List of Course Outcomes:

Course Code and Course Name	Course Outcomes
MME 602 Electronic, Magnetic and Dielectric Materials	CO1: An understanding about the nature of electrical conduction in metals and semiconductors.
	CO2: Insight about the modern techniques for fabrication / synthesis of semiconductor materials.
	CO3: Understanding about the various important semiconductor devices such metal oxide semiconductors, pn junctions, transistors like BJT's and FET'S.
	CO4: Understanding of magnetic properties of materials and their application.
	CO5: Knowledge about the latest dielectric materials and their application.
	CO6: Insight about the new developments / trends in electronic, magnetic and dielectric materials used in various fields particularly Energy sector and Biomedical applications.

Condensed Matter Physics
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Lecture - 9
The Free Electron Theory of Metals

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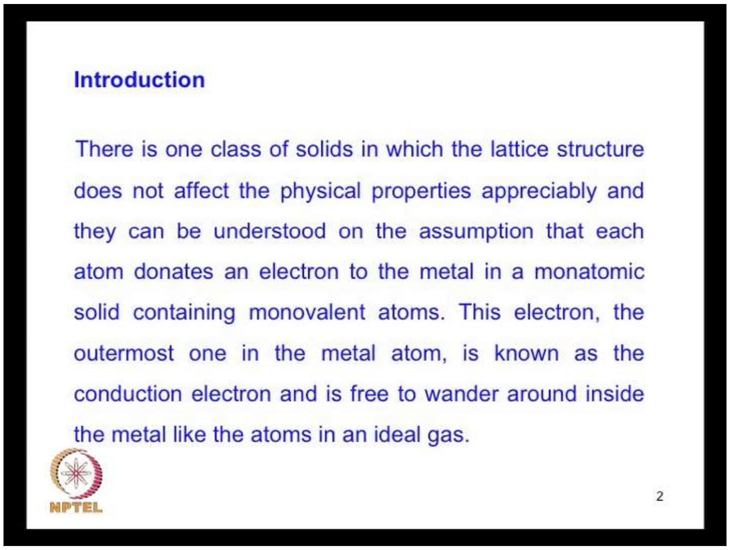

Introduction

There is one class of solids in which the lattice structure does not affect the physical properties appreciably and they can be understood on the assumption that each atom donates an electron to the metal in a monatomic solid containing monovalent atoms. This electron, the outermost one in the metal atom, is known as the conduction electron and is free to wander around inside the metal like the atoms in an ideal gas.

We saw in the last session how the physical properties of solids depend rather strongly on this symmetric properties; however there is 1 class of solids in which the details in the lattice structure does not play a very big role on the physical properties, these are metals such as gold silver copper and so on. This metals their behavior can be understood on the assumption that each atom donates in the case of mono valid metal one-electron to the metal, and this electron is usually the outermost 1 in the metal atom.

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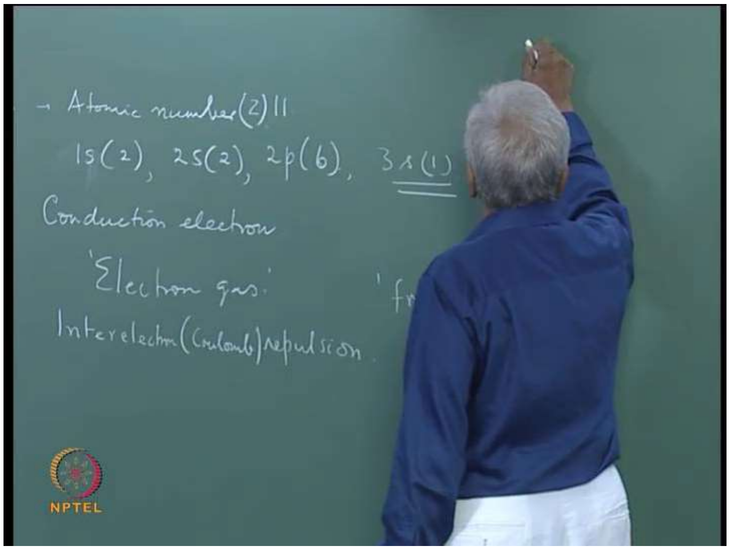

For example, in the case of sodium which has an atomic number atomic number is the number of electrons of leaven z is the usual symbol. There are leaven electrons in the sodium atom of which 10 of them go into this so-called 1 s 2 electrons go into 1 s shell and then 2 electrons go into the 2 s shell and then six electrons go into the 2 p sell. So, this is the so-called close shell structure out of these leaven.

Electrons ten of them go into the close shells leaving only one-electron in the outermost three s shell. So, this the electron which is the outermost in the metal atom this is just an example similarly 1 can look at any metal atom and then analysis the outermost electron is available for conduction, because it is rather weekly bound to the parent atom and therefore, can be ionized rather readily. And this becomes this outermost electron is known as the conduction electron because this gets ionized and this electron becomes available and is free to wander around inside the metal. So, it is the very much like the atoms and molecules in an ideal guess.

So, one speaks of an electron gas in this case. So, this means that even though the metal is the conduction this system a condensed matter a solid, but the electrons inside are behaving very much like the atoms. And molecules in an ideal gas be one made ask what happens to the coulomb repulsion between the 2 electrons pars of electronics this intel electron repulsion is rather week in comparison to the attraction between the electrons and the positive ions which are left behind after the ionization. So, 1 has 1 neglects the first approximation inter electron are coulomb repulsion. If overlooked ignore to start with. So, that one can think of free electrons which are not strongly interacting free electron for free in the sense that the free-for conduction to carry electricity insight, that is why metals are such good conductors of electricity only thing is these electrons the ideal gas molecules are atoms are classical particles.

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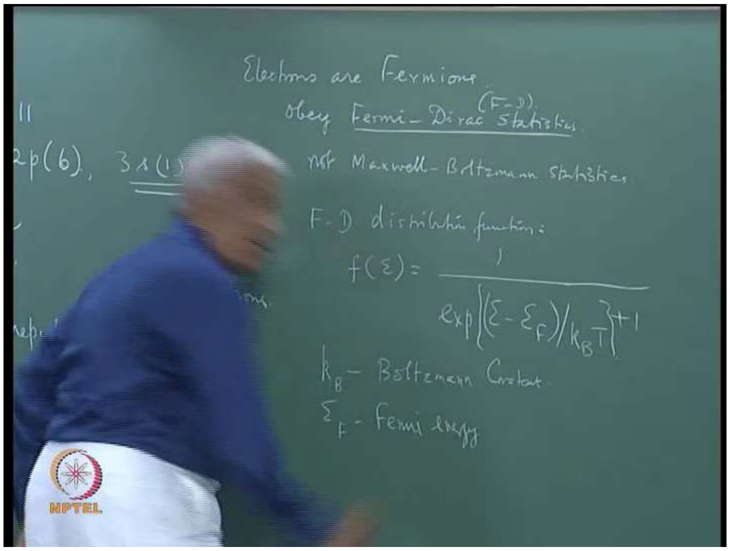

Electrons are Fermions.

obey Fermi–Dirac (F-D) statistics

not Maxwell-Boltzmann statistics

F-D distribution function:

$$f(\varepsilon) = \frac{1}{\exp\{(\varepsilon - \varepsilon_F)/k_B T\} + 1}$$

k_B – Boltzmann Constant

ε_F – Fermi energy

Whereas electrons are quantum particles which obey electrons are known as fermions fermions means they obey so-called for me the dirac statistics rather than not Maxwell Boltzmann statistics. So, there collective behavior is not describe by classical Maxwell Boltzmann the statistics which are which is obey it by ideal gas molecules and atoms, but in then we discuss the properties of this electron gas we have to take count of the fact that they obey fermi dirac statistics. So, we have to use fermi dirac statistics in order to describe.

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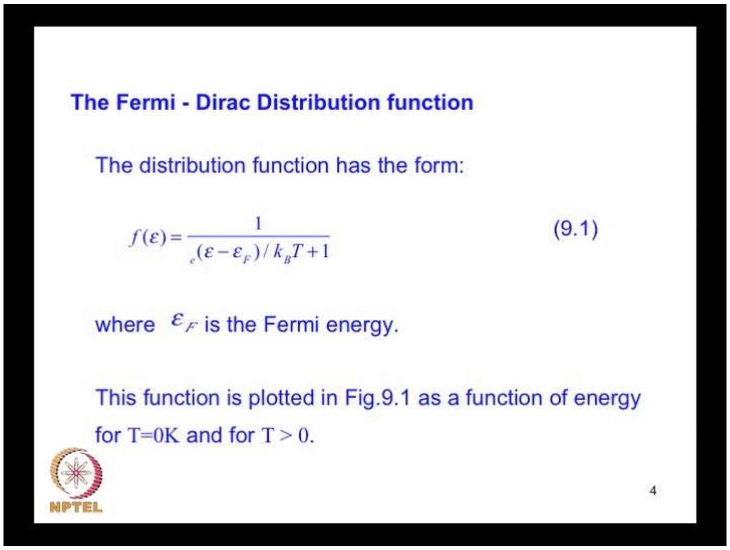

The Fermi - Dirac Distribution function

The distribution function has the form:

$$f(\varepsilon)=\frac{1}{e^{(\varepsilon-\varepsilon_F)/k_BT}+1} \qquad (9.1)$$

where ε_F is the Fermi energy.

This function is plotted in Fig.9.1 as a function of energy for $T=0K$ and for $T > 0$.

They are collective behavior this is are other important factor up the fermi direct distribution function I will write it as a f t for short the fermi direct distribution function as the following firm f of e that is the distribution function which describes how the electrons are distributed into the various energy states. So, this system of electrons has different energy levels the electron energies are different. And therefore, the electrons occupy these energies and the way we are distributed energy is given by this function 1 by a exponential e by the e f by kb t plus 1, where kb is the Boltzmann constant and the e f is known as the fermi energy k b is the universal constant as you know. And the fermi energy is a characteristic of the metal now everything will depend the collective behavior will depend on the statistical distribution how the electrons are distributed an energy.

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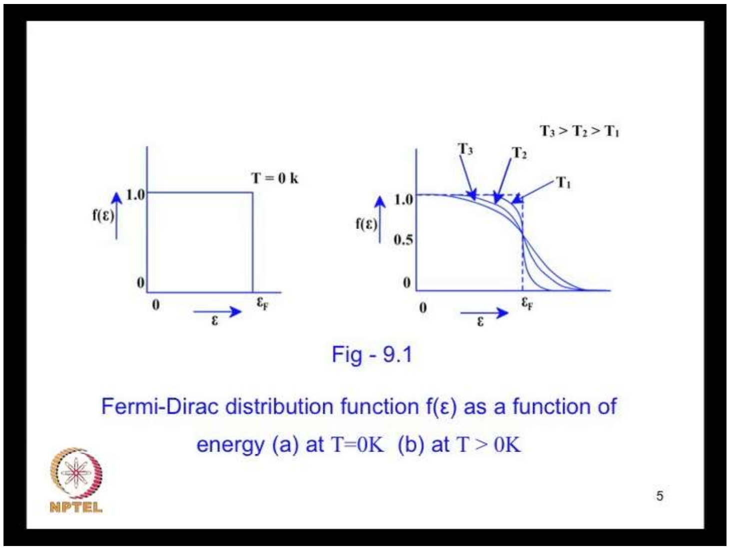

Fig - 9.1

Fermi-Dirac distribution function f(ε) as a function of energy (a) at T=0K (b) at T > 0K

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Therefore let us look at how this function looks, this function is plotted in this figure.

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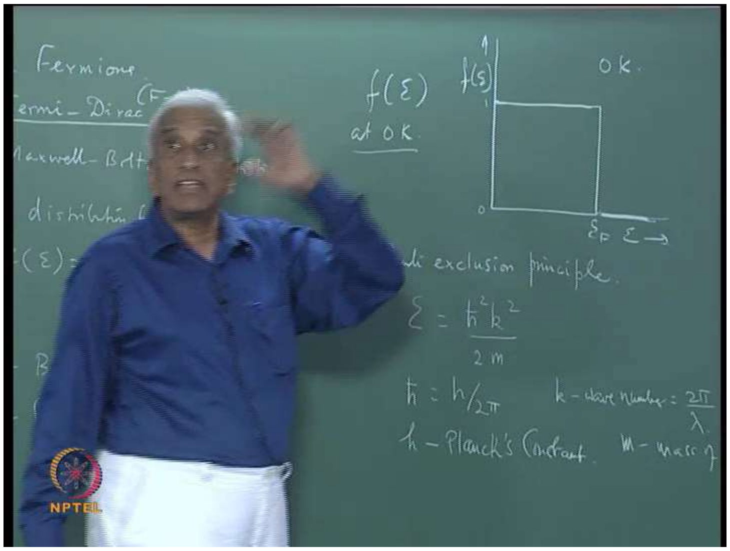

Let us look at the figure on the left side, which gives the value this function plotted at absolute 0 lets discussed the behavior of the metal at absolute 0 and then we can go to finite temperatures this simpler. So, you can see that this function looks like this. So, if I as the fermi energy here than this is 0 this is one. So, that is the behavior of this function at absolute 0. So, this is at 0 k what is this there the physical meaning of this picture is that if you look at all state's all energies which are less than the fermi energy. If you look to the left that this ef in the graph on the energy access all this states are occupy with a probability of unity. In the sense that this mean that they are fully occupied the states are all completely occupied by the electrons none of the state's is empty all the states below e f are all occupy by electrons this. Whereas all the state above ef the fermi energy are completely empty they have 0 probability the f of e is 0.

So, the probability of occupation of the state about the fermi energy at absolute 0 is 0 that mean that they are completely an occupy. This is because the electron obey what is known as Pauli is crucial principle that is way they are fermions this means that it if 1 state are 1 energy level is occupied by an electron then another electron cannot be found in the same state it is excluded from occupying the same state. So, each state is occupied by an electron, and you have all the states below e f occupy well this picture is slightly modified at finite temperature, but we will come to that a little latter the it is this is enough for as…

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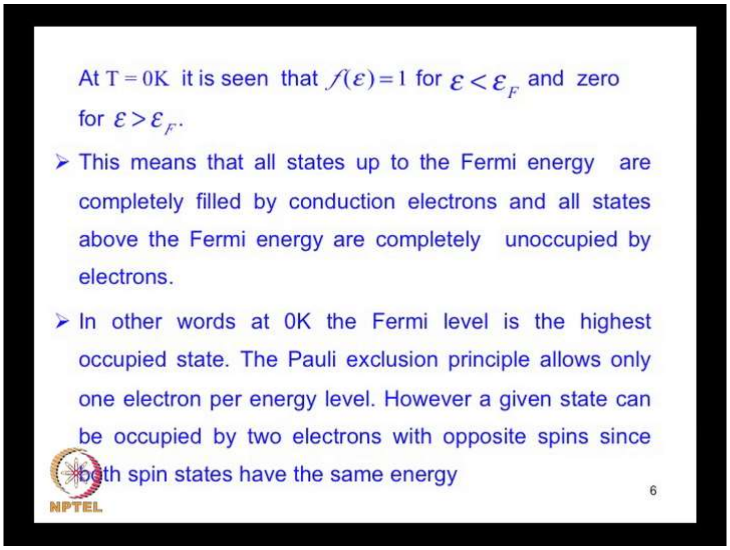

At $T = 0K$ it is seen that $f(\varepsilon) = 1$ for $\varepsilon < \varepsilon_F$ and zero for $\varepsilon > \varepsilon_F$.

- This means that all states up to the Fermi energy are completely filled by conduction electrons and all states above the Fermi energy are completely unoccupied by electrons.
- In other words at 0K the Fermi level is the highest occupied state. The Pauli exclusion principle allows only one electron per energy level. However a given state can be occupied by two electrons with opposite spins since both spin states have the same energy

Now, So, if this is. So, at 0 kelvin the fermi level e f is the highest occupied state now of course, then I say that each state is occupied by one-electron according to the Pauli principle what I mean is that we do not consider this spin of electron if you consider the spin of the electron. Then we know that electron can have has a spin of half and. So, can occupied 2 states with parlor or anti parallel spin beer given direction in space therefore, these 2 electrons with opposite spins both have the same energy. And so each of the states can be occupied by through electrons with opposite spins without violating only principle.

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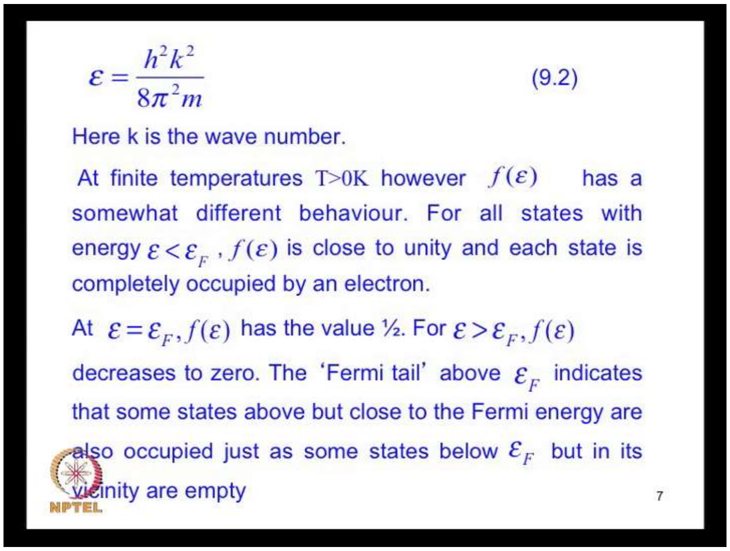

$$\varepsilon = \frac{h^2 k^2}{8\pi^2 m} \qquad (9.2)$$

Here k is the wave number.

At finite temperatures T>0K however $f(\varepsilon)$ has a somewhat different behaviour. For all states with energy $\varepsilon < \varepsilon_F$, $f(\varepsilon)$ is close to unity and each state is completely occupied by an electron.

At $\varepsilon = \varepsilon_F, f(\varepsilon)$ has the value ½. For $\varepsilon > \varepsilon_F, f(\varepsilon)$ decreases to zero. The 'Fermi tail' above ε_F indicates that some states above but close to the Fermi energy are also occupied just as some states below ε_F but in its vicinity are empty

You will remember this, but this spatial energy of these electron is simply given by the kinetic energy, which is h cross square k square by 2 m there h cross is h by 2 pi h is the planck's k is the wave number which is equal to 2 pi by lambda we already talked about lambda broglie wavelength. And m is the mass the electron. So, the energies of the electron in the state is given by the wave vector k, and this is just the kinetic energy h cross square k square by 2 m.

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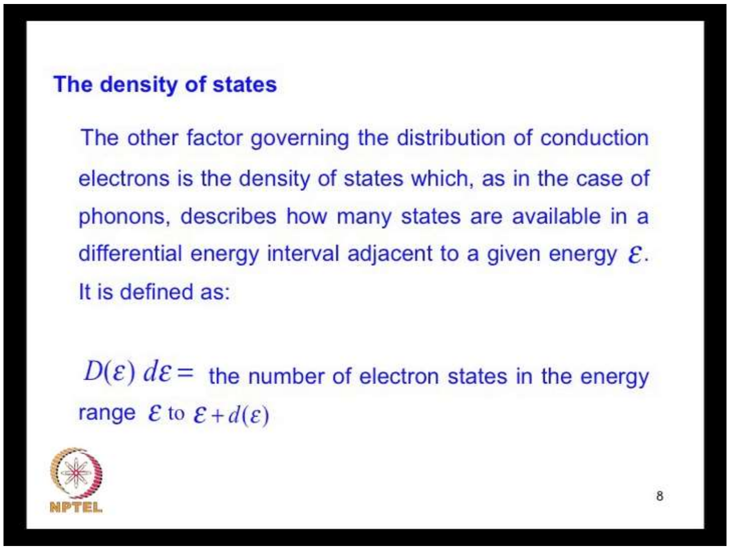

The density of states

The other factor governing the distribution of conduction electrons is the density of states which, as in the case of phonons, describes how many states are available in a differential energy interval adjacent to a given energy ε. It is defined as:

$D(\varepsilon)\, d\varepsilon =$ the number of electron states in the energy range ε to $\varepsilon + d(\varepsilon)$

Now, if we why do we need this we need this information united calculatefor example, the number of electrons conduction electrons inside a metal the metal is now somewhat like a box with in which this electron gases free to wonder around, but the electron is not a allow to escape out of the better. So, that is a the only constraint on the electrons. So, within the metal they are free to wander around very much like the atoms and molecules of a gas.

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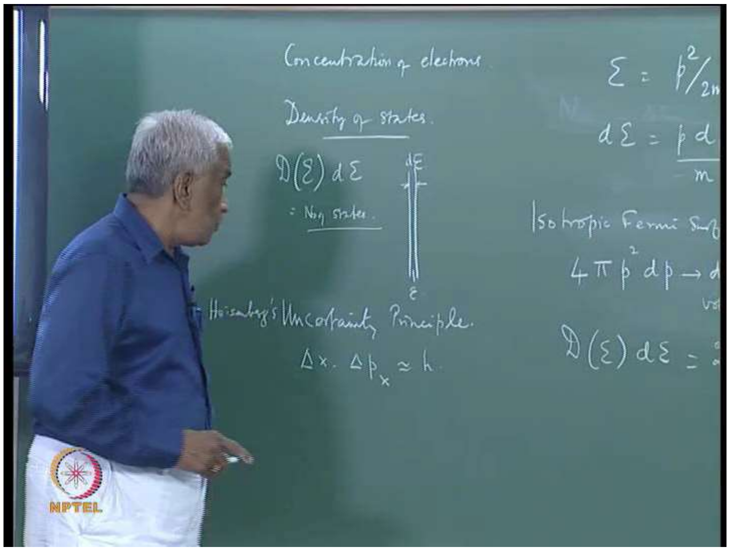

So, next we should to calculate the concentration of electrons which is the number of electrons for unit volume can I say electron I only mean the conduction electrons in order to find this t we have to also consider in addition to the distribution function. We have to consider what is known as the density of states this is because the distribution function tells us how the electrons are distributed in the energy, but as you can see from this equalization connecting the energy and the wave vector are the wave number it is the wave number which decides that the electrons state.

So, we want to also know how the hold me a conduction electrons are distributed indifferent states corresponding to a given energy. So, this is given by what is known as the density of states. So, it tells us how many states are available in a differentia energy interval agents to a given energy. So, if I look at a particular energy. So, I would loot look at an infinite this month d e around a given energy. So, if I take this infinity dismal energy interval we d f e is the density of a state function which described the d f e d e gives the the number of steps in this energy interval.

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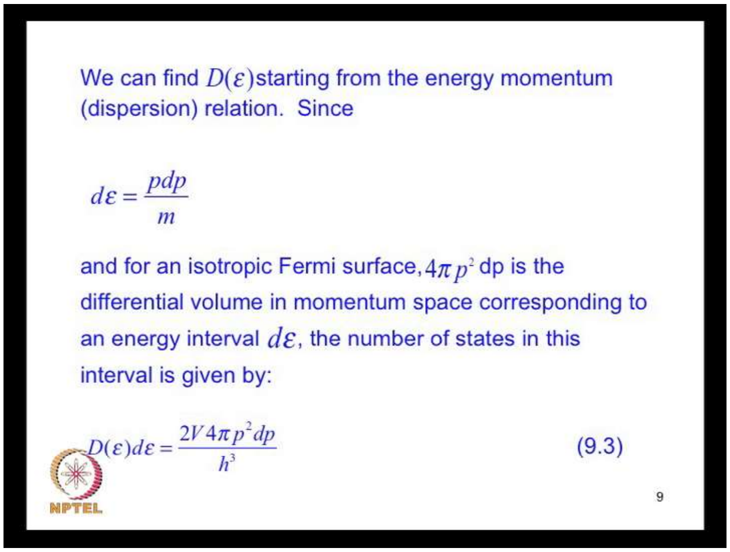

We can find $D(\varepsilon)$ starting from the energy momentum (dispersion) relation. Since

$$d\varepsilon = \frac{pdp}{m}$$

and for an isotropic Fermi surface, $4\pi p^2$ dp is the differential volume in momentum space corresponding to an energy interval $d\varepsilon$, the number of states in this interval is given by:

$$D(\varepsilon)d\varepsilon = \frac{2V4\pi p^2 dp}{h^3} \qquad (9.3)$$

So, we wish to find out this density of states together the distribution function ff e and the density of the state function d f e d e together will determine the average this statistical properties are this electron gas how do you find this density of states function we will just discuss this next.

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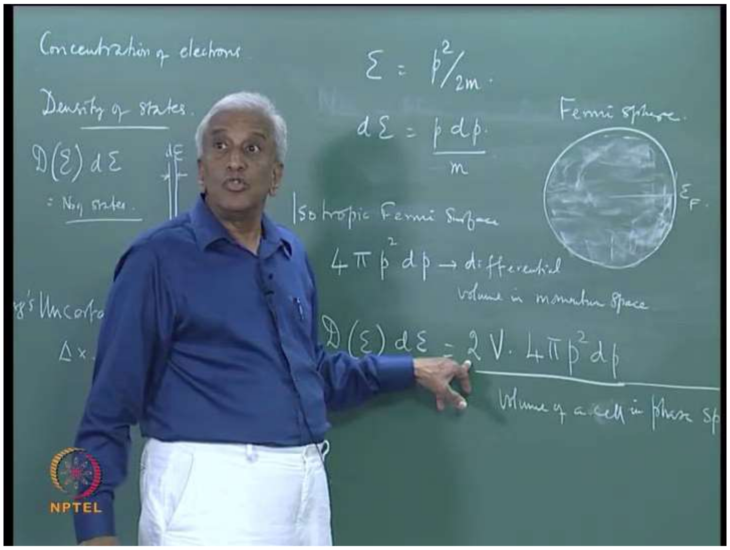

So, we have we know that the energy is just p-square by 2 m because the electron have only kinetic energy. So, d e is p d p by m now if I look at the momentum space and if I regard the fermi energy as corresponding to a value which corresponds to an isotropic fermi surface which means it is fermi surface. So, it is the spear with radios e f in energy space. So, that is the fermi spear and all the inside state inside this or occupy by electron gas. So, we know that radios the volume of this will differential volume is four pi p square d p.

This is the differential volume in momentum space position and momentum together define a state in statically physics. So, this is the differential volume in momentum space if we take the number. Now, we count the number or state in this interval by writing d f e d e e equals v the actual volume in real physical space the position space multiplied by the differential volume in momentum space times 2 the factor 2. In order to take it account this spin and divide this by the volume of f s cell in phase space sell means state each cell each of the cell correspond to 1 state of the electron as we discussed already according to the pauli principle.

Now, this volume of a cell in phase space is given by the so-called uncertainty principle in quantum mechanics as I already told you the electrons are quantum particles. So, we have discussed as statistical behavior according to the quantum statistics and fermi dirac statistics is a quantum statistics. Now the main feature of quantum behavior comes from the so-called uncertainty principle due to Haisonbag this principle states that the product in uncertainties of position. And momentum is of the order of the planks constant and therefore, this is in 1 by mention therefore, we can write the volume of a cell in phase space as the product of the uncertainty you cannot look it a particle beyond this accuracy in quantum mechanics. So, this is the minimum uncertainties.

So, this is the spatial and momentum, extent the extension in space and a real space and momentum is given is order of the planks constant. So, if we use the same argument for all the three dimensions and in real space and all the three components of linear momentum then they get this volume is h cube this is h for each dimensions. So, there are three dimensional. So, each time it is multiplied. So, get h cube and that is the uncertainty to which you can locate a given state in phase space in quantum mechanics therefore, that corresponds. So, this space the phase space is quantum mechanics is course grain and this is the volume occupied by a a state in phase space. So, you derive the total volume available physical volume v times the differential volume in momentum space times the factor 2 due to spins state and divide the whole thing by h cube.

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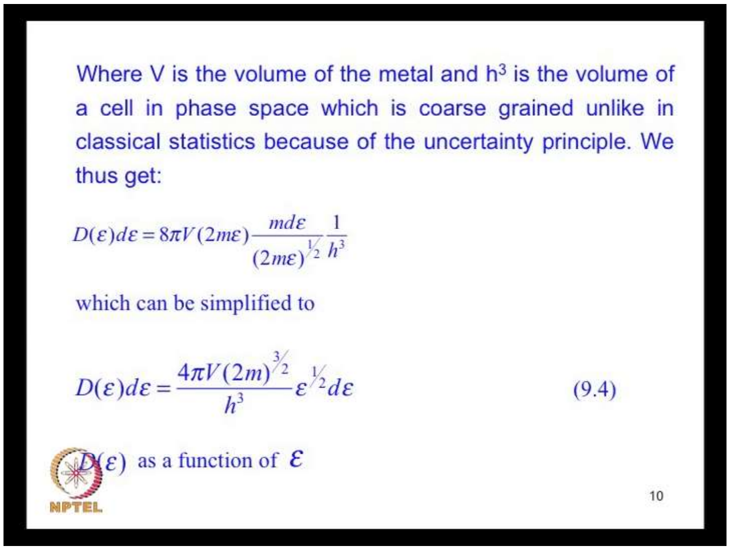

Where V is the volume of the metal and h^3 is the volume of a cell in phase space which is coarse grained unlike in classical statistics because of the uncertainty principle. We thus get:

$$D(\varepsilon)d\varepsilon = 8\pi V(2m\varepsilon)\frac{m\,d\varepsilon}{(2m\varepsilon)^{1/2}}\frac{1}{h^3}$$

which can be simplified to

$$D(\varepsilon)d\varepsilon = \frac{4\pi V(2m)^{3/2}}{h^3}\varepsilon^{1/2}d\varepsilon \qquad (9.4)$$

$D(\varepsilon)$ as a function of ε

That will give the number are state which is intern to the given by d f e d e. So, this gives as the way to calculate density of state function therefore, we just substitute p square is just 2 m e.

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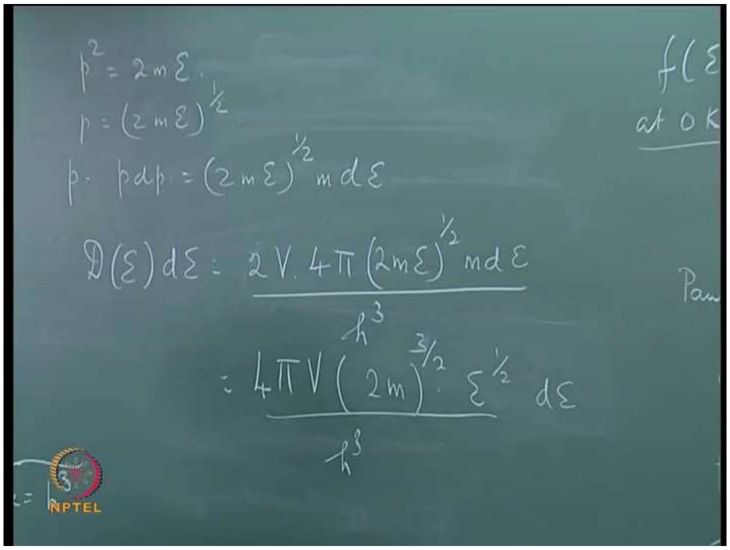

$$p^2 = 2m\mathcal{E}$$

$$p = (2m\mathcal{E})^{1/2}$$

$$p \cdot p\,dp = (2m\mathcal{E})^{1/2}\, m\, d\mathcal{E}$$

$$\mathcal{D}(\mathcal{E})\,d\mathcal{E} = \frac{2V \cdot 4\pi (2m\mathcal{E})^{1/2}\, m\, d\mathcal{E}}{h^3}$$

$$= \frac{4\pi V (2m)^{3/2}}{h^3}\, \mathcal{E}^{1/2}\, d\mathcal{E}$$

So, 4 pi. So, p is 2 m e to the power half. So, here I have p square d p which I can write as p times p d p p d p already I have as m d e. So, 2 m e to the power half times m p e therefore, substituting here d f e d e 2 v into four pi into p square d p which is here to m e to the power half into m d e pi h cube. So, this some simplification gives you the density of space function as four pi v.

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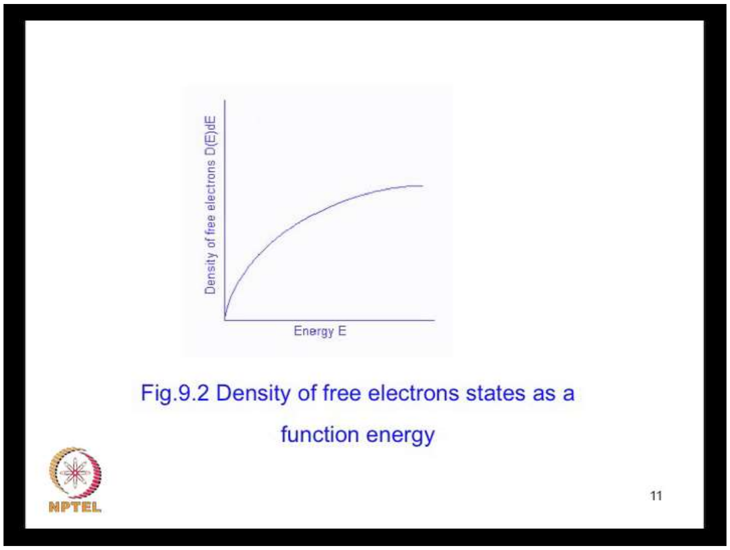

Fig.9.2 Density of free electrons states as a function energy

So, you can see that this is the density of state function which is plotted these together. So, you can see the density of state goes as e power half.

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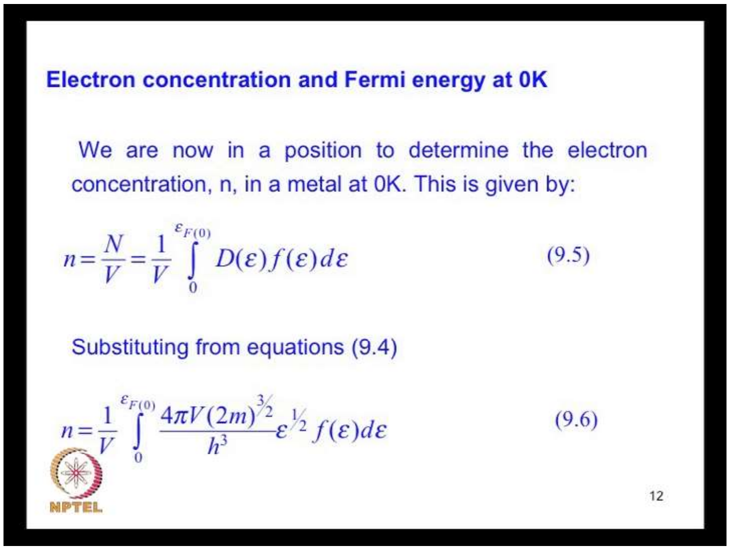

Electron concentration and Fermi energy at 0K

We are now in a position to determine the electron concentration, n, in a metal at 0K. This is given by:

$$n = \frac{N}{V} = \frac{1}{V}\int_0^{\varepsilon_{F(0)}} D(\varepsilon) f(\varepsilon)\, d\varepsilon \qquad (9.5)$$

Substituting from equations (9.4)

$$n = \frac{1}{V}\int_0^{\varepsilon_{F(0)}} \frac{4\pi V (2m)^{3/2}}{h^3}\varepsilon^{1/2} f(\varepsilon)\, d\varepsilon \qquad (9.6)$$

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Now, we have a all the we have developed all the things that we need 2 evaluate the electron concentration at 0-kelvin let us do this now.

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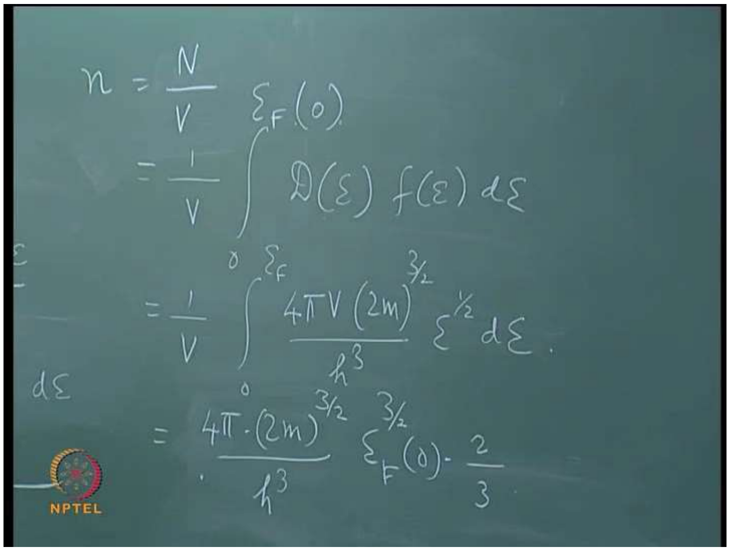

$$n = \frac{N}{V} = \frac{1}{V}\int_0^{\varepsilon_F(0)} D(\varepsilon)\, f(\varepsilon)\, d\varepsilon$$

$$= \frac{1}{V}\int_0^{\varepsilon_F} \frac{4\pi V (2m)^{3/2}}{h^3}\, \varepsilon^{1/2}\, d\varepsilon.$$

$$= \frac{4\pi \cdot (2m)^{3/2}}{h^3}\, \varepsilon_F(0)^{3/2} \cdot \frac{2}{3}$$

So, the number of electrons in unit volume is the total number divided by volume and that will be the total is what is given by this. So, I have 1 by integral of e f of e d e comes 0 to e f this is because of ff e gives you how the electrons are distributed in energy. And d f e gives you use you how the energies are distributed at in states and therefore, the product of these 2 integrated over an energy interval from 0 to fermi energy up to the all states are completely occupied rest of them are completely empty. So, it is enough if I integrated over all the energies from 0 to e f let me write e f at 0 in order to remind ourselves of the fact, that we have calculating it at 0 kelvin. So, if I substituted the this 1 by b 0 to e f, then I have this four pi v into 2 m to the power three by 2 by h cube e power half d e and I have removed f of e because this is going to be 1 for all the states. So, it is going to have a value 1 at absolute 0.

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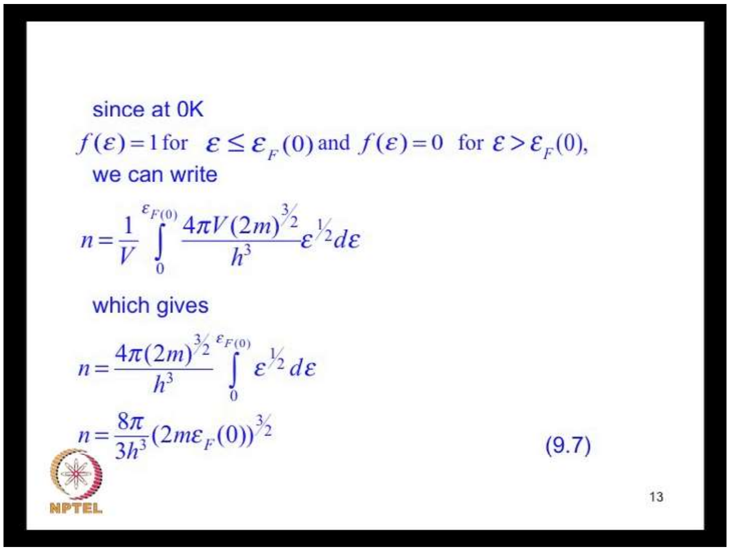

since at 0K

$f(\varepsilon)=1$ for $\varepsilon \le \varepsilon_F(0)$ and $f(\varepsilon)=0$ for $\varepsilon > \varepsilon_F(0)$,

we can write

$$n=\frac{1}{V}\int_0^{\varepsilon_{F(0)}} \frac{4\pi V(2m)^{3/2}}{h^3}\varepsilon^{1/2}d\varepsilon$$

which gives

$$n=\frac{4\pi(2m)^{3/2}}{h^3}\int_0^{\varepsilon_{F(0)}} \varepsilon^{1/2}\,d\varepsilon$$

$$n=\frac{8\pi}{3h^3}(2m\varepsilon_F(0))^{3/2} \qquad (9.7)$$

So, we can write all these constants can be back out v cancels for 4 pi 2 m to the power 3 by 2 by h cube e f 0 to the power 3 by 2 into 2 by 3 as a result of integration.

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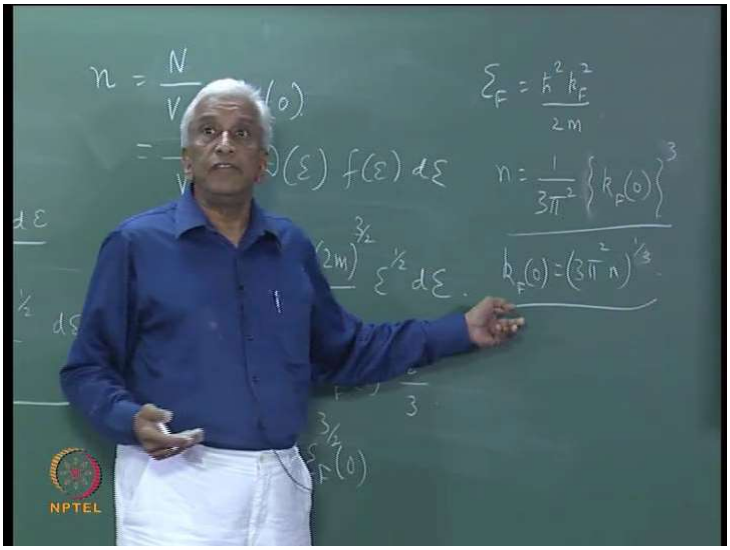

So, that gives me final result as using this and using ef as we already saw e f is nothing, but the kinetic energy up to the wave vector at fermi energy h cross square k f square by 2 m therefore, we get n s. So, that gives you rather compact relationship between the fermi wave vector at absolute 0 and the electron concentration n now me assume that because for example, in a metal like sodium each atom donates 1 electron to the conduction band. So, if we have a moral a gram atom of this solid then this will contain as is well known and number of atoms. So, that correspond to the number of electrons donate at a conduction electron and do not donated.

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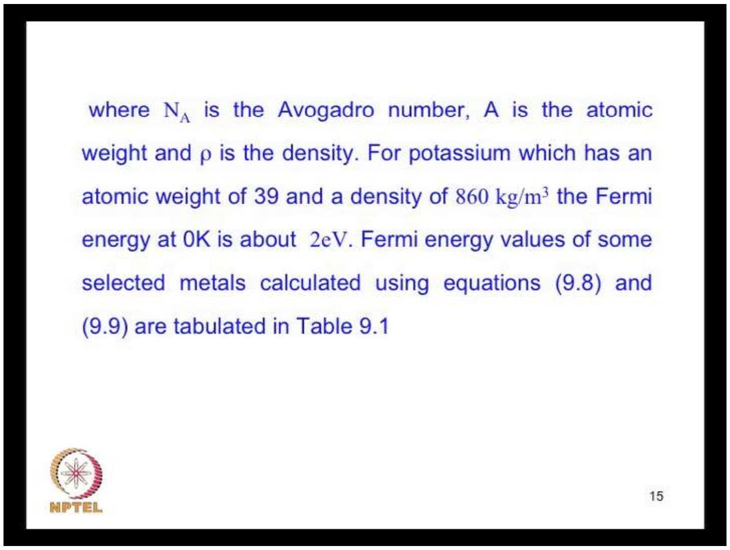

where N_A is the Avogadro number, A is the atomic weight and ρ is the density. For potassium which has an atomic weight of 39 and a density of 860 kg/m^3 the Fermi energy at 0K is about 2eV. Fermi energy values of some selected metals calculated using equations (9.8) and (9.9) are tabulated in Table 9.1

So, if you take number and divide by the atomic wait.

