive Index)



* definition for index of refraction

$$n = \left(\frac{\sin \beta}{\sin \alpha} \right)^{-1}$$

* Another definition:

$$n = \frac{c}{v}$$

* During refraction from vacuum/material to another medium:

Constants	E, ν	frequency Energy
Things that change	v, λ	wavelength speed

NOTE: Visible light range: 400 - 700 nm
Violet Red

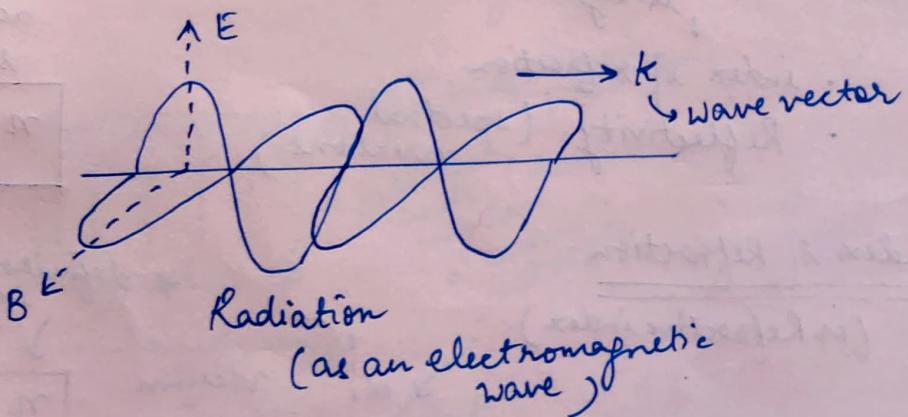
Our discussion will also cover:

{ Radio waves
X-rays
 γ -rays
UV
IR
Microwaves

LECTURE - 19

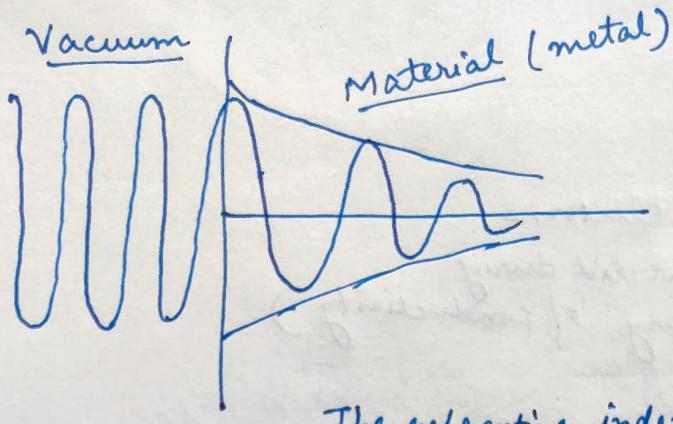
62] Optical properties

- (i) Index of Refraction (n) → discussed previously
- (ii) Damping constant (k)



When radiation passes through a metal

it undergoes damping → controlled by the damping constant



The refractive index
also varies as:

$$n^* = n - ik$$

↓ ↓ ↓
 real part iota imaginary part
 $(\sqrt{-1})$

From this we can obtain:

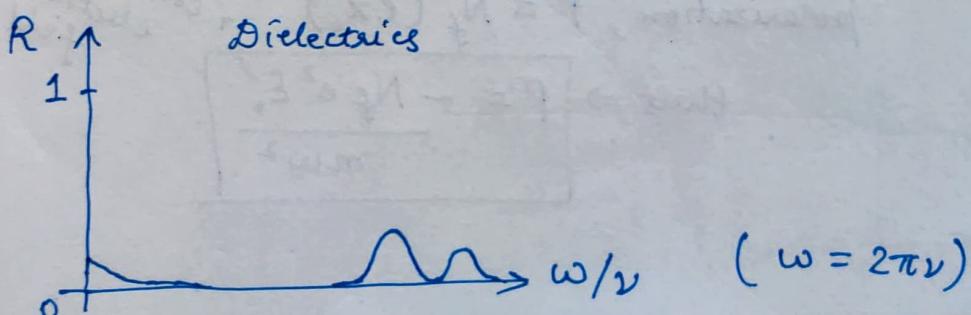
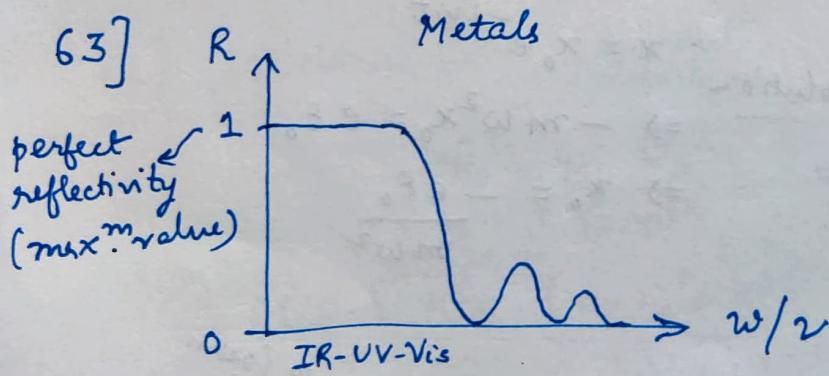
$$\epsilon^* = \underbrace{\epsilon_1}_{\text{real}} - i \underbrace{\epsilon_2}_{\text{imaginary}} \quad (\epsilon \text{ is dielectric constant here})$$