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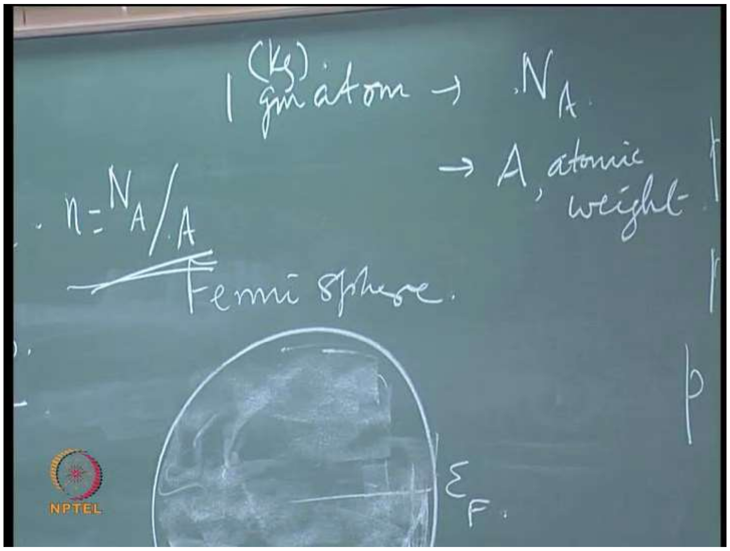

So, that gives me in 1 gram atom are kilogram atom correspond to n a number of atoms and I have each atom gives you 1 electron in a monatomic solid. So, this is the number of electrons. So, this correspond to your weight of a where this is atomic weight therefore, the number of electron is just in 1 mole is n a by a times.

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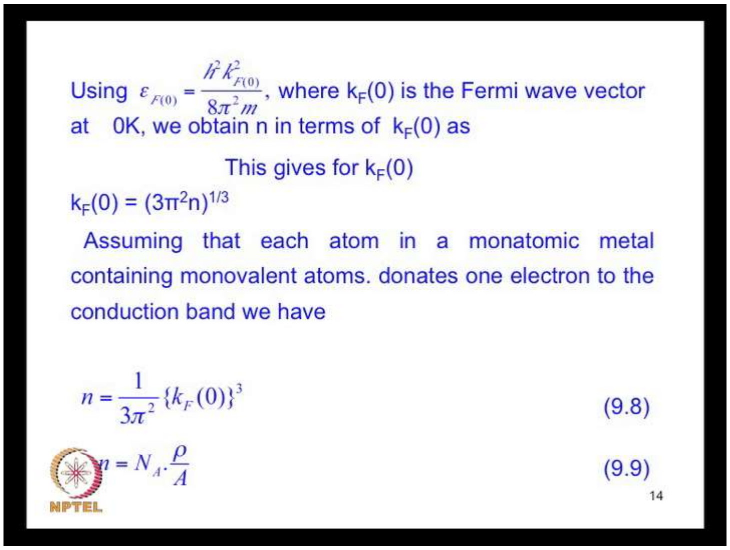

Using $\varepsilon_{F(0)} = \frac{h^2 k^2_{F(0)}}{8\pi^2 m}$, where $k_F(0)$ is the Fermi wave vector at 0K, we obtain n in terms of $k_F(0)$ as

This gives for $k_F(0)$

$k_F(0) = (3\pi^2 n)^{1/3}$

Assuming that each atom in a monatomic metal containing monovalent atoms. donates one electron to the conduction band we have

$$n = \frac{1}{3\pi^2}\{k_F(0)\}^3 \quad (9.8)$$

$$n = N_A \cdot \frac{\rho}{A} \quad (9.9)$$

They have to we are forgetting the fact that we have also row because it this gives you the number half electrons per unit mass, and then we have to multiply this by the density.

So, we can calculate n and therefore, calculate the fermi wave vector and inurn the fermi energy. So, we have way of calculating the fermi energy from this formula.

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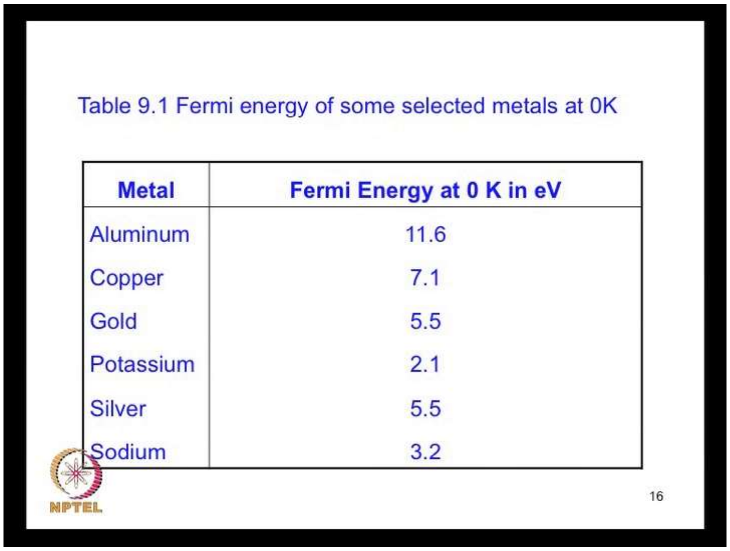

Table 9.1 Fermi energy of some selected metals at 0K

Metal	**Fermi Energy at 0 K in eV**
Aluminum	11.6
Copper	7.1
Gold	5.5
Potassium	2.1
Silver	5.5
Sodium	3.2

So, the fermi energy values calculated in this way are also shown in the table. So, the fermi energy at 0 kelvin the values are given in an electron volt which is a convenient unit in a the case of atomic physics. This gives you the energy of an electron when is accelerated through a potential of 1 volte, now the various metals aluminum copper gold potassium silver sodium.

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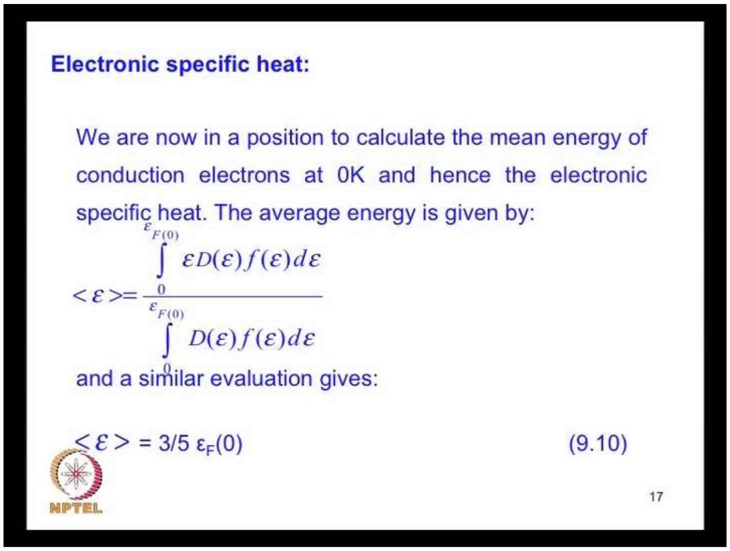

Electronic specific heat:

We are now in a position to calculate the mean energy of conduction electrons at 0K and hence the electronic specific heat. The average energy is given by:

$$<\varepsilon> = \frac{\int_0^{\varepsilon_{F(0)}} \varepsilon D(\varepsilon) f(\varepsilon) d\varepsilon}{\int_0^{\varepsilon_{F(0)}} D(\varepsilon) f(\varepsilon) d\varepsilon}$$

and a similar evaluation gives:

$$<\varepsilon> = 3/5\ \varepsilon_F(0) \qquad (9.10)$$

You can see the fermi energy the various from something like eleven points six electron volts to the three-point to electron volts in any case all of the order of electron volts. So, this is a very important idea because if you converted by using Boltzmann constant to equal intemperate this will be a the order of ten to the power of four kelvin. So, a very high temperature. So, the energies the fermi energy corresponds to be a very high temperature the corresponding temperature in temperature units. Now we will use these concepts to calculate an important thermal property namely be electronic specific heat this means that this electron gas, if you inject some heat and energy into it they electron absorbs this energy. And that temperature goes up though these this specific heat is defined as the rate of change of the mean internally energy of the conduction electron at 0 k with respect to temperature.

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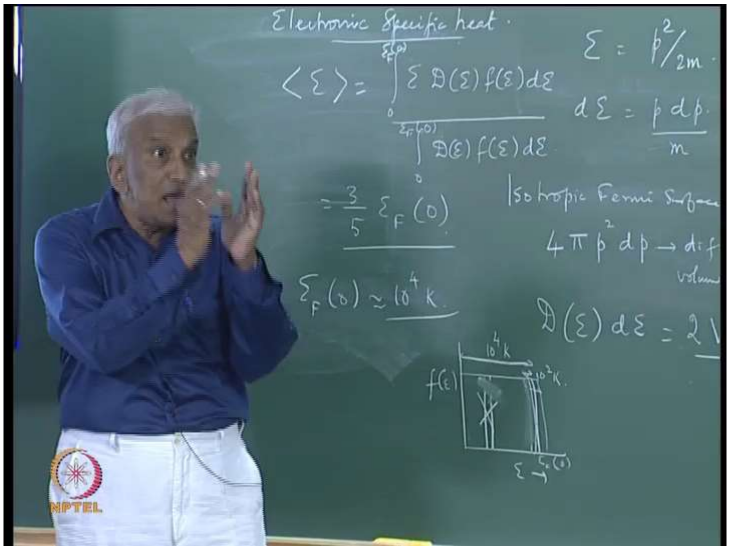

So, the electronic specificate can be calculated that by calculating the average energy of this electron gas which is simply done by again at absolute 0. This is done by integrating from 0 to e f 0 of e d f e f f e d e by 0 to e f 0 of e f e f of e d. So, this gives going by the same procedure they arrive at the result this is three fifth of e f 0.

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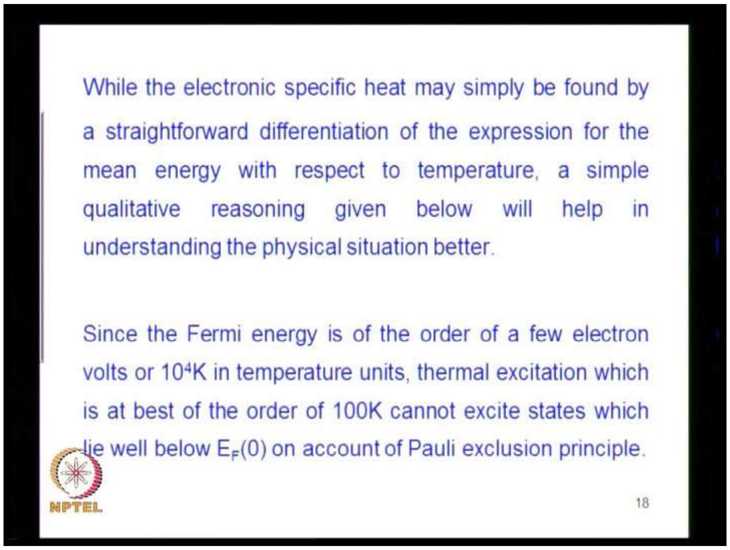

While the electronic specific heat may simply be found by a straightforward differentiation of the expression for the mean energy with respect to temperature, a simple qualitative reasoning given below will help in understanding the physical situation better.

Since the Fermi energy is of the order of a few electron volts or 10^4K in temperature units, thermal excitation which is at best of the order of 100K cannot excite states which lie well below $E_F(0)$ on account of Pauli exclusion principle.

The average energy is three fifth of fermi energy at absolute 0 now the electronics specific heat having got the average energy, we can simply differentiate this expression fermi energy with respect to temperature that gives you the electronic specific heat. Now we will first qualitatively see what kind results that we are going to get or this calculation the electronic specific heat, since we said that the e f 0 is the order of ten to the power four kelvin in temperature units.

So, if you thermal exited usually thermal excitation is at best of the order of hundred kelvin. So, it is a very small if you go back to the energy distribution this is e f 0 if you go back to this this is of the order of this in temperature e units is that the the order of ten thousand kelvin, but our energy excitations thermal energy excitation is only at the order of a hundred kelvin. So, it is small temperature window. So, the exhibition is going to shift states from this to this, but the state's are all remember that they are all completely occupied and are subject to the electron for subject pauli is crucial that mean if state is completely occupying already you can put another electron.

So, this exhibition from this one occupy state to another occupy state in this whole range is not going to be possible even though you give with excitation, the electrons cannot be exited fermi occupied state here into another occupied state which is not empty. So, this is only pass only at this edge this is not possible and the thermal exhibition is one only possible here here. So, this is of the order of ten to the power four Kelvin, and this is order of ten square. So, this is only possible across this fermi energy if it bring it here.

So, it can excite across in to 1 of the empty state here. So, only the a fraction of the electron which occupy a stated within this ten hundred kelvin in the neighborhood of the fermi energy only they will be able to get excited. So, what is this fraction they are k b t by k b t r k b t f corresponds to all the states the electrons not the energy scale and response b t corresponds to the energy of the thermal excitation.

So, this is the fraction which is t by t f that is the fraction of electrons excited exited thermally and each of them has an exhibition of order of k b t therefore, the excitation energy is as the order of k b t square by t f, so d by d t I of this use this specific. So, these are the order of k b t. So, this tells me that the electronic specific is the order of k b t it is proportional to the temperature t. So, the electronic heat capacity r c e electronic specific heat is plus equal to the constant times the temperature. So, that is the basic results that we get for the electronic specific heat of the conduction electronic gas, so you get this is the value at absolute 0.

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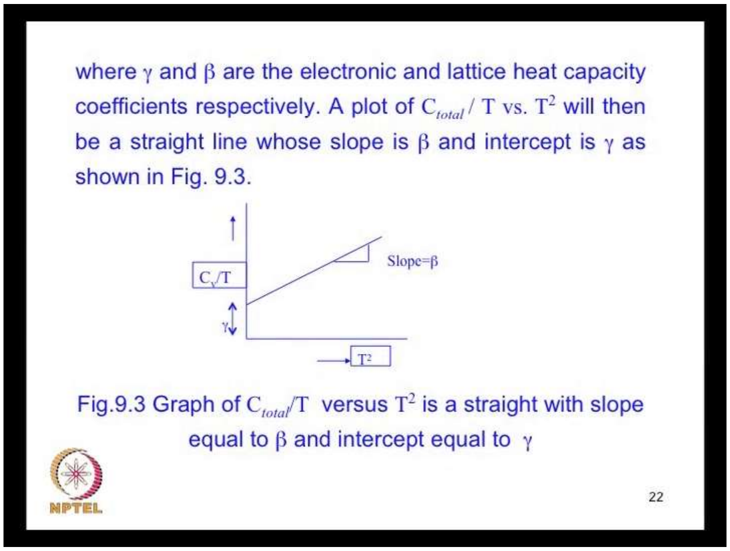

where γ and β are the electronic and lattice heat capacity coefficients respectively. A plot of C_{total} / T vs. T^2 will then be a straight line whose slope is β and intercept is γ as shown in Fig. 9.3.

Fig.9.3 Graph of C_{total}/T versus T^2 is a straight with slope equal to β and intercept equal to γ

So, this is shown graphically. So, in figure of course, you will never be able to measure the electronic heat capacitance alone it will be also the specific with includes the contribution from the electron. And also from the lattice of ions are the atoms in the solid and that as we will see later is given by the may be theory specificate and that temperature depend is a t q dependence. So, the overall behavior is given off by a relation of this time c total and therefore, if you brought c by t verses p-square that would be a straight line that is what is shown in figure. So, from the intercept of this we can get the heat capacity question gamma, we have discussed everything at absolute 0, but the question arises w what happens? Then you have an electron at a finite temperature the this the bit more difficult to calculate, we will not go through the details at this calculation here, but I will just roughly.

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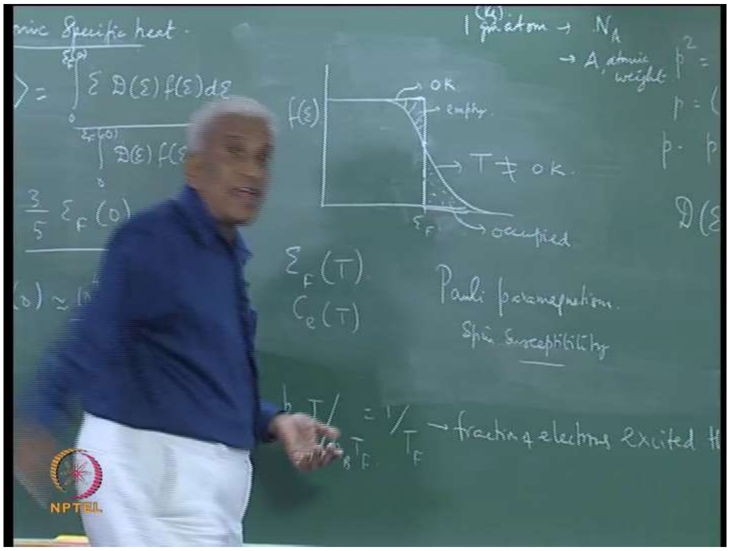

It what happens by looking at the distribution function. So, at a finite temperature the fermi dirac distribution function this at a finite temperature which is not 0. So, the distribution function, now deviate from the behavior at absolute 0, this is at 0 kelvin as we have already seen, and at finite temperature, this reduces to something like this. That is the behavior here at the not equal to 0 at any finite temperature it the f f e decreases from the value 1 to something like of fermi energy. And then it goes on beyond it is non-zero even beyond the ef this means that some of this state or empty even before even below the fermi energy, and some on the state or above the fermi energy are occupy and these the number occupied states goes on increasing.

So, this is the behavior and this will modify the fermi energy the fermi energy will be a function of temperature. Now and the heat capacity equation which is still found to be a linear function of temperature, but but the constant the linear heat capacity question is slightly different. We will not calculate this this is the overall behavior now electron gas also processes many other interesting properties the electron have a magnetic moment because that that is been and this contributes to magnet. So, this is known as Pauli paramagnets or this is a spin susceptibility this is the magnetic susceptibility which arises from the fact that the electron Aspin's, and therefore a magnetic moment. So, this is another important characteristic of the conduction electron gas in metals in addition the metals most important characteristic is that metal is a very good contact to have electricity. Now we would like to have an expression far the electrical conductivity of a metal.

And how it depends on for example, temperature and not only the electrical conductivity the a metal is also a good conductor of heat. So, we would like to know how the thermal conductivity is determined by the behavior electron gas, we also know that there is such a thing called thermo electric power the phenomenon the thermo electricity in which metal junction used in order to produce the thermo electricity and e m f. So, we would also like to know how the thermoelectric power of a good conductor is determined by the behavior the electron gas these are things we will discuss in next lecture.

Condensed Matter Physics
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Lecture - 09
The Free Electron Theory of Metals-Worked Examples

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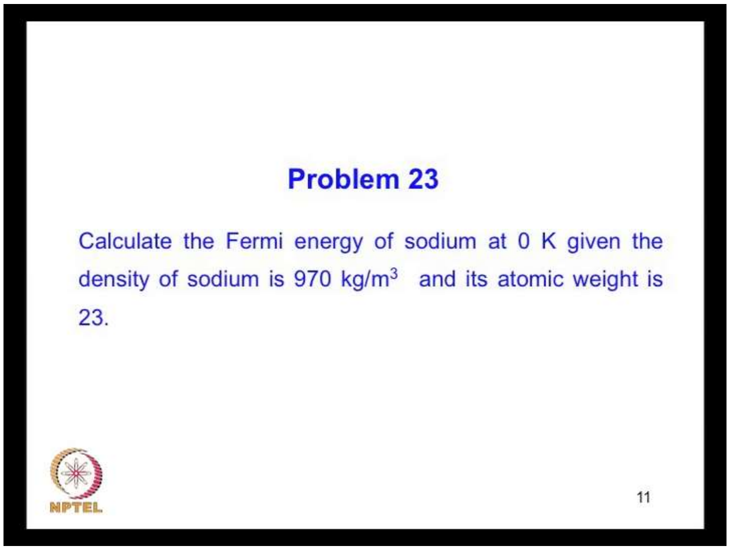

Problem 23

Calculate the Fermi energy of sodium at 0 K given the density of sodium is 970 kg/m^3 and its atomic weight is 23.

Now, we will move on to some questions relating to electrons in solids, the free electrons in metals in particular.

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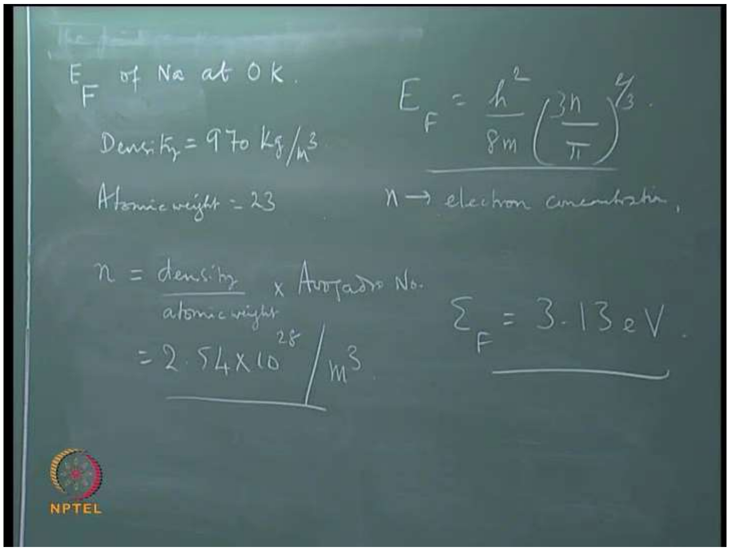

E_F of Na at 0 K.

Density = 970 kg/m^3

Atomic weight = 23

$$E_F = \frac{h^2}{8m}\left(\frac{3n}{\pi}\right)^{2/3}.$$

$n \rightarrow$ electron concentration,

$$n = \frac{\text{density}}{\text{atomic weight}} \times \text{Avogadro No.}$$

$$= 2.54 \times 10^{28} / m^3.$$

$$\Sigma_F = 3.13 \text{ eV}.$$

The problem that we will discuss is we are asked to calculate the Fermi energy of sodium at 0 k, where given the density of sodium is 970 kilograms per meter cube, and the atomic weight is 23 as we know. We know that the basic expression for the Fermi energy is h square by 8 m into n by pi to the power 2 by 3, where n is the electron concentration, 3 n by pi.

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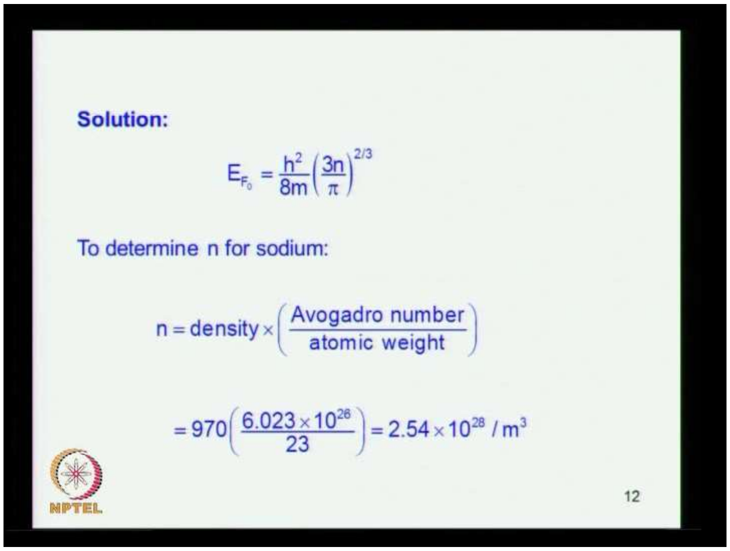

Solution:

$$E_{F_0} = \frac{h^2}{8m}\left(\frac{3n}{\pi}\right)^{2/3}$$

To determine n for sodium:

$$n = \text{density} \times \left(\frac{\text{Avogadro number}}{\text{atomic weight}}\right)$$

$$= 970\left(\frac{6.023 \times 10^{26}}{23}\right) = 2.54 \times 10^{28}\ /\ m^3$$

So, we are required to find n for which we take the density and divide by the atomic weight and multiplied by Avogadro number. And that the density and the atomic weight are given here, Avogadro number is known the result of this calculation is 2.54 into 10 to the power 28 electron per meter cube. We are assuming that is in sodium is monovalant that this is really the number of atoms per in unit value and assuming that each atoms donates one conduction electron, we get the number of electrons per unit volume as this.

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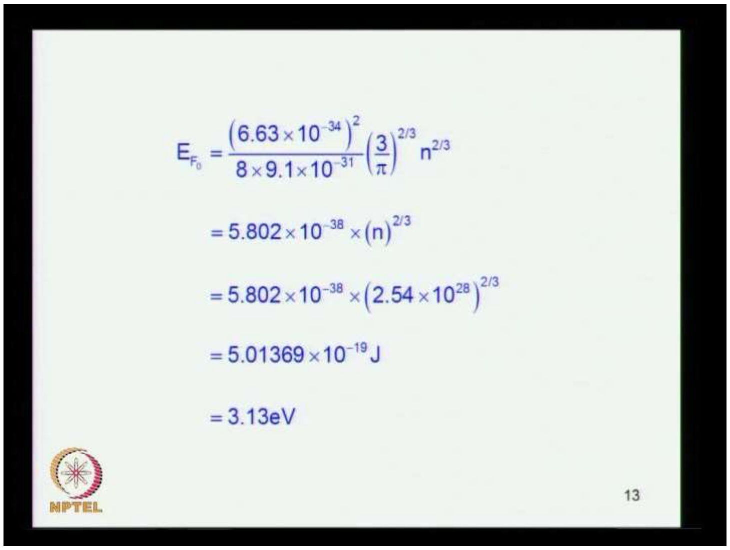

$$E_{F_0} = \frac{\left(6.63\times10^{-34}\right)^2}{8\times9.1\times10^{-31}}\left(\frac{3}{\pi}\right)^{2/3} n^{2/3}$$

$$= 5.802\times10^{-38}\times(n)^{2/3}$$

$$= 5.802\times10^{-38}\times\left(2.54\times10^{28}\right)^{2/3}$$

$$= 5.01369\times10^{-19}\,\mathrm{J}$$

$$= 3.13\,\mathrm{eV}$$

And therefore, substituting this value of n, we get the Fermi energy as 3.13 electron volts this is a just a question of substituting this expression is. So, that is the Fermi energy of sodium at zero Kelvin.

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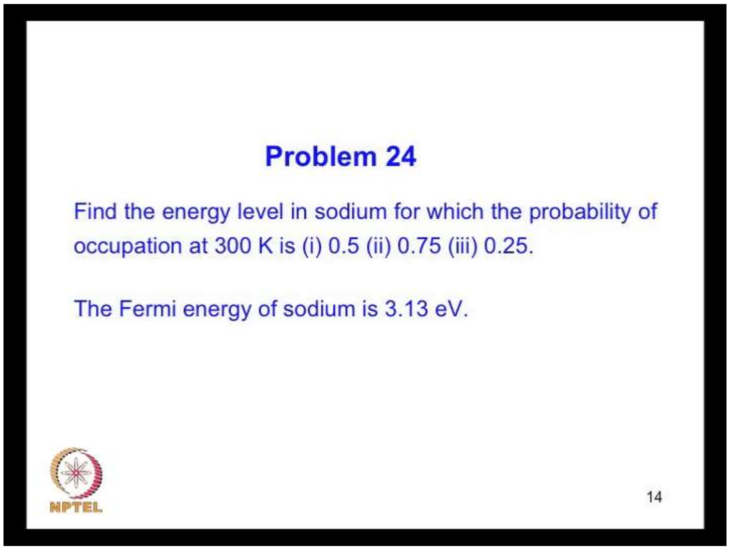

Problem 24

Find the energy level in sodium for which the probability of occupation at 300 K is (i) 0.5 (ii) 0.75 (iii) 0.25.

The Fermi energy of sodium is 3.13 eV.

In the next problem, we again deal with sodium we are asked to find the energy level in sodium at absolute zero, no, not at absolute zero.

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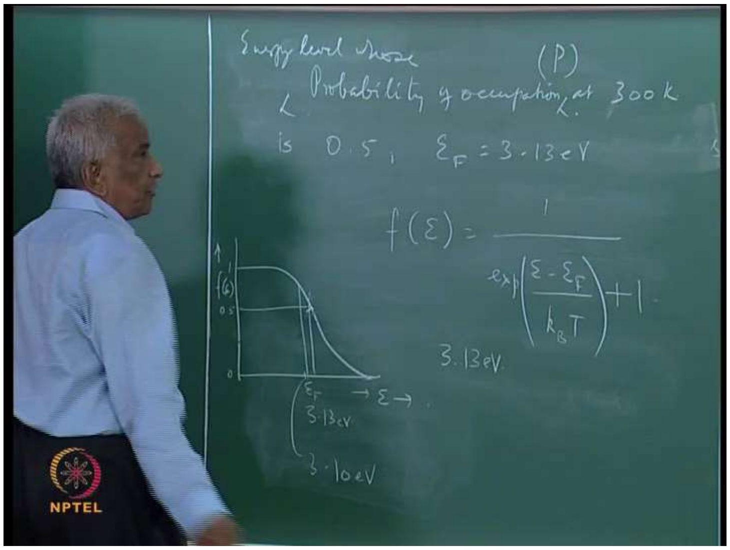

But probability of occupation of this energy level at a temperature of 300 Kelvin is 0.5. Energy level whose probability of occupation since here from given the result of the previous problem that E f the Fermi energy at zero k is at 3.13 electron volts. For this we go back to the Fermi Dirac distribution function which finite temperatures as they form like this, we have discussed all these already. So, that is the shape of Fermi Dirac distribution function and therefore, we know that the probability of occupation at 300 k becomes half exactly at the Fermi level.

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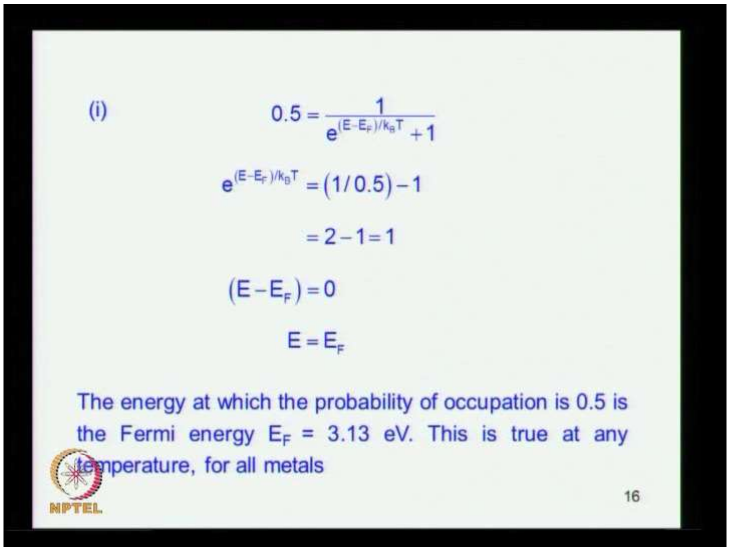

(i)

$$0.5 = \frac{1}{e^{(E-E_F)/k_B T}+1}$$

$$e^{(E-E_F)/k_B T} = (1/0.5)-1$$

$$= 2-1=1$$

$$(E-E_F)=0$$

$$E=E_F$$

The energy at which the probability of occupation is 0.5 is the Fermi energy E_F = 3.13 eV. This is true at any temperature, for all metals

So, we can find this we can readily see that this has to be at an energy of 3.13 electron volts.

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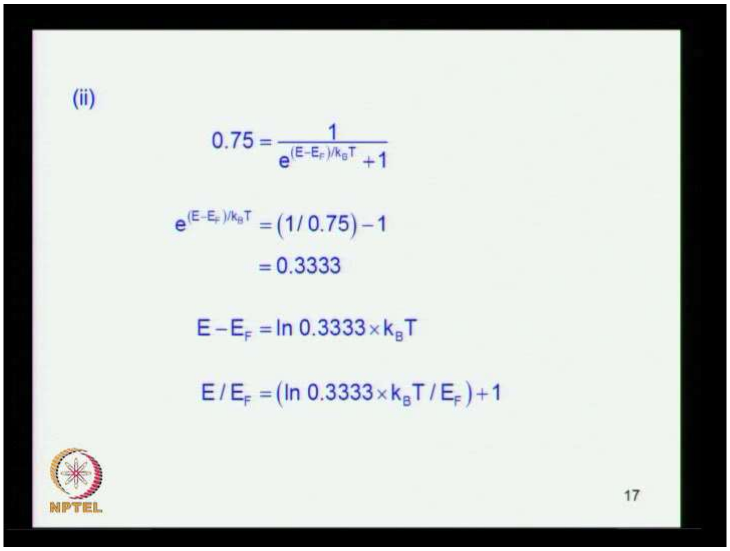

(ii)

$$0.75 = \frac{1}{e^{(E-E_F)/k_BT}+1}$$

$$e^{(E-E_F)/k_BT} = (1/0.75)-1$$
$$= 0.3333$$

$$E-E_F = \ln 0.3333\times k_BT$$

$$E/E_F = (\ln 0.3333\times k_BT/E_F)+1$$

This is true in general of all metals. The value of half for the probability of half occupation occurs at the Fermi energy. In the same way, we can find the values energy at which the probability of occupation becomes for example, 0.75.

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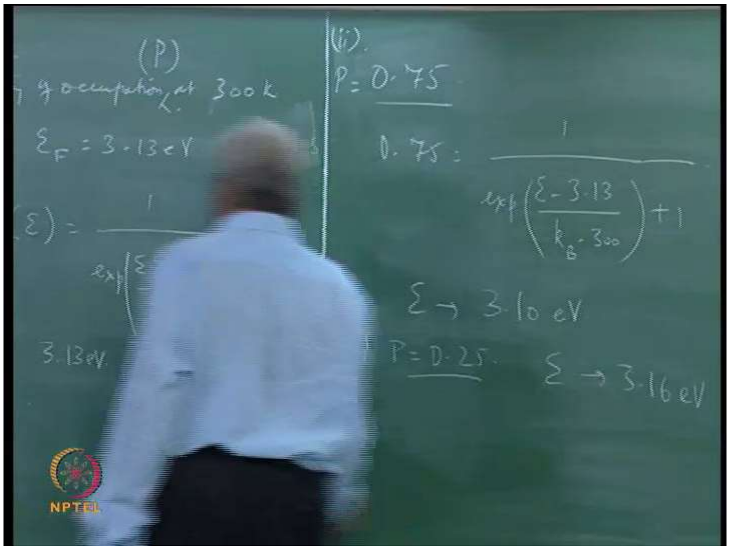

So, that is the second question we have to find. So, substituting 0.75 equal to 1 by exponential e minus 3.13 by k B into 300 plus 1 substituting in this we can readily see that the E happens to be something like 3.10 electron volts.

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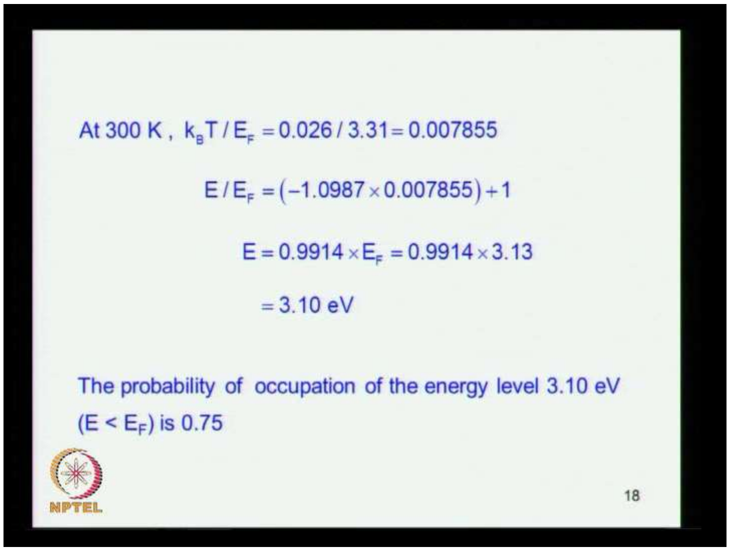

At 300 K , $k_B T / E_F = 0.026 / 3.31 = 0.007855$

$$E / E_F = (-1.0987 \times 0.007855) + 1$$

$$E = 0.9914 \times E_F = 0.9914 \times 3.13$$

$$= 3.10 \text{ eV}$$

The probability of occupation of the energy level 3.10 eV ($E < E_F$) is 0.75

And that would be this is 3.13, and this will be somewhere here 3.10 electron volts in which we have a probability of occupation of 0.75. The next question concerns the same value for energy level for which the probability is 0.25.

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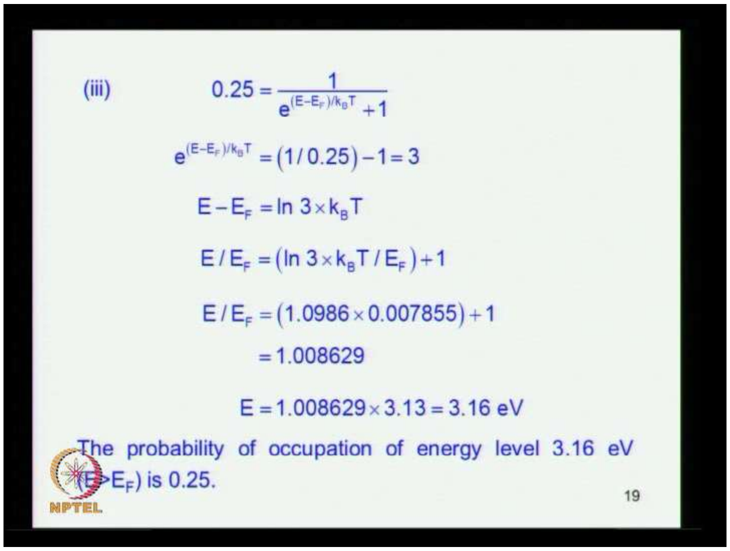

(iii) $$0.25 = \frac{1}{e^{(E-E_F)/k_B T} + 1}$$

$$e^{(E-E_F)/k_B T} = (1/0.25) - 1 = 3$$

$$E - E_F = \ln 3 \times k_B T$$

$$E / E_F = (\ln 3 \times k_B T / E_F) + 1$$

$$E / E_F = (1.0986 \times 0.007855) + 1$$

$$= 1.008629$$

$$E = 1.008629 \times 3.13 = 3.16 \text{ eV}$$

The probability of occupation of energy level 3.16 eV ($E > E_F$) is 0.25.

And for following same procedure, we find the corresponding energy is 3.16 electron volts. In other words, we have the Fermi tail here and it is slightly above the Fermi level this is 3.16 electron volts and that is where the probability reduces further from 0.5 to 0.25, but still it is non-zero. So, states here are occupied with a probability of one-fourth.

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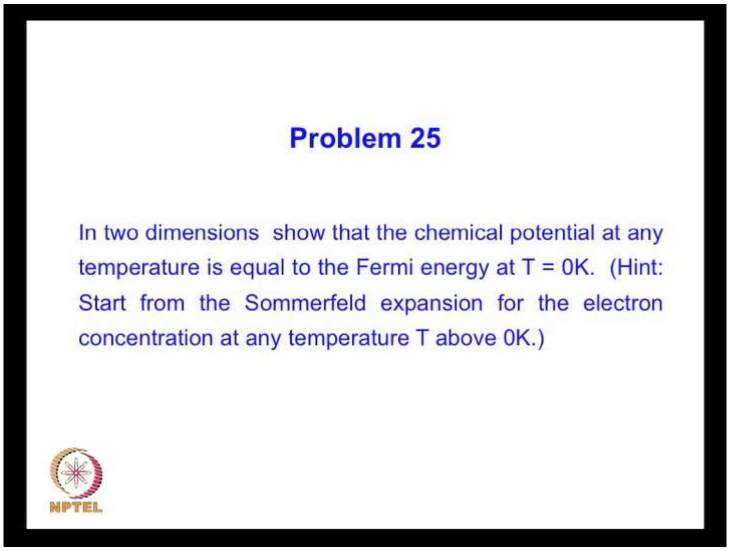

Problem 25

In two dimensions show that the chemical potential at any temperature is equal to the Fermi energy at T = 0K. (Hint: Start from the Sommerfeld expansion for the electron concentration at any temperature T above 0K.)

The next problem is about the chemical potential in two dimensions are at any temperature for the electron gas.

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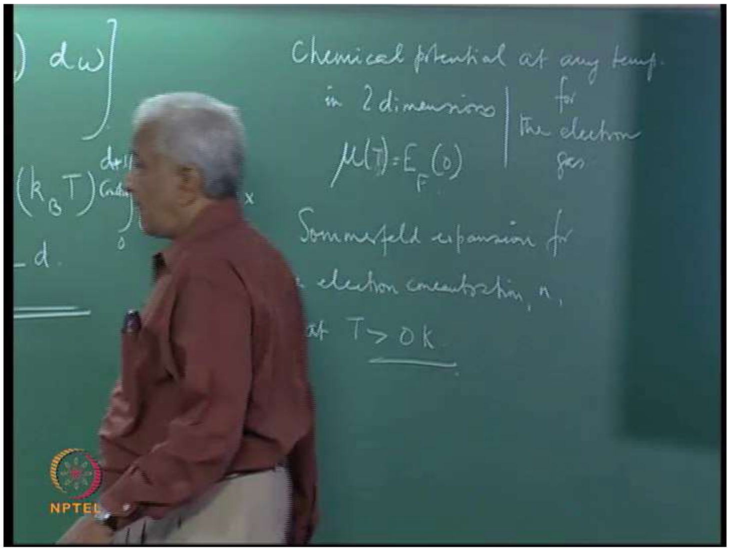

Chemical potential at any temp.
in 2 dimensions | for the electron gas
$\mu(T) = E_F(0)$

Sommerfeld expansion for
electron concentration, n,
at $T > 0K$

And we are required to prove this is the standard symbol, for this is mu and this is we are required to prove that this is equal to E f zero at this is the Fermi energy at T equal to zero k this is mu of t mu at any temperature. So, in order to prove this, we have to start from the slope called Sommerfeld expansion for the electron concentration in at any temperature T.

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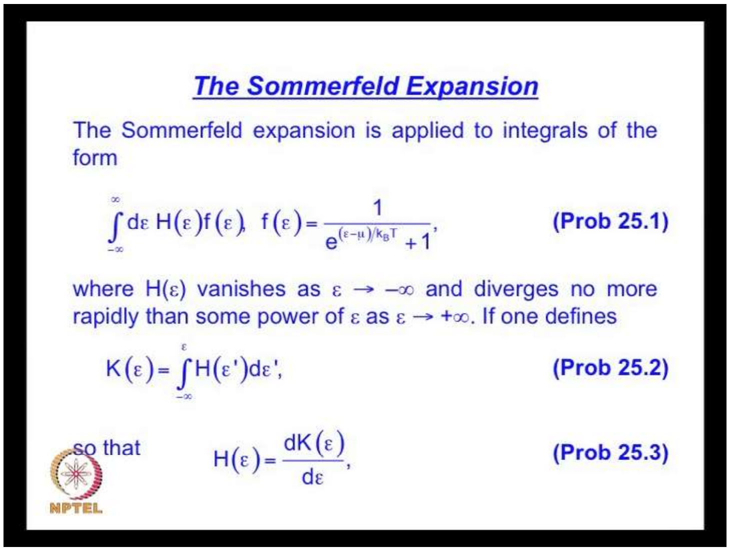

The Sommerfeld Expansion

The Sommerfeld expansion is applied to integrals of the form

$$\int_{-\infty}^{\infty} d\varepsilon\, H(\varepsilon) f(\varepsilon), \quad f(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/k_B T} + 1}, \qquad \textbf{(Prob 25.1)}$$

where $H(\varepsilon)$ vanishes as $\varepsilon \to -\infty$ and diverges no more rapidly than some power of ε as $\varepsilon \to +\infty$. If one defines

$$K(\varepsilon) = \int_{-\infty}^{\varepsilon} H(\varepsilon')\, d\varepsilon', \qquad \textbf{(Prob 25.2)}$$

so that

$$H(\varepsilon) = \frac{dK(\varepsilon)}{d\varepsilon}, \qquad \textbf{(Prob 25.3)}$$

So, what is the Sommerfeld expansion?

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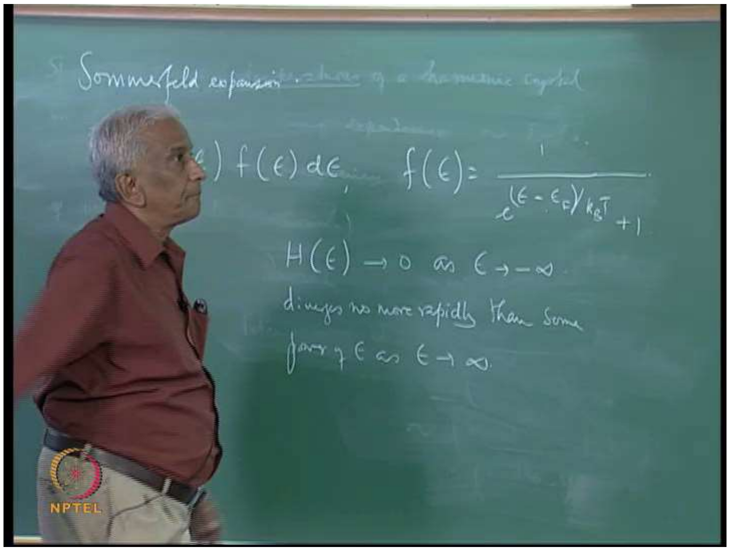

Let us consider this before answering the question. So, let us discuss the Sommerfeld expansion. In order to use this the concerned integrals of the form H of E F of E d E from minus infinity to plus infinity, where F of E is the Fermi derived distribution function and the function F of E tends to zero or vanishes as E tends to minus infinity, and diverges no more rapidly than some power of epsilon as epsilon tends to infinity.

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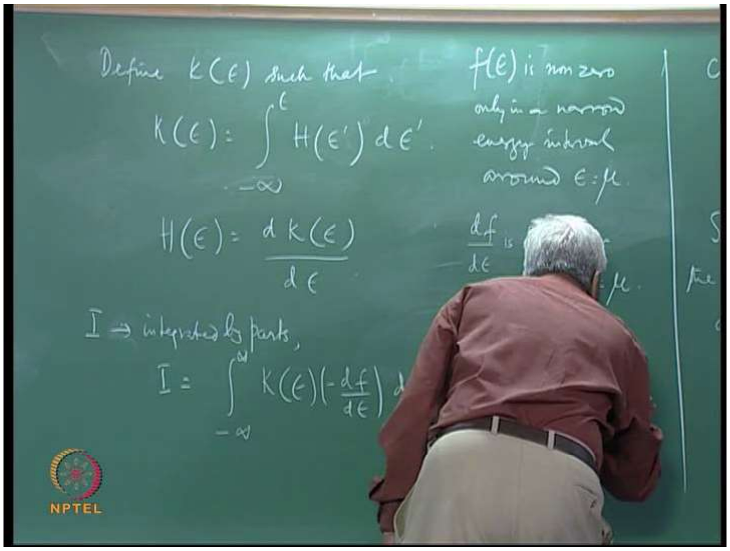

Define $k(\epsilon)$ such that

$$k(\epsilon) = \int_{-\infty}^{\epsilon} H(\epsilon')\, d\epsilon'.$$

$$H(\epsilon) = \frac{d\,k(\epsilon)}{d\epsilon}$$

$I \Rightarrow$ integrated by parts,

$$I = \int_{-\infty}^{\infty} k(\epsilon)\left(-\frac{df}{d\epsilon}\right) d$$

$f(\epsilon)$ is non zero only in a narrow energy interval around $\epsilon = \mu$.

$\frac{df}{d\epsilon}$ is

μ.

So, if it is so then let us define another function k of function epsilon define function k of epsilon such that k of epsilon equals integral zero to epsilon H of epsilon prime d epsilon prime. In other words, H of epsilon is just d k of epsilon by d epsilon. With this definition, now let us go back to let us call this integral I, then this integral maybe integrated by parts, and get we get I equal to the first term will go to zero. So, we will have integral minus infinity two plus infinity k of e into minus d f by d e times d e. Therefore, the d f by d e is large only around e equal to mu.

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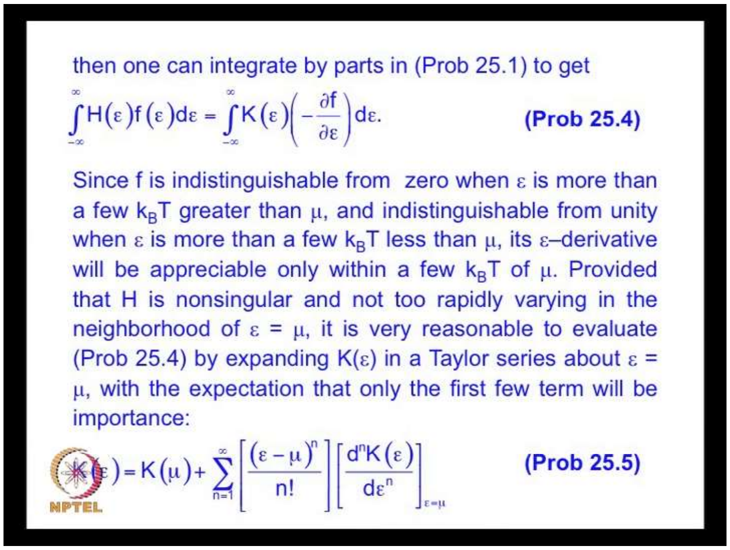

then one can integrate by parts in (Prob 25.1) to get

$$\int_{-\infty}^{\infty} H(\varepsilon) f(\varepsilon)\, d\varepsilon = \int_{-\infty}^{\infty} K(\varepsilon)\left(-\frac{\partial f}{\partial \varepsilon}\right) d\varepsilon. \qquad \textbf{(Prob 25.4)}$$

Since f is indistinguishable from zero when ε is more than a few $k_B T$ greater than μ, and indistinguishable from unity when ε is more than a few $k_B T$ less than μ, its ε–derivative will be appreciable only within a few $k_B T$ of μ. Provided that H is nonsingular and not too rapidly varying in the neighborhood of $\varepsilon = \mu$, it is very reasonable to evaluate (Prob 25.4) by expanding $K(\varepsilon)$ in a Taylor series about $\varepsilon = \mu$, with the expectation that only the first few term will be importance:

$$K(\varepsilon) = K(\mu) + \sum_{n=1}^{\infty} \left[\frac{(\varepsilon-\mu)^n}{n!}\right]\left[\frac{d^n K(\varepsilon)}{d\varepsilon^n}\right]_{\varepsilon=\mu} \qquad \textbf{(Prob 25.5)}$$

Therefore what do we do, we expand therefore, expand k of e as in a Taylor series at epsilon equal to mu in this integral I.

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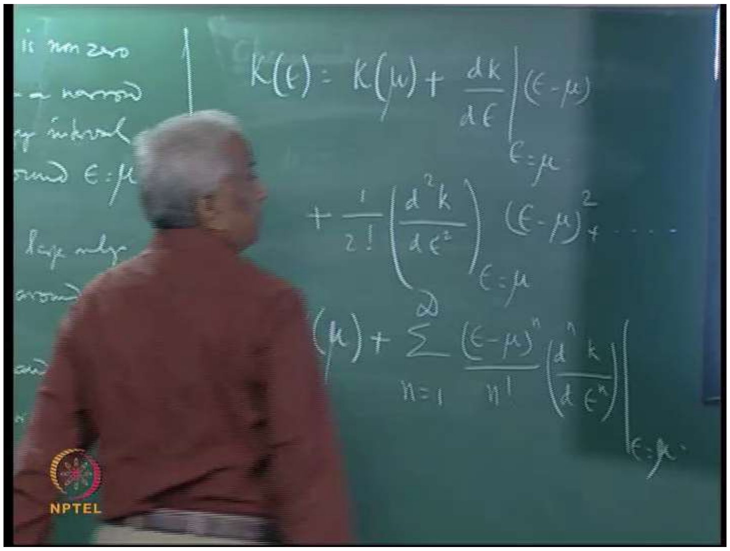

So if we do this, we get things like K of e equals K of mu plus d K by d epsilon e equal to mu times epsilon minus mu plus 1 by 2 factorial d square k like d epsilon square at epsilon equal to mu times epsilon minus mu hole square plus terms like this. So, in general, we can write this as k of mu plus the sum from over n equal to one to infinity of epsilon mu minus mu to the power l by n factorial into d n k by d epsilon n evaluated at epsilon equal to mu.

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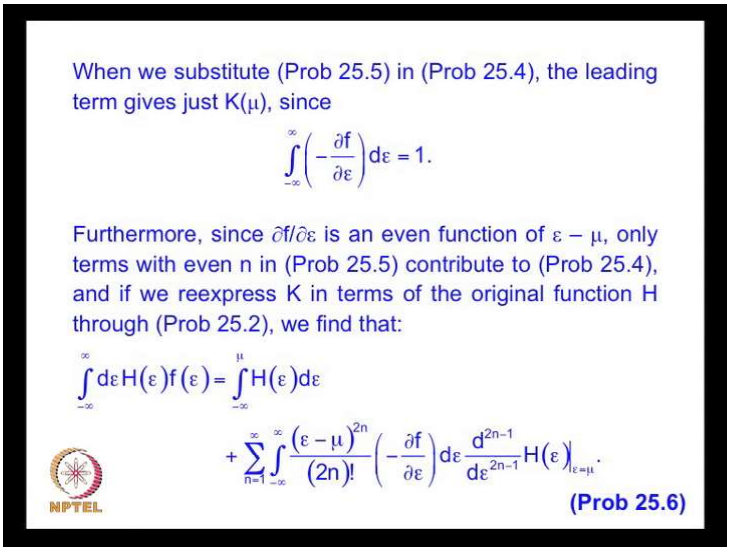

When we substitute (Prob 25.5) in (Prob 25.4), the leading term gives just $K(\mu)$, since

$$\int_{-\infty}^{\infty}\left(-\frac{\partial f}{\partial \varepsilon}\right)d\varepsilon = 1.$$

Furthermore, since $\partial f/\partial \varepsilon$ is an even function of $\varepsilon - \mu$, only terms with even n in (Prob 25.5) contribute to (Prob 25.4), and if we reexpress K in terms of the original function H through (Prob 25.2), we find that:

$$\int_{-\infty}^{\infty} d\varepsilon\, H(\varepsilon) f(\varepsilon) = \int_{-\infty}^{\mu} H(\varepsilon)\, d\varepsilon + \sum_{n=1}^{\infty}\int_{-\infty}^{\infty}\frac{(\varepsilon-\mu)^{2n}}{(2n)!}\left(-\frac{\partial f}{\partial \varepsilon}\right)d\varepsilon\, \frac{d^{2n-1}}{d\varepsilon^{2n-1}}H(\varepsilon)\Big|_{\varepsilon=\mu}.$$

(Prob 25.6)

So, this is what we are going to substitute here.

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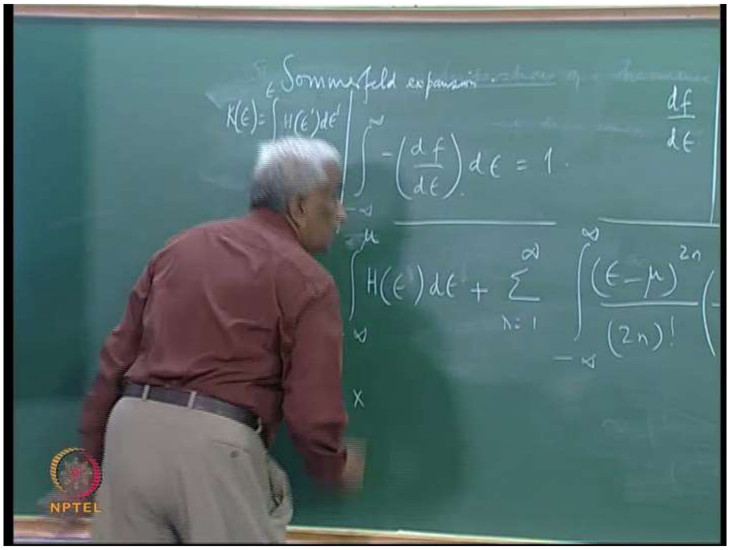

In integral has we also take into account, in fact, this is the delta function with a value one from minus infinity to plus infinity, this is an even function.

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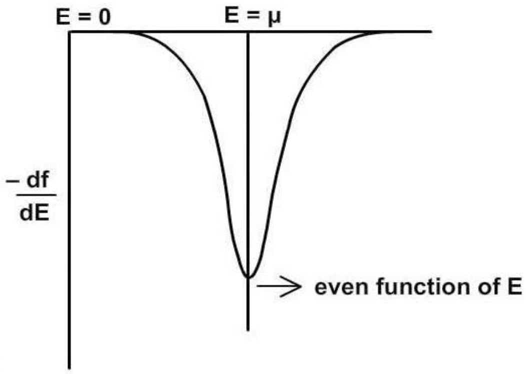

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So it is look like this, so that would be d f by strictly it becomes in the related becomes delta function. So, we use this property therefore, it is a even function of epsilon. Therefore, in this integration over E, we have only left with terms, which are even n. So, taking only those terms we can write the integral required integral as we have the definition that k of E is integral using that. So, the first term will be k of mu. So, this will be a minus infinity to mu that will be the first term plus sigma n equal to 1 to infinity of the integral minus infinity to plus infinity epsilon minus mu, we considered only even terms. So, with the power 2 n and 2 n factorial here into minus d f by d E into d 2 n minus 1 by d epsilon 2 n minus 1 of k evaluated at epsilon equal to mu, times and this is H because I have written 2 n minus one here. So, this is the final result which we can now integrate.

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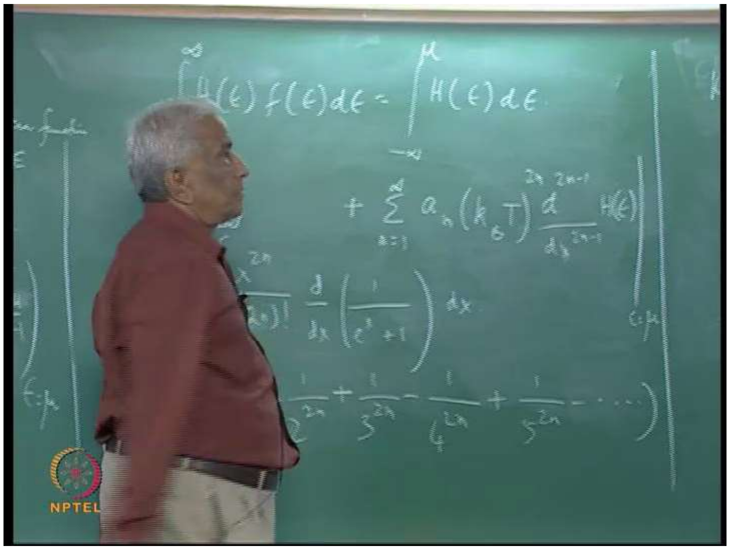

So, we finally, make the substitution epsilon minus mu by k b t as x because that is what is occurring in the derivative of the Fermi Dirac function.

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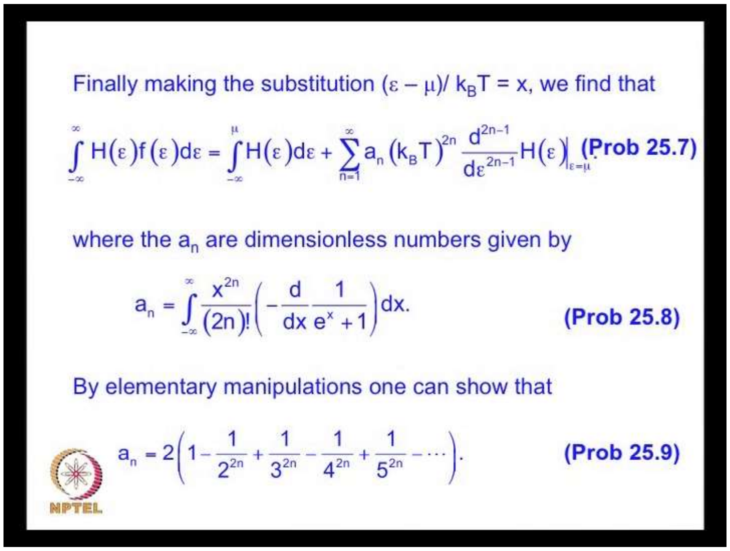

Finally making the substitution $(\varepsilon - \mu)/ k_B T = x$, we find that

$$\int_{-\infty}^{\infty} H(\varepsilon) f(\varepsilon) d\varepsilon = \int_{-\infty}^{\mu} H(\varepsilon) d\varepsilon + \sum_{n=1}^{\infty} a_n (k_B T)^{2n} \frac{d^{2n-1}}{d\varepsilon^{2n-1}} H(\varepsilon)\Big|_{\varepsilon=\mu} \quad \textbf{(Prob 25.7)}$$

where the a_n are dimensionless numbers given by

$$a_n = \int_{-\infty}^{\infty} \frac{x^{2n}}{(2n)!} \left(-\frac{d}{dx} \frac{1}{e^x + 1} \right) dx. \quad \textbf{(Prob 25.8)}$$

By elementary manipulations one can show that

$$a_n = 2\left(1 - \frac{1}{2^{2n}} + \frac{1}{3^{2n}} - \frac{1}{4^{2n}} + \frac{1}{5^{2n}} - \cdots \right). \quad \textbf{(Prob 25.9)}$$

Therefore, we get the integral finally as integral minus infinity H of e F of e d e equals plus sigma n equal to 1 to infinity of a n times k B T to the power 2 n into d to the power 2 n minus 1 by d x to the power 2 n minus 1 of H of e epsilon evaluated at epsilon equal to mu. Where a n as the integral of the form x to the power 2 n by 2 n factorial into d by d x of 1 by e to the power x plus 1 d x . So, one can show that this this integral can be evaluated and we arrive at 2 into 1 minus 1 by 2 to the power n 2 n plus 1 by 3 to the power 2 n minus 1 by 4 to the power 2 plus 1 by 5 to the power 2 n and so on. This is a standard result, which we will assume here.

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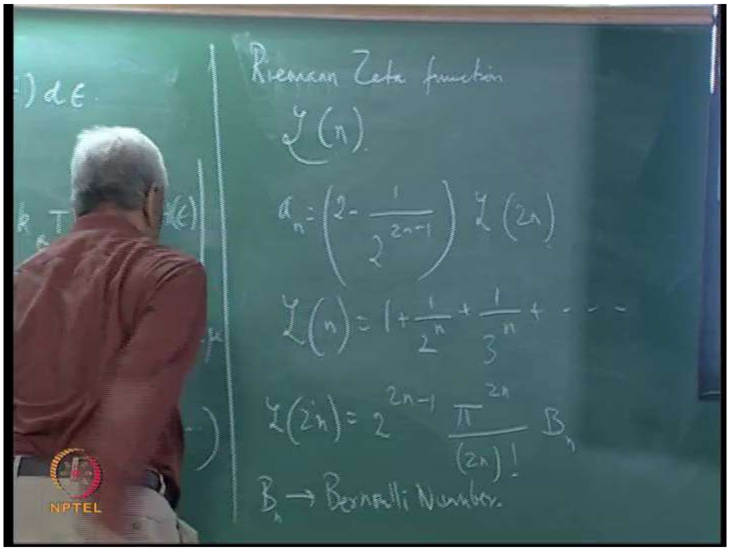

So, this is written usually in terms Riemann zeta function.

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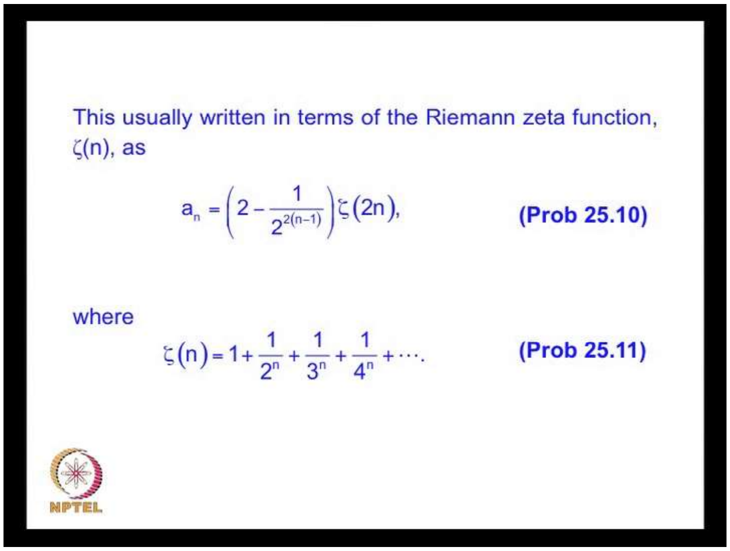

This usually written in terms of the Riemann zeta function, ζ(n), as

$$a_n = \left(2 - \frac{1}{2^{2(n-1)}}\right) \zeta(2n), \qquad \textbf{(Prob 25.10)}$$

where

$$\zeta(n) = 1 + \frac{1}{2^n} + \frac{1}{3^n} + \frac{1}{4^n} + \cdots. \qquad \textbf{(Prob 25.11)}$$

Zeta of n, so we write a n as 2 minus 1 by 2 to power 2 n minus 1 into zeta of 2 n. Where zeta n is 1 plus 1 by 2 to the power n plus 1 by 3 to the power n plus etcetera.

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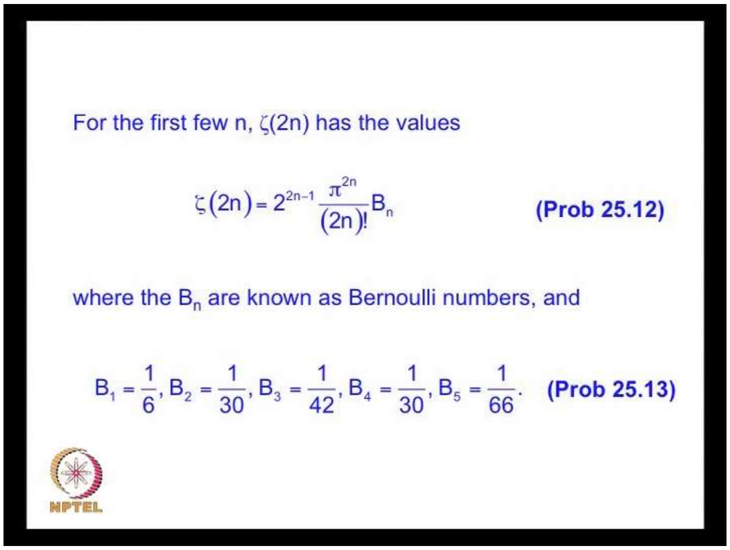

For the first few n, $\zeta(2n)$ has the values

$$\zeta(2n) = 2^{2n-1}\frac{\pi^{2n}}{(2n)!}B_n$$ **(Prob 25.12)**

where the B_n are known as Bernoulli numbers, and

$$B_1 = \frac{1}{6}, B_2 = \frac{1}{30}, B_3 = \frac{1}{42}, B_4 = \frac{1}{30}, B_5 = \frac{1}{66}.$$ **(Prob 25.13)**

So, this can be evaluated, so zeta 2 n in general as the form 2 to the power 2 n minus 2 times pi to the power 2 n by 2 n factorial into B n, where B n is known as the Bernoulli number.

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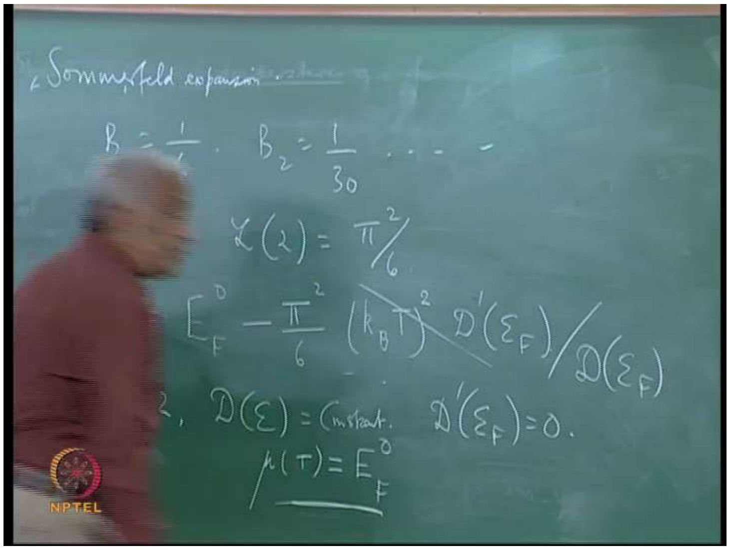

So, this Bernoulli number as the following values B 1 for n equal to 1 is just 1 6; B 2 is 1 by 30 and so on. So, these are known standard results. So, in most practical calculations in metal physics, we need to know rarely more than zeta two zeta 2 the Riemann's zeta function is just pi square by 6.

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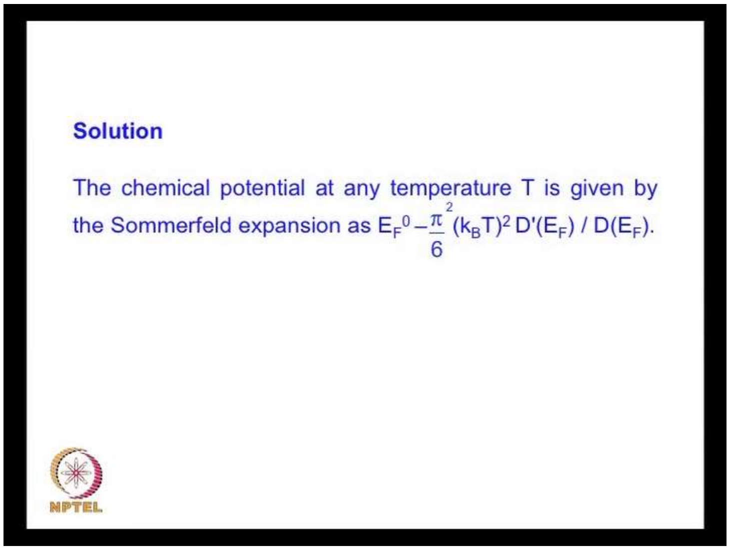

Solution

The chemical potential at any temperature T is given by the Sommerfeld expansion as $E_F{}^0 - \frac{\pi^2}{6}(k_B T)^2 D'(E_F) / D(E_F)$.

So, using this result we get the chemical potential mu at any temperature T as E F 0, the chemical potential or the Fermi energy and absolute zero minus using the expansion Sommerfeld expansion and truncating it in the first term pi square by 6 k B T whole square into D of E F where D of E F is the density of states D dash by D E F. Where D dash D E F is derivative with respect to the energy.

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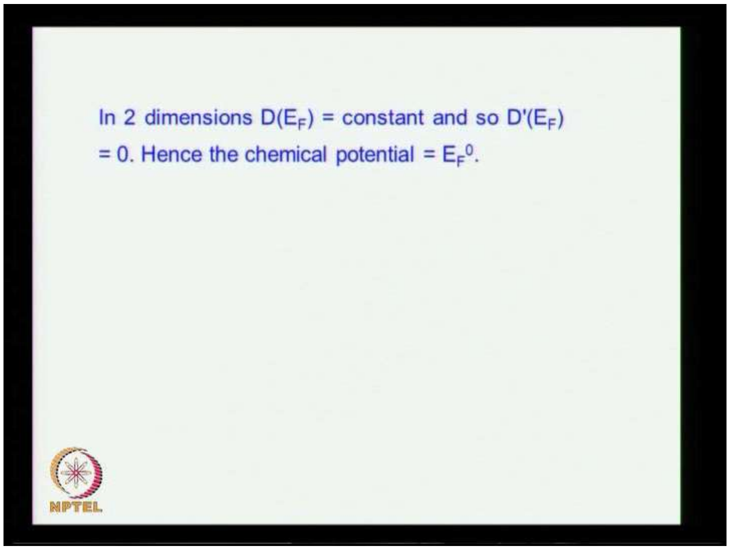

In 2 dimensions $D(E_F)$ = constant and so $D'(E_F)$ = 0. Hence the chemical potential = $E_F{}^0$.

So, we arrive at this result for the chemical potential in two dimensions, the question was about chemical potential in two dimensions, for D equal to 2, we know that the density of states d of e is constant this is the reason which we have considered already. Therefore, D dash E F is zero. Therefore, mu of t the chemical potential at any temperature T above zero k is just the Fermi energy at T equal to zero k, because this term vanishes, so that is the result that we are required to prove.

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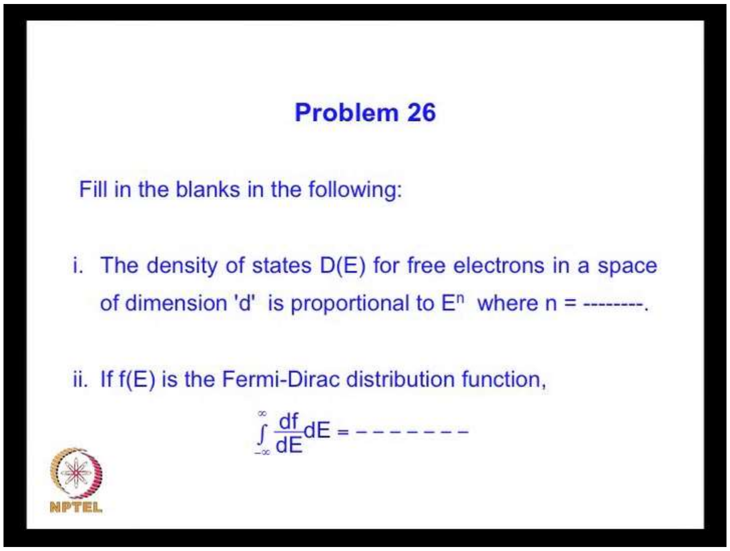

Problem 26

Fill in the blanks in the following:

i. The density of states D(E) for free electrons in a space of dimension 'd' is proportional to E^n where n = --------.

ii. If f(E) is the Fermi-Dirac distribution function,

$$\int_{-\infty}^{\infty} \frac{df}{dE} dE = -------$$

The next question is given in the form of a fill in the blanks, fill in the blanks are straightforward.

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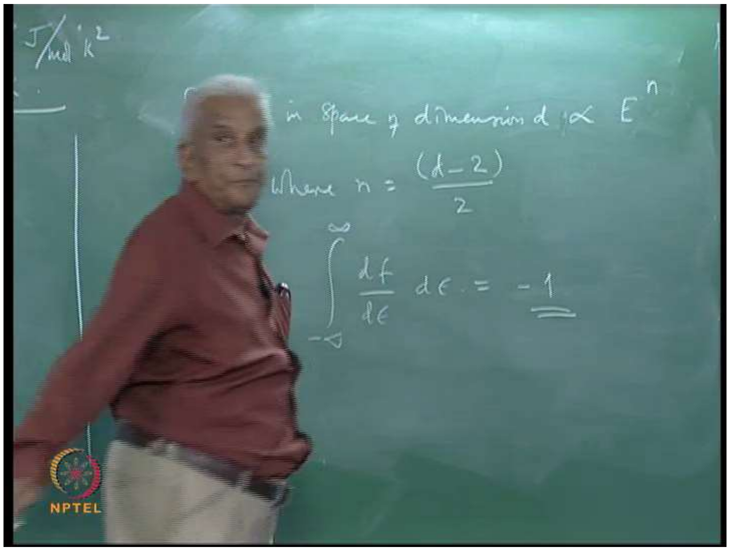

The density of states d of e for free electrons in the space of dimension d in space of dimension d is proportional to the energy to the power n where n is the answer; obviously, we have considered this already the answer is; obviously, d minus 2 by 2. And the next question is about Fermi Dirac distribution function, if the f of e is the Fermi Dirac distribution function integral d f by d e time d e over minus infinity to plus infinity is the answer obviously, minus 1.

Condensed Matter Physics

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Lecture - 10

The Free Electron Theory of Metals - Electrical Conductivity

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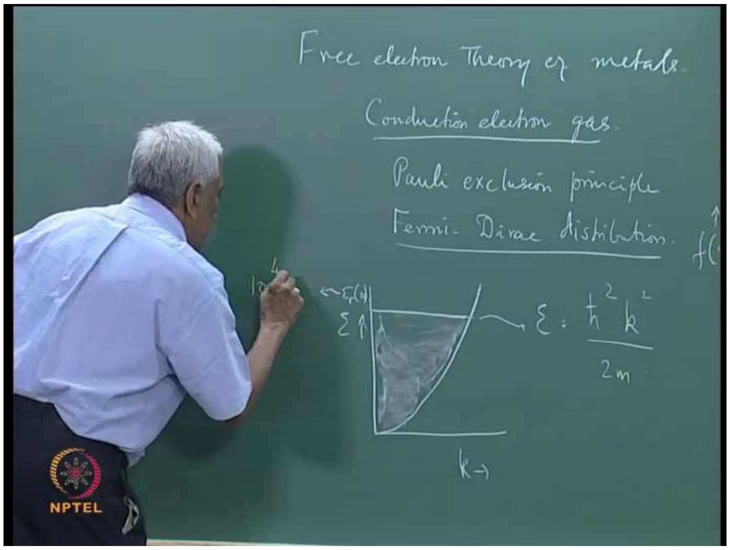

In the last lecture we discussed the free electron theory of metals in this connection we noted that metals constitute a particularly simple kind of solids in which most of the conduction properties and other related thermal behaviour all these are determined by the. So, called conduction electrons which behave very much like an ideal gas atoms or molecules except that the electron gas obeys in subjected to Pauli exclusion principle and therefore, satisfy fermi dirac distribution.

So, even though the metal is a solid crystalline solid it is mainly the electron gas which decides these physical properties like electrical transport heat transport of heat specific heat all these properties are determined by of course, there is a role from the ions the conduction electrons are formed by ionisation of the atoms of the metal. So, that you have positive ions. And then into which there is a free electron gas which is free to wander around as long as it is within the metal it is confined to the metal as a whole the metallic bond is something that binds the electron gas to the metal it is not able to escape it and become completely free.

So, except that they are free to wander around inside the metal under the influence of applied electric or magnetic fields applied heat thermal gradients and so on. So, it is this behaviour of this electron gas which is profoundly different from.

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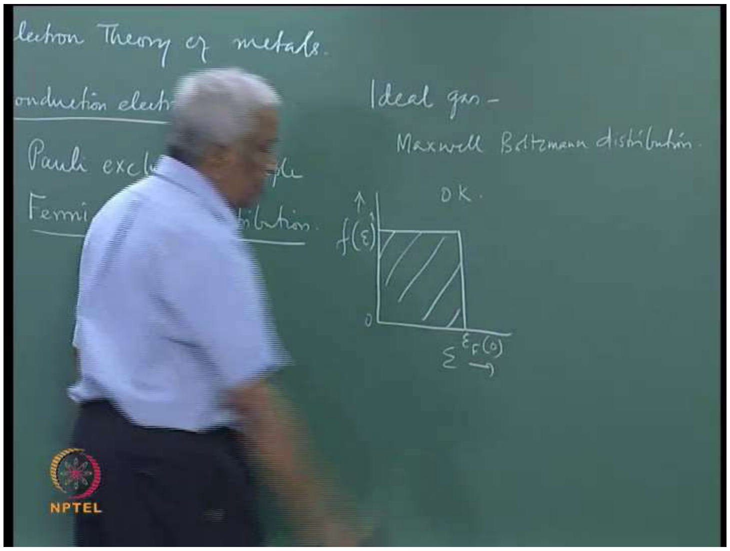

That of an ideal gas atom or molecule because the molecules are atoms of an ideal gas a classical ideal gas or satisfied the or governed by the Maxwell Boltzmann distribution this is familiar already to all of us, but the electron gas is subjected to the fermi dirac distribution. This is because the electrons are quantum mechanical particles and fermi dirac distribution is different from the Maxwell Boltzmann distribution because of the quantum behaviour of the electrons which are determined by the pauli exclusion principle the essence of the pauli exclusion principle is that. If there is an energies level and an electron occupies this energy level then no other electrons can come and occupy the same energy level. So, that is why it is called the exclusion principle and this profoundly affects the way the electrons are distributed in energy and we saw the precise form of the fermi dirac distribution which at absolute zero the distribution function goes like this as a value one here to zero and it is like this and this is known as the fermi energy ef this is f zero kelvin.

So, all these states within for energies less than the fermi energy the states are completely occupied each state being occupied by a given single electron and all these states above the fermi level are completely empty. So, the fermi energy at absolute zero is the highest energy level which is occupied in the case of a metal. And therefore, this will modify the way there are electrons are distributed in energy and this is again given by the dispersion curve of the electron, which is the e versus k curve and this is governed by the kinetic energy of the electrons which is h cross square k square by 2 m. And therefore, this will be a parabolic curve which will look like this. So, that is a and states up to the fermi energy are filled these are all these states are completely filled.

So, what happens is that we discussed last time the behaviour of the contribution of these electrons to the specific heat, because when there is a thermal excitation the electrons are going to observe this heat. And therefore, there's going to be specific heat contribution due to this electron gas. Now this contribution we saw is like the hound in the hound of baskervilles is the dog that did not bark at night. So, the electronic in specific heat does not appear, it is not a dominant contribution that is the overall result of this, that is because this fermi energy is at the order of 10 to the power four Kelvin. Whereas normal thermal elicitations are of the order of thermal excitation is at the order of ten to the power two kelvin.

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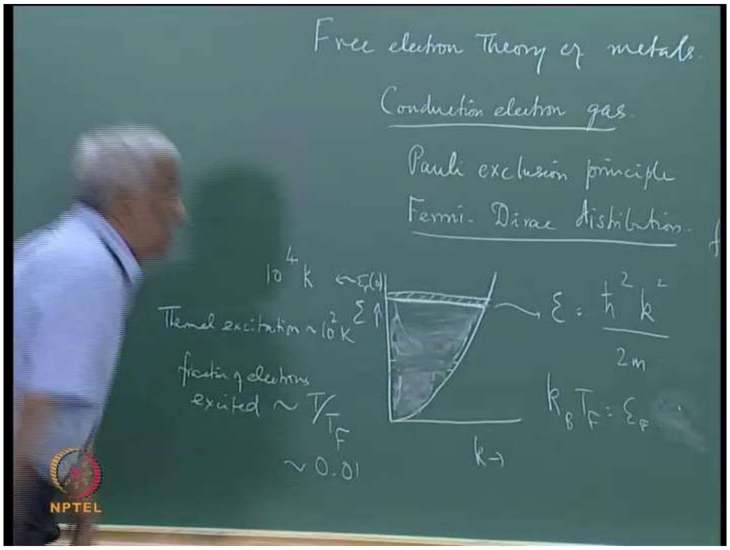

So, it is a very small quantity in comparison to this. So, if you have a small temperature window here which say this is the energy initial energy, and the thermal excitation suppose it takes the electron to this now this is the initial. And final states are all already occupied and therefore, the electron cannot go into this state. So, even though you excite it these electrons which are deep within the energy scheme the occupied energy level they are unable to participate in the thermal excitation it is only the electrons which are the fringe which are here in a small skin layer around the fermi energy these are the fraction of electrons which will be able to contribute to the specific heat by being thermally excited. So, it is this fraction and this fraction as you can see is about a hundredth this ratio of this temperatures is one in hundredth. So, it is only a fraction of point zero one or one in hundred of total of number of electron, which can get excited and therefore, contribute to this specific heat it is for this reason. So, the fraction of electrons excited is of the order of t by t f, where t f is given by k b t f equals e f zero or e f. So, this fraction is only at the order of 0.0.

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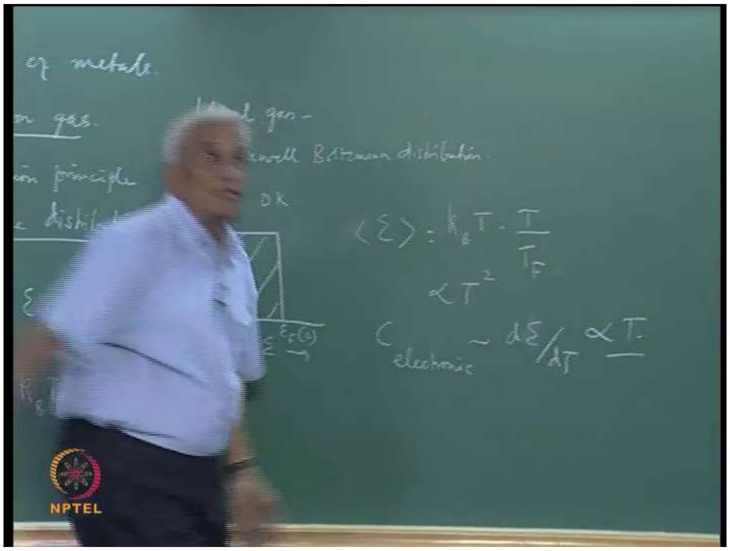

One and this fraction of electron each electron will be excited by an amount k b t by Boltzmann's equipartition theorem therefore, the total contribution is T f, that is the mean energy of these electrons, which are excited since this goes as t square. So, the specific heat c electronic the specific heat which is the e by d t is proportional to the absolute temperature.