Thus, optical and
electrical properties
are related (relations
can be derived)

* refer to Griffiths
Electromagnetism

NOTE: $R \rightarrow$ reflectivity

(You can also derive the
relation b/w n and R)



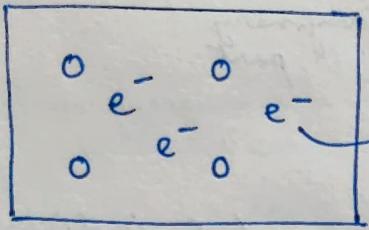
64] Free approximation

i.e. assuming material to have free electrons

(similar to how we did during classical theory of conductivity)

The difference here is

Electric field will vary with time (in an oscillatory manner)



we will look at the effect of radiation on motion of any single e^-

Using Newton's 2nd Law:

$$m \frac{dv}{dt} = e E(t)$$

$$\Rightarrow m \frac{d^2x}{dt^2} = e E(t)$$

This can be written as: $m \frac{d^2x}{dt^2} = e E_0 e^{-i\omega t}$

(This is eqn for forced oscillator)

We can pick a trial solution: $x = x_0 e^{-i\omega t}$
 $\Rightarrow -m\omega^2 x_0 = e E_0$
 $\Rightarrow x_0 = -\frac{e E_0}{m\omega^2}$

Now, we know:

polarization, $P = N_f (e x_0)$ comes from electric field

thus $\Rightarrow P = -\frac{N_f e^2 E_0}{m\omega^2}$

NOTE: { $D = \epsilon_0 E + P$
 $D = \epsilon E$
 \downarrow
 Here, $\epsilon = K \epsilon_0$

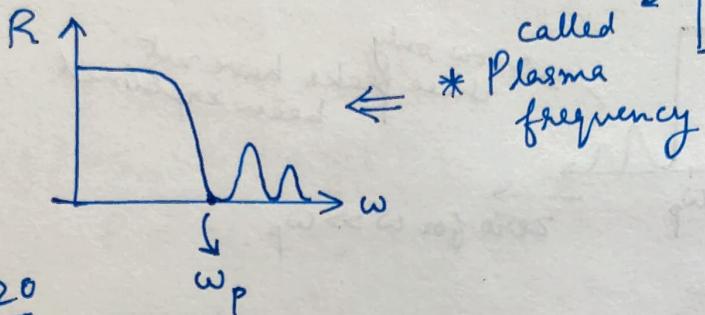
Thus, $K = 1 + \frac{P}{\epsilon_0 E} = 1 - \frac{N_f e^2}{m \omega^2 \epsilon_0} = 1 - \frac{\omega_p^2}{\omega^2}$

this
is dielectric
constant

electric
field

such that

$$\omega_p^2 = \frac{N_f e^2}{\epsilon_0 m}$$



LECTURE-20

NOTE: Both dielectric constant (ϵ) and Reflectivity (R) can be complex quantities.

We will use 'hat' notation (^) to denote complex no.s.

65] So we have:

$$\hat{\epsilon} = 1 - \frac{\omega_p^2}{\omega^2}$$

Complex quantity

, and also: $\hat{\epsilon} = \epsilon_1 - i\epsilon_2$
 $\hat{n} = n - ik$

(where k is damping constant)

66] We obtain (showing without derivation):

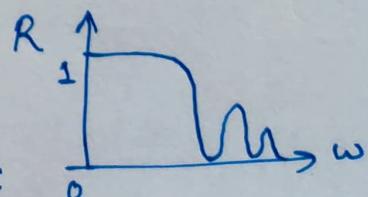
$$\hat{n}^2 = 1 - \frac{\omega_p^2}{\omega^2} \Rightarrow \text{for } \omega \ll \omega_p \quad \hat{n}^2 \approx -\frac{\omega_p^2}{\omega^2}$$

i.e. real part (n) = 0

$$\text{Also } \Rightarrow R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$$

$$\Rightarrow R = 1 *$$

Hence this explains initial part of this curve:



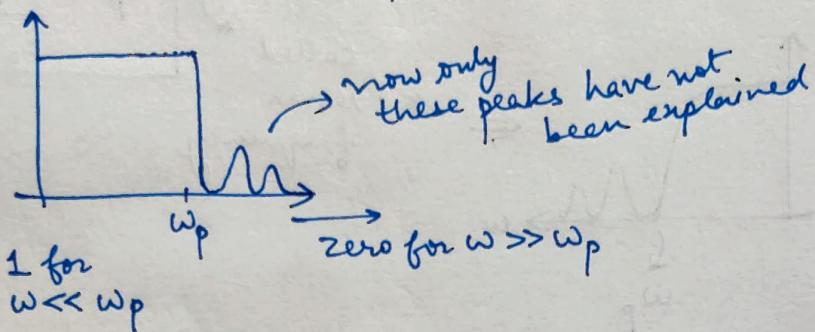
For the case $\omega \gg \omega_p$:

$$\hat{n}^2 \approx 1 \rightarrow \text{thus, } \hat{n} = 1 \quad (-1 \text{ is rejected})$$

thus, $R = 0$ *

Similarly, at $\omega = \omega_p$, we get $\hat{n} = 0$ and $R = 1$

(NOTE: When we actually solve for R , we see that the curve falls abruptly after ω_p)



67] Forced Damped Oscillations

We have the equation:

$$m \frac{d^2x}{dt^2} + \gamma \frac{dx}{dt} = eE$$

(Forced damped oscillator)

In steady state, velocity becomes constant:

$$\therefore \frac{d^2x}{dt^2} \rightarrow 0$$

and we get: $\gamma v = eE$

$$\text{We can also write, } v = \frac{j}{N_e} = \frac{\sigma - E}{N_e}$$

$$\text{thus, } \gamma = \frac{N_f e^2}{\sigma}$$

So we have the following:

$$m \frac{d^2x}{dt^2} + \frac{N_f e^2}{\sigma} \frac{dx}{dt} = eE_0 e^{-i\omega t}$$

$$\begin{aligned} \text{Taking } x &= x_0 e^{-i\omega t} \\ \Rightarrow -m\omega^2 x_0 e^{-i\omega t} - i\omega x_0 \gamma e^{-i\omega t} &= eE_0 e^{-i\omega t} \\ \Rightarrow (-m\omega^2 - i\omega\gamma) x_0 &= eE_0 \\ \Rightarrow x_0 &= \frac{-eE_0}{m\omega^2 + i\omega\gamma} \end{aligned}$$

$$\text{i.e., } x_0 = \frac{-eE_0}{m\omega^2 + i\frac{N_f e^2 \omega}{\sigma}}$$

Using this, we can get :

$$\begin{aligned} P &= N_f e x_0 \\ &= -N_f e^2 E_0 \\ &\quad \frac{m\omega^2 + i\frac{N_f e^2 \omega}{\sigma}}{} \end{aligned}$$

$$\text{Using this we can also get, } \hat{\epsilon} = 1 + \frac{P}{E_0 E}$$

$$\text{and we also have the relation: } \hat{n}^2 = \hat{\epsilon}$$

$$\Rightarrow \hat{n}^2 = 1 + \frac{-N_f e^2}{E_0 (m\omega^2 + i\frac{N_f e^2 \omega}{\sigma})}$$

$$\text{For simplification, taking } \omega_p^2 = \frac{N_f e^2}{m E_0}$$

$$\begin{aligned} \Rightarrow \hat{n}^2 &= 1 - \frac{N_f e^2}{m\omega^2 E_0 + i\frac{\omega E_0 N_f e^2}{\sigma}} \\ &= 1 - \frac{1}{\omega^2/\omega_p^2 + i\frac{\omega}{(\sigma/E_0)}} \end{aligned}$$

↓ real part:
 $n^2 - k^2$
 ↓ Imag. part:
 $\frac{2nk}{\omega}$

* Now for the case: $\omega \ll \omega_p$

(I) Also taking $\frac{\sigma}{\epsilon_0 \omega} \ll 1$ and using this we get:

$$\hat{n}^2 = 1 - \frac{1}{i \frac{\sigma}{\epsilon_0 \omega}} = 1 + i \frac{\sigma}{\epsilon_0 \omega}$$

$$\text{i.e.} \Rightarrow \hat{n}^2 \approx 1$$

$$\text{thus, } R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \approx 0$$

(II) Also taking $\frac{\sigma}{\epsilon_0 \omega} \gg 1$

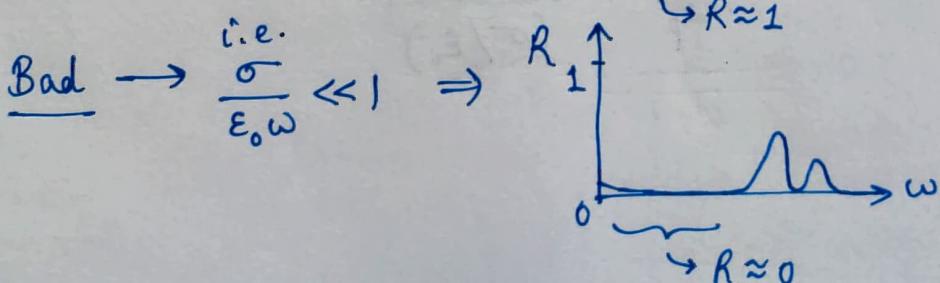
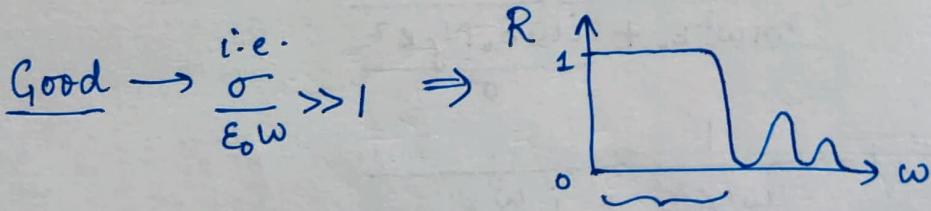
$$\text{So we get: } \hat{n}^2 \approx 1 - \frac{1}{\omega^2 / \omega_p^2}$$