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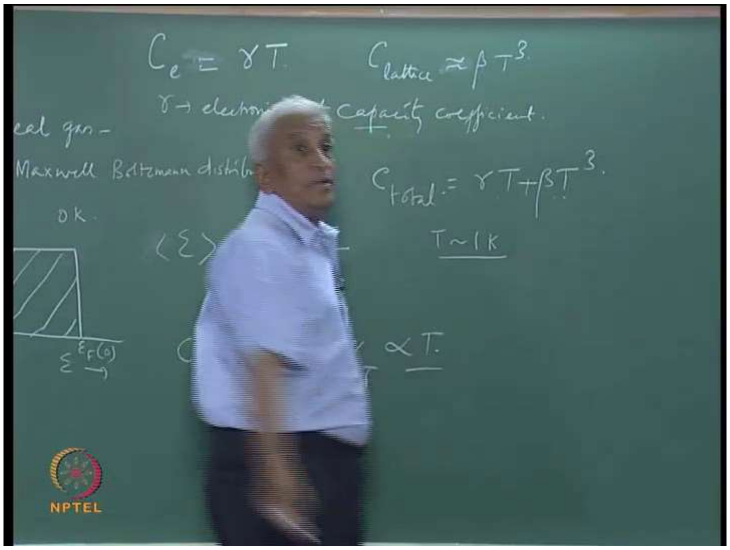

So, that is what we write as c e equals it goes as gamma t where gamma is the electronic heat capacity coefficient. So, it is the Pauli exclusion principle and the fermi dirac distribution which profoundly modify the behaviour of the electronic system, and prevent it from absorbing thermal excitation energy to a large extent and confine only a small fraction t by T f of the total number of electron to be thermally excited. And therefore, contribute only a term or the order of gamma t as we will see later the lattice the crystal lattice of a ions in a metal will have a contribution which goes as t cube the cube of the absolute temperature and therefore, the total specific heat will be of the form gamma t plus beta t cube.

So, at high temperatures it is this term which will dominate therefore, this will be negligible, and you cannot even detect it it is only when you go to temperatures as the order of one Kelvin, which is an extremely low temperature it is only at such low temperature. These two terms will become comparable and then you can detect the electronic contribution. So, this is the important concept that we developed last time.

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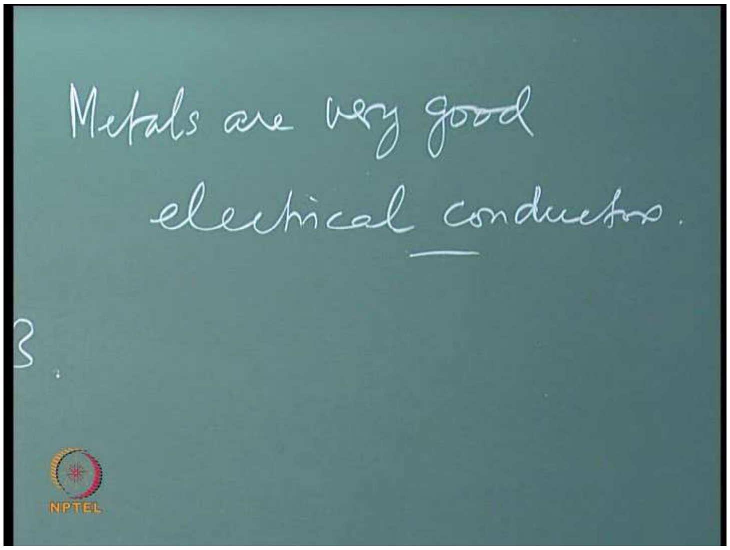

Metals are very good electrical conductors.

3.

Now, we move on to discuss how this picture of conduction electron gas in a metal is going to lead to the very well-known behaviour of metals namely that they are very good electrical conductors. So, we would like to know how and why a metal like silver or gold or copper they are very good conductors of electricity this is a very important characteristic of a metal which we would like to understand in the frame work of the free electron gas picture. So, this is our next aim. So, what do we do we just take this conduction electron gas consider it and then apply an electric field a dc electric field.

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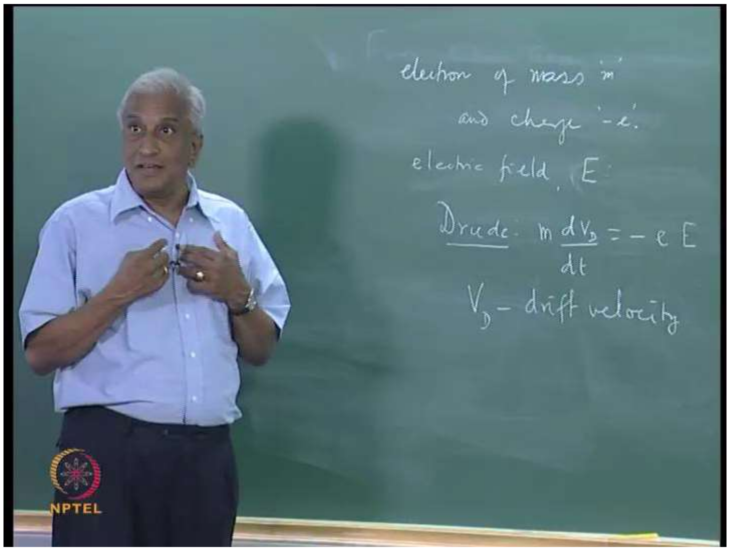

electron of mass 'm' and charge '-e'.

electric field, E

Drude: $m \frac{dV_D}{dt} = -eE$

V_D – drift velocity

So, let us first start looking by looking at the behaviour of a single electron of electronic charge electron of mass m and charge minus e. So, let us look at what happens to these electron when we apply a dc electrical field of strength e. So, we know that we can this is a very simple situation. And we will to start with use a classical picture which was due to which was first proposed by a person named Drude. So, this is known as the Drude theory of electrical conductivity this is an extremely simple picture where I have a particle of mass m, but a charged particle carrying the charge minus e and therefore, in an electric field the force on it will be minus e e and that will be equal to this is the force.

So, Newton's law of motion tells us that this should be because this v d, because v d is known as the drift velocity of the electron why do we call it drift velocity. This is because normally if you do not have an applied electric field what happens to these electrons, they are still moving around they they are very much like as we said they are very much like the atoms on a ideal gas. So, they are not keeping quite. So, they are free to move around. And therefore, they do move does it mean that they there will be a conductivity there will be electrical conduction whenever an electron moves somewhere there should be a current and therefore, there should be a conduction, but this question is answered because in the classical picture these electrons are free to move around.

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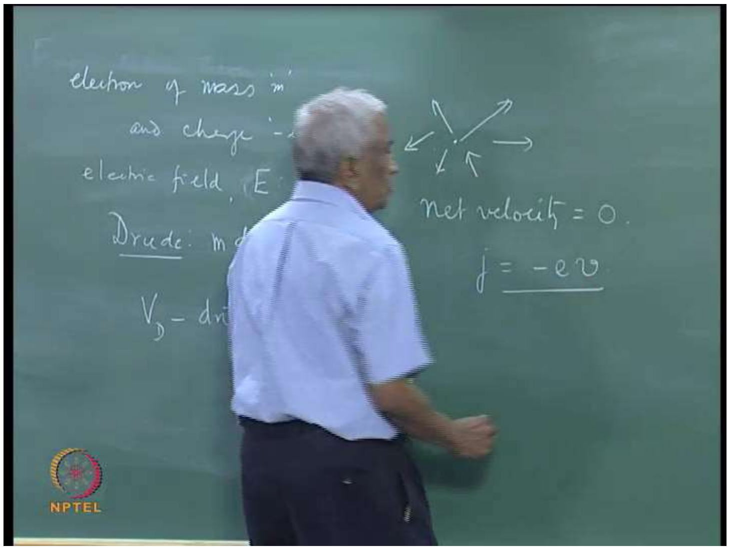

But they more around in perfectly a random fashion very much like what is said in the kinetic theory of gases. So, they are moving around a given electron is moving around in all possible directions randomly with equal probability. Therefore, this electron is very much like a drunkard what does a drunkard do a drunkard stands here he is under the influence of liquor. So, you watch him he is moving a few steps in this way and then talks to himself and comes, and moves a few steps this way and then this way. So, what happens even after a few hours, if you watch him he if he is standing in a place is moving this moving this way moving this way moving everywhere all the time, but the where is the net displacement he is where is was a few hours ago. So, it is a drunkard who walks all the time, but with no net displacement there is no net displacement. So, in the same way the electrons when they are simply diffusing like the atoms of a gas then the net velocity in any given direction when there is no field vanishes identically it is zero and therefore, when there is these current density is just given by minus ev. So, this velocity is zero.

So, it vanishes. So, there is no conduction even though the electrons are moving around they are bumping around in all possible directions, but nothing happens, if you are cannot focusing on a particular direction and trying to measure the conduction conductivity in that direction. So, it vanishes in the absence of an applied electric field, but when you put an applied electric field in then this electric field forces the electron to move in a direction opposite to the applied electric field. Therefore, there is a net drift in a given direction that is why this is called a drift velocity, and this gives you the rate at which this distribute this this drift velocity changes with time and gets accelerated by the applied electric field. So, that is the equation of motion well if this is all there is to head.

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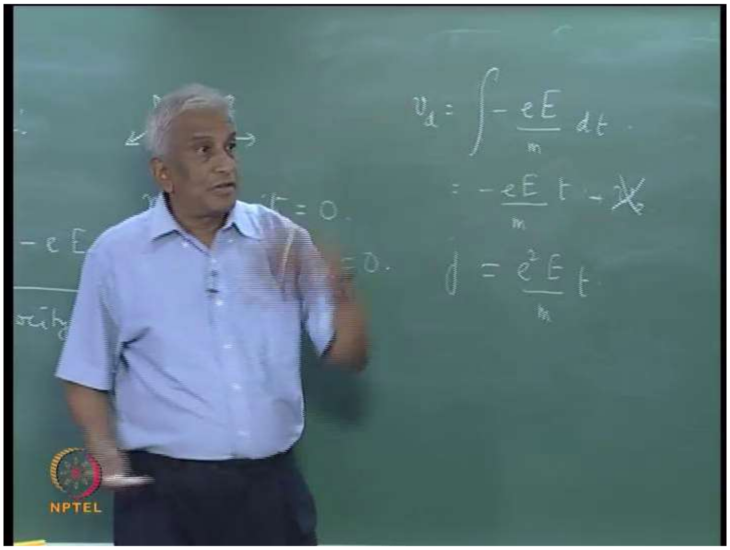

Let us see what happens therefore, integrating this we will see that v d is integral minus e e by m d t. Therefore, this is by t plus a constant v zero the initial speed which is zero to start with there was no velocity when there was no electric field. So, if we start from rest this is the net, and the j the current density will go as e square e by m into t from this equation so; that means, there will be a current build up. And as time passes on the current will go on increasing monotonically, and it will eventually if you wait long enough it can even blow up and become infinitely large, but we all know that this does not happen in any conductor there is a finite current. If you apply a certain voltage producing a certain electric field it produces a certain amount of current which is given by ohm's law, this is the observation that we are all familiar with, but this model does not explain that instead it predicts a current density which goes on increasing monotonically with time.

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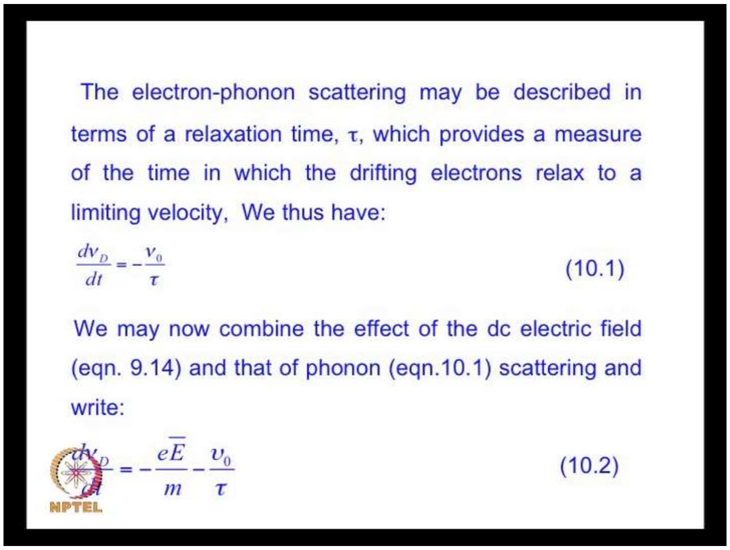

The electron-phonon scattering may be described in terms of a relaxation time, τ, which provides a measure of the time in which the drifting electrons relax to a limiting velocity, We thus have:

$$\frac{dv_D}{dt} = -\frac{v_0}{\tau} \qquad (10.1)$$

We may now combine the effect of the dc electric field (eqn. 9.14) and that of phonon (eqn.10.1) scattering and write:

$$\frac{dv_D}{dt} = -\frac{e\overline{E}}{m} - \frac{v_0}{\tau} \qquad (10.2)$$

If you wait long enough you can get an infinite current from a finite electric field which is up surd, this is because there is something that we ignored you are not taken into account these electrons this is the behaviour of one electron. And even if you have ten thousand or ten to the power 24 electrons the behaviour can be described by a simple addition or super position of these current contributions.

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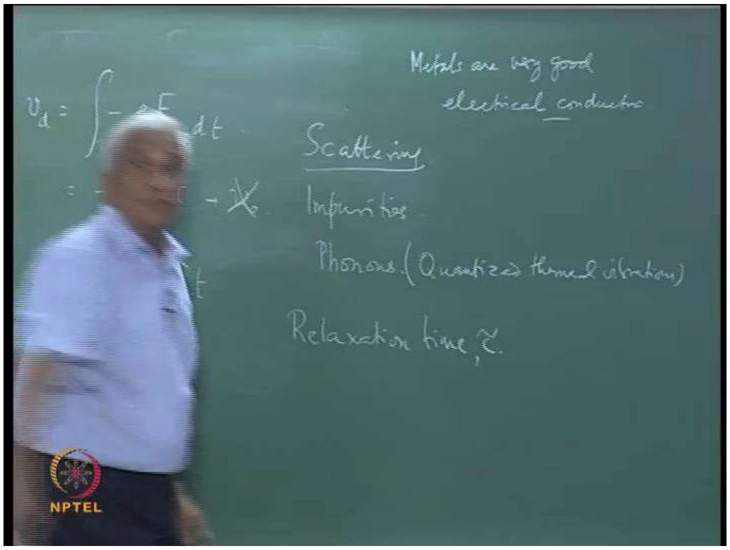
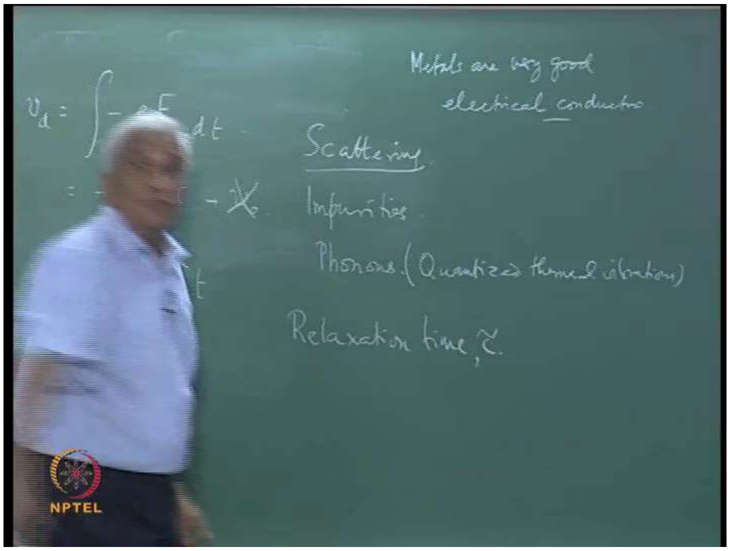


But this gas is being when it is moving when it is drifting under the influence of an electric field, there are other things that are happening on the path these electrons gets scattered by various obstacles on their way. For example, in a in a metallic lattice there are many impurities impurity atoms, there are also the positive ions and then there are defects of various kinds like dislocations stacking walls grain boundaries and. So, on all these act as scattering centres. So, this scattering can arise from impurities also these atoms are ions in a crystalline solid are not at rest there are vibrating all the time there are thermal vibrations at any finite temperatures and these thermal vibrations increase as temperature increases.

So, it is a even if you think that these vibrations are simple harmonic there will be an effect due to these vibrations vibrating atoms and therefore, they can act as scattering centres the vibrating ions in the crystal lattice in the metallic crystal lattice. So, these thermal vibrations when they are quantise, they are called phonons we will discuss them a little later for our present discussion, it is enough to know that these are quantised thermal vibrations of the solid.



So, there can be scattering due to phonons, which will increase with temperature unlike the impurities the phonon scattering will depend on the temperature. So, these scattering events have to be considered in order to decide what will be the drift velocity of a given electron the way this scattering is taken into account is by its thinking that suppose there is no scattering of a given electron is scattered at a particular instant of time. Then the entire distribution is affected the distribution of the electrons momentarily, but then this distribution if you leave this like this. And look at only the scattering even immediately after the scattering the entire distribution will relax back to its original value there is an equilibrium distribution. And then that is momentarily disturbed by the scattering of the electrons and then after a little time this disturbed distribution will relax back to the original equilibrium distribution function. So, this is model which is called the relaxation time model.

So, if this takes as an amount of frame tau tau is known as the relaxation time the characteristic time in which the drifting electron relax back to an equilibrium configuration, when there will be a limiting velocity not a unlimited velocity like that. Then this is described mathematically by any equation of this form these are simple first order differential equation which as you all know will produce a solution which gives you a velocity which decays exponentially with a characteristic time. So, this will a drift velocity which goes as. So, that is why this tau is known as the characteristic time of relaxation through which describes this exponential relaxation process. So, this can now be combined. So, there are two processes one the applied electric field accelerates the electron, and then the electrons which gets scattered by the various scattering centres in the solid they produce a relaxation at the distribution function towards an equilibrium or limiting value.

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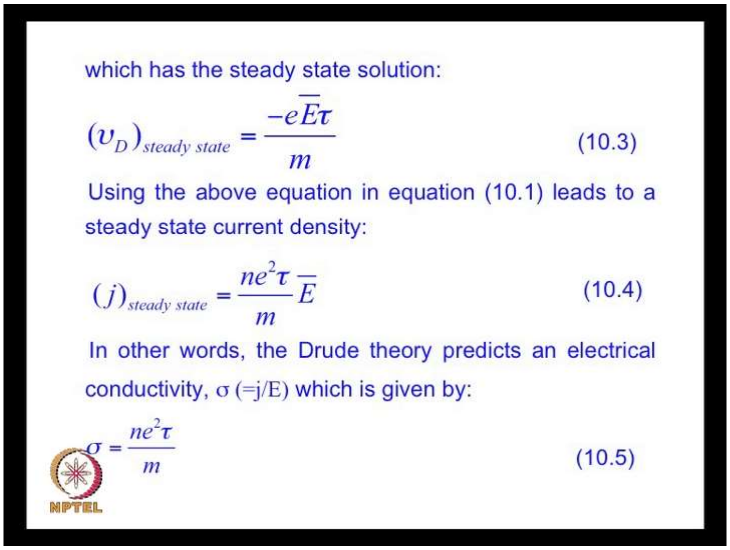

which has the steady state solution:

$$(v_D)_{steady\ state} = \frac{-e\overline{E}\tau}{m} \qquad (10.3)$$

Using the above equation in equation (10.1) leads to a steady state current density:

$$(j)_{steady\ state} = \frac{ne^2\tau}{m}\overline{E} \qquad (10.4)$$

In other words, the Drude theory predicts an electrical conductivity, σ (=j/E) which is given by:

$$\sigma = \frac{ne^2\tau}{m} \qquad (10.5)$$

And therefore, we have to consider both of these equations together to describe the rate of change in time of the drift velocity.

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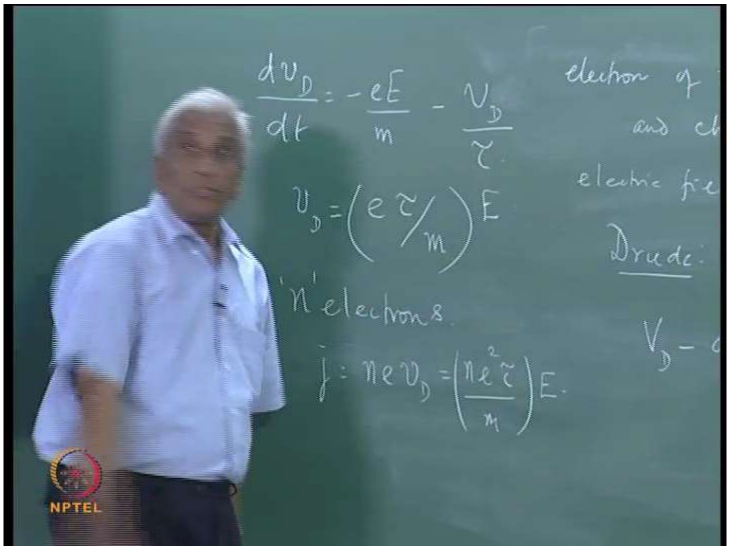

So, when you do this you get an equation a combined equation which is of this form eE by m like this plus an additional term. So, that equation is that is the equation will describe the time rate of change, and when you solve this first order differential equation this will give you a steady state solution which will give you something like. And therefore, if there are if there is a number n electrons if if n is the electron concentration then j is n e v d, and this will be n e square tau by m times e and since by ohm's law this is equal to sigma e where sigma is the conductivity.

So, we get the electrical conductivity as n e square tau by m; that is the drude expression for the electrical conductivity of a metal having a concentration n of conduction electrons each carrying a charge e. And a mass having a mass m, which are drifting under the influence of an electric field getting scattered by the various scattering centres inside the metal. And relax with a characteristic in time tau towards an equilibrium value. So, for such a situation the drude theory, which is a purely classical theory which does not take into account the quantum nature as electrons this is a very old theory, but which gives a remarkably accurate expression for the electrical conductivity. If you we already saw how we can calculate the electron concentrations using fermi dirac distribution, and if you plug in the value one finds a very nice way to describe the electrical resistivity or conductivity behaviour of simple metals well.

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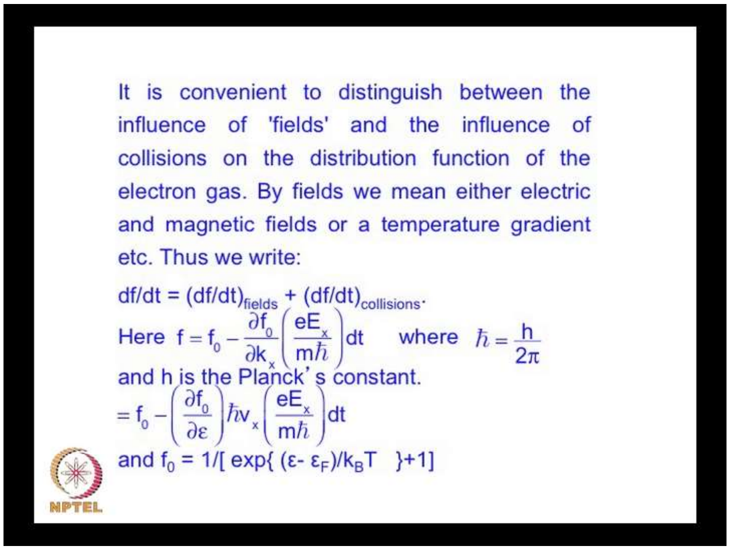

It is convenient to distinguish between the influence of 'fields' and the influence of collisions on the distribution function of the electron gas. By fields we mean either electric and magnetic fields or a temperature gradient etc. Thus we write:

$df/dt = (df/dt)_{\text{fields}} + (df/dt)_{\text{collisions}}$.

Here $f = f_0 - \frac{\partial f_0}{\partial k_x}\left(\frac{eE_x}{m\hbar}\right)dt$ where $\hbar = \frac{h}{2\pi}$

and h is the Planck's constant.

$= f_0 - \left(\frac{\partial f_0}{\partial \varepsilon}\right)\hbar v_x\left(\frac{eE_x}{m\hbar}\right)dt$

and $f_0 = 1/[\exp\{(\varepsilon - \varepsilon_F)/k_BT\}+1]$

This is all very well, but the question is can we use classical behaviour a classical description the answer is no as we already saw in the connection with the electronic heat capacity. So, we have to require that the electrons obey fermi dirac statistics. So, we have to write the equilibrium distribution function in the presence of scattering, and in the presence of an applied electric field in order to do this we make use of a formalism which was again developed by Boltzmann.

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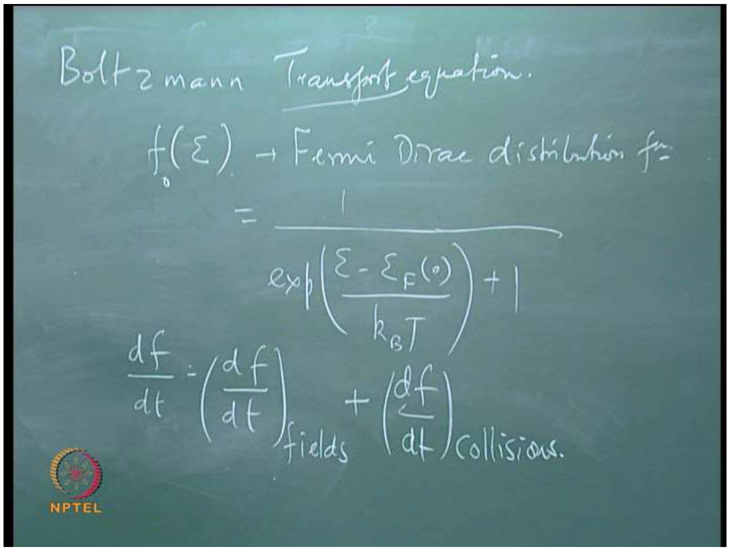

Boltzmann Transport equation.

$f_0(\mathcal{E}) \rightarrow$ Fermi Dirac distribution fn

$$= \frac{1}{\exp\left(\frac{\mathcal{E} - \mathcal{E}_F(0)}{k_BT}\right) + 1}$$

$$\frac{df}{dt} = \left(\frac{df}{dt}\right)_{\text{fields}} + \left(\frac{df}{dt}\right)_{\text{collisions}}$$

This is known as the Boltzmann transport equation the Boltzmann transport equation says tells us what happens to the distribution function in the presence of an applied electric field, and also in the presence of scattering mechanisms. So, we talk about again the distribution function f of e, which is the fermi dirac standard fermi dirac distribution function but we will call it f zero when it is when there are no applied electric fields, and there are now scattering mechanism. We will call it f zero, that is the equilibrium distribution function, which has we know has the form one by we saw this last time.

So, this is a standard equilibrium distribution function in the absence of applied electric fields and scattering mechanisms, but now the Boltzmann's transport equation tells us how to write the distribution function in the presence of fields and collisions due to scattering. So, the distribution function changes the f of e changes with time. And now we have to it is convenient to distinguish between the influence of fields fields can be electric fields it can be magnetic fields it can be even temperature gradient. So, depending, if it is an electric field the transfer to the electrons is determined by the electrical conduction mechanism, if it is a thermal gradient then this is determined by the thermal conduction.

So, you can have via this formalism we can at the same time describe electrical as well as thermal conduction and many other processes as you see which come under the general category of transport processes, that is why this equation is known as the transport equation. So, the change in the distribution function with time has two contributions one due to fields and another due to collisions. So, we will evaluate them separately.

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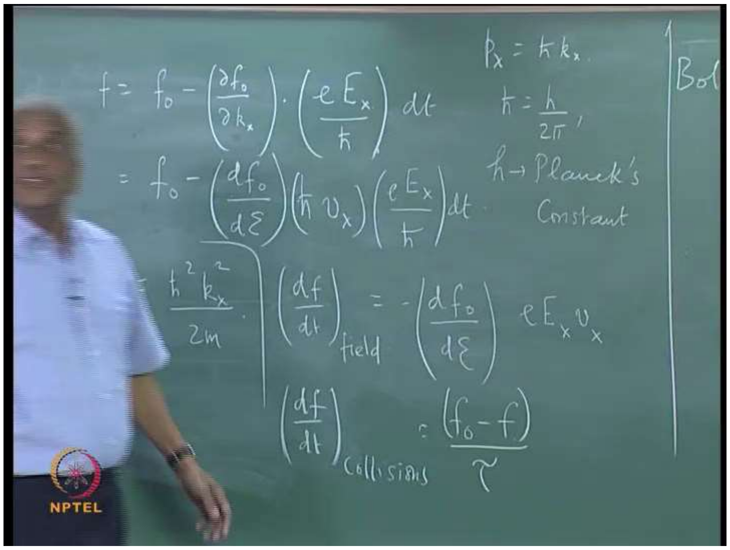

$$f = f_0 - \left(\frac{\partial f_0}{\partial k_x}\right) \cdot \left(\frac{eE_x}{\hbar}\right) dt$$

$$= f_0 - \left(\frac{df_0}{d\varepsilon}\right)(\hbar v_x)\left(\frac{eE_x}{\hbar}\right) dt$$

$p_x = \hbar k_x$.

$\hbar = \frac{h}{2\pi}$,

$h \rightarrow$ Planck's Constant

$$\varepsilon = \frac{\hbar^2 k_x^2}{2m}$$

$$\left(\frac{df}{dt}\right)_{\text{field}} = -\left(\frac{df_0}{d\varepsilon}\right) eE_x v_x$$

$$\left(\frac{df}{dt}\right)_{\text{Collisions}} = \frac{(f_0 - f)}{\tau}$$

So, how do we do this. So, this will be implying this f nought minus I can write this as in terms of the energy using the energy momentum relationship. Therefore, I can write de by d k x here, which will give me h cross v x, you can check this up times e ex by h cross d t where v x is the corresponding speed. So, this is k x square by two m. So, this simplifying this we will find now differentiating this d f by d t field.

And now f nought is the equilibrium distribution function in the absence of the fields, and therefore that will not change the fields do not affect the equilibrium configuration the value the way they are distributed under equilibrium in steady state. So, the change is coming only from this and that is given as please note that I am writing the x component of the applied electric field in terms of e in this form, and the energy is written by represented by e in this form. So, please distinguish these two let us keep these two separately not mix them up. So, this gives you this term and the df by dt due to collisions you have already seen how it goes by the velocity and therefore, this is a similar form very much similar to what happens in the case of the drift velocity.

So, the distribution from this describe this equation describes the exponential relaxation at the distribution function to the equilibrium value f nought with the characteristic time tau. So, these two have to be combined in order to get the total rate of change. So, that will give me f as taking f in this, and combining these two equations the results here, we arrive at the net distribution function in the presence of the applied field into...

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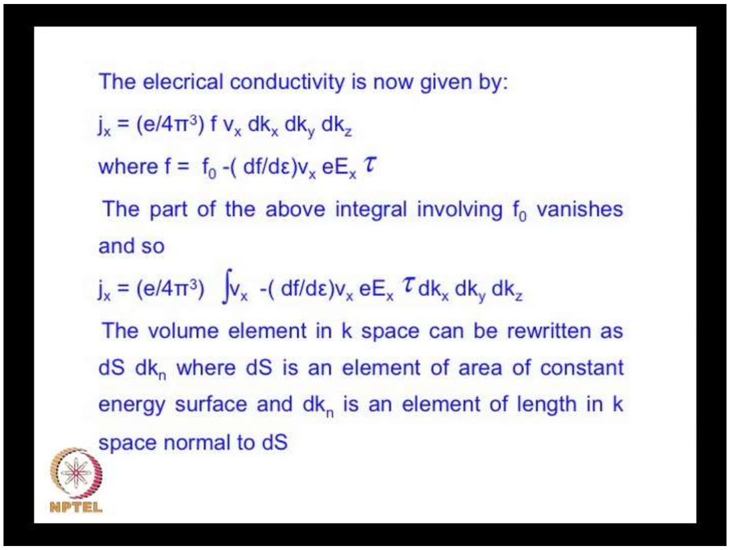

The elecrical conductivity is now given by:

$j_x = (e/4\pi^3)\ f\ v_x\ dk_x\ dk_y\ dk_z$

where $f = f_0 - (df/d\varepsilon) v_x\ eE_x\ \tau$

The part of the above integral involving f_0 vanishes and so

$j_x = (e/4\pi^3) \int v_x\ -(df/d\varepsilon) v_x\ eE_x\ \tau\ dk_x\ dk_y\ dk_z$

The volume element in k space can be rewritten as dS dk_n where dS is an element of area of constant energy surface and dk_n is an element of length in k space normal to dS

So, we have to now use this distribution function the new distribution function to describe the average behaviour of various quantities such as the current density.

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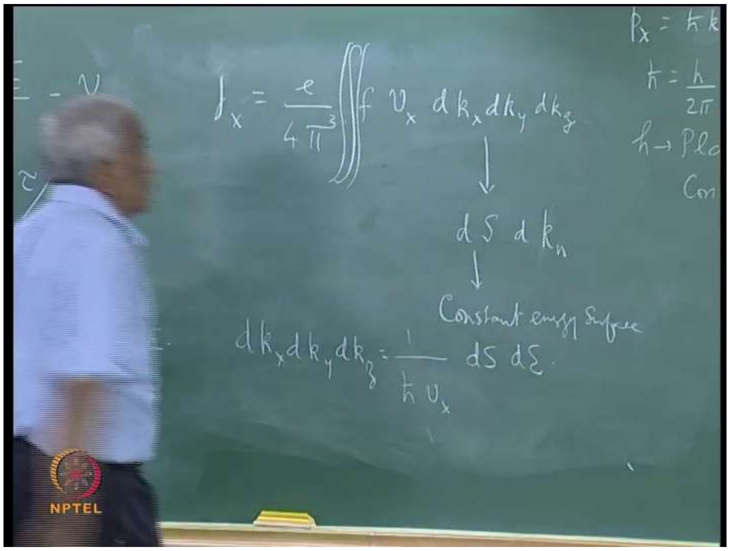

So, the evaluation of the current density proceeds in the same way as before j x equals e by four pi cube f v x d k x d k y d k z integral a triple integral in k's place, where f is what we have on the other side. Now this has two contribution from f naught and d f naught by de now this contribution due to the part involving f nought vanishes, because it is the equilibrium configuration. And it is a as we have already seen under steady state equilibrium in the absence of applied fields this contribution to the current density vanishes because the electron has a random motion. So, it is only the other term which contributes to this in order to evaluate this integral the usual procedure is to consider this volume element in k's place which can be written rewritten. We rewrite this part as d s times d k n, where d s is an element of area of constant energy surface and k n d k n is a length element in the direction normal to this constant energy. So, we evaluate this integral using this relationship.

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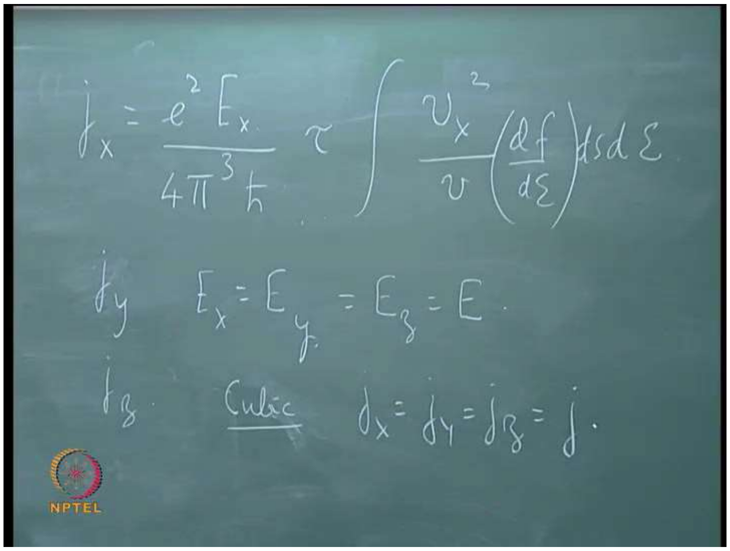


$$j_x = \frac{e^2 E_x}{4\pi^3 \hbar} \tau \int \frac{v_x^2}{v} \left(\frac{df}{d\varepsilon}\right) ds\, d\varepsilon$$

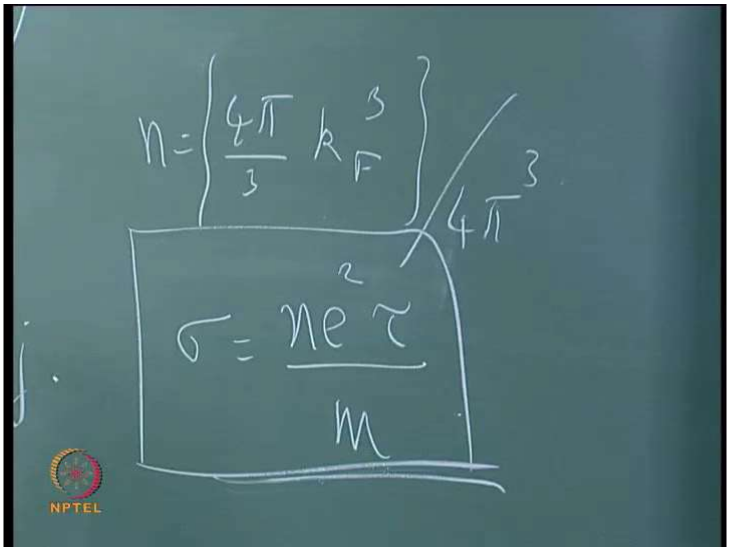
j_y $E_x = E_y = E_z = E$.

j_z. Cubic $j_x = j_y = j_z = j$.

So, that I can write d k x d k y d k z as one by h cross v x d s de, so replacing this and calculating this we arrive at the final result j x equals evaluating all this e square e x by four pi cube h cross tau integral v x square by v d s de into d f by d t. Now we left ex we would like to not only calculate j x, but we will also like to calculate it along with three principle directions xyz. So, we would like to evaluate j y and j z.

Under the influence of electric fields directed along the y and z directions setting ex to be equal to e y to be equal to e z, that is we apply the same electric field and we assume that this metal is a cubic metal having cubic symmetry. So, that j x equal to j y equal to j z equal to j in other words we for the moment we ignore the anisotropic of a solid and consider the metal as an isotropic conductor, which has the same behaviour in all the three directions. If we do this and simplify this integral we get the relation connecting j to e, and and using ohm's law j equal to sigma e we can write the conductivity as e square by 12 pi cube h cross to tau integral v square by v.

(Refer Slide Time: 41:33)



$$n = \left\{ \frac{4\pi}{3} k_F^3 \right\} \Big/ 4\pi^3$$

$$\boxed{\sigma = \frac{n e^2 \tau}{m}}$$

So, which is v d s and evaluating this and using the relation n equal to four pi by three k f cube divided by four pi cube, that is the electron concentration. We get back we find that simplifying we find again the same relation the old drude formula for the electrical conductivity this means that the application of the fermi dirac distribution does not change the form in the drude's formula. And we get this this expression gives you a very nice way to determine the a calculate the electrical conductivity of a metal. We will continue in the next lecture to see how we can describe other transport process like thermal conduction using the same formulation.

Free electron model

is article needs additional citations for verification.

Learn more

In solid-state physics, the **free electron model** is a simple model for the behaviour of charge carriers in a metallic solid. It was developed in 1927,[1] principally by Arnold Sommerfeld who combined the classical Drude model with quantum mechanical Fermi–Dirac statistics and hence it is also known as the **Drude–Sommerfeld model**.

Given its simplicity, it is surprisingly successful in explaining many experimental phenomena, especially

- the Wiedemann–Franz law which relates electrical conductivity and thermal conductivity;
- the temperature dependence of the electron heat capacity;
- the shape of the electronic density of states;
- the range of binding energy values;
- electrical conductivities;
- the Seebeck coefficient of the thermoelectric effect;

- thermal electron emission and field electron emission from bulk metals.

The free electron model solved many of the inconsistencies related to the Drude model and gave insight into several other properties of metals. The model considers that metals are composed of a quantum electron gas where ions play almost no role. The model can be very predictive when applied to alkali and noble metals.

Ideas and assumptions

In the free electron model four main assumptions are taken into account:

- Free electron approximation: The interaction between the ions and the valence electrons is mostly neglected, except in boundary conditions. The ions only keep the charge neutrality in the metal. Unlike in the Drude model, the ions are not necessarily the source of collisions.
- Independent electron approximation: The interactions between electrons are ignored. The electrostatic fields in metals are weak because of the screening effect.
- Relaxation-time approximation: There is some unknown scattering mechanism

such that the electron probability of collision is inversely proportional to the relaxation time τ, which represents the average time between collisions. The collisions do not depend on the electronic configuration.

- Pauli exclusion principle: Each quantum state of the system can only be occupied by a single electron. This restriction of available electron states is taken into account by Fermi–Dirac statistics (see also Fermi gas). Main predictions of the free-electron model are derived by the Sommerfeld expansion of the Fermi–Dirac occupancy for energies around the Fermi level.

The name of the model comes from the first two assumptions, as each electron can be treated as free particle with a respective quadratic relation between energy and momentum.

The crystal lattice is not explicitly taken into account in the free electron model, but a quantum-mechanical justification was given a year later (1928) by Bloch's theorem: an unbound electron moves in a periodic potential as a free electron in vacuum, except for the electron mass m_e becoming an effective mass $m*$ which may deviate considerably from m_e (one can even use negative effective mass to describe conduction by electron holes). Effective masses can be derived from band structure computations that were not originally taken into account in the free electron model.

From the Drude model

Many physical properties follow directly from the Drude model as some equations do not depend on the statistical distribution of the particles. Taking the classical velocity distribution of an ideal gas or the velocity distribution of a Fermi gas only changes the results related to the speed of the electrons.

Mainly, the free electron model and the Drude model predict the same DC electrical conductivity σ for Ohm's law, that is

$$\mathbf{J} = \sigma \mathbf{E} \quad \text{with} \quad \sigma = \frac{ne^2\tau}{m_e},$$

where $\mathbf{J}$ is the current density, $\mathbf{E}$ is the external electric field, n is the electronic density (number of electrons/volume) and e is the electron electric charge.

Other quantities that remain the same under the free electron model as under

Drude's are the AC susceptibility, the plasma frequency, the magnetoresistance, and the Hall coefficient related to the Hall effect.

Properties of an electron gas

Many properties of the free electron model follow directly from equations related to the Fermi gas, as the independent electron approximation leads to an ensemble of non-interacting electrons. For a three-dimensional electron gas we can define the Fermi energy as where is the reduced Planck constant. The Fermi energy defines the Fermi level, *i.e.* the maximal energy an electron in the metal can have at zero temperature. For metals the Fermi energy is in the order of units of electronvolts.[2]

In three dimensions, the density of states of a gas of fermions is proportional to the square root of the kinetic energy of the particles.

Density of states

The 3D density of states (number of energy states, per energy per volume) of a non-interacting electron gas is given by:

where is the energy of a given electron. This formula takes into account the spin degeneracy but does not consider a possible energy shift due to the bottom of the conduction band. For 2D the density of states is constant and for 1D is inversely proportional to the square root of the electron energy.

Chemical potential

Additionally the Fermi energy is used to define chemical potential . Sommerfeld expansion is a technique used to calculate the chemical potential for higher energies, that is

where is the temperature and we define as the Fermi temperature (is Boltzmann constant). The perturbative approach is justified as the Fermi temperature is usually of about 10^5 K for a metal, hence at room temperature or lower the Fermi energy and the chemical potential are practically equivalent.

Compressibility of metals and degeneracy pressure

The total energy per unit volume (at) can also be calculated by integrating over the phase space of the system, we obtain

which does not depend on temperature. Compare with the energy per electron of an ideal gas: , which is null at zero temperature. For an ideal gas to have the same energy as the electron gas, the temperatures would need to be of the order of the Fermi temperature. Thermodynamically, this energy of the electron gas corresponds to a zero-temperature pressure given by

where is the volume and

is the total energy, the derivative performed at temperature and chemical potential constant. This pressure is called the electron degeneracy pressure and does not come from repulsion or motion of the electrons but from the restriction that no more than two electrons (due to the two values of spin) can occupy the same energy level. This pressure defines the compressibility or bulk modulus of the metal

This expression gives the right order of magnitude for the bulk modulus for alkali metals and noble metals, which show that this pressure is as important as other effects inside the metal. For other metals the crystalline structure has to be taken into account.