But we initially took $\omega \ll \omega_p$ as well,

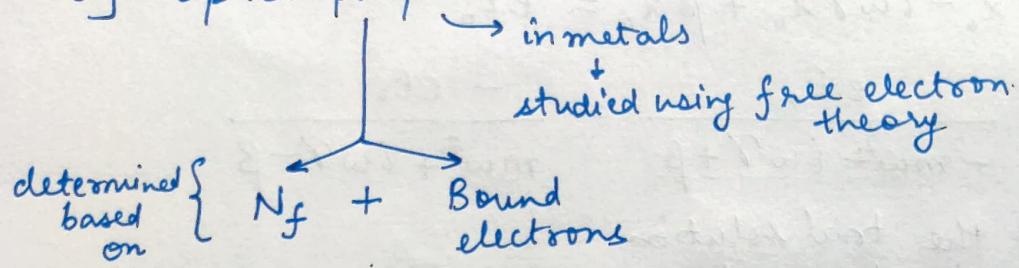
$$\therefore \hat{n}^2 \approx -\frac{\omega_p^2}{\omega^2}$$

So in this case we obtain, $R \approx 1$

* Hence, this give us an understanding for the case of both good and bad conductors



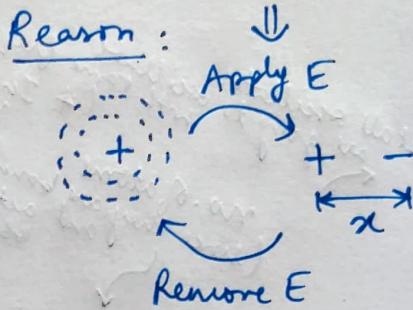
68] Optical properties



Till now we have focused mainly on N_f (i.e. free e⁻s)

But now we will be considering * Bound e⁻s for discussion of dielectrics *

Here we will consider model of forced damped simple harmonic oscillator



Thus this system behaves like a spring:

$$m \frac{d^2x}{dt^2} + \gamma \frac{dx}{dt} + \beta x = eE \quad \leftarrow \text{Hence the model is:}$$

β ("spring constant")

this term is introduced for Dielectrics

We have:

$$m \frac{d^2x}{dt^2} + \gamma \frac{dx}{dt} + \beta x = eE_0 e^{-i\omega t}$$

$$\text{Taking } x = x_0 e^{-i\omega t}$$

$$\Rightarrow -m\omega^2 x_0 e^{-i\omega t} - i\omega \gamma x_0 e^{-i\omega t} + \beta x_0 e^{-i\omega t} = eE_0 e^{-i\omega t}$$

(we will keep the terms γ and β as it is)

bcoz we do not know if there are free e⁻s or not, so γ and β cannot be replaced

$$\Rightarrow -m\omega^2 x_0 - i\gamma\omega x_0 + \beta x_0 = eE_0$$

$$\Rightarrow x_0 = \frac{eE_0}{-m\omega^2 - i\gamma\omega + \beta} = \frac{-eE_0}{m\omega^2 + i\gamma\omega - \beta}$$

LECTURE-21

But in this case the trial solution is not perfect.

* From Appendix A : We find the solution to that eqⁿ as : $x = \frac{eE_0 e^{i(\omega t - \phi)}}{\sqrt{m^2(\omega_0^2 - \omega^2) + \gamma^2 \omega^2}}$

We are assuming that all oscillators are going to oscillate with same freq. (* In reality not necessarily true)

No. of atoms (since they are bound and act as oscillators)

$$\text{where, } \tan \phi = \frac{\gamma \omega}{m(\omega_0^2 - \omega^2)}$$

$$\text{and } \omega_0 = \sqrt{\frac{\beta}{m}}$$

$$\text{Now, } P = \frac{N_a e^2 E e^{-i\phi}}{\sqrt{m^2(\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2}}$$

$$\hat{\epsilon} = 1 + \frac{N_a e^2 e^{-i\phi}}{\epsilon_0 \sqrt{m(\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2}}$$

$$\text{Using } e^{-i\phi} = \cos \phi - i \sin \phi$$

$$\hat{\epsilon} = 1 + \frac{N_a e^2 (\cos \phi - i \sin \phi)}{\epsilon_0 \sqrt{m^2(\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2}}$$

$$\hat{\epsilon} = \epsilon_1 - i \epsilon_2$$

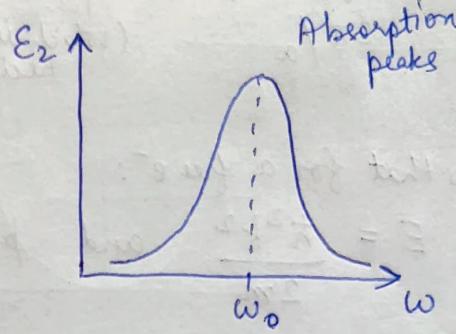
$$\therefore \Rightarrow \epsilon_1 = 1 + \frac{N_a e^2 \cos \phi}{\epsilon_0 \sqrt{m^2(\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2}}$$

$$\cos \phi = \frac{1}{\sqrt{1 + \tan^2 \phi}} \quad \text{and} \quad \sin \phi = \frac{\tan \phi}{\sqrt{1 + \tan^2 \phi}}$$

Thus, we get:

$$\epsilon_1 = 1 + \frac{e^2 m N_a (\omega_0^2 - \omega^2)}{\epsilon_0 (m^2 (\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2)}$$

$$\epsilon_2 = \frac{e^2 N_a \gamma \omega}{\epsilon_0 (m^2 (\omega_0^2 - \omega^2)^2 + \gamma^2 \omega^2)}$$



(∴ ϵ_2 gives an idea about absorption
↓
and at ω_0 Resonance
takes place)

Here we assumed that all oscillators are oscillating with some freq
but in general there will be multiple such frequencies
this leads to the formation of multiple peaks

(* The one major drawback of the classical theory)

was the inability to explain the peaks in R vs ω plot for high ω values



This will be explained with the help of Quantum theory

69] Quantum Theory

Band Structure

We will discuss

Interband

Intraband

direct band structure

indirect band structure

e.g.: insulators, semiconductors, metals

metals

explained using momentum conservation

LECTURE-22

* NOTE: We will be using a concept called
"Reciprocal Space" (i.e. k -space)

... in $\Rightarrow x$ -space
 a

... in $\Rightarrow k$ -space
 $2\pi/a$ (which is the reciprocal space)

70] We know that for a free e^- :

$$E = \frac{\hbar^2 k^2}{2m} \quad \text{and} \quad p = \hbar k$$

We are here discussing the situation

when a photon hits a solid
and thus electrons in the
crystal get excited
to a higher energy level

(given that such unoccupied
energy levels are
available)

For these transitions

momentum of electrons and photons
must remain constant

(by Conservation of
Momentum)

Now, for optical frequencies

$p_{\text{photon}} \ll p_{\text{electron}}$

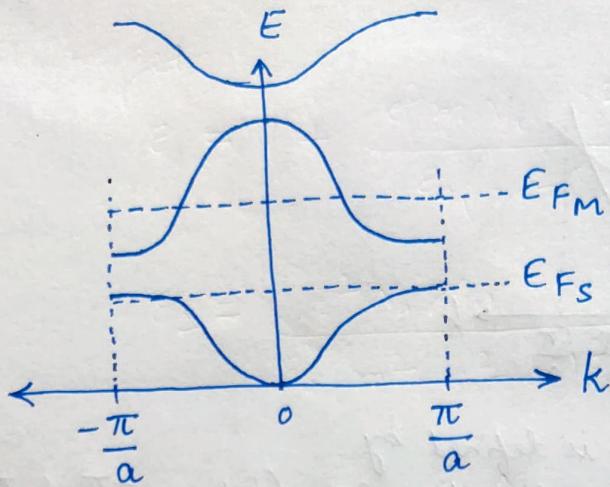
$$\text{and since, } k_{\text{photon}} = \frac{p_{\text{photon}}}{\hbar} \Rightarrow k_{\text{photon}} \ll \frac{\pi}{a}$$

By Momentum Conservation $\Rightarrow k$ remains constant

thus when we draw the
energy transition in
the E -vs- k plot

we only see a
vertical transition

called Direct transitions *

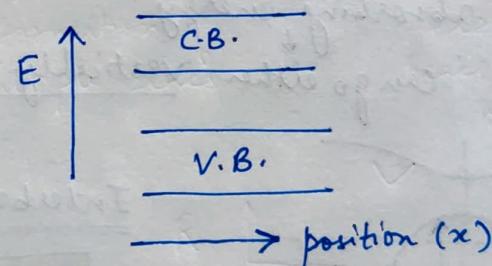


- 71] Interband transitions → * these explain the "Bound" e⁻s of Classical theory
- direct indirect
↓
makes use of concept of phonons

- 72] Intraband transitions
- (i) Occur in metals
 - (ii) Continuous range of absorptions
 - (iii) It represents the Quantum counterpart of the Free e⁻s in Classical theory *