Additional predictions

Heat capacity

One open problem in solid-state physics before the arrival of the free electron model was related to the low heat capacity of metals. Even when the Drude model was a good approximation for the Lorenz number of the Wiedemann-Franz law, the classical argument is based on the idea that the volumetric heat capacity of an ideal gas is

.

If this was the case, the heat capacity of a metal could be much higher due to this electronic contribution. Nevertheless, such a large heat capacity was never measured, rising suspicions about the argument. By using Sommerfeld's expansion one can obtain corrections of the energy density at finite temperature and obtain the volumetric heat capacity of an electron gas, given by:

,

where the prefactor to is considerably smaller than the 3/2 found in , about 100 times smaller at room temperature and much smaller at lower . The good estimation of the Lorenz number in the Drude model was a result of the classical mean velocity of electron being about 100 larger than the quantum version, compensating the large value of the classical heat capacity. The free electron model calculation of the Lorenz factor is about twice the value of Drude's and its closer to the experimental value. With this heat capacity the free electron model is also able to predict the right order of magnitude and temperature dependence at low T for the Seebeck coefficient of the thermoelectric effect.

Evidently, the electronic contribution alone does not predict the Dulong–Petit law, i.e. the observation that the heat capacity of a metal is constant at high temperatures. The free electron model can be improved in this sense by adding the lattice vibrations contribution. Two famous schemes to include the lattice into the problem are the Einstein solid model and Debye model. With the addition of the later, the volumetric heat capacity of a metal at low temperatures can be more precisely written in the form,

,

where and are constants of related to the material. The linear term comes from the electronic contribution while the cubic term comes from Debye model. At high temperature this expression is no longer correct, the electronic heat capacity can be neglected, and the total heat capacity of the metal tends to a constant.

Mean free path

Notice that without the relaxation time approximation, there is no reason for the electrons to deflect their motion, as there are no interactions, thus the mean free path should be infinite. Drude model considered the mean free path of electrons to be close to the distance between ions in the material, implying the earlier conclusion that the diffusive motion of the electrons was due to collisions with the ions. The mean free paths in the free electron model are instead given by (where is the Fermi speed) and are in the order of hundreds of ångströms, at least one order of magnitude larger than any possible classical calculation. The mean free path is then not a result of electron-ion collisions but instead is related to imperfections in the material, either due to defects and impurities in the metal, or due to thermal fluctuations.[3]

Inaccuracies and extensions

The free electron model presents several inadequacies that are contradicted by experimental observation. We list some inaccuracies below:

> **Temperature dependence**
> The free electron model presents several physical quantities that have the wrong temperature dependence, or no dependence at all like the electrical conductivity. The thermal conductivity and specific heat are well predicted for

alkali metals at low temperatures, but fails to predict high temperature behaviour coming from ion motion and phonon scattering.

Hall effect and magnetoresistance

The Hall coefficient has a constant value $R_{\mathrm{H}} = -1/(ne)$ in Drude's model and in the free electron model. This value is independent of temperature and the strength of the magnetic field. The Hall coefficient is actually dependent on the band structure and the difference with the model can be quite dramatic when studying elements like magnesium and aluminium that have a strong magnetic field dependence. The free electron model also predicts that the traverse magnetoresistance, the resistance in the direction of the current, does not depend on the strength of the field. In almost all the cases it does.

Directional

The conductivity of some metals can depend of the orientation of the sample with respect to the electric field. Sometimes even the electrical current is not parallel to the field. This possibility is not described because the model does not integrate the crystallinity of metals, i.e. the existence of a periodic lattice of ions.

Diversity in the conductivity

Not all materials are electrical conductors, some do not conduct electricity very well (insulators), some can conduct when impurities are added like semiconductors. Semimetals, with narrow conduction bands also exist. This diversity is not predicted by the model and can only by explained by analysing the valence and conduction bands. Additionally, electrons are not the only charge carriers in a metal, electron vacancies or holes can be seen as quasiparticles carrying positive electric charge. Conduction of holes leads to an opposite sign for the Hall and Seebeck coefficients predicted by the model.

Other inadequacies are present in the Wiedemann-Franz law at intermediate temperatures and the frequency-dependence of metals in the optical spectrum.

More exact values for the electrical conductivity and Wiedemann-Franz law can be obtained by softening the relaxation-time approximation by appealing to Boltzmann transport equations or Kubo formula.

The spin is mostly neglected in the free electron model and its consequences can lead to emergent magnetic phenomena like Pauli paramagnetism and ferromagnetism.

An immediate continuation to the free electron model can be obtained by assuming the empty lattice approximation, which forms the basis of the band structure model known as the nearly free electron model.

Adding repulsive interactions between electrons does not change very much the picture presented here. Lev Landau showed that a Fermi gas under repulsive interactions, can be seen as a gas of equivalent quasiparticles that slightly modify the properties of the metal. Landau's model is now known as the Fermi liquid theory. More exotic phenomena like superconductivity, where interactions can be attractive, require a more refined theory.

See also

- Bloch wave
- Electronic entropy
- Tight binding
- Two-dimensional electron gas
- Bose–Einstein statistics
- Fermi surface

- White dwarf

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Condensed Matter Physics
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Lecture - 34
Energy Bands in Solids

The free electron theory, which was successful in explaining the physical properties of metallic materials has its serious limitations.

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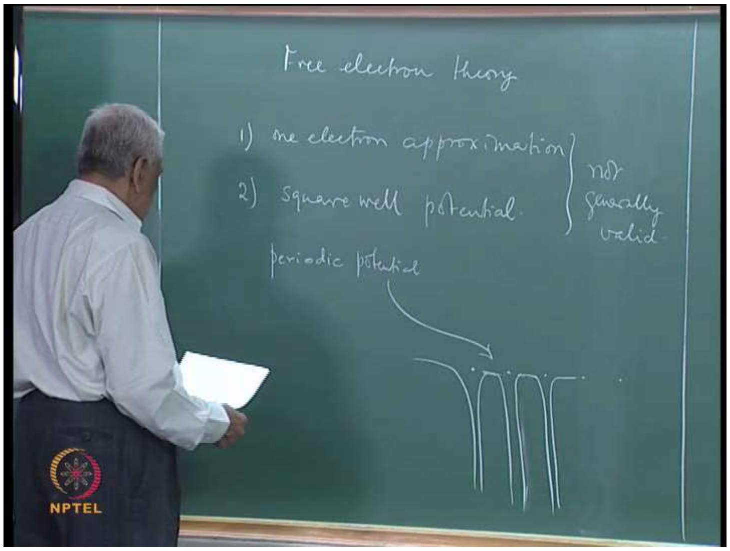

Because it is based on the free electron theory is based on one - one electron approximation, which means that we look at one electron and considered the effect of all the other conductional electrons on it in the form of a square well potential, which is constant throughout the metal. And to which this electron is subject and which prevent it from getting out of the metal as whole. These are the two approximation and they are not generally valid.

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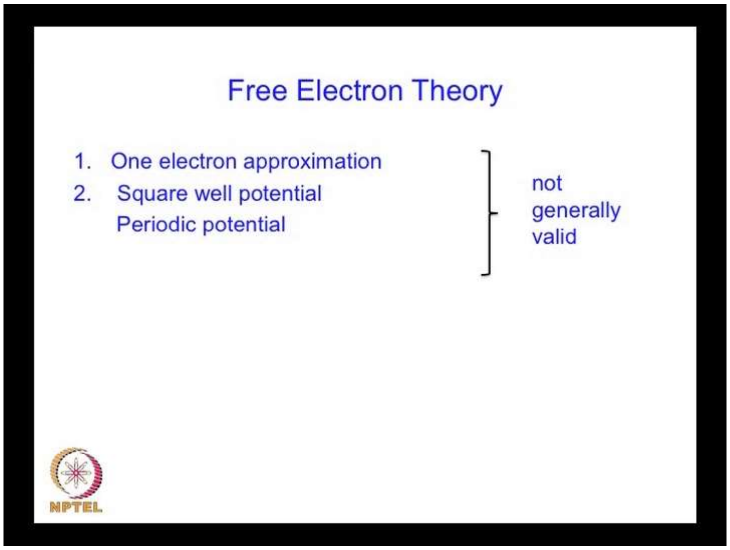

Free Electron Theory

1. One electron approximation
2. Square well potential
   Periodic potential

not generally valid

So, in order to make further progress, it is necessary to go beyond this approximation mainly consider the more realistic situation in which we consider the periodic potential experienced by an electron due to all the ion cores in the lattice - crystal lattice. So, there are ion cores which are regularly arranged in a crystal lattice in all three dimension, I am showing one-dimensional situation. So, the potential is something like there will be…

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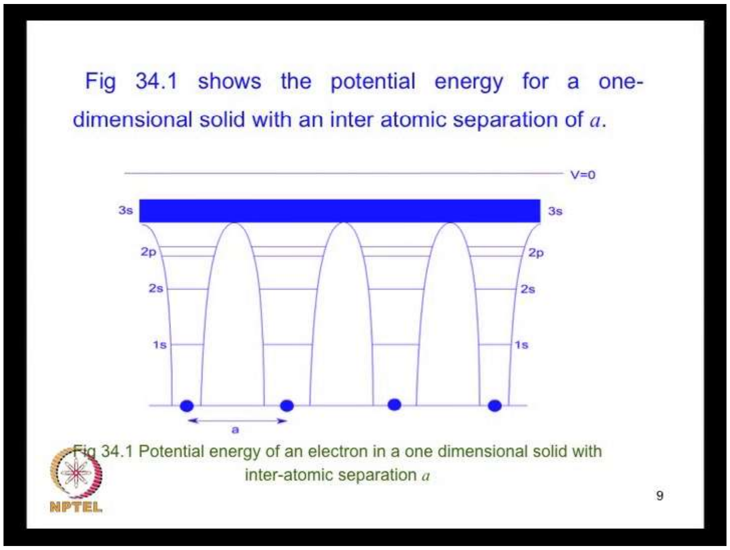

Fig 34.1 shows the potential energy for a one-dimensional solid with an inter atomic separation of a.

Fig 34.1 Potential energy of an electron in a one dimensional solid with inter-atomic separation a

So, and this will repeated self everywhere so and so on. So, this is the periodic potential which we are talking about. This potential has a periodicity of the crystal lattice. So we have to consider the motion of the electron subject to this given by the Schrodinger equation in quantum mechanics.

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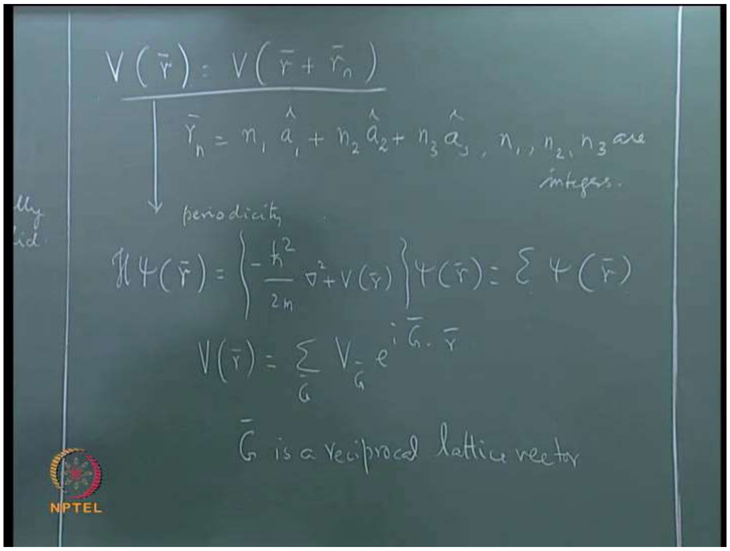

$$V(\bar{r}) = V(\bar{r} + \bar{r}_n)$$

$\bar{r}_n = n_1 \hat{a}_1 + n_2 \hat{a}_2 + n_3 \hat{a}_3$, n_1, n_2, n_3 are integers.

periodicity

$$\mathcal{H} \psi(\bar{r}) = \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V(\bar{r}) \right\} \psi(\bar{r}) = E \psi(\bar{r})$$

$$V(\bar{r}) = \sum_{\bar{G}} V_{\bar{G}} e^{i \bar{G} \cdot \bar{r}}$$

$\bar{G}$ is a reciprocal lattice vector

Subject to this periodic potential V of r, which has the periodicity of the crystal lattice. In other words V of r equals where r n is a general lattice vector n 1 a 1 plus n 2 a 2 plus n 3 a 3 and n 1 n 2 n 3 are integers and a 1 a 2 a 3 are the basic translation vectors.

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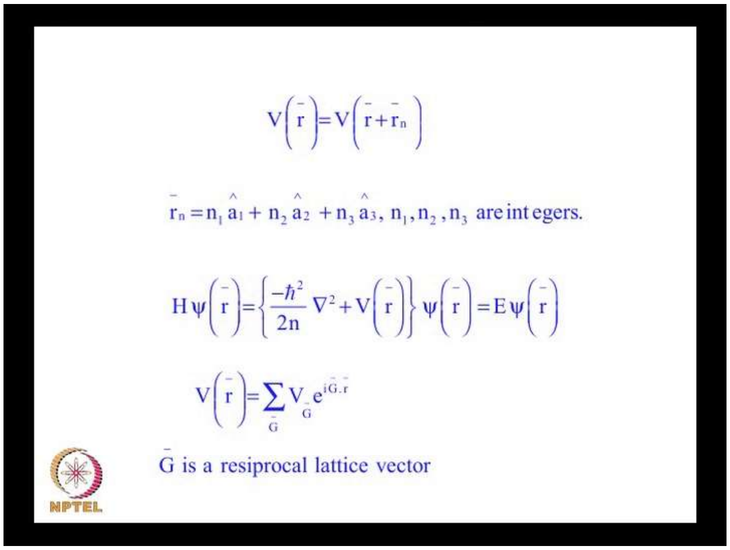

$$V(\bar{r}) = V(\bar{r} + \bar{r}_n)$$

$\bar{r}_n = n_1 \hat{a}_1 + n_2 \hat{a}_2 + n_3 \hat{a}_3$, n_1, n_2, n_3 are integers.

$$H\psi(\bar{r}) = \left\{ \frac{-\hbar^2}{2n} \nabla^2 + V(\bar{r}) \right\} \psi(\bar{r}) = E\psi(\bar{r})$$

$$V(\bar{r}) = \sum_{\bar{G}} V_{\bar{G}} e^{i\bar{G}.\bar{r}}$$

$\bar{G}$ is a resiprocal lattice vector

So, this is simply the condition of periodicity that the potential remains same at any given lattice point, and it is equal to the value of potential at any other lattice point given by the position vector r plus r n. So, this is the condition and we have to solve the Schrodinger equation H psi of r equals minus H cross by a by 2 m del square plus V of r psi of r equal to E psi of r. So, we have to find energy Eigen values E by solving this Schrodinger equation subject to this. And because of the periodicity, it is possible to expand this in the Fourier series of the lattice periodic potential in the form where G is a reciprocal lattice vector we already consider this well discussing diffraction of x-rays by a crystal lattice.

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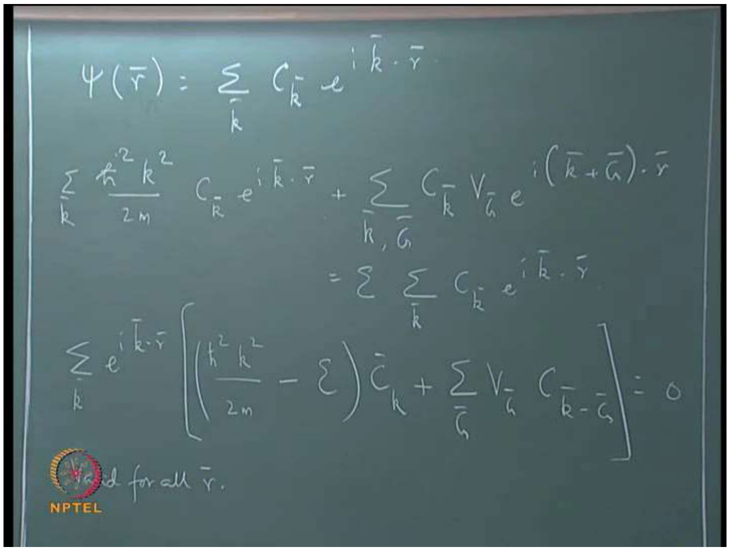

$$\psi(\bar{r}) = \sum_{\bar{k}} C_{\bar{k}} e^{i\bar{k}\cdot\bar{r}}$$

$$\sum_{\bar{k}} \frac{\hbar^2 k^2}{2m} C_{\bar{k}} e^{i\bar{k}\cdot\bar{r}} + \sum_{\bar{k},\bar{G}} C_{\bar{k}} V_{\bar{G}} e^{i(\bar{k}+\bar{G})\cdot\bar{r}} = \mathcal{E} \sum_{\bar{k}} C_{\bar{k}} e^{i\bar{k}\cdot\bar{r}}$$

$$\sum_{\bar{k}} e^{i\bar{k}\cdot\bar{r}} \left[\left(\frac{\hbar^2 k^2}{2m} - \mathcal{E} \right) \bar{C}_{k} + \sum_{\bar{G}} V_{\bar{G}} C_{\bar{k}-\bar{G}} \right] = 0$$

d for all $\bar{r}$.

And we can also expand the plain psi of r in the form of plain waves where k is the wave vector of z electron. So, using this substituting this and this we get equals E sigma k c k a to the power I k dot r.

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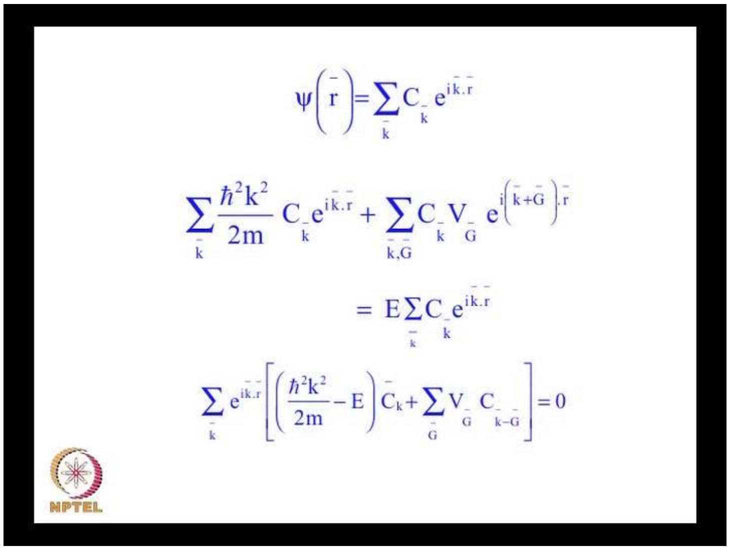

$$\psi\left(\bar{r}\right)=\sum_{\bar{k}} C_{\bar{k}}\, e^{i\bar{k}.\bar{r}}$$

$$\sum_{\bar{k}} \frac{\hbar^2 k^2}{2m} C_{\bar{k}}\, e^{i\bar{k}.\bar{r}} + \sum_{\bar{k},\bar{G}} C_{\bar{k}} V_{\bar{G}}\, e^{i\left(\bar{k}+\bar{G}\right).\bar{r}}$$

$$= E\sum_{\bar{k}} C_{\bar{k}}\, e^{i\bar{k}.\bar{r}}$$

$$\sum_{\bar{k}} e^{i\bar{k}.\bar{r}}\left[\left(\frac{\hbar^2 k^2}{2m}-E\right)\bar{C}_k+\sum_{\bar{G}} V_{\bar{G}}\, C_{\bar{k}-\bar{G}}\right]=0$$

That will be the equation that we have to solve and this can be written also in the form factoring out a to the power I k dot r we can write this as which is valued for all are which means the square bracket at quantity should vanish.

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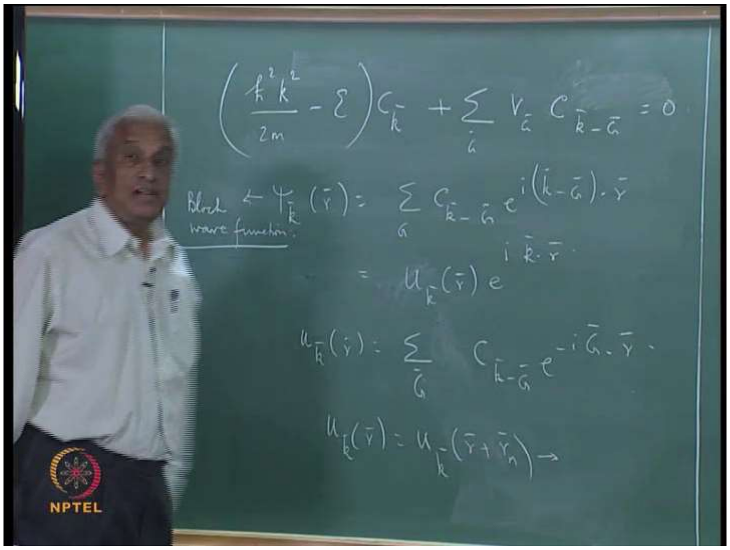

$$\left(\frac{\hbar^2 k^2}{2m}-\varepsilon\right)C_{\bar{k}} + \sum_{\bar{G}} V_{\bar{G}}\, C_{\bar{k}-\bar{G}} = 0$$

Bloch wave function ← $\psi_{\bar{k}}(\bar{r}) = \sum_{G} C_{\bar{k}-\bar{G}}\, e^{i(\bar{k}-\bar{G}).\bar{r}}$

$$= u_{\bar{k}}(\bar{r})\, e^{i\bar{k}.\bar{r}}$$

$$u_{\bar{k}}(\bar{r}) = \sum_{\bar{G}} C_{\bar{k}-\bar{G}}\, e^{-i\bar{G}.\bar{r}}$$

$$u_{k}(\bar{r}) = u_{\bar{k}}(\bar{r}+\bar{r}_n) \rightarrow$$

So, we get. So, that we can therefore, write psi k of r as sigma g c k minus g E to the power I k minus g dot r.

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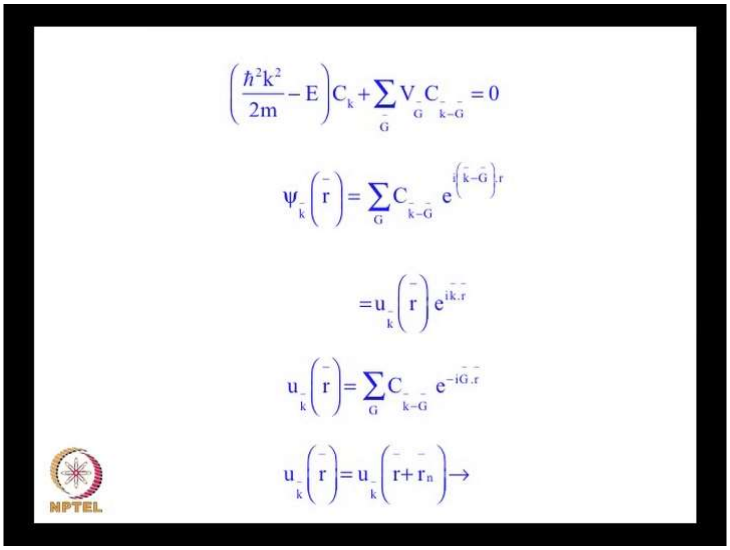

$$\left(\frac{\hbar^2 k^2}{2m} - E\right) C_{k} + \sum_{\bar{G}} V_{\bar{G}} C_{\bar{k}-\bar{G}} = 0$$

$$\psi_{\bar{k}}\left(\bar{r}\right) = \sum_{G} C_{\bar{k}-\bar{G}}\, e^{i\left(\bar{k}-\bar{G}\right).r}$$

$$= u_{\bar{k}}\left(\bar{r}\right) e^{i\bar{k}.\bar{r}}$$

$$u_{\bar{k}}\left(\bar{r}\right) = \sum_{G} C_{\bar{k}-\bar{G}}\, e^{-i\bar{G}.\bar{r}}$$

$$u_{\bar{k}}\left(\bar{r}\right) = u_{\bar{k}}\left(\bar{r}+\bar{r}_n\right) \rightarrow$$

Which can also be written as u k of r a to the power i k dot r where u k of r is. So, we get the automatic property that the wave function psi k of r this modulator is a free electron wave function E to the power i k dot r modulator by the function u k of r such that u k of r equals u k of r plus r n. So, this as the modulating function as the periodicity of the lattice and so this is known as black wave function. So, the consequences of translational invariance of the periodic crystalline lattice is that the wave function psi k r is no longer the free electron plane wave function E to the power i k dot r that E to the power i k dot r modulated by the u k of r which is also translational invariance. And this is the form of the black wave function which we should use in our description of the energy Eigen values of an electron moving in a perfectly periodic potential. So, this is step one this is one important result which we will use in our discussion of the formation of so-called energy bands in solids.

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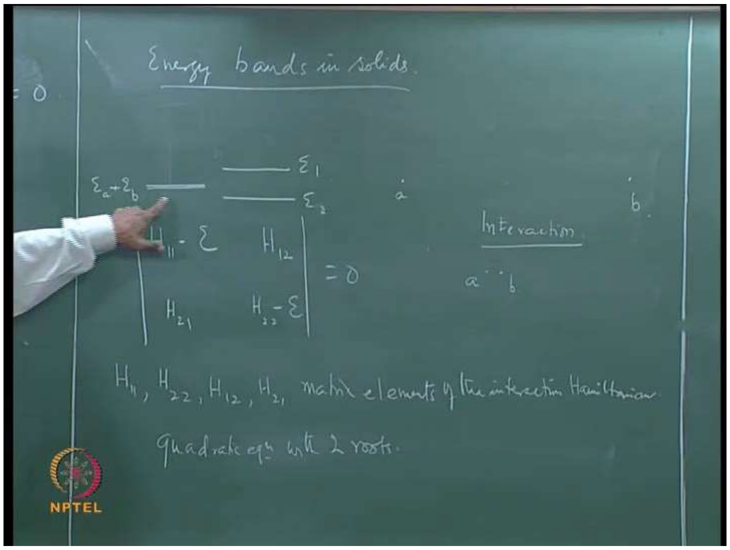

So, we move on to the discussion of energy bands in solids. In this discussion, we have to answer the question how bands f found the already saw in our discussion of the energetic of a homo nuclear diatomic molecule that if you have two molecule which are a far apart and therefore, non-interacting. The energy Eigen value of the two atom system is just twice the energy of the individual atoms and I am showing them together here in the form in which they are regenerate. So, this is energy of E a plus E b wave a and b are atoms which are no interacting now as the atoms are brought together we saw that the atom start interacting we turn on an interaction interact atomic interaction the electronic and nucleolus the electron and nucleates start interacting by as a coulomb potential. So, this interaction many it turn on and the two molecules come close together then we saw that the energy Eigen value is going to be given by the secular determinant where H 1 1 H 2 2 H 1 2 and H 2 1 are matrix elements of the interaction potential. Or interaction Hamiltonians between the individual atomic states represented by psi 1 psi 2. So, solving this we see that we get a quadratic equation with two root.

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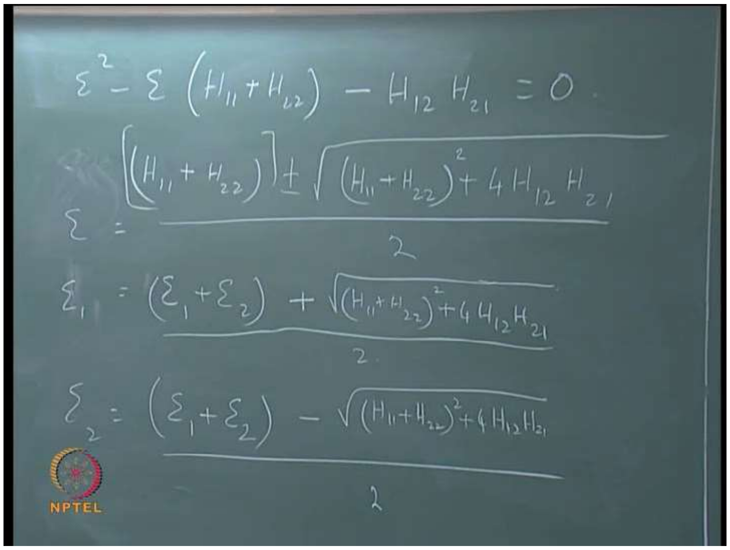

$$\varepsilon^2 - \varepsilon(H_{11} + H_{22}) - H_{12} H_{21} = 0$$

$$\varepsilon = \frac{[(H_{11} + H_{22})] \pm \sqrt{(H_{11} + H_{22})^2 + 4 H_{12} H_{21}}}{2}$$

$$\varepsilon_1 = \frac{(\varepsilon_1 + \varepsilon_2) + \sqrt{(H_{11} + H_{22})^2 + 4 H_{12} H_{21}}}{2}$$

$$\varepsilon_2 = \frac{(\varepsilon_1 + \varepsilon_2) - \sqrt{(H_{11} + H_{22})^2 + 4 H_{12} H_{21}}}{2}$$

So, these quadratic equation has this form for which the roots are. So, this shows this will be this is the H 1 1 plus H 2 2 is what we call E 1 plus E 2 these are the energies of individual non interacting atoms and the resulting energy. Now in the presents of the interaction one of this is E one is plus square root of H 1 1 plus H 2 2 square plus 4 k 1 2 H 2 1.

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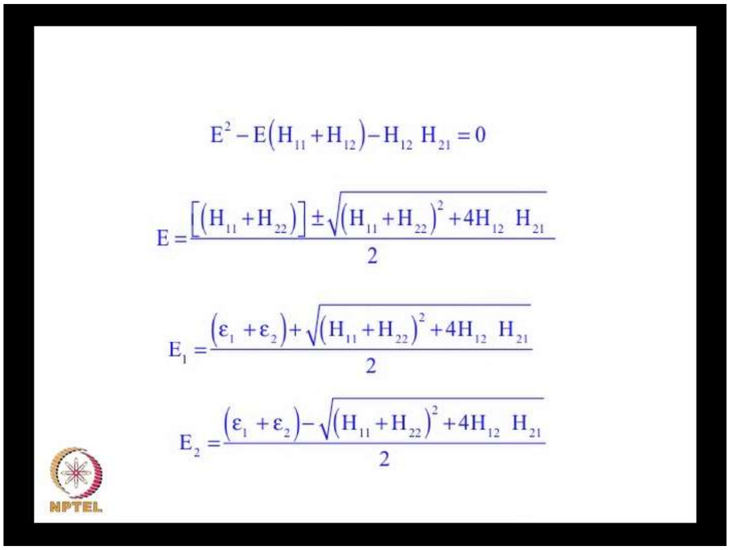

$$E^2 - E(H_{11} + H_{12}) - H_{12}\, H_{21} = 0$$

$$E = \frac{[(H_{11} + H_{22})] \pm \sqrt{(H_{11} + H_{22})^2 + 4H_{12}\ H_{21}}}{2}$$

$$E_1 = \frac{(\varepsilon_1 + \varepsilon_2) + \sqrt{(H_{11} + H_{22})^2 + 4H_{12}\ H_{21}}}{2}$$

$$E_2 = \frac{(\varepsilon_1 + \varepsilon_2) - \sqrt{(H_{11} + H_{22})^2 + 4H_{12}\ H_{21}}}{2}$$

Yes and the other one will be E 2 will be minus. So, there are two routes one corresponding to a lower value corresponding to the negative sign there, and a higher energy value corresponding to… So, these are the E 2 E 1. So, you see that any interaction when it is stand on the two atom systems the energy level are split into in a such a way, the two fold degenerate is lifted and there are two non-degenerated energy levels one the higher energy Eigen value, and another with the lower energy Eigen value. Now this is the situation when two atoms interact. We are now considering the periodic potential due to the entire lattice of all the ten to power 23 electrons. So, these are going to give you a large number of interaction of the same kind the solid is after all large molecule.

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So, we are going to have a large number of splitting in this. So, of this finally, becomes a quasi I continuum when the number of interaction is very large so. This is a quasi I continuum. So, this continuum what we call an energy band in the presence of the perfectly periodic crystalline potential the electron energy going to sprodon into the form of energy bands. So, this is the mechanism of energy bands in order to discuss the detailed nature of the energy band.

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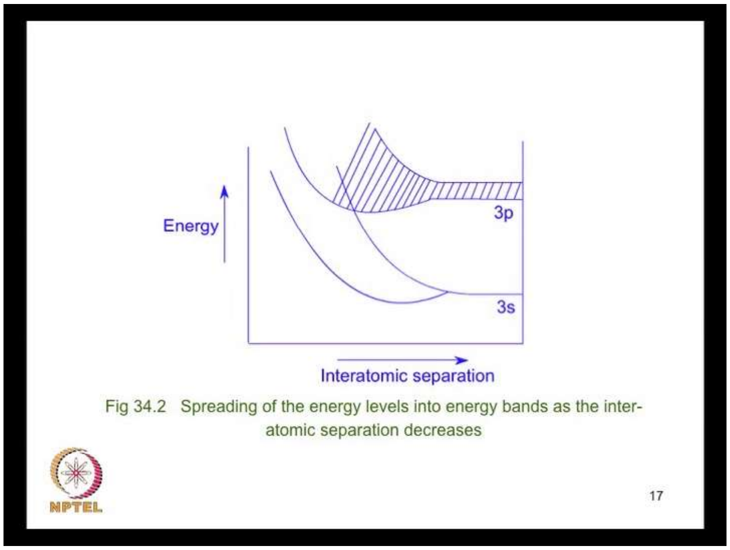

Fig 34.2 Spreading of the energy levels into energy bands as the interatomic separation decreases

Energy band it is necessary to go a little for other this is only a qualitative description of the interaction. Now let us consider a specific model in which we will be position to calculate the energy band structure.

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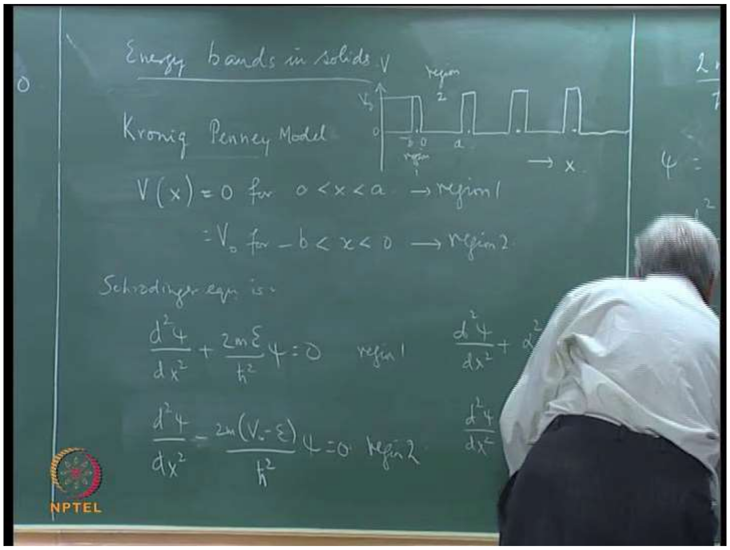

Energy bands in solids

Kronig Penney Model

$V(x) = 0$ for $0 < x < a$ → region 1

$= V_0$ for $-b < x < 0$ → region 2

Schrodinger eqn is:

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad \text{region 1}$$

$$\frac{d^2\psi}{dx^2} - \frac{2m(V_0 - E)}{\hbar^2}\psi = 0 \quad \text{region 2}$$

$$\frac{d^2\psi}{dx^2} + \alpha^2$$

$$\frac{d^2\psi}{dx^2}$$

So, this model is simplify one-dimensional model known as Kronig-Penney model. This discusses the motion of the electron in is one-dimensional potential which is 0 for 0 less than X less than area.

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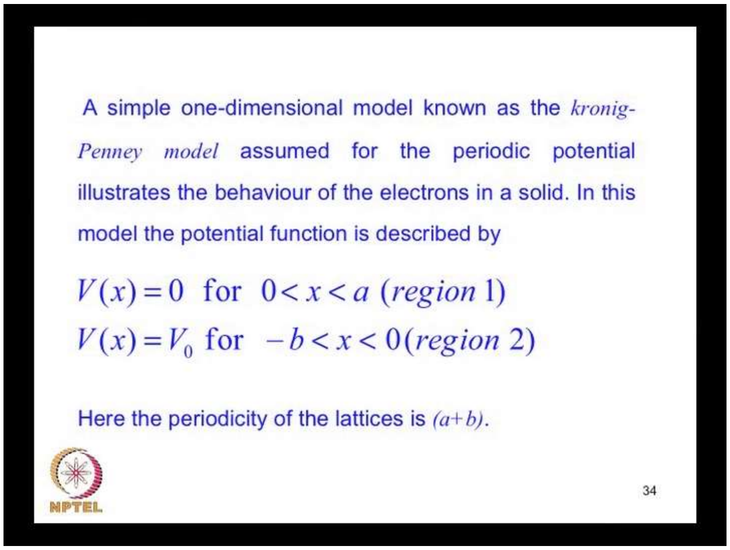

A simple one-dimensional model known as the *kronig-Penney model* assumed for the periodic potential illustrates the behaviour of the electrons in a solid. In this model the potential function is described by

$$V(x) = 0 \text{ for } 0 < x < a \ (region\ 1)$$

$$V(x) = V_0 \text{ for } -b < x < 0 (region\ 2)$$

Here the periodicity of the lattices is $(a+b)$.

And equals V 0 for minus b less than a less than a. So this is known as less than 0 region one, this is region two pictorially this mean that we have atoms which are situated like this.

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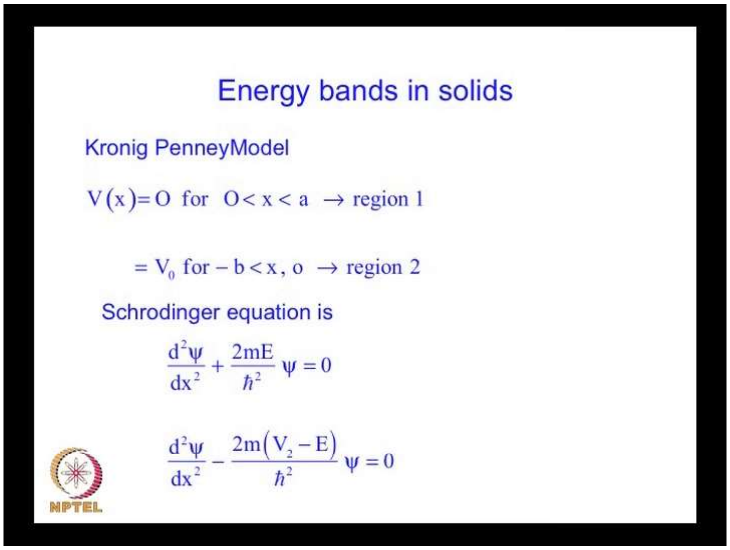

Energy bands in solids

Kronig PenneyModel

$$V(x) = O \text{ for } O < x < a \rightarrow \text{region 1}$$

$$= V_0 \text{ for } -b < x, o \rightarrow \text{region 2}$$

Schrodinger equation is

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

$$\frac{d^2\psi}{dx^2} - \frac{2m(V_2 - E)}{\hbar^2}\psi = 0$$

And then you have a potential which is 0 here potentially is represented here which is 0 and when it is reaches the neighborhood of ion core then the potential goes up like that. So, this is V 0 this is minus b this is 0 this is a.

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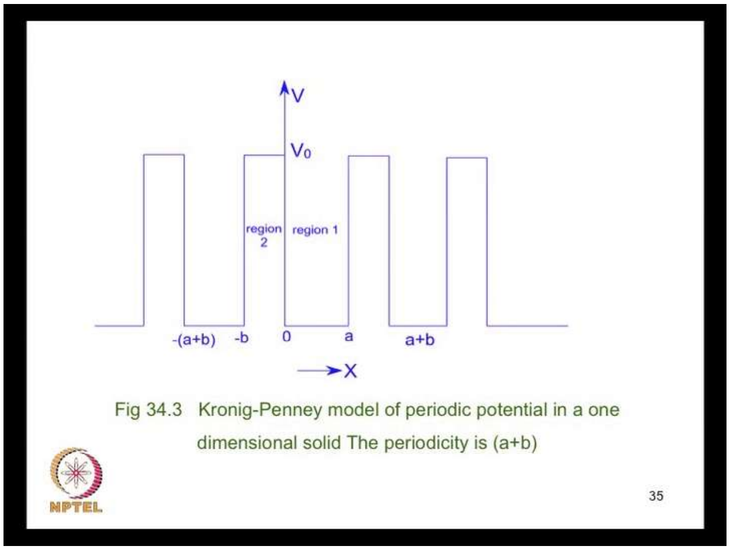

Fig 34.3 Kronig-Penney model of periodic potential in a one dimensional solid The periodicity is (a+b)

So, in the torsion the Schrodinger equations in one-dimensional d square psi d x square 2 two m V by H cross square psi equal 0 this is region one where V of x is 0 then. So, this is region one this is region 2 this region one this is region 2 let us first short and write 2 m E by H cross square.

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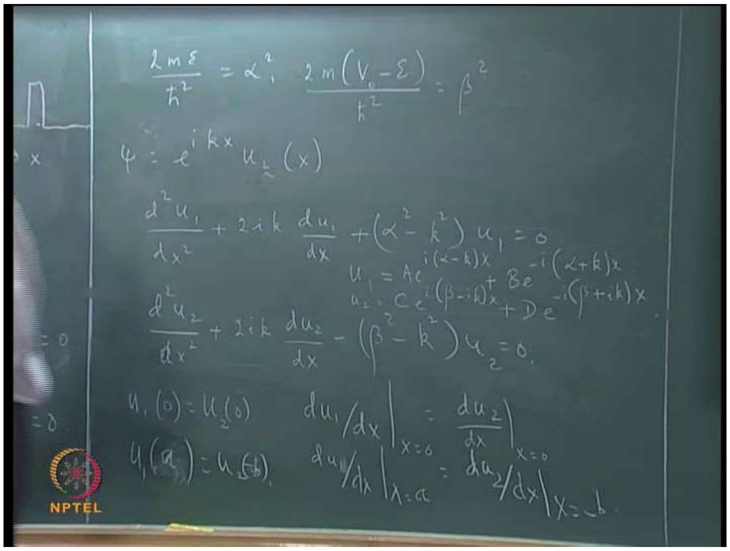

$$\frac{2mE}{\hbar^2} = \alpha^2; \quad \frac{2m(V_0 - E)}{\hbar^2} = \beta^2$$

$$\psi = e^{ikx} u_k(x)$$

$$\frac{d^2u_1}{dx^2} + 2ik\frac{du_1}{dx} + (\alpha^2 - k^2)u_1 = 0$$

$$u_1 = Ae^{i(\alpha-k)x} + Be^{-i(\alpha+k)x}$$

$$u_2 = Ce^{i(\beta-ik)x} + De^{-i(\beta+ik)x}$$

$$\frac{d^2u_2}{dx^2} + 2ik\frac{du_2}{dx} - (\beta^2 - k^2)u_2 = 0.$$

$$u_1(0) = u_2(0) \quad du_1/dx\Big|_{x=0} = \frac{du_2}{dx}\Big|_{x=0}$$

$$u_1(a) = u_2(-b), \quad du_1/dx\Big|_{x=a} = du_2/dx\Big|_{x=-b}.$$

Yes alpha square and two m into V naught minus E by H cross square as beta square. So, that this becomes and this is now we have the black solution the black form which we discuss already in the form. So, that substituting this and making differentiation and substitute that we get the two equation these equation become and there u r, u 2 are the function u here in the region 1 2. So, these are the equation to be satisfy solved for u and u 2 the solution u and u 2 should satisfy boundary condition which are such that at the interface were at minus b at 0 and a they have to be matched in other words u 1 of 0. They matched two wave function match at x equal to 0.