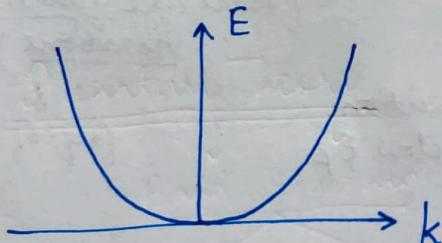
73] Quantum Mechanical Model

We have Energy bands of Silicon:



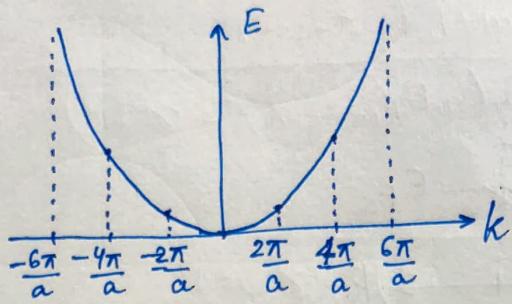
Using 'k' vector and 'p' momentum:
for a moving e⁻ we have

$$E = \frac{\hbar^2 k^2}{2m} \text{ and } p = \hbar k$$

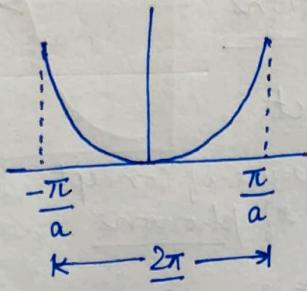


{ NOTE: As discussed previously:
 $\frac{2\pi}{a} \dots \rightarrow$ This is x-space
 $\frac{2\pi}{a} \dots \rightarrow$ This is k-space (Reciprocal space) }

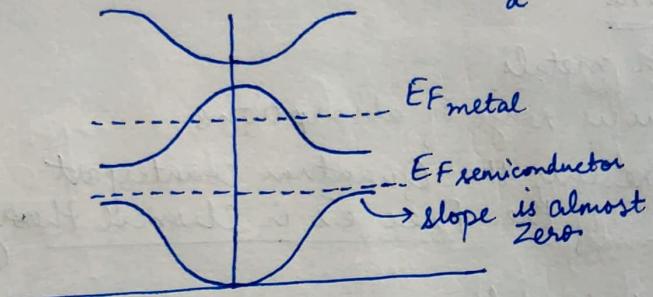
Thus, based on this:



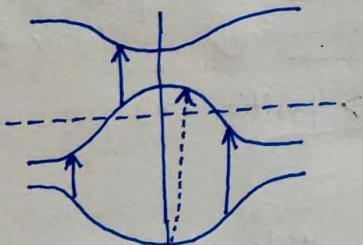
* The 1st Brillouin zone is defined by the region of diameter $\frac{2\pi}{a}$ (between $-\frac{\pi}{a}$ to $\frac{\pi}{a}$):



* NOTE:



74] After absorbing \downarrow energy
can go either vertically up or at some angle



Interband transitions

Direct

* No momentum cost associated
 \downarrow

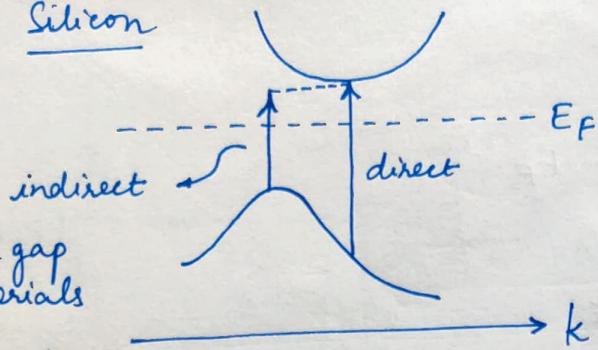
- (i) Availability of
- (ii) only vertical transition can not come below E_F

Indirect

\downarrow phonons
(these are quantized vibrations)

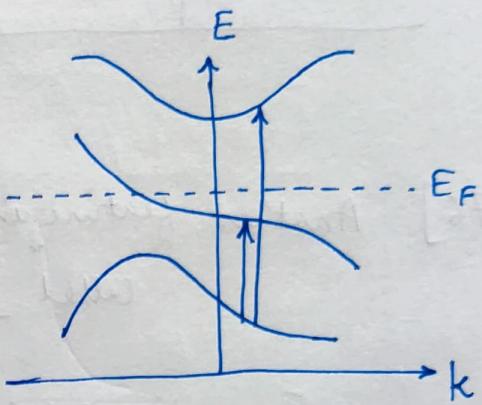
\downarrow freq. of ω_{ph}

Silicon

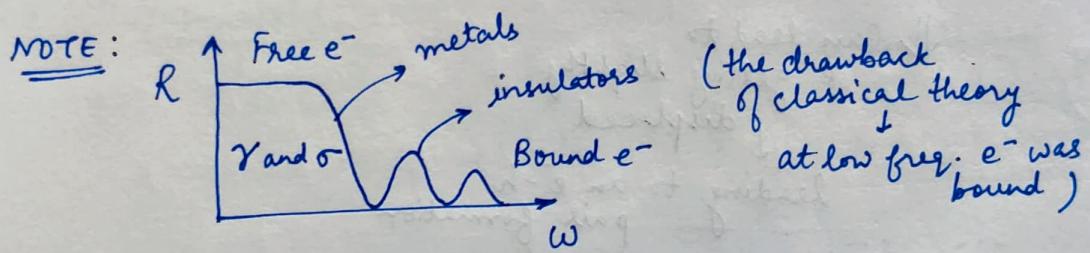


* (band gap materials
+ need extra momentum
↓ provided by phonons)

NOTE: Probability of indirect



NOTE: Intraband transition
↓ Continuous range → only in metals



LECTURE-23

75]

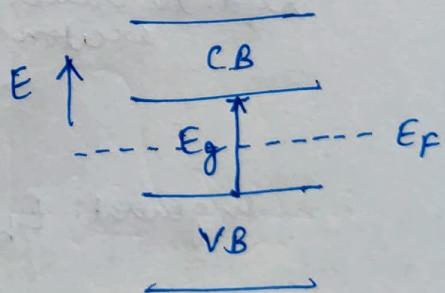
Semiconductors

We have discussed
2 types of transitions

Interband
↓
transition
with the
bond itself

Interband
↓
Only this is
allowed

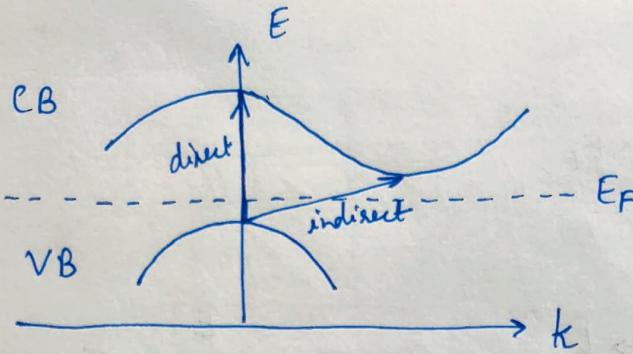
* Not allowed
in semiconductor



(indirect transition) ↓ The smallest transition will be of E_g (band gap)

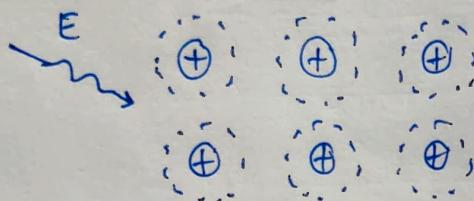
$$Si \sim 0.7 \text{ eV}$$

$$Ge \sim 1.1 \text{ eV}$$

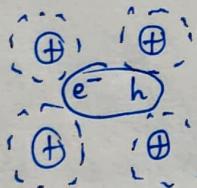


76] Another feature in Semiconductors

called Excitons * → an e^- -hole pair



↓ can lead to
 e^- getting slightly
 ↓ displaced
 leading to an e^- -h
 pair formation



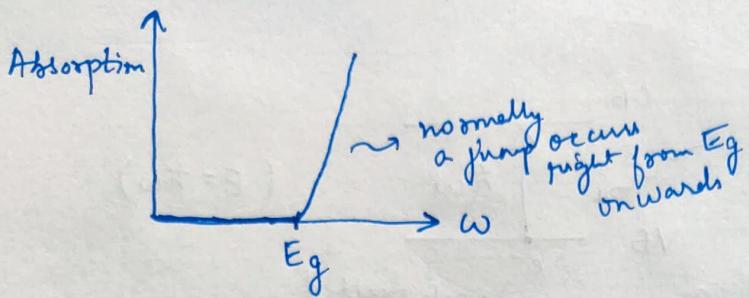
The energy
 reqd. to create → E_b
 exciton ↓

it is material specific

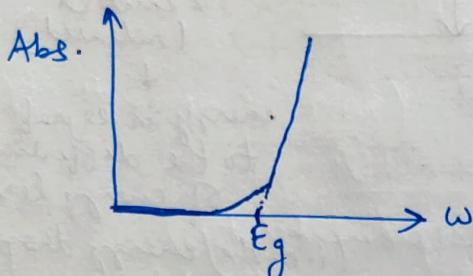
↳ i.e.
 mainly depends
 on Dielectric
 constant (ϵ)

$$\text{In general: } E_b \propto \frac{1}{\epsilon^2}$$

NOTE: It is possible for excitonic waves to propagate through
 ↓ the material
 leading to excitonic states of energy



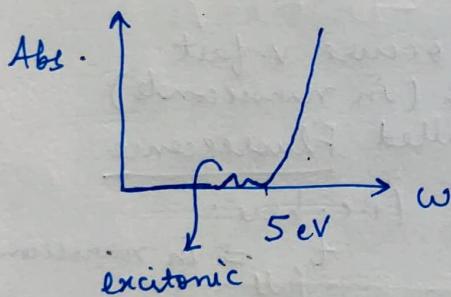
But if Excitons are present
slight increase happens
just before E_g as well:



77] Insulators

↓
Interband
↓
band gap of $\sim 5 \text{ eV}$

* (typically insulators
only have direct transition
and not usually
indirect)



78] Phonon excitation by photons

... - O - α - O - α - O - spring constant - O - ...