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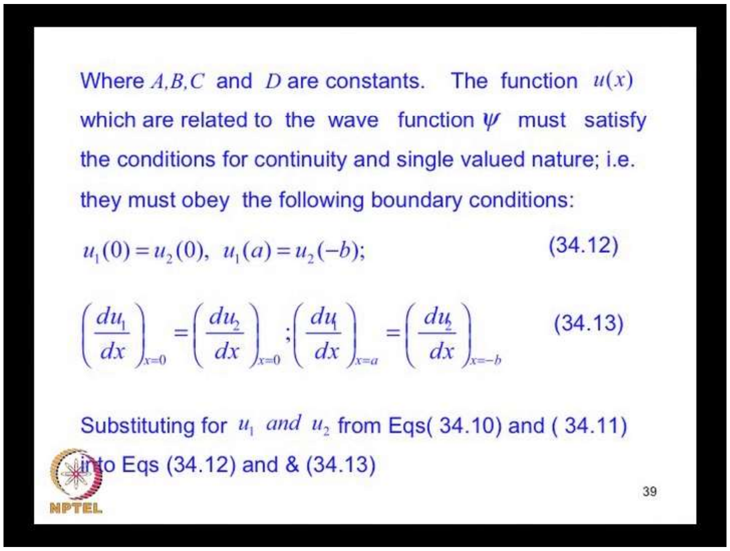

Where A, B, C and D are constants. The function $u(x)$ which are related to the wave function ψ must satisfy the conditions for continuity and single valued nature; i.e. they must obey the following boundary conditions:

$$u_1(0) = u_2(0), \quad u_1(a) = u_2(-b); \qquad (34.12)$$

$$\left(\frac{du_1}{dx}\right)_{x=0} = \left(\frac{du_2}{dx}\right)_{x=0}; \left(\frac{du_1}{dx}\right)_{x=a} = \left(\frac{du_2}{dx}\right)_{x=-b} \qquad (34.13)$$

Substituting for u_1 *and* u_2 from Eqs(34.10) and (34.11) into Eqs (34.12) and & (34.13)

And there are again match at u 1 of minus B equals u 2 of a for u 1 of a. These 2 minus B this a consequent of translation in variance and also condition on the derivatives d u one d x at the x equal to 0 matches d u 2 by d x at x is equal to 0. And a similar condition on d u 1 by d x x equal to a equals d u 2 by d x at x equal to minus b. If I take the forms this gives forms u 1 equals a E to the power i alpha minus k x plus d E to the power of minus i alpha plus k x. And u 2 is c to the power I beta prime by k x plus d E to the power minus i beta plus i k x. So, we required the solution u 1 and u 2 to satisfied this condition and that gives you a determinant which a 4 by 4 determinant because 4 conditions there and which when expanded leads to the following condition to be satisfied.

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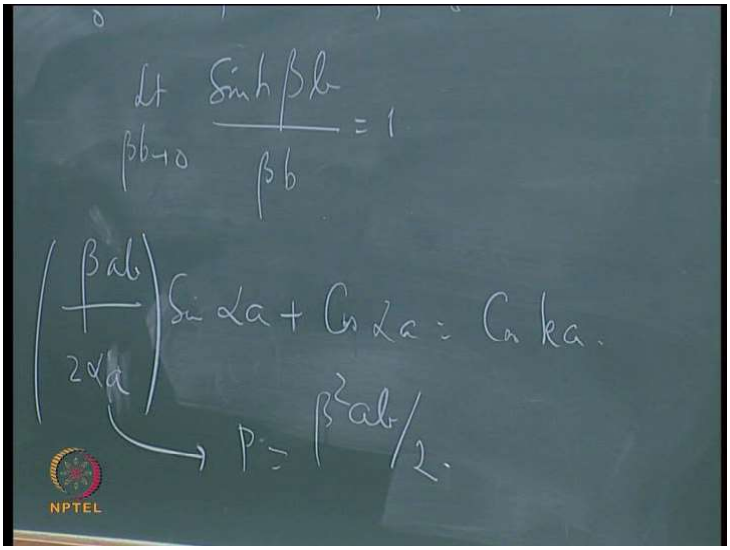

$$\underset{\beta b\to 0}{Lt}\ \frac{\sinh \beta b}{\beta b} = 1$$

$$\left(\frac{\beta ab}{2\alpha a}\right) \sin \alpha a + \cos \alpha a = \cos ka.$$

$$\xrightarrow{\quad} P = \beta^2 ab/2.$$

Namely beta square by alpha square by 2 alpha beta sin alpha a sin H of beta b plus cos alpha a cosign hyperbolic beta b equal to cos k a plus b. So, that will be the condition to be satisfied which is got by a expanding by the four by four determinants now we specify to the situation where V naught tends to infinity and b tends to 0 in other words it is extremely thin barrier it is infinitely high.

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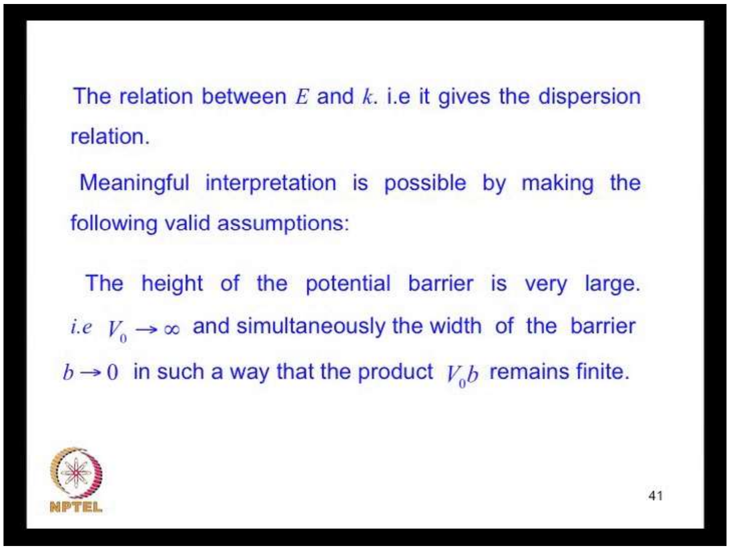

The relation between E and k. i.e it gives the dispersion relation.

Meaningful interpretation is possible by making the following valid assumptions:

The height of the potential barrier is very large. i.e $V_0 \to \infty$ and simultaneously the width of the barrier $b \to 0$ in such a way that the product $V_0 b$ remains finite.

Such that V naught b remains this case we get limit beta b 10 into 0 sin H beta b by b equal to 1 and therefore, the derivative condition b sin alpha a plus cos alpha a equals cos k a.

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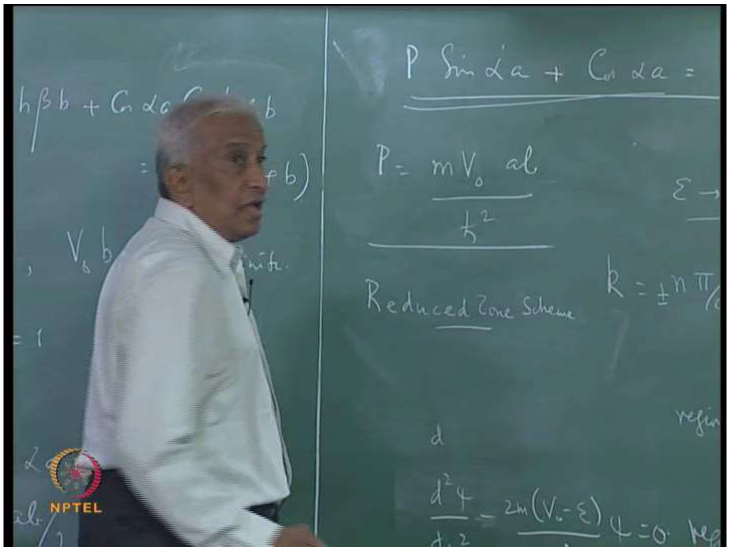

So, this p is nothing but m V naught a b by H cross square. So, this is the parameter which involves the highest of the potential barrier and the thickness of the potential barrier. So, this is the basic condition which determines the energy Eigen values.

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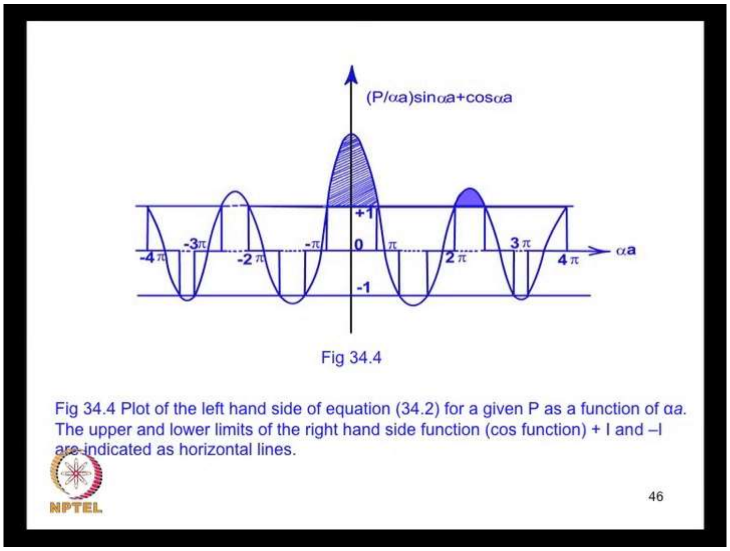

Fig 34.4

Fig 34.4 Plot of the left hand side of equation (34.2) for a given P as a function of αa. The upper and lower limits of the right hand side function (cos function) + I and –I are indicated as horizontal lines.

We can see the nature of this energy band s by looking at the graphical representation of these energy bands. So, the figure shows the plate of the right hand side this side of this equation for a given value of p as a function of alpha a. So, we can see that there shaded portions left hand side is plotted since the right hand side is just cosign function. So, it cannot go beyond the value is a plus one of minus one and therefore, you find shaded regions in the figure correspond to such values of cosign k a which are unreasonable and therefore, are forbidden they are not allowed. So, you find that energy values get into two in two regions one the un shaded one corresponding to the allowed energy values and the shaded regions which corresponds to the forbidden regions the energy Eigen values.

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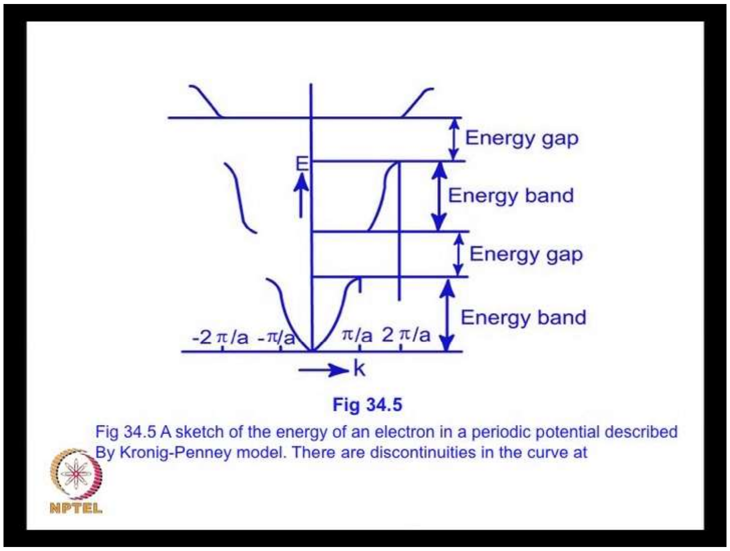

Fig 34.5

Fig 34.5 A sketch of the energy of an electron in a periodic potential described By Kronig-Penney model. There are discontinuities in the curve at

So, these energy Eigen values when plotted look like this they are shown the energy E versus k curve we shown in. So, this gives the energy versus the wave vector for an electron in a periodic potential described by the chronic penny model. So, you can see that there are discontinuities at k equal to pi by a and k equal to minus pi by a and then k equal to two pi by a k equal to minus q pi by a and so on. So, in general, for all k equal to n pi by a plus or minus there are discontinuities in a energy. So, the energy Eigen value goes from the value suddenly it is this and all the energy Eigen values in this region are not allowed.

So, these are the allowed energy Eigen values these are the forbidden energy Eigen values in the gap region again these are allowed set up Eigen values then followed by energy gap again in the next band so on for the third band and so on. So, this goes on and we find that this can be represented a bit more effectively in the. So, called reduced zones scheme this only means that the states k and k plus or minus in into 2 pi by a n into pi by a.

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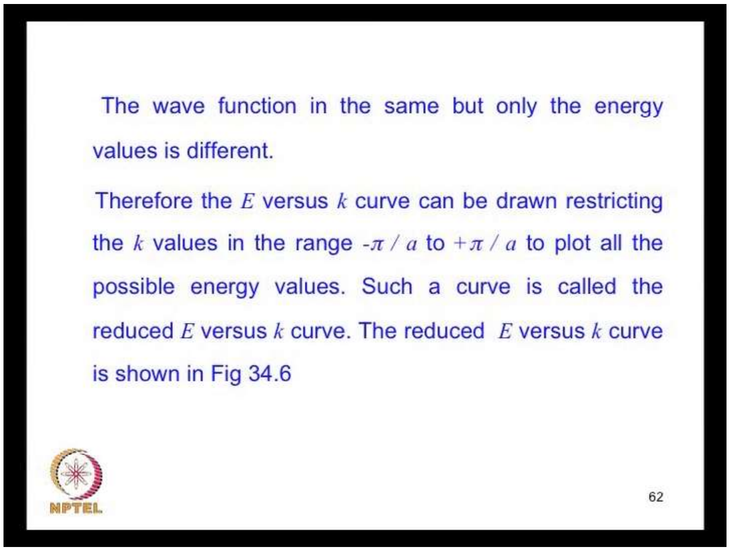

The wave function in the same but only the energy values is different.

Therefore the E versus k curve can be drawn restricting the k values in the range $-\pi / a$ to $+\pi / a$ to plot all the possible energy values. Such a curve is called the reduced E versus k curve. The reduced E versus k curve is shown in Fig 34.6

These are all equal and they are identical functions while the functions while the energies are different. So, the energies are different, but they are discovered by the same function. So, these verses k curve can be done by restricting the k values in the range minus pi by a to plus pi by a

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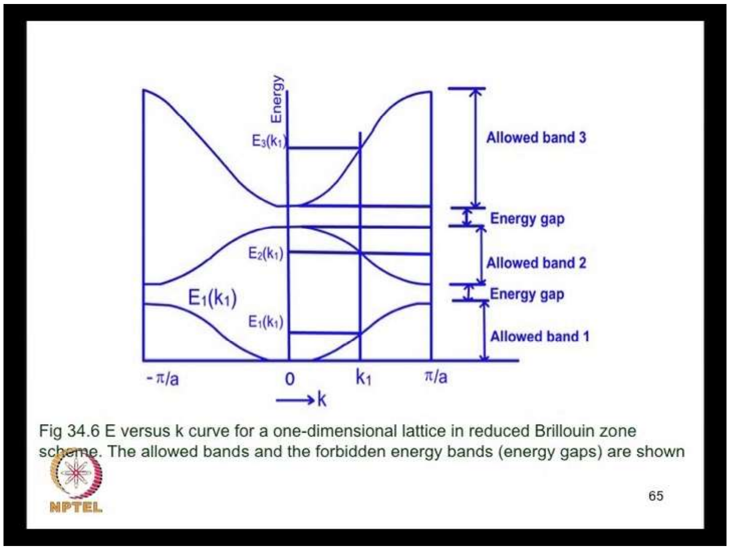

Fig 34.6 E versus k curve for a one-dimensional lattice in reduced Brillouin zone scheme. The allowed bands and the forbidden energy bands (energy gaps) are shown

And all the energy values can be plotted within this region. So, such a plot issue shown in figure where the first band as energies shown in the lowermost curve these are we allowed value and then E two is the corresponding energy values for the second band plotted in the reduced came therefore, there is a gap between these two. So, there is an energy gap and then the next allowed band comes here that is the two k and similarly E three k with a gap here. So, this shows the entire energy band structure within this first Brillouin zone which is the region between minus pi by a and plus pi by a. So, this is this describe the band structure the typical band structure. So, the Kernig-Penny model gives as an easy way to understand the formation of energy bands in periodic solid.

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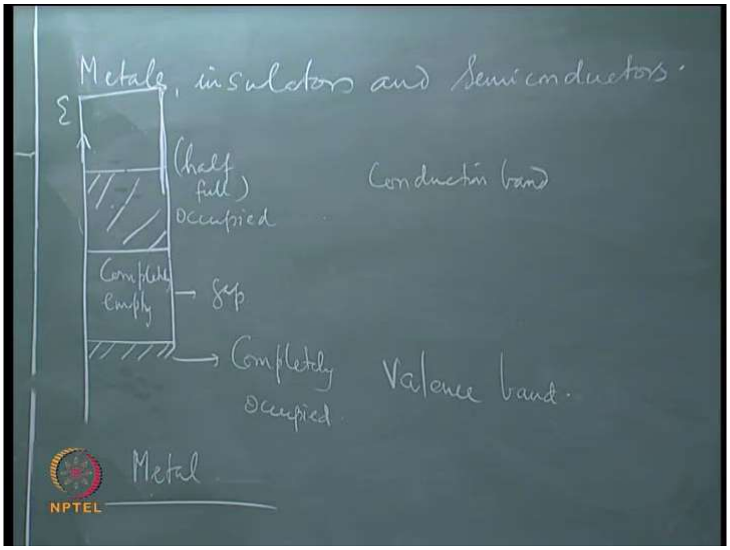

And this is very important in a discussion of the property of metals insulators and semiconductor these are new clause of materials which we are going to discuss from now on in a unified way hoe do you discuss this the matter let me just sketch the band structure in a simple way. So, this is the E energy and this is the band structure in a very crude form.

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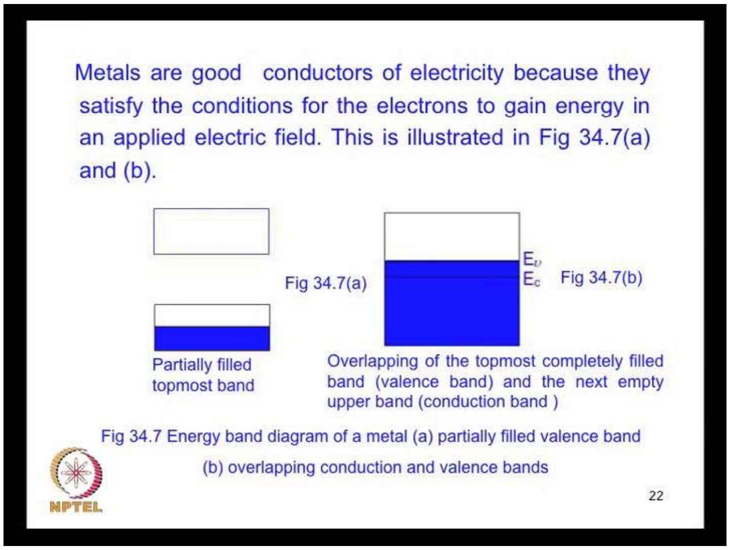

Metals are good conductors of electricity because they satisfy the conditions for the electrons to gain energy in an applied electric field. This is illustrated in Fig 34.7(a) and (b).

Fig 34.7 Energy band diagram of a metal (a) partially filled valence band (b) overlapping conduction and valence bands

So, we have states laying here this is empty and there are states here. So, these are states which are occupy and these are states which are forbidden and therefore, this states allow forbidden an occupy empty and this is an occupied band the bands. And of course, the extent of to this energy value and it is only of full this band is completely occupy the lower bands and this is completely empty this is the gap. So, this is the picture of a metal in a metal there is a completely occupy band separated from a partially occupied or of full conduction band this is known as the valance band and this is the conduction band. So, the valance band is completely occupied whenever a band is completely occupied states are free for an electron to get into because of Pawley's fusion principle and. So, conduction in a such a band is not possible the electron cannot move on one state to another similarly if there is a completely empty band that is also something in which there are no electrons therefore, is there is no conduction.

So, for conduction to be possible in a material request have a band structure with an uppermost band which is only partially feel in this case the metal is only of filled and therefore, of the band is empty and off of the band is occupied. So, the electrons the conduction electron is can move from the occupied states into the empty states there by facilitating conduction. So, conduction is possible. So, this is the band structure which renders a metal conducting coming to the case of an insulators and insulators how is its band structure.

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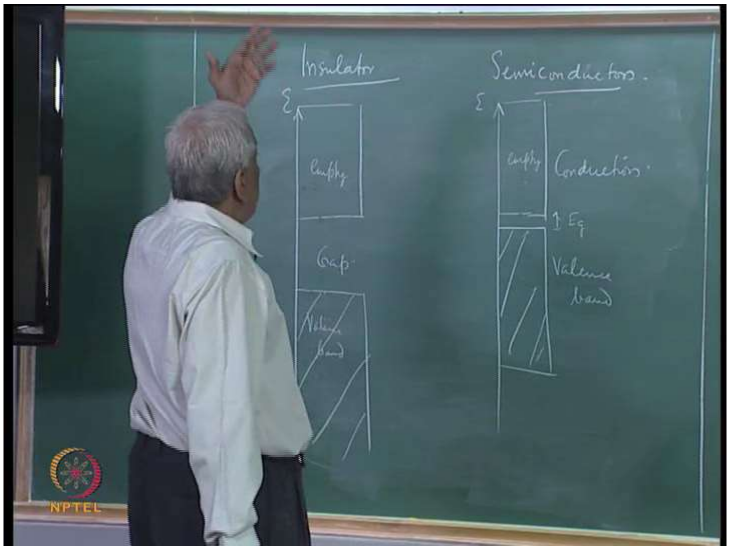

Band structure again we shown in schematically in this way. So, you have a upper band and a lower band this is a gap. So, this is the valence band which is completely occupied and a conduction band which is empty, but separated The conduction band which is empty is separated from the valance band which is completely occupy by a very large gap energy gap. So, for carriers to into this empty band from in the occupied band they have to cross overcome this barrier produced by these energy gap and they have to get in from the state in the valance band they have to get into the state in the empty unoccupied band upper band. So, this is possible only there as the energy which is more than the gap energy and then an insulators is does not happen and therefore this is not conducting.

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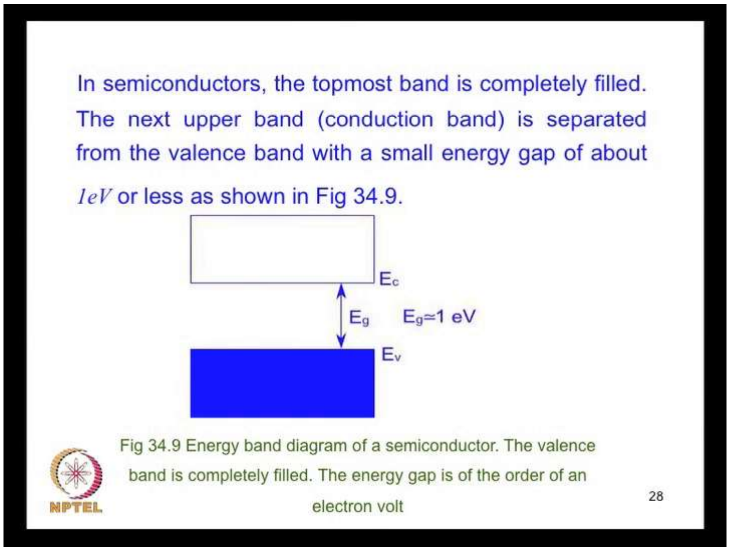

In semiconductors, the topmost band is completely filled. The next upper band (conduction band) is separated from the valence band with a small energy gap of about $1eV$ or less as shown in Fig 34.9.

Fig 34.9 Energy band diagram of a semiconductor. The valence band is completely filled. The energy gap is of the order of an electron volt

Now we come to an another interesting class of material which we have not talked about so far which is known as semiconductors. So, here the band structure is very similar that of an insulator. And there is an valance band below which is completely occupied with an energy gap which in contrast to an insulator the energy gap is as a very small value. In other words, the occupied valance band is separated from the unoccupied conduction band only by an extremely small amount of energy of the order of an electron hole. So, it is easily possible for carriers to get excited across the gap from getting to conduction band. Therefore, they neither an insulator nor a metal like this, but they are semiconducting.

So, this is the new class of material, which will be discussing from now on. And the band structure theory, the theory of energy band provides a convenient mechanism or convenient way to understand the difference between an insulators, a metal and a semiconductor from the point of view of their band structures. And there relate these electronic band structure to the nature of the conduction band in these material. We will discuss semiconductors in the next session.

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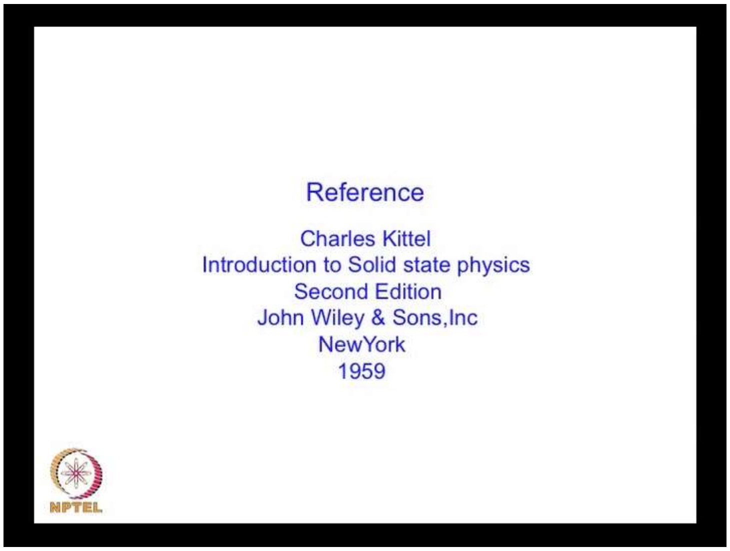

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Magnetic and Dielectric materials in Material science

We know that current through a circular coil produces magnetic moment along the axis of the coil. When the electrons revolve around the positive nucleus, orbital magnetic moment arises. Similarly when the electron spins, spin magnetic moment arises. Magnetism arises from the magnetic moment or magnetic dipole of the magnetic materials. Any material that can be magnetized by application of external magnetic field is called a magnetic material.

Types of Magnetic materials :

1. Diamagnetic
2. Paramagnetic
3. Ferro –magnetic
4. Anti Ferromagnetic
5. Ferromagnetic

Important terms used in magnetism :

Magnetic flux density (B) :

Magnetic flux density (B) in any material is the number of lines of magnetic force passing through unit area perpendicularly.

Unit : Wb/m^2 or Tesla

Magnetic field intensity (H) :

Magnetic field intensity at any point in the magnetic field is the force experienced by an unit north pole placed at that point.

Unit : A/m

$$\boxed{B = \mu_0 H}$$

Where μ_0 = permeability of free space (vacuum)

$$\boxed{\mu_0 = 4\pi \text{ x } 10^{-7}\ H_1 m^{-1}}$$

Instead of vacuum, it the field is applied in a solid medium, the magnetic induction in the solid is given by

$$\boxed{B = \mu H}$$

where μ = permeability of the solid material through which the magnetic lines of force pass

$$\boxed{\mu = \frac{B}{H}}$$

Hence the magnetic permeability (μ) of any material is the ratio of the magnetic induction in the sample to the applied magnetic field intensity.

Relative permeability,

$$\boxed{\mu_r = \frac{\mu}{\mu_o}}$$

The intensity of magnetization (M)

The intensity of Masgnetisation of a sampkle of a material is the magnetic moment per unit volume.

Unit : A/m

M & H are related by magnetic succeptibility x.

$$x = \frac{M}{H}$$

Magnetic Susceptibility (x) :

Magnetic susceptibility (x) of a material is the ratio of the intensity of magnetization produced in the sample to the magnetic field intensity which produces the magnetization. It has no units. Momentic induction (B) is given by

$$B = \mu_o (H + M)$$

Hence

$$\mu_o = \frac{B}{H+m}$$

Relative permeability, μ_r= 1 + x

Classification of Magnetic materials.

- If the atoms do not carry permanent magnetic dipoles, those materials are called diamagnetic.
- If the atoms of the material carry permanent magnetic dipoles, further classification is based on the interaction between the individual dipoles.
- If the permanent dipoles do not interact among themselves, the material is paramagnetic.
- If the interaction among the permanent dipoles is strong such that all the dipoles line up in parallel, the material is ferromagnetic.
- If the permanent dipoles line up in antiparallel direction, and are equal the material is antiferromagnetic and the magnetization vanishes.
- If the magnitudes of permanent dipoles aligned antiparallel are not equal thus exhibiting magnetization then the material is ferrmagnetic.

Different sources of permanent magnetic moment are

1. The orbital magnetic moment of the electrons.
2. The spin magnetic moment of the electrons $
3. The spin magnetic moment of the nucleus.

Properties of diamagnetic materials. :

1. Permanent dipoles are absent.
2. Effect is weak and often marked by other kinds of magnetism.
3. When placed inside a magnetic field, magnetic lines of force are repeled.
4. Magnetic susceptibility is negative.
5. Magnetic susceptibility is independent of applied magnetic field strength.
6. Relative permeability is slightly less than unity.

Properties of paramagnetic materials. :

1. They posses permanent magnetic dipoles.
2. These dipoles are non-interacting
3. The dipoles are randomly oriented and hence in the absence of external applied magnetic field, the net magnetization in any given direction is zero.
4. When placed inside a magnetic field, it attracts the magnetic lines of force.
5. Paramagnetic succeptibility is positive and depends greatly on temperature.

Bohr Magneton :

When the atom is placed in a magnetic field, the orbital magnetic moment of the electrons is quantized.

A quantum of magnetic moment of an atomic system is known as Bohr magneton.

$$\mu_B = \frac{eh}{4\pi m}$$

Curie Law :

Langevin showed that classical paramagnetic susceptibility (x) due to the alignment of magnetic moments along field direction is given by

$$x = \frac{h_o N \mu^2}{3kT} = \frac{C}{T}$$

where C = Curie constant and the relation is known as Curie Law

Curie – Weiss Law :

Ferromagnetic materials exhibit spontaneous magnetization below a characteristic temperature called the ferromagnetic curie temperature. Above this temperature, the substance becomes paramagnetic and obey Curie – Weiss Law.

$$x = \frac{C}{T-\theta}$$

where c is Curie constant

q is paramagnetic Curie temperature

Heisenberg theory of Ferromagnetism :

The molecular field based on simple dipole – dipole interaction was found to be less and hence cannot account for the existence of ferromagnetism.

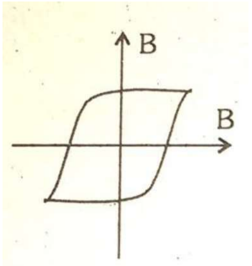
Heisenberg removed this discrepancy by assuming the quantum exchange interaction between the electrons spins instead of dipole – dipole interaction.

Domain theory of ferromagnetism :

According to Weiss, a virgin specimen of ferromagnetic material consists of a number of regions or domains which are spontaneously magnetized due to parallel alignment of all magnetic dipoles. The direction of spontaneous magnetization varies from domain to domain.

Hysteresis in magnetic materials :

The hysteresis of ferromagnetic material refers to the log of magnetization behind the magnetising field. It is irreversible B-H characteristic curve of ferromagnetic or ferromagnetic materials.



Hysteresis loss :

Hysteresis loss is the loss of energy in taking a ferromagnetic body through a complete cycle of magnetization. This loss is represented by the area enclosed by the hysteresis loop.

Properties of hard and soft magnetic materials.

Properties	Hard	soft
1. Area of hysteresis loop	Large	Small
2. Hysteresis loss	Large	Small
3. Domain wall movement	Difficult	Relatively earlier
4. Coercivity	Large	Small
5. Retentivity	Large	Small
6. Magnetization & Demagnetization	Not easy	Easy
7. Magnetostatic energy	Large	Small
8. Permeability & Susceptibility	Small	Large
9. Type of magnet that could be made	Permanent magnet	Electro-magnets

Antiferromagnetism :

In antiferromagnetism, electron spin of neighbouring atoms are aligned antiparallel. Anti-ferromagnetic susceptibility is small and positive and it depends greatly on temperature.

Ferrites :

In a material of the magnitudes of permanent dipoles aligned antiparallel are not equal, such an uncompensated antiferromagnetism is known as ferrimagnetism and the corresponding materials are said to be ferromagnetic or ferrites.

Applications of Ferrites :

1. They are used in transformer cores for high frequencies upto microwaves.
2. They are used in radio receivers to increase the sensitivity and selectivity of the receiver.
3. Ferrites are used in digital computers and data processing circuits as magnetic storage elements.
4. They are used as isolator.

uses in Transformer cores :

Ferrites are used as transformer cores for frequencies upto microwaves. This is because the eddy current problem preventing penetration of magnetic flux into the material is much less severe in ferrites than in iron.

Magneto Resistance Effect :

In some magnetically soft materials the electrical resistance changes when the material is magnetized. The resistance goes back to its original value when the magnetizing field is turned off. This effect is called magneto resistance effect.

Importance of magnetic materials :

Magnetic materials used for high density data storage. some materials are easily magnetized when placed in a weak magnetic field. When the field is turned off, the material rapidly demagnetizes. These materials are called soft magnetic materials.

In Hard magnetic materials through strong field is required for magnetization, they retain their magnetization even on removal of the field.

In some materials, the electrical resistance varies on magnetization. This effect is called Magneto Resistance Effect.

These effects are utilized in manufacture of magnetic recording heads for write and read the date for storage and retrival.

Basic parts of a digital magnetic – tape system :

i) Magnetic tape : Flexible plastic tape with their ferromagnetic material coating.

ii) Tape Transport : Mechanism to run the tape part the recording / reading head.

iii) Translators : Electronic part to convert given analog signal into digital for recording purposes and digital into analog for reading purposes.

iv) Reading / writing Heads : Magnetic read / write heads to record / retrieve the data in / from the magnetic tape.

v) switching and buffering equipment : This is to select the correct tape mechanism and to provide tasks such as winding /rewinding of the tape etc.

Bubble storage :

Data can be stored in this crystals of canted antiferromagnetic oxides ($B_aFe_{12}O_{19}$, $YFeo_3$), or in amorphous alloyed films (Gd-Co, Gd-Fe), or in ferromagnetic materials such as Yttrium –iron – garnet ($Y_3Fe_5O_{12}$). They are tiny cylindrical regions called bubbles (as small as 1 mm in diameter) having a reversed momentisation compared to the matrix.

Hole burning :

The recording medium consists of an inert crystal host (such as Y_2SiO_5 with a low concentration of rare-earth impurity ions (such as Eu^{3+}) distributed randomly.

Information is stored in the impurity ions by absorption of light resulting in a mechanism called hole burning.

Stimulated echo ;

The recorded information is retrieved by a mechanism called the stimulated echo-when the recorded crystal is illuminated by another lager beam called the read pulse, coherent radiation is emitted from the already recorded impurity ion. This phenomenon is called stimulated echo.

Dielectrics :

Dielectrics are insulating materials. In dielectrics all the electrons are bound to their parent molecules and there are no free charges. Even with normal voltage or thermal energy, electrons are not released. Dielectrics are non-metallic materials of high specific resistance and have negative temperature coefficient of resistance.

Dielectric constant 'ε_r' :

The dielectric characteristics of a material are determined by the dielectric constant or relative permittivity 'ε_r'. Of that material. It is the ratio between the permittivity of the medium and the permittivity of free space.

$$\varepsilon_r = \frac{\varepsilon}{\varepsilon_o}$$

ε_r has no unit.

It is a measure of polarization in the dielectric material.

Electric Plarization :

Let us consider an atom placed inside an electric field. The centre of positive charge is displaced along the applied field direction while the centre of negative charge is displaced in the opposite direction. Thus a dipole is produced. When a dielectric material is placed inside an electric filed such dipoles are created in all the atoms inside. This process of producing electric dipoles which are oriented along the field direction is called polarization in dielectrics.

Polarizability (α) :

When the strength of the electric field E is increased the strength of the induced dipole also increases. Thus the induced dipole moment is proportional to the intensity of the electric field.

i.e. $\mu = \alpha$ E

where α , the constant of proportionality is called polarizability.

Electric flux density (D) :

The electric flux density D at a point in a material is given by

$D = \varepsilon_r \varepsilon_o E$

where E is the electric field strength.

e_o – dielectric constant or permittivity of free space (vacuum)

e_r – relative dielectric constant or relative permittivity of the material.

Electric Susceptibility (X_e) :

Polarization vector p can be written as

$P = \varepsilon_o X_e E$

where the constant X_e is the electric susceptibility.

There $X_e = \frac{P}{\varepsilon_o E} = \frac{\varepsilon_o (\varepsilon_r - 1)E}{\varepsilon_o E}$

∴ $X_e = (\varepsilon_r - 1)$

Polarization process ;

Polarization occurs due to several atomic mechanisms. when the specimen is placed inside a d.c. electric field, polarization is due to four types of processes.

a) electronic polarization
b) ionic polarization
c) orientation polarization &
d) Space charge polarization

Electronic polarization :

The displacement of the positively charged nucleus and the electrons of an atom in opposite directions on application of an electric field is called electronic polarization.

Dielectric loss ;

When a dielectric material is subjected to the a.c. voltage, the electrical energy is absorbed by the material and is dissipated in the form of heat. This dissipation of energy is called dielectric loss.

Loss angle :

In a perfect insulator polarization is complete during each cycle and there is no consumption of energy and the charging current leads the applied voltage by 90° But for commercial dielectrics this phase angle is less then 90° by an angel δ called dielectric loss angle. Tan δ is taken as measure of dielectric loss and is known as loss tangent.

Also $\tan\delta = \frac{\varepsilon_r''}{\varepsilon_r'}$

Dielectric brak down :

When a dielectric material loses its resistivity and permits very large current to flow through it, then the phenomenon is called dielectric breakdown.

Different dielectric breakdown mechanisms :

i) Intrinsic breakdown
ii) Thermal breakdown
iii) Discharge breakdown
iv) Electrochemical breakdown
v) Defect breakdown

Piezoelectrics and pyroelectrics are the two active dielectrics.

Piezoelectrics such as Barium titanate ($B_a T_i O_3$), Pottassium dihydrogen phosphate (KPP), Lithium Niobate ($LiNbO_3$) are used for making pressure transducers, ultrasonic transducers and microphones. Pyroelectrics such as Barium titanate (BaTiOe), Triglycine suplhate (TGS) and Lithium Niobate ($LiNbo_3$) are used to make high sensitive infrared detectors.

Requirement of good insulating materials ;

i) high electrical resistivity
ii) high dielectric strength
iii) Sufficient mechanical strength to withstand vibration &
iv) good heat conducting property

Classification of insulating materials ;

a) Solid insulating materials
b) Liauid insulating materials
c) Gaseous insulating materials

a) Solid insulating materials :

1. Mica
2. Ceramics

3. Asbestos
4. Rubber
5. PVC materials

b) Liquid insulating materials :

i) Mineral insulating oil,
 1. Transformer oil
 2. Cable oil
 3. Capacitor oil
ii) synthetic insulating oil
iii) Miscellaneous insulating oils
 1. Vegetable oil
 2. Vaseline
 3. Silicon liquids

c) Gaseous insulating materials :

i) Air
ii) Nitrogen
iii) Inert gases
iv) Sulphur hexafluoride

Important applications of dielectric materials:

i) Electical conductors made of aluminium or copper which are used for electric wiring are insulated with a outer jacket of plastic or rubber.

ii) In heater coils ceramic beads are used to avoid short circuiting as well as to insulate the outer body from electric current.

iii) In electric iron, mica or asbestos insulation is provided to prevent the flow of electric current to the outer body of the iron

iv) In transformers as well as in motor and generator windings vanished cotton is used as insulator.

Condensed Matter Physics

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Lecture - 36
Semiconductors

We will start a discussion of semiconductors one of the most important class of materials in solids which have a wide range of technological application. In fact progress in semiconductor technology has revolutionized the area of modern electronics. Semiconductors are materials, which have electrical conductivities, as it is obvious from the name lying between the electrical conductivity of a good conductor like a metal and a perfect insulator.

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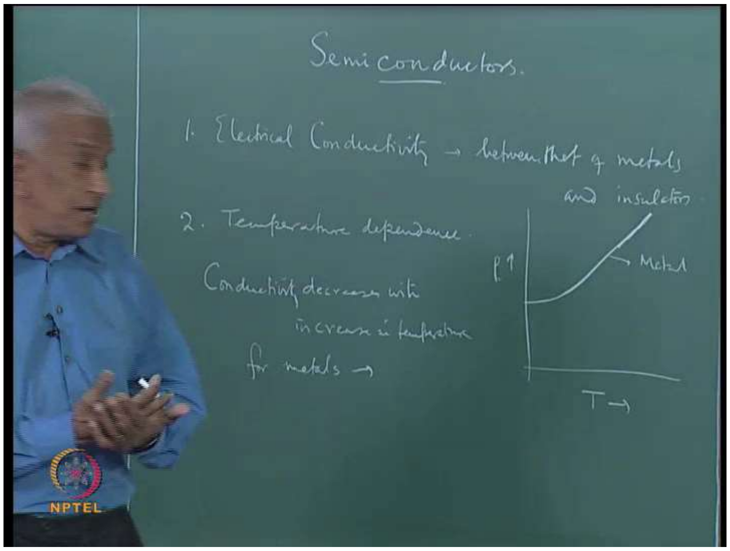

So, conductivities - electrical conductivity between that of metal and insulators.

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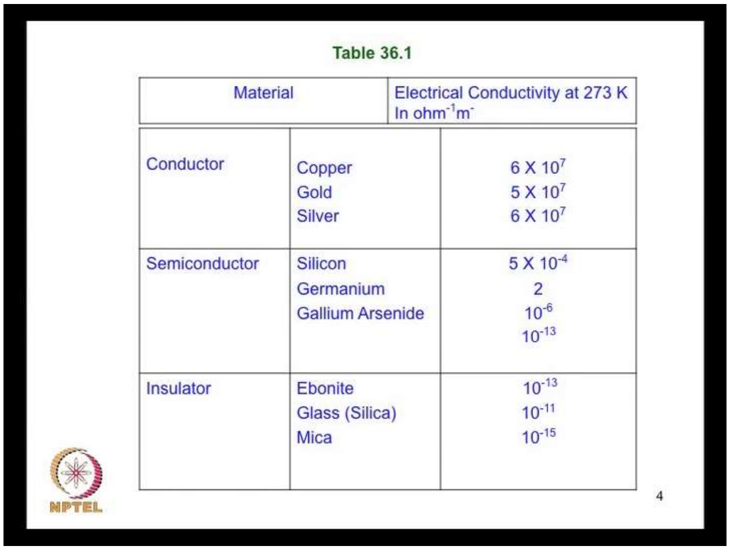

Table 36.1

Material		Electrical Conductivity at 273 K In ohm^{-1}m^{-}
Conductor	Copper Gold Silver	6 X 10^{7} 5 X 10^{7} 6 X 10^{7}
Semiconductor	Silicon Germanium Gallium Arsenide	5 X 10^{-4} 2 10^{-6} 10^{-13}
Insulator	Ebonite Glass (Silica) Mica	10^{-13} 10^{-11} 10^{-15}

For example, we have given in table form. The conductivities of good conductors such as copper, gold and silver; insulators like ebonite, glass and mica; and semiconductors - the standard semiconductors are silicon, germanium and gallium arsenide. The electrical conductivity values at 0 degree Celsius or 273 Kelvin is given in the last column, and it is clear that the conductors have conductivity values of which are very high compared to those a semiconductor which in turn are very high compared to those are insulators. So, the electrical conductivities spans something like from the 18, 19 orders of magnitude among common materials. So, this is a very remarkable variation that is the first feature.

The second feature is that you have a temperature dependence of the electrical conductivity or resistors. We all know that indicates of a metal, electrical resistance versus temperature is linear and then becomes non-linear and become this is for a metal. So, it has a linear variation and then the resistivity decreases with temperature; as the temperature is decrease, the resistivity decreases. So, you see that the resistivity increases, therefore the conductivity decreases electrical conductivity decreases decreases with increasing temperature for a metal, so there are said to have the resistivity increases. Whereas in the case of a semiconductor conductivity increases with increasing temperature.

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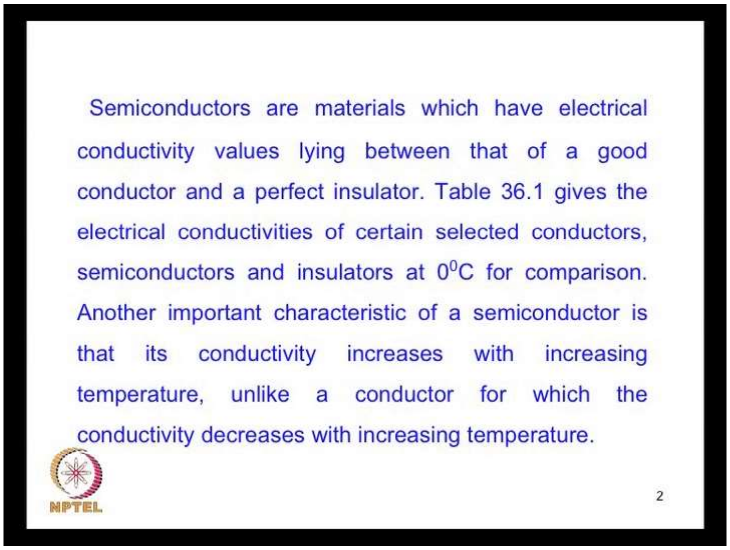

Semiconductors are materials which have electrical conductivity values lying between that of a good conductor and a perfect insulator. Table 36.1 gives the electrical conductivities of certain selected conductors, semiconductors and insulators at 0^0C for comparison. Another important characteristic of a semiconductor is that its conductivity increases with increasing temperature, unlike a conductor for which the conductivity decreases with increasing temperature.

Unlike whereas, semiconductor conductivity increases, so this is called a positive temperature coefficient. So, this has a positive temperature coefficient of resistance. So, this is known as ptc. Whereas, the metals is known as ntc, it has a negative temperature coefficient. So, this is another important difference between the behavior way temperature variation of the conductivity of a semiconductor versus that of a metal.

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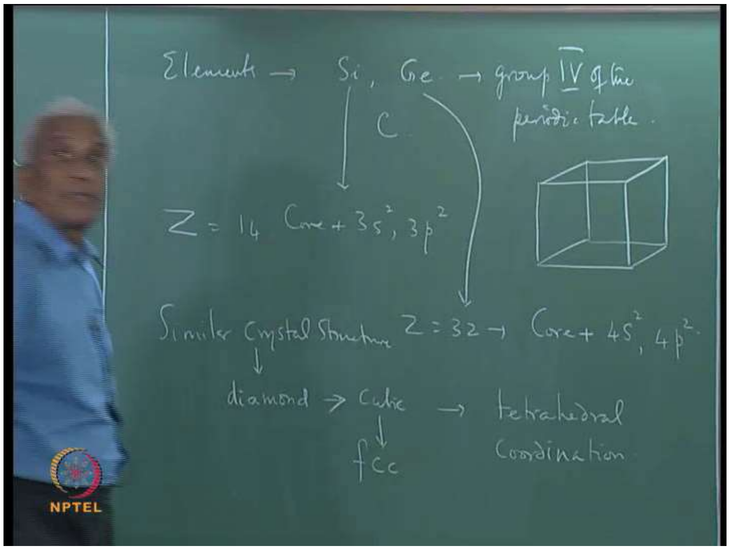

Now, what are semiconductors? The typical semiconductor elements are as I already mentioned silicon and germanium. Both these elements belongs to the group four of the periodic table. Another important element, which form is in the group four is carbon. So, carbon, silicon, germanium have identical electronic configuration. And this is the reason why all of them behave like semiconductors. For example, silicon has an atomic number fourteen, therefore, it has an electronic configuration in which there are four electron with outermost 3S 2 core plus 3S 2 and 3P 2 electrons.

Germanium has an atomic number of 32, germanium has an atomic number of 32 and that as an electron configuration which is 4 s 2 and 4 p 2. Essential thing is this is the 3 s and 3 p shell this is 4 s and 4 p shell, but in both cases the s and p outermost s and p shall are occupied by 2 electrons each. So, that is why the electron configurations are similar. So, that is why there has similar physical and chemical properties, they have indeed similar crystal structure. In fact, it is also similar to that of carbon, but in its form as diamond. So, this crystal structure is that of diamond which is nothing but carbon, so the diamond has a cubic crystal structure. So, this diamond structure is shown in a picture.

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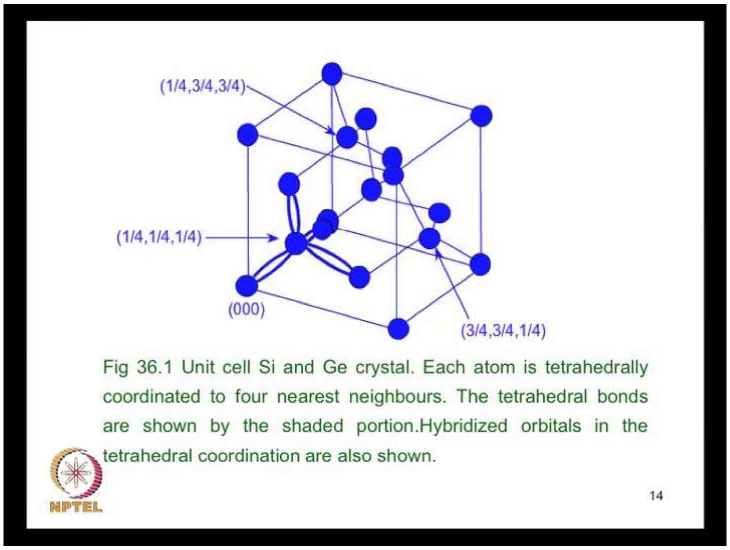

Fig 36.1 Unit cell Si and Ge crystal. Each atom is tetrahedrally coordinated to four nearest neighbours. The tetrahedral bonds are shown by the shaded portion.Hybridized orbitals in the tetrahedral coordination are also shown.

So, figure shows the unit cell of silicon and germanium crystal. In this, we will discuss this in great detail, but this is the main feature. Each atom of silicon is tetrahedrally coordinate, have a cube and each atom of silicon is tetrahedrally coordinated, auto four near neighbor - tetrahedrally coordinates. Tetrahedron means the near neighbor is 4. So, each silicon is coordinated to 4 near neighbor silicon. So, there are tetrahedral bonds which are shown by shaded portions.

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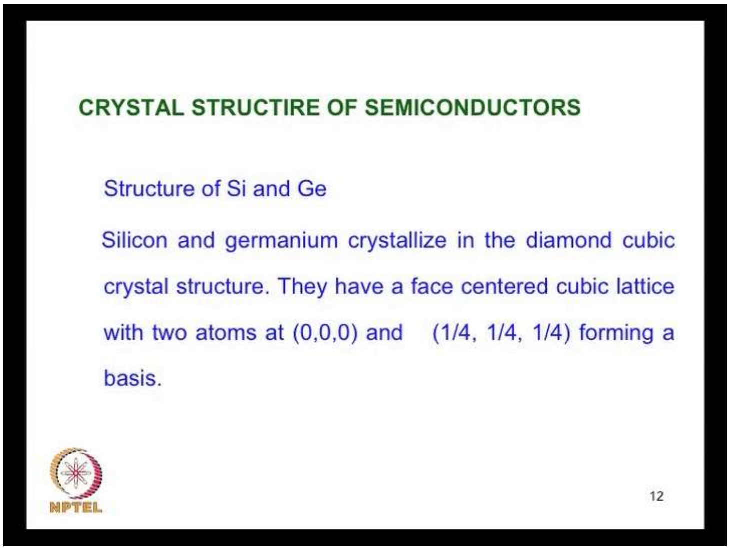

CRYSTAL STRUCTIRE OF SEMICONDUCTORS

Structure of Si and Ge

Silicon and germanium crystallize in the diamond cubic crystal structure. They have a face centered cubic lattice with two atoms at (0,0,0) and (1/4, 1/4, 1/4) forming a basis.

So, this structure is basically a face centered cubic – FCC. What does it mean that; that means, that there are times not only here, but all so at the face centred, and it is these are atoms which are tetrahedrally coordinate. So, the basis is a simple cubic lattice with two molecules in the unit cell one here and another at one-forth, one-fourth, one-forth. These are the two atoms, which form the basis, so this is what gives you the tetrahedral coordination. So, the tetrahedral mean the angle is 109 degrees 46 minutes.

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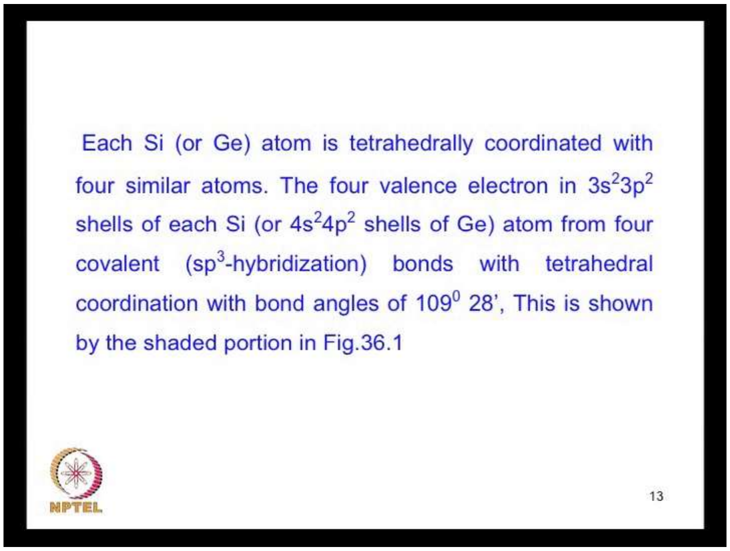

Each Si (or Ge) atom is tetrahedrally coordinated with four similar atoms. The four valence electron in $3s^2 3p^2$ shells of each Si (or $4s^2 4p^2$ shells of Ge) atom from four covalent (sp^3-hybridization) bonds with tetrahedral coordination with bond angles of 109^0 28’, This is shown by the shaded portion in Fig.36.1

So, these bonds are shown, basically what is happening is that you have two electrons here, one of these get electrons get promoted.

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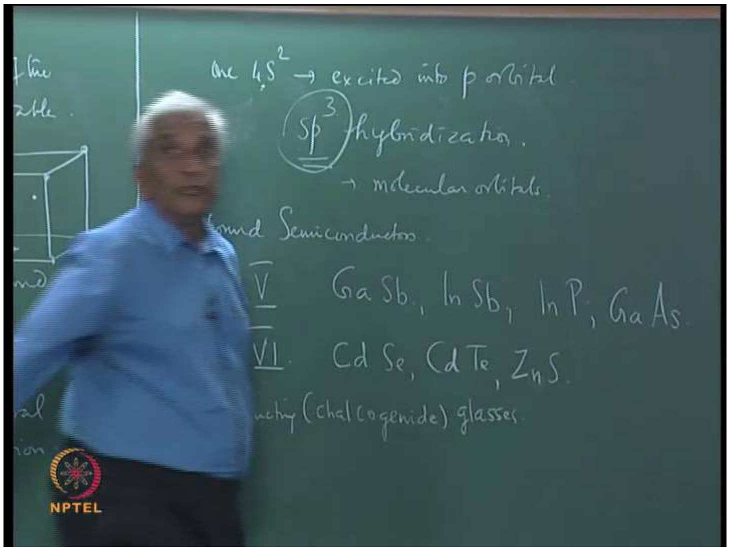

In the molecular orbital picture of the bond formation, you have one 4 S 2 electron excited into P orbital, and then you have one electron here 4 s 1. And then you have three electron and forming on S p 3 hybridization that is this electron which is excited joints with these and you have this electron with three electrons in the p shell including the one electron which is excited into the p shell. And you have the remaining electron and 3 p electrons combine together to form S P 3 hybridized molecular orbital. These are the ones; we form covalent bonds, which are shown by the shaded region in the figure.

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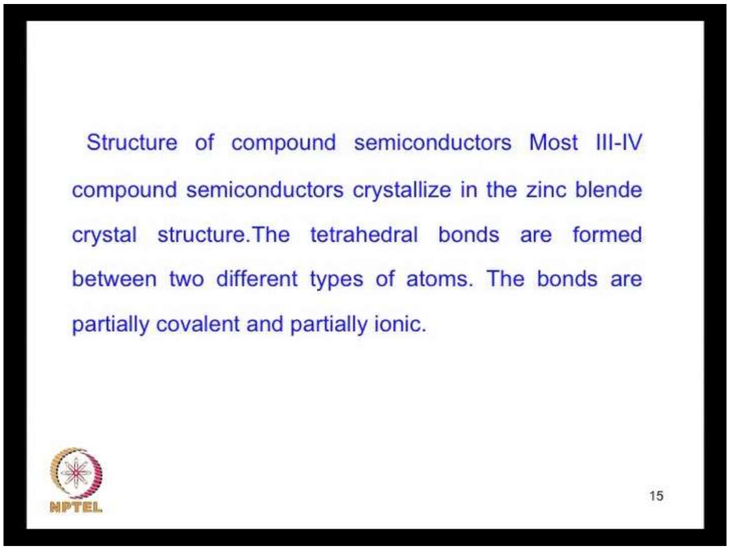

Structure of compound semiconductors Most III-IV compound semiconductors crystallize in the zinc blende crystal structure.The tetrahedral bonds are formed between two different types of atoms. The bonds are partially covalent and partially ionic.

This is also the case with most compounds semiconductors, the compound semiconductors are formed by combining a group three element with a group five element or a group two element with a group six element.

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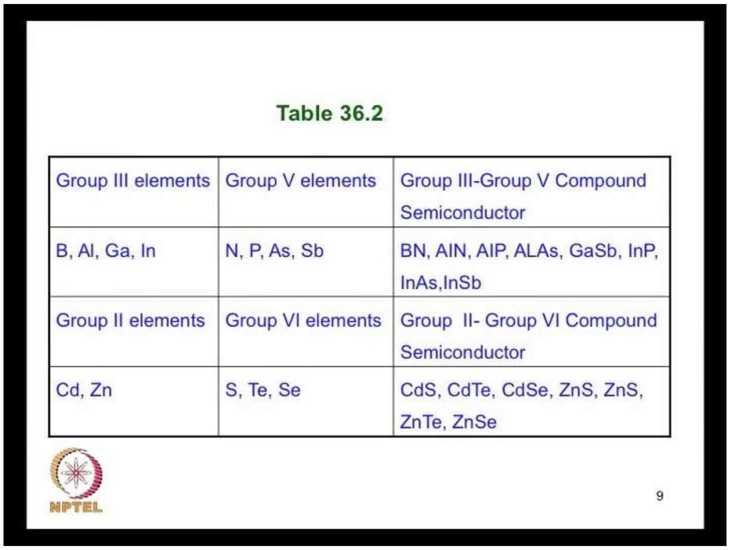

Table 36.2

Group III elements	Group V elements	Group III-Group V Compound Semiconductor
B, Al, Ga, In	N, P, As, Sb	BN, AlN, AlP, ALAs, GaSb, InP, InAs,InSb
Group II elements	Group VI elements	Group II- Group VI Compound Semiconductor
Cd, Zn	S, Te, Se	CdS, CdTe, CdSe, ZnS, ZnS, ZnTe, ZnSe

So, both are compound semiconductors. The table shows these. So, you have group two elements and group three elements and group five elements giving you things like gallium, antimonite, indium, antimonite and so on. Indium phosphate, gallium arsenide things like that, so these are all three-five compounds. In the other case two six compounds it is materials like cadmium selenite, cadmium telluride and so on, zinc sulphide, usually sulphur selenium, tellurium form the sixth group, so cadmium, zinc etcetera are in the second group. So, forming compounds of this kind, so these are the two-six compound semiconductors. These also have similar crystal structure.

You also have classes the compound semiconductors prepared in glass c form chalcogens, the sulphur selenium solarium are known as chalcogens and therefore, these are known also has chalcogenide glasses. So, preparing glassy form they are the class called the semiconducting glasses they have also acquired a lot of technological importance. So, that is regarding the basic structure and basic chemistry chemical and nature of these various kinds of semiconductor now we also have two important classes of semiconductors.

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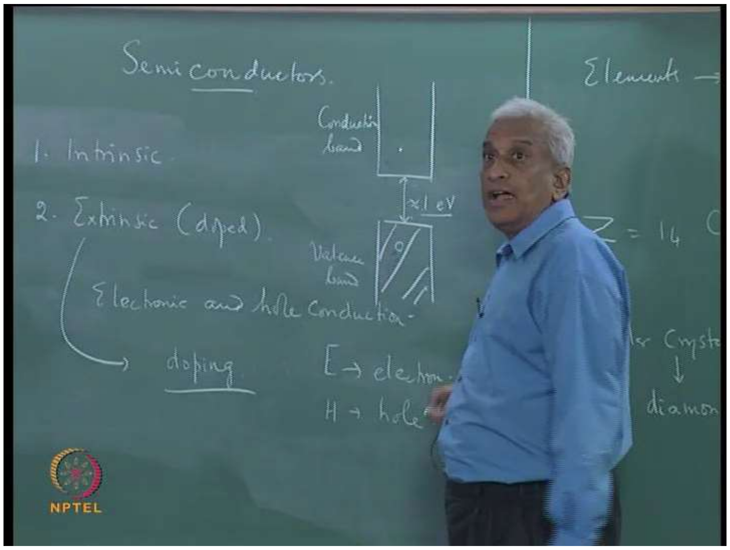

There are one is known as intrinsic semiconductor, second-class is extrinsic or doped semiconductor, because we have seen from our discussion of the energy band structure that the band structure electronic structure consist of an occupied valence band and an unoccupied conduction band, and the energy gap is rather low it is of the order of one electron volt say. So, the energy gap is such that it is sufficiently small for carriers to be a as already discuss, carriers can be excited across this the energy gap even thermally by at sufficiently high temperatures.

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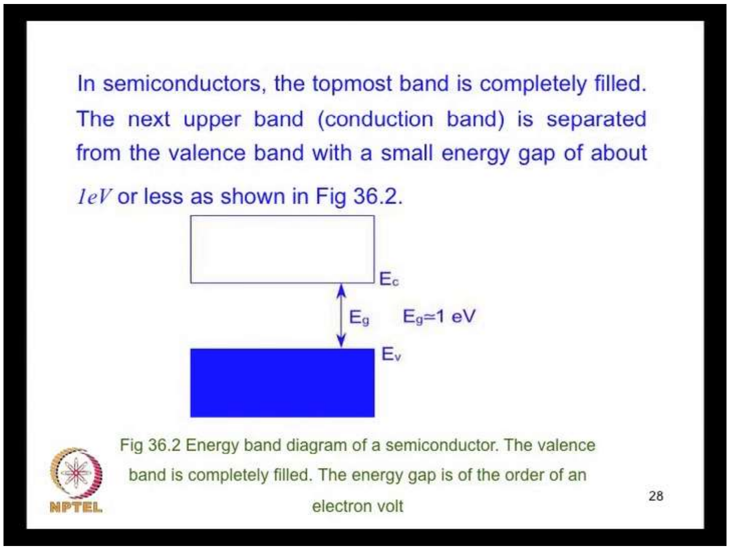

In semiconductors, the topmost band is completely filled. The next upper band (conduction band) is separated from the valence band with a small energy gap of about $1eV$ or less as shown in Fig 36.2.

Fig 36.2 Energy band diagram of a semiconductor. The valence band is completely filled. The energy gap is of the order of an electron volt

For example, room temperature and above, the carriers can be excited thermally some of the carriers. So, the intrinsic conductivity depends on the thermal activation of these carriers across the energy gap. So, then there are is an electron excited into the empty conduction band and a hole left behind in the valence band. Both the electron and hole move in opposite direction producing conduction. So, you have an electronic conduction and if hole conduction in a semiconductor, this is another major difference.

So, you have electronic and hole conduction; how do we know this we know these by performing hall effect measurements. This is why in an intrinsic semiconductor, the conduction is produced thermally or by natural means automatically without doing anything by just thermal activation. Whereas, in the case of an extrinsic semiconductor, the electrical properties are controlled by adding impurities in extremely small concentration, so you call that doping, controlled impurities in an extremely pure material. Specific impurities are added we will discuss this later in detail.

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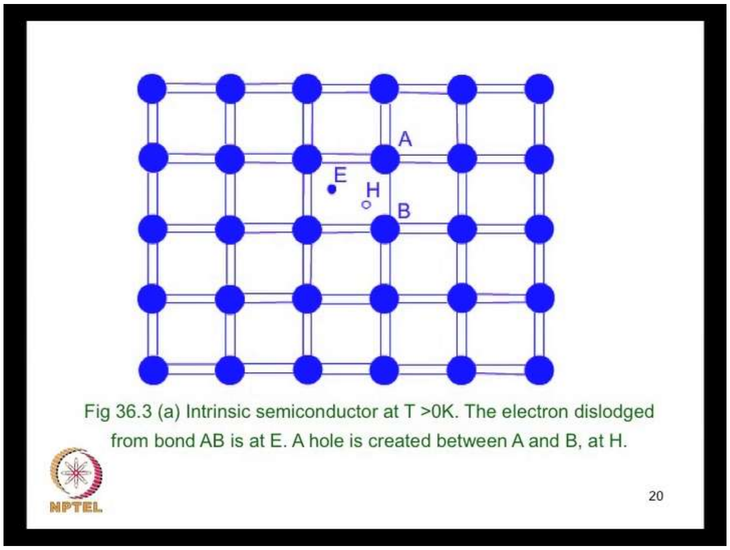

Fig 36.3 (a) Intrinsic semiconductor at T >0K. The electron dislodged from bond AB is at E. A hole is created between A and B, at H.

In order to understand what happened let us look at the intrinsic semiconductor at a finite temperature which is above 0 Kelvin. Let us look at a particular site where there are see all the bonds here are shown by two dashes two lines. And this means the number of bonds, the number of lines is equal to the number of bonds. Now suppose we consider an electron, yes that is marked E, now because this electron has been lost by the atom A and therefore, you have only one line. So, you have what is shown here is just the tetrahedral arrangement in three dimensions is projected onto two-dimensions. So, the four tetrahedral bonds are shown schematically in this manner.

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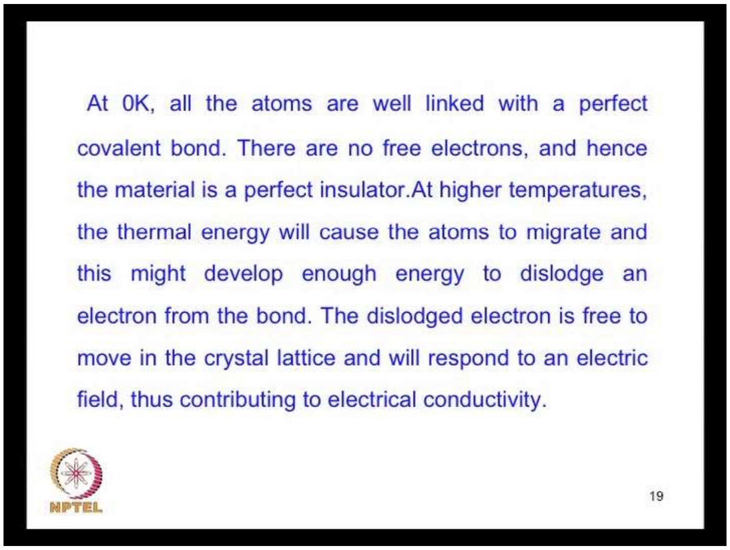

At 0K, all the atoms are well linked with a perfect covalent bond. There are no free electrons, and hence the material is a perfect insulator.At higher temperatures, the thermal energy will cause the atoms to migrate and this might develop enough energy to dislodge an electron from the bond. The dislodged electron is free to move in the crystal lattice and will respond to an electric field, thus contributing to electrical conductivity.

At 0 Kelvin all the atoms are well linked with a perfect covalent bond. And there are no free electron, there is no conduction, the semiconductor is a perfect insulator. But as the temperature is increased the thermal energy will cause the atoms to migrate. Once the electron gains enough thermal energy, it gets dislodged from this bond. So, the dislodged electron is now free to move in the crystal lattice, and this electron will now respond to an electric field, thus contributing to electrical conductivity.

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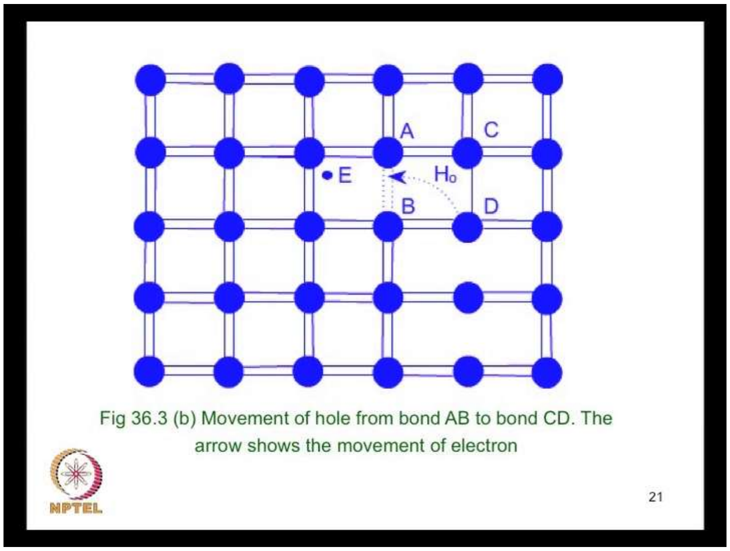

Fig 36.3 (b) Movement of hole from bond AB to bond CD. The arrow shows the movement of electron

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Now in this figure the dislodged electron where shown by the letter E. So, the bond A B as last one electron. So, it has only a single link. So, between A and B, there is a missing link or a missing electron. A missing electron is shown as a hole H by the letter H. The electron these by the letter E in the figure, while H is for hole. So, when the electric field is applied, the electron moves in the direction opposite to that of the applied field, while the hole moves in the opposite direction. Now the missing link in the bond A B may be restored, if it captures another electron from a neighboring bond and then the hole moves on to that new side.

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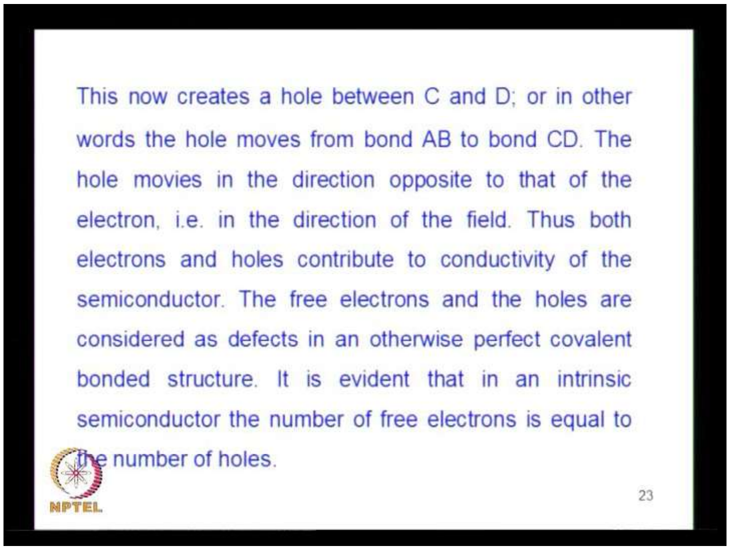

This now creates a hole between C and D; or in other words the hole moves from bond AB to bond CD. The hole movies in the direction opposite to that of the electron, i.e. in the direction of the field. Thus both electrons and holes contribute to conductivity of the semiconductor. The free electrons and the holes are considered as defects in an otherwise perfect covalent bonded structure. It is evident that in an intrinsic semiconductor the number of free electrons is equal to the number of holes.

So, this creates a hole now if it moves between c and d rather than from A and B because A B as captured an electron. So, the hole moves in the direction opposite to that of the electron it is along the direction of the field both the electrons and holes contribute to the conductivity the free electron and the holes are considered as defects in an otherwise perfect covalent bonded structure. So, in an intrinsic semiconductor the number of holes and the number of electrons are equal this is an important concept. Whereas, in the case of an extrinsic semiconductor as we already saw we have to add impurities or doped with impurities.

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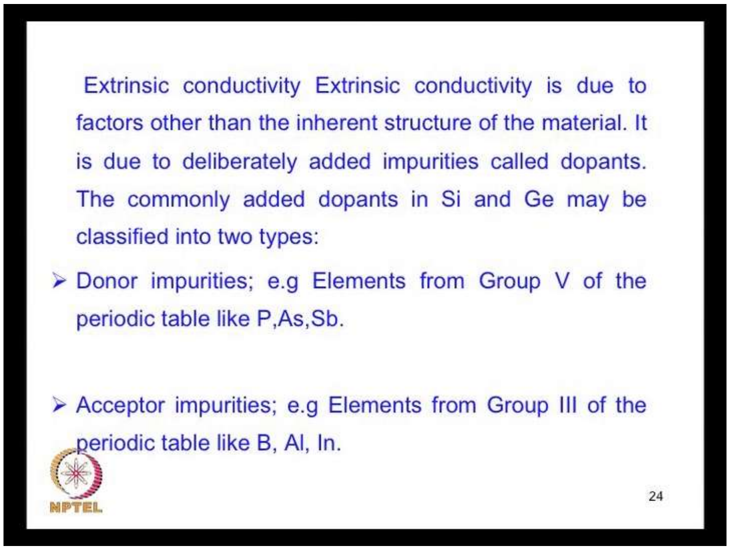

Extrinsic conductivity Extrinsic conductivity is due to factors other than the inherent structure of the material. It is due to deliberately added impurities called dopants. The commonly added dopants in Si and Ge may be classified into two types:

- Donor impurities; e.g Elements from Group V of the periodic table like P,As,Sb.

- Acceptor impurities; e.g Elements from Group III of the periodic table like B, Al, In.

Now, the impurities can be of two types. The impurities which are added can be either donor impurities or acceptor impurities. A donor impurity is one which donates an electron for example, an element from group 5 in the periodic table, we already saw these elements like phosphorus, arsenic and tumanic; whereas, acceptor impurities are one which are from an element from group 3 such as bismuth, aluminum, indium. So, these are added in extremely small quantities in at the part per million.

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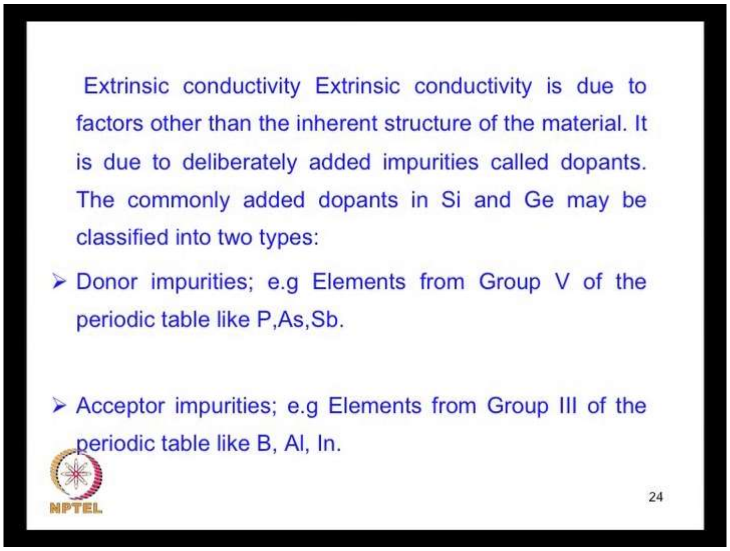

Extrinsic conductivity Extrinsic conductivity is due to factors other than the inherent structure of the material. It is due to deliberately added impurities called dopants. The commonly added dopants in Si and Ge may be classified into two types:

- Donor impurities; e.g Elements from Group V of the periodic table like P,As,Sb.
- Acceptor impurities; e.g Elements from Group III of the periodic table like B, Al, In.

If it is a donor impurity, you added an electron, so it is said to give n type conductivity because it is electronic conduction since in charge on the electron is negative it is called n type semiconductors. When you doped a pure material semiconductor silicon or germanium with a controlled amount of donor impurities from group 5 of the periodic table, for example, give result in an n-type semiconductor. Whereas, if you have and acceptor, this will give me p-type semiconductor, because it accepts an electron and thus creates a hole. So, the conduction is by an excess of holes and the hole has a positive charge, it moves in the direction opposite to that of the electron in a electric field. So, this is usually from these. So, therefore, you have n-type semiconductors and p-type semiconductors.

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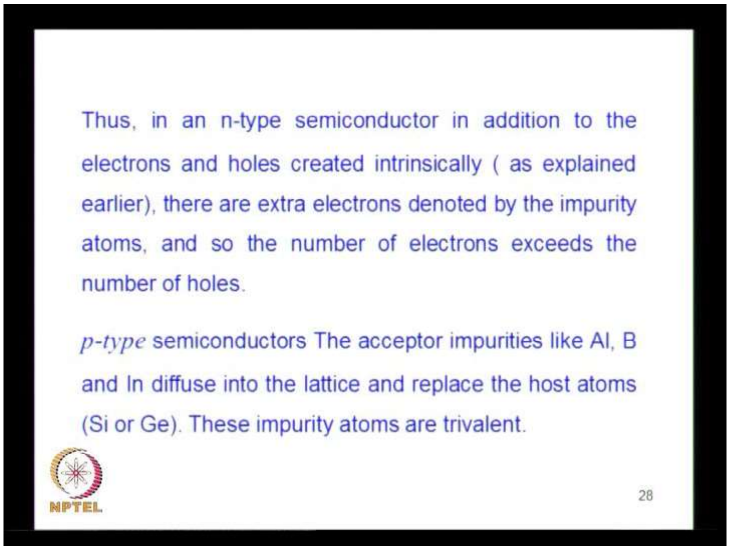

Thus, in an n-type semiconductor in addition to the electrons and holes created intrinsically (as explained earlier), there are extra electrons denoted by the impurity atoms, and so the number of electrons exceeds the number of holes.

p-type semiconductors The acceptor impurities like Al, B and In diffuse into the lattice and replace the host atoms (Si or Ge). These impurity atoms are trivalent.

So, in an n-type semiconductor, in addition to the electrons and holes which are created intrinsically by say thermal activation, there are additional electrons which are donated by the impurity atoms. And so, the number of electrons exceeds the number of holes, here n e - the electron concentration is greater than n h - the hole concentration. So, electrons are known as the majority carriers. Whereas, in a p-type semiconductor, the number of holes exceeds the number of electron, and therefore, holes are the majority carriers. Therefore, holes in an n-type material are also known as minority carriers; similarly, here the electrons are minority carriers. Each impurity atom creates a hole in the case of a p-type semiconductor, and the holes move in the direction of an applied field contributing to a hole conduction, so the number of holes exceeds that of electron. The amount of donor or acceptor impurities usually added is extremely small 10 to 100 phosphor ppm - parts per million, so that is the usual concentration. In order to do this, it is very important that we have an extremely pure basic most crystal material, silicon or germanium to which a controlled amount is added.

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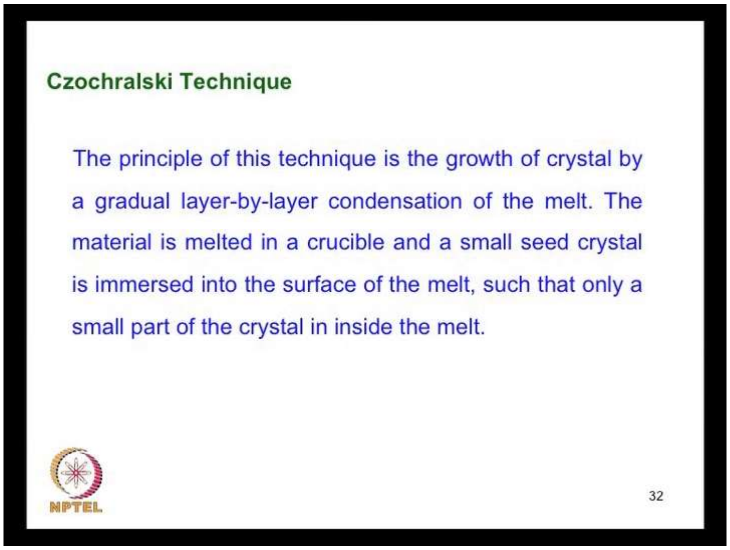

Czochralski Technique

The principle of this technique is the growth of crystal by a gradual layer-by-layer condensation of the melt. The material is melted in a crucible and a small seed crystal is immersed into the surface of the melt, such that only a small part of the crystal in inside the melt.

So, this is very important and that is why the production of semiconductors is an extremely difficult operation involving very importance techniques of crystal growth such as these Czochralski technique, zone refining and so on. We will not going to these technical aspects. So, the crystal growth crystallization of this pure semiconductor is a technology by itself.

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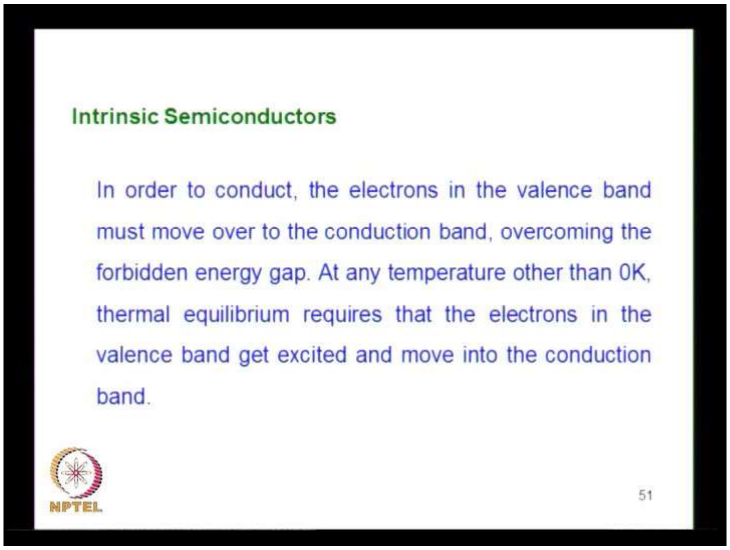

Intrinsic Semiconductors

In order to conduct, the electrons in the valence band must move over to the conduction band, overcoming the forbidden energy gap. At any temperature other than 0K, thermal equilibrium requires that the electrons in the valence band get excited and move into the conduction band.

Now if you want to understand the nature of conduction in a quantitative manner, we have two discuss a in terms of for an intrinsic semiconductor will go by carrier concentration, how to determine the carrier concentration in an intrinsic semiconductor.

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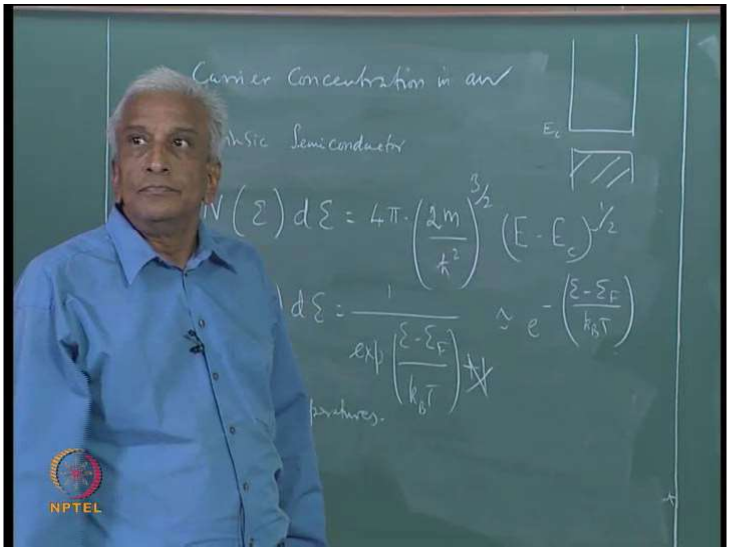

In order to know this, we have to know the number of electrons and holes. So, for this we have to go back to is so-called electron density a states.

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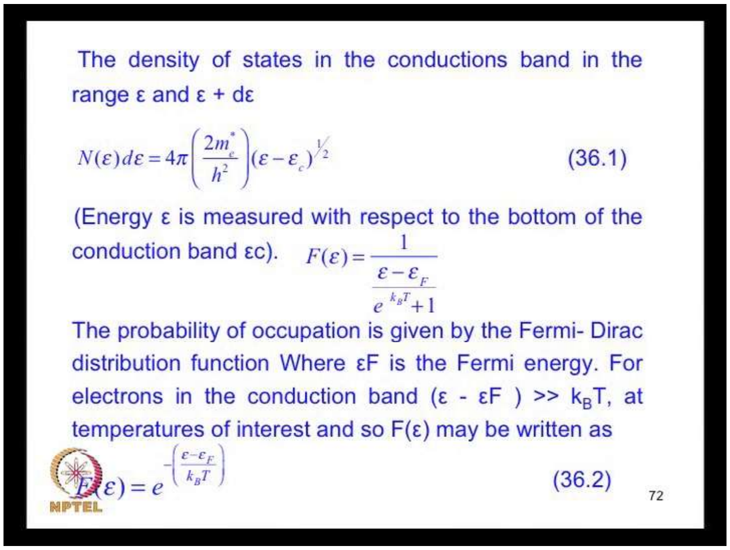

The density of states in the conductions band in the range ε and ε + dε

$$N(\varepsilon)d\varepsilon = 4\pi\left(\frac{2m_e^*}{h^2}\right)(\varepsilon-\varepsilon_c)^{1/2} \qquad (36.1)$$

(Energy ε is measured with respect to the bottom of the conduction band εc). $F(\varepsilon) = \frac{1}{e^{\frac{\varepsilon-\varepsilon_F}{k_BT}}+1}$

The probability of occupation is given by the Fermi- Dirac distribution function Where εF is the Fermi energy. For electrons in the conduction band (ε - εF) >> k_BT, at temperatures of interest and so F(ε) may be written as

$$F(\varepsilon) = e^{-\left(\frac{\varepsilon-\varepsilon_F}{k_BT}\right)} \qquad (36.2)$$

So, in order to find the concentration of carriers, we have to go to the number density of states N of e de which is 4 phi times 2 m by h cross squire to the power 3 by 2 times e minus e c to the power half this is because in the band structure of a semiconductor. This is taken off the bottom of the conduction band is taken as e and the energy is major from this, so that is why the energy term becomes e minus. In addition, we have the Fermi Dirac distribution function, which is 1 by exponential e minus e F by k B T plus 1. But at high temperatures, when the temperature is sufficiently high that e minus e F by k B T, the exponential is large compared to this. We can forget about this and this can be written as e to the power minus e minus e F by k B T combining these two expressions.