(Oscillated by ω_0)

$E = E_0 e^{-i\omega t}$ falls on it:

We get:

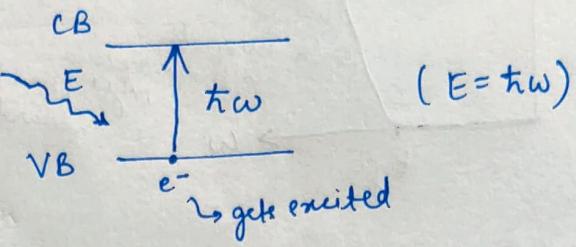
$$m \frac{d^2x}{dt^2} + \gamma \frac{dx}{dt} + \alpha x = q E_0 e^{-i\omega t}$$

* NOTE: One big difference b/w this and what we did earlier for bound e's
(i.e. coupled oscillators)
(thus α is different) earlier it was of e^- and nucleon
here spring is b/w atoms

[Also m and q are different]

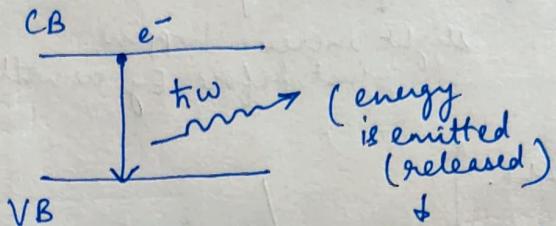
79] Emission

In the phenomena of absorption :



$$(E = \hbar\omega)$$

But in emission case
(here no photon is present)



+
energy is equal to the difference of energy levels

(i.e. the energy drop that has taken place)

Types of Emissions

80] 1. Spontaneous emission

+
emission that occurs bcz e^-

↓ falls down on its own from higher to lower state
(nothing is reqd. to make this happen)

also called
Luminescence

+
If this drop occurs v. fast
↓ (in nanoseconds)

called Fluorescence

(i.e. here:

$t_{\text{fall}} = \text{in nanoseconds}$)

If occurs when e^- stays in the higher state for $\mu s - ms$

↓
called Phosphorescence

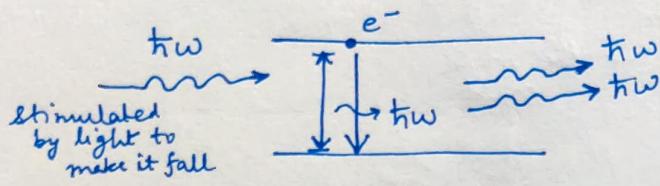
(i.e. $t_{\text{after which fall starts}} = \mu s \text{ to } ms$)

{ * NOTE: Both phosphorescence and Fluorescence may happen in (i.e. may be supported) the same material }

{ although usually this doesn't happen }

2. Stimulated Emission → eg: LASERS

(Light Amplification by Stimulated Emission of Radiation)



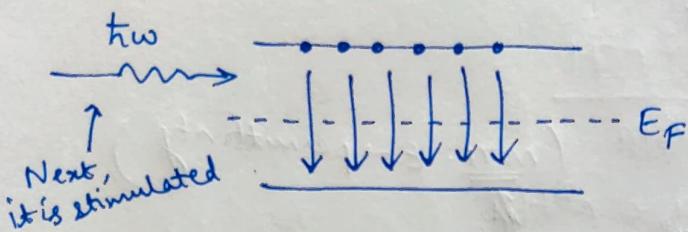
(e^- are stuck for some amount of time)

↓
can be explained based on

Uncertainty principle:
 $\Delta E \Delta t \approx \hbar$

Process is as follows:

* First → Population inversion is made to occur



i.e.

all e^- s are pushed

above Fermi (or in general, just to a higher state)

⇒ this is the principle/process behind LASERS

Thus LASERS cannot be made in case of spontaneous emission

since it cannot be controlled

as e^- s will fall at any time on their own

eg: Materials used for LASERS commonly → Nd: Neodymium

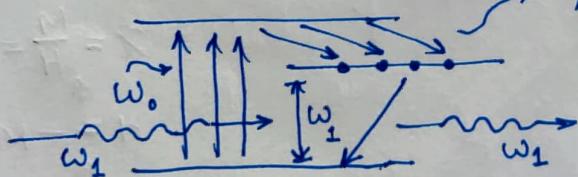
Nd YAG
in solid state

He-Ne gas

{ NOTE: The phenomenon of pushing the e^- s to higher state → called * Optical pumping }

Another level of complexity is

↳ 3-level LASER *



here spontaneous emission occurs onto this level just below the high state

thus, population inversion occurs here

and later can be stimulated to produce LASERS

(The advantage of this is * that Spontaneous and Stimulated emissions are not competing)