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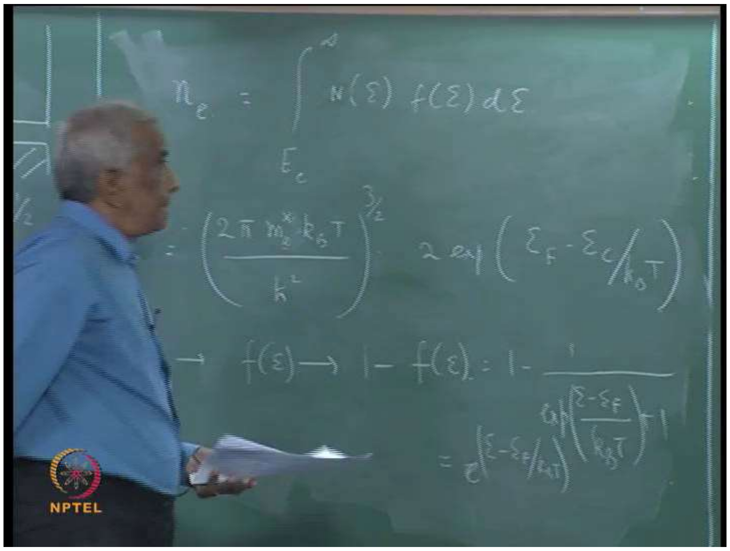

We get the expressions for the number of electrons in an energy interval e t by de and if I integrate it from E C to infinity that will give the number of electrons. So, if we carry out the integration, we arrive at the result 2 phi m k B T by h cross squire 3 power 3 by 2 into 2 exponential E F minus E C by k B T that will be the carrier concentration. Here of course, we do not write m as the mass of the free electrons since this electron e is in the periodic potential, we replace it by the m star, the effective mass. And we denote this as the effective mass of the electron by writing me star. Similarly we can calculate the hole concentration where we have to write instead of f of e should be replaced by 1 minus f of e, because this dependence on the probability of a state e not occupied or unoccupied when it is empty then the electron get in to it. And therefore, this depends on the number of vacancies, so it will be one minus f of e and that again gives you 1 minus 1 by and that will give you e to the power e minus e F by… So, they should be use in order to find the hole concentration, and we be integrate from the minus infinity to their top of the valence band, because that is where the holes exists. So, this is from minus infinity to the top of the valence band e V.

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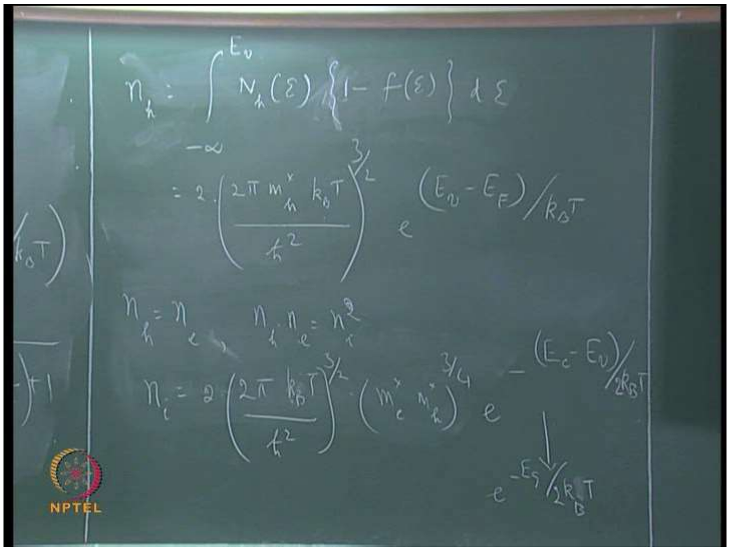

$$n_h = \int_{-\infty}^{E_v} N_h(\varepsilon)\{1 - f(\varepsilon)\}\, d\varepsilon$$

$$= 2\left(\frac{2\pi m_h^* k_B T}{\hbar^2}\right)^{3/2} e^{(E_v - E_F)/k_B T}$$

$$n_h = n_e, \quad n_h \cdot n_e = n_i^2$$

$$n_i = 2\left(\frac{2\pi k_B T}{\hbar^2}\right)^{3/2} (m_c^* m_h^*)^{3/4}\, e^{-(E_c - E_v)/2k_B T}$$

$$\downarrow$$

$$e^{-E_g/2k_B T}$$

So, n h is integral and that use the result m h star k B T y h cross square 3 by 2 into e to the power and E v minus E F by k B T. So, the number of holes and the number of electrons whenever the hole is created here then electrons gets exacted automatically. So, that number of holes at the number of electrons are equal in an intrinsic semiconductor. Therefore, n h times n e is what I call an i square in intrinsic carriers concentration, so that from these relation can find the intrinsic carriers concentration has with a bit of algebra this can be shown to be and what is C minus e v that is nothing but a energy gap. So, this becomes just exponential minus E g by 2 k B T.

Now we are taking the square root. So, we can see that the conductivity which we proportional to the carrier concentration in intrinsic carrier concentration will depend exponentially on the argument E g by 2 k B T. So, if the energy gap, which is usually as the order of one electron volt that is the energy gap. So, and the temperature 300 k, this will be the sort of this leads to the known exponential dependence as well as the known positive temperature coefficient of a semiconductor.

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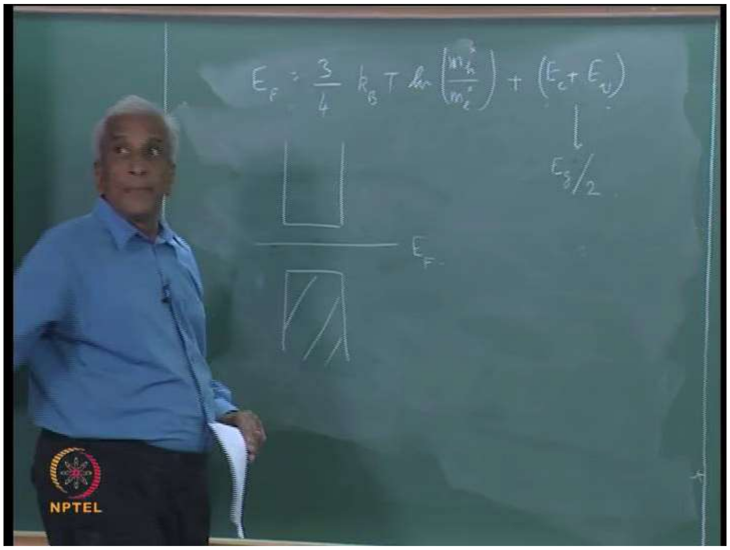

Inverting this, we can also find the Fermi energy, it turns out that the Fermi energy is three-fourth k B T m h star by m e star plus E c plus E v. If the hole and electron as the same effect you mass than this term will become 0 leaving all this and this will be E g by 2, the average of E c and E v. So, the Fermi energy lies midway between the conduction band and the valance band in a semiconductor.

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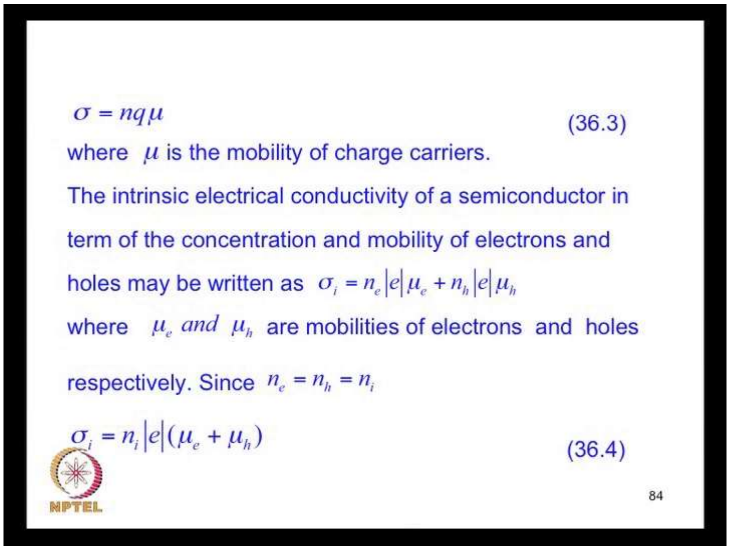

$\sigma = nq\mu$ (36.3)

where μ is the mobility of charge carriers.

The intrinsic electrical conductivity of a semiconductor in term of the concentration and mobility of electrons and holes may be written as $\sigma_i = n_e|e|\mu_e + n_h|e|\mu_h$

where μ_e *and* μ_h are mobilities of electrons and holes respectively. Since $n_e = n_h = n_i$

$\sigma_i = n_i|e|(\mu_e + \mu_h)$ (36.4)

So, the intrinsic carrier concentration goes the exponential minus E g by 2 k B T.

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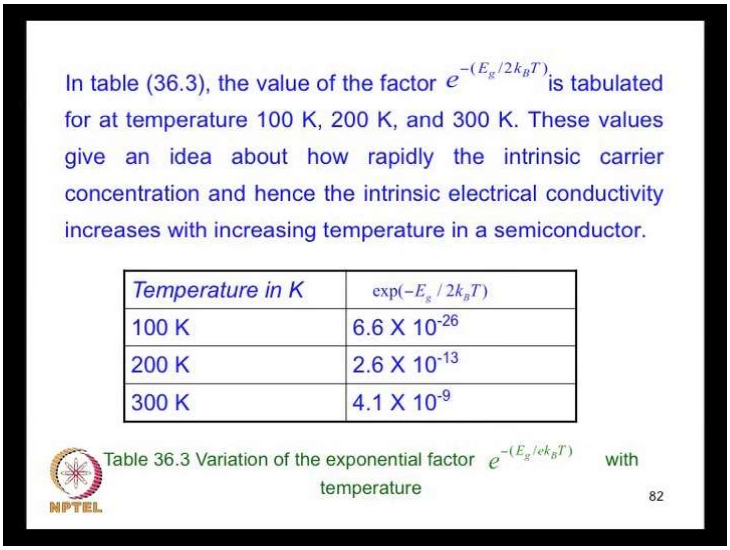

In table (36.3), the value of the factor $e^{-(E_g/2k_BT)}$ is tabulated for at temperature 100 K, 200 K, and 300 K. These values give an idea about how rapidly the intrinsic carrier concentration and hence the intrinsic electrical conductivity increases with increasing temperature in a semiconductor.

Temperature in K	$\exp(-E_g/2k_BT)$
100 K	6.6×10^{-26}
200 K	2.6×10^{-13}
300 K	4.1×10^{-9}

Table 36.3 Variation of the exponential factor $e^{-(E_g/ek_BT)}$ with temperature

This temperature dependent exponential term table shows the variation temperature dependence on the factor. So, the intrinsic electrical and conductivity will consist of two terms one involving the electron and another involving the hole. Well we can similarly in discuss the concentration of majority carriers in an extrinsic semiconductor, we will do that next time.

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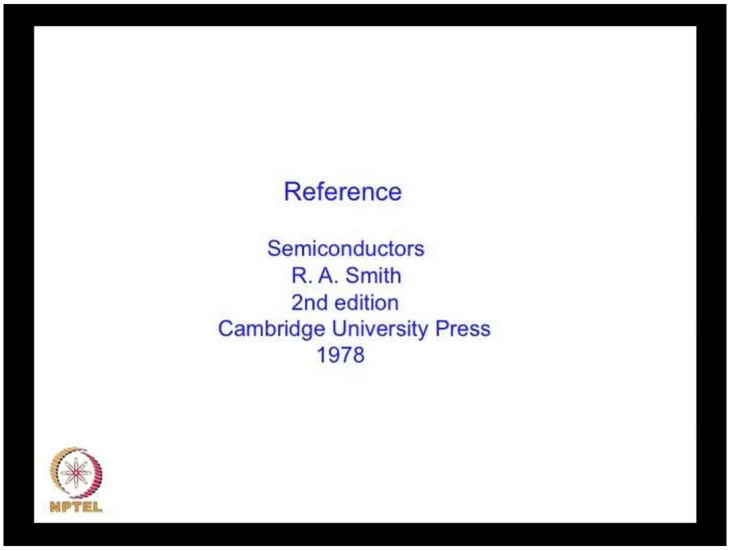

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Prof. G. Rangarajan
Department of Electrical Engineering
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Lecture - 37
Semiconductors (Continued)

Last time, we discussed the carrier concentration and conduction in intrinsic semiconductors, but the crucial thing about semiconductors is the possibility to precisely control the carrier concentrations through controlled doping of a very pure sample of semiconductor. In other words, the entire interest from the point of view of devices and semiconductor electronics is based on the fact that there exist extrinsic semiconductors contrasted with intrinsic semiconductors which we discussed last time.

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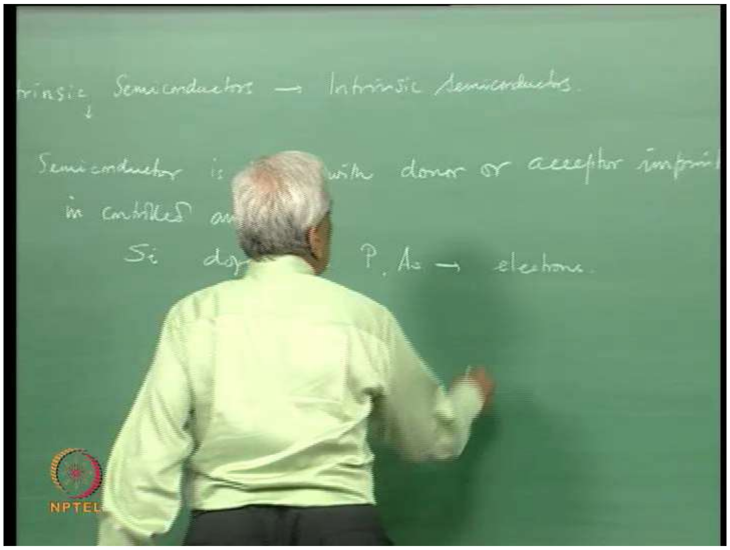

We will discussed the carrier transport in an extrinsic semiconductor in this lecture. It has already been mentioned that an extrinsic semiconductor is one in which as semiconductor, which is extremely pure is doped with donor or acceptor impurities in controlled amounts. For example, a sample a silicon is doped with an impurity like phosphorous arsenic etcetera to give a donor impurity which modifies the behavior of semiconductor completely and which gives the possibility to control this behavior and use it in various kinds of physical situations. So, similarly there can be acceptor impurities which also inject controlled amounts of holes this inject controlled amounts of electronics whereas, l acceptor impurity provides a hole.

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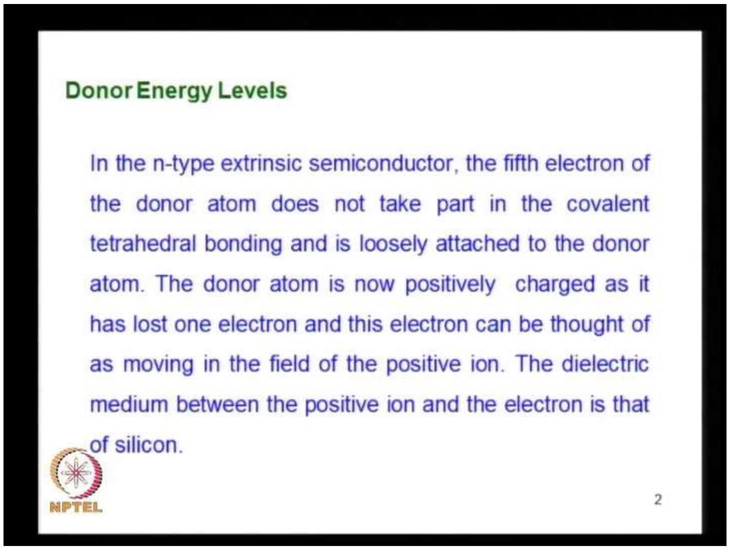

Donor Energy Levels

In the n-type extrinsic semiconductor, the fifth electron of the donor atom does not take part in the covalent tetrahedral bonding and is loosely attached to the donor atom. The donor atom is now positively charged as it has lost one electron and this electron can be thought of as moving in the field of the positive ion. The dielectric medium between the positive ion and the electron is that of silicon.

So, we will discuss this mechanism of how to calculate the carrier concentration which is the basic information required for technical exploitation of these materials.

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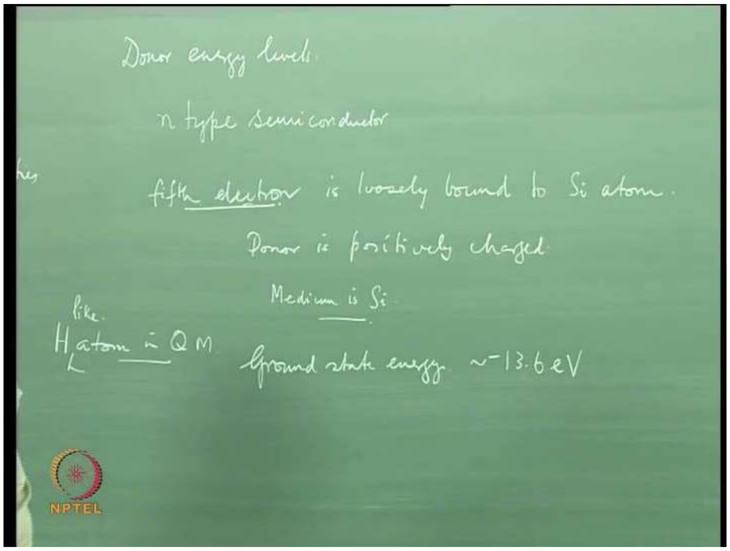

Donor energy levels.

n type semiconductor

fifth electron is loosely bound to Si atom.

Donor is positively charged.

Medium is Si.

like.

H atom in QM

Ground state energy ~ -13.6 eV

In order to do this, we will start considering the energy levels of a donor impurity in an extrinsic semiconductor this is called an n type semiconductor. So, the fifth electron in a pentavalent impurity is not able to get tetrahedral bounded to the silicon arbiters know that is because the tetrahedral bounding allows four electron. So, the fifth electron is loosely bound to the silicon atom the donor such as phosphorous or arsenic is now positively charge because it is donated on electron. This loosely bound fifth electron can be thought as moving in the never hood of this positively charged atom or ion to be more specific the dielectric medium in which this motion takes place is that of silicon. So, we consider this in the framework favor of the wee known theory of the hydrogen atom or hydrogen like atoms in quantum mechanics.

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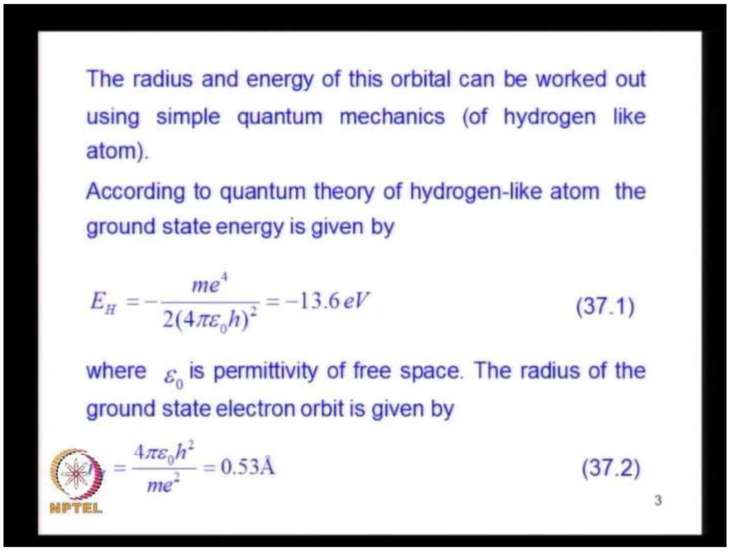

The radius and energy of this orbital can be worked out using simple quantum mechanics (of hydrogen like atom).

According to quantum theory of hydrogen-like atom the ground state energy is given by

$$E_H = -\frac{me^4}{2(4\pi\varepsilon_0 h)^2} = -13.6\,eV \qquad (37.1)$$

where ε_0 is permittivity of free space. The radius of the ground state electron orbit is given by

$$= \frac{4\pi\varepsilon_0 h^2}{me^2} = 0.53\text{Å} \qquad (37.2)$$

And borrow the results for this which is well known the ground state energy of such a hydrogen like atom is 13.6 electron volts negative because it is a binding energy and this is got from the expression minus m E to the power 4 by 2 into 4 pi epsilon naught x square. Now, in this case the moss of the electron is known to be the effective moss m star in the semiconductor and epsilon naught is replaced by the relative dielectric constant epsilon r of silica and the radius of this orbit of this electron that the radius is given by.

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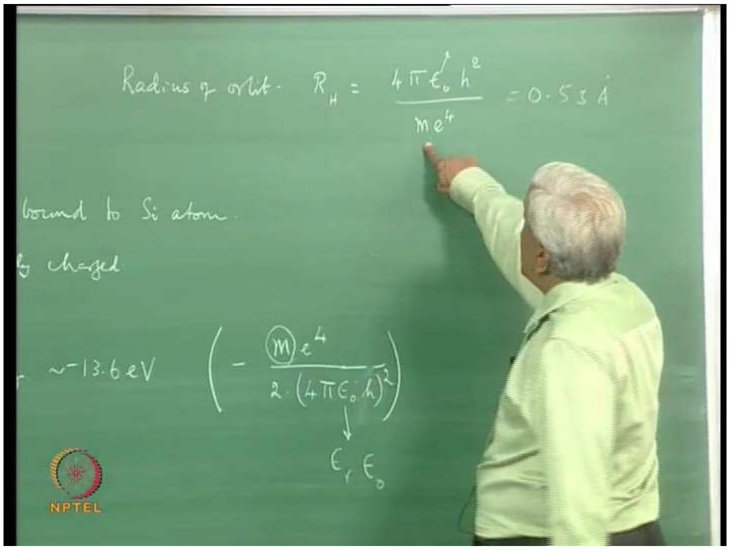

And that works out to be 0.53 in a hydrogen like atom now these things again are modified by the replacement of the dielectric permittivity by epsilon R epsilon naught, where epsilon R is the characteristic relative dielectric constant of silicon and also the replacement of m the electronic moss by the effect moss in the semiconductor.

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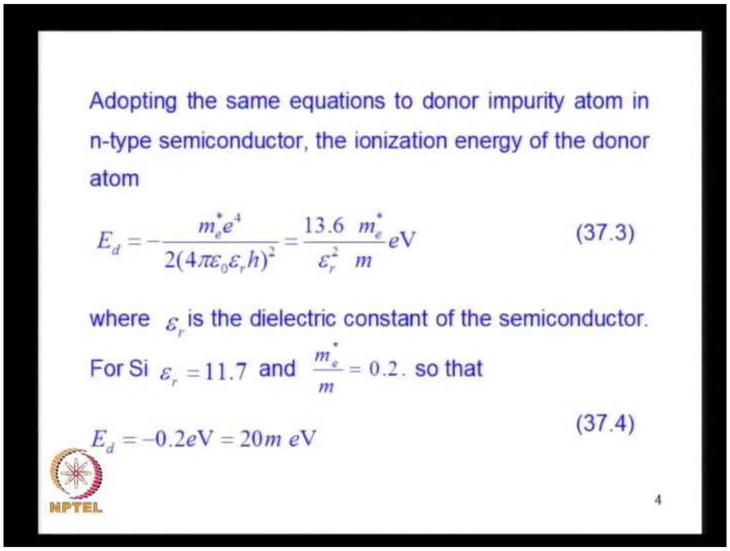

Adopting the same equations to donor impurity atom in n-type semiconductor, the ionization energy of the donor atom

$$E_d = -\frac{m_e^* e^4}{2(4\pi\varepsilon_0\varepsilon_r h)^2} = \frac{13.6}{\varepsilon_r^2}\frac{m_e^*}{m}\text{eV} \qquad (37.3)$$

where ε_r is the dielectric constant of the semiconductor.

For Si $\varepsilon_r = 11.7$ and $\frac{m_e^*}{m} = 0.2$. so that

$$E_d = -0.2\text{eV} = 20m\ eV \qquad (37.4)$$

4

So, there donor energy can therefore, be readily calculated using these expressions and using known values at the effective moss and the dielectric constant.

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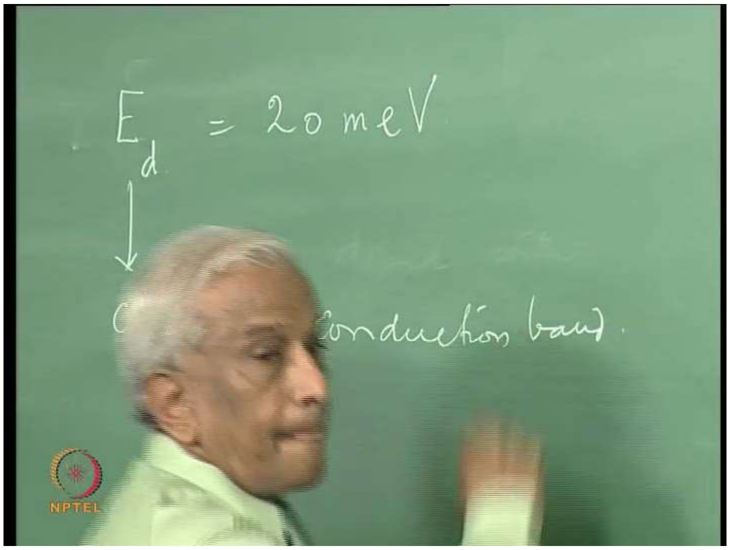

So, this works out to be E d the energy of the donor atom using the well known result for hydrogen atom the 13.6 electron volts this works out to be 20 million electron volt.

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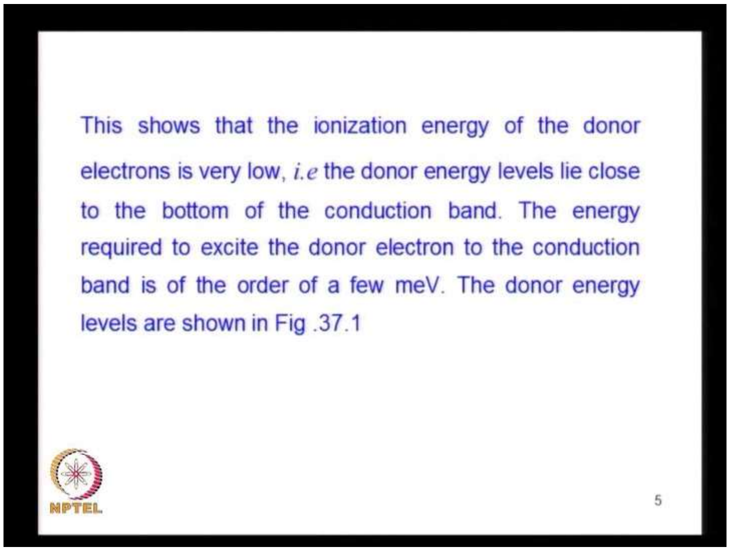

This shows that the ionization energy of the donor electrons is very low, *i.e* the donor energy levels lie close to the bottom of the conduction band. The energy required to excite the donor electron to the conduction band is of the order of a few meV. The donor energy levels are shown in Fig .37.1

Which is an extremely small quantity and the bore orbit is also rather large. So, the donor energy levels lie very close they are very close they are very close to the conduction band.

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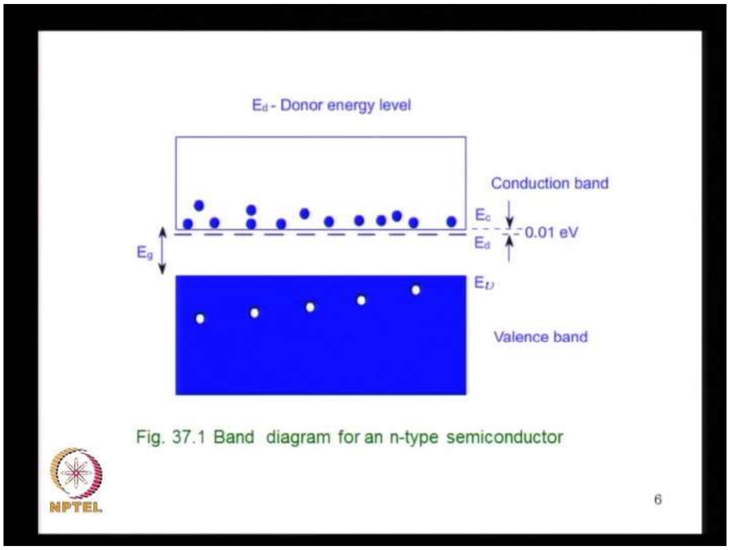

Fig. 37.1 Band diagram for an n-type semiconductor

So, this is shown in the figure you have the conduction band.

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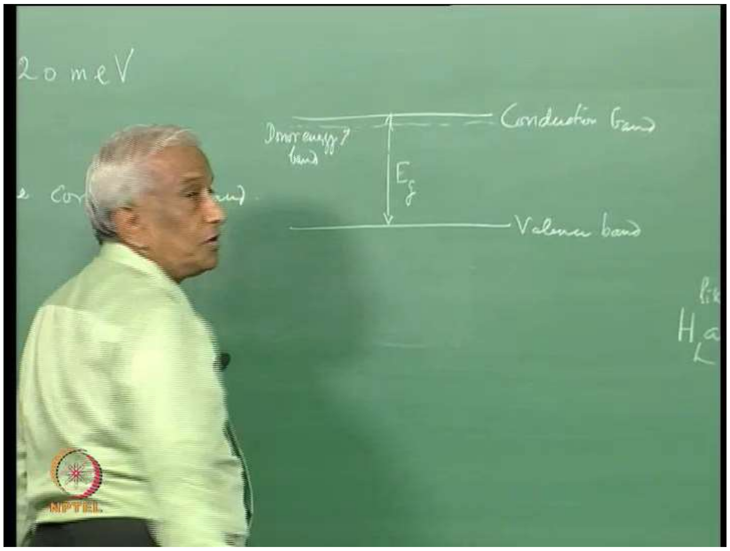

The bottom of the conduction band and the top of the valance band with an energy gap here and the donor energy level band likes very close donor energy band it is an extremely small quantity the distance between them.

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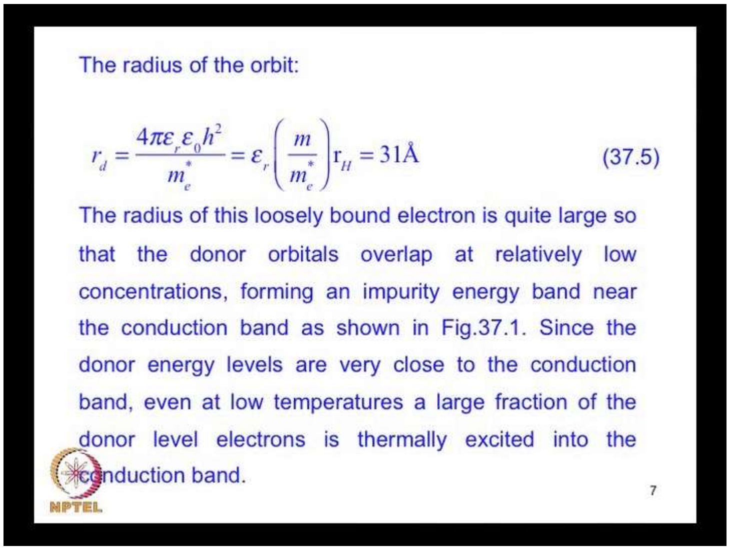

The radius of the orbit:

$$r_d = \frac{4\pi\varepsilon_r\varepsilon_0 h^2}{m_e^*} = \varepsilon_r\left(\frac{m}{m_e^*}\right)\mathrm{r}_H = 31\text{Å} \qquad (37.5)$$

The radius of this loosely bound electron is quite large so that the donor orbitals overlap at relatively low concentrations, forming an impurity energy band near the conduction band as shown in Fig.37.1. Since the donor energy levels are very close to the conduction band, even at low temperatures a large fraction of the donor level electrons is thermally excited into the conduction band.

And the radius of this orbit is also very large. So, that is a big boler lap between the orbits of the neighboring ions and therefore, this form a a donor band. So, this is a, so close to the cut bottom of the conduction band that thermal excitation can provide a very convenient way of exciting the electrons from the donor levels into the conduction band.

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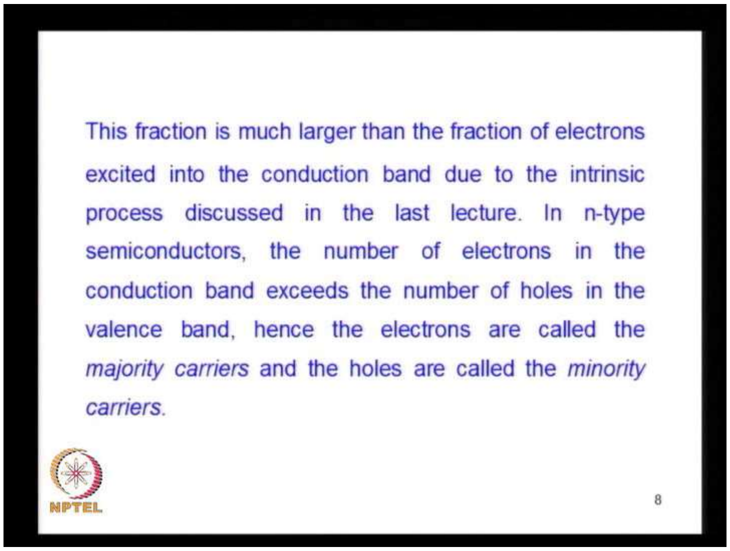

This fraction is much larger than the fraction of electrons excited into the conduction band due to the intrinsic process discussed in the last lecture. In n-type semiconductors, the number of electrons in the conduction band exceeds the number of holes in the valence band, hence the electrons are called the *majority carriers* and the holes are called the *minority carriers*.

Their by facilitating conduction. So, the fraction of electrons thus exited thermally or otherwise from the donor band to the conduction band is relatively large in comparison to the fraction which is exited across the energy gap from the valance band. So, and these are due to the whole states in the valance band.

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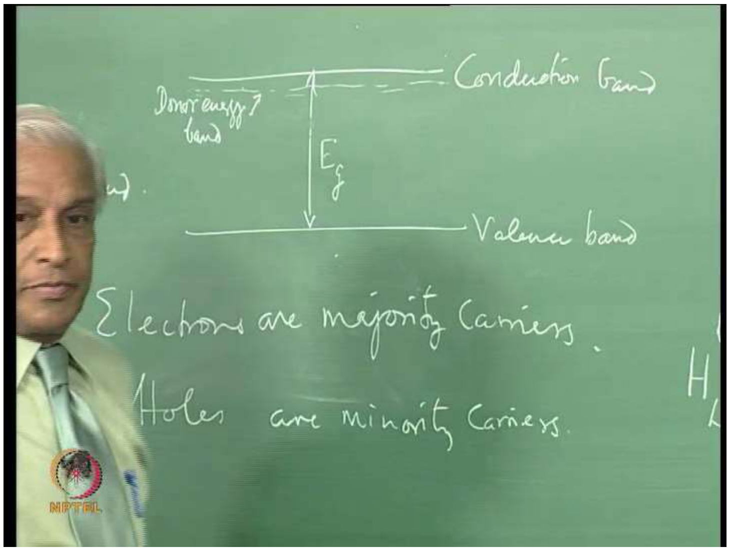

Electrons are majority carriers.

Holes are minority carriers.

So, the electrons from the donor are the so called majority carriers, because they are in very large numbers; whereas, the holes from the valance band are minority carriers in an n type semiconductor by following the same argument.

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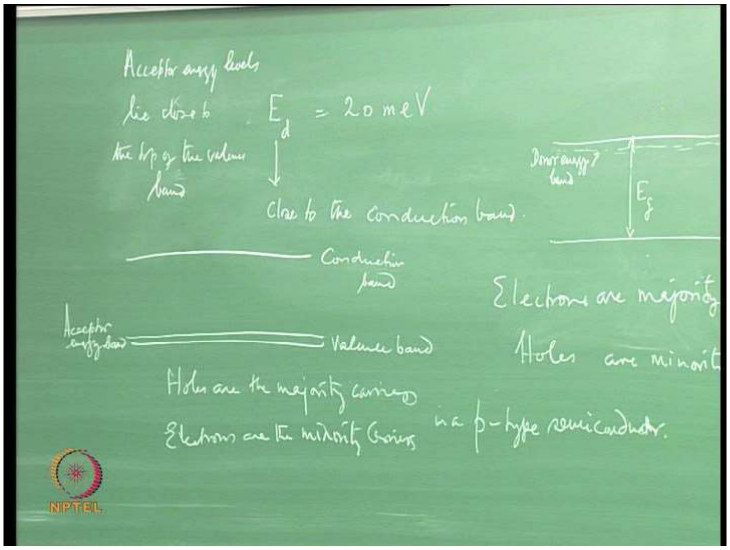

Holes are the majority carriers

Electrons are the minority carriers in a p-type semiconductor.

Electrons are majority

Holes are minorit

One can also see that the acceptor energy levels lay very close to the top of the valance band. So, this picture gives like this is the conduction band this is the valance band and we have acceptor energy band.

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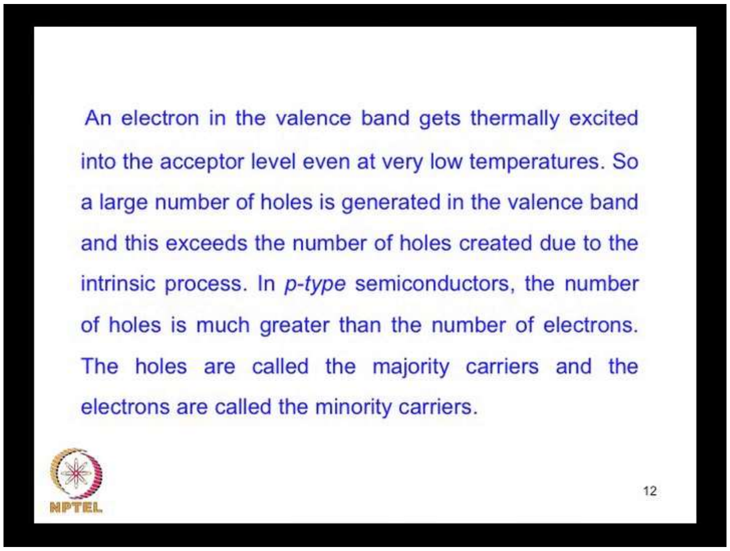

An electron in the valence band gets thermally excited into the acceptor level even at very low temperatures. So a large number of holes is generated in the valence band and this exceeds the number of holes created due to the intrinsic process. In *p-type* semiconductors, the number of holes is much greater than the number of electrons. The holes are called the majority carriers and the electrons are called the minority carriers.

Which lies extremely growth to the top of the valance band and because of this we have the majority carriers are holes in this case while electrons are the minority carriers in a p type semiconductor. So, this is the overall situation and now we have already see in that electron concentration.

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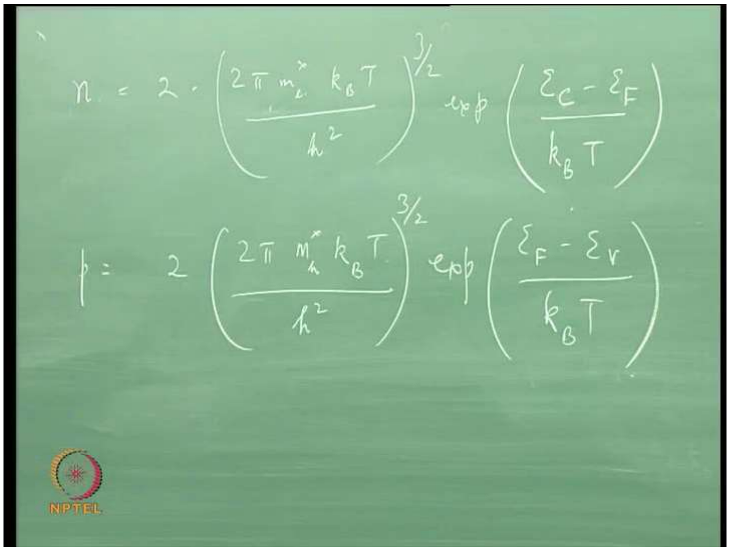

$$n = 2 \cdot \left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2} \exp\left(\frac{\varepsilon_C - \varepsilon_F}{k_B T}\right)$$

$$p = 2 \left(\frac{2\pi m_h^* k_B T}{h^2}\right)^{3/2} \exp\left(\frac{\varepsilon_F - \varepsilon_V}{k_B T}\right)$$

The electron concentration is given as n and that is two into two pi m square k b T by square hole to the power 3 by 2 exponential E f minus E f. Similarly, the whole concentration is given by a similar expression where it is effective moss of the hole T is the temperature.

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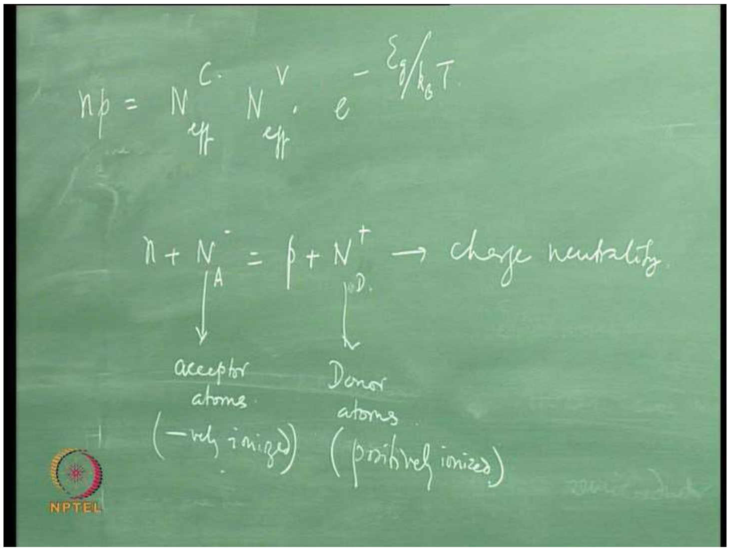

$$np = N_{eff}^{C} \, N_{eff}^{V} \cdot e^{-\mathcal{E}_g/k_B T}$$

$$n + N_A^- = p + N_D^+ \rightarrow \text{charge neutrality}$$

acceptor atoms (−vely ionized)

Donor atoms (positively ionized)

So, the product of these two becomes N times p is considering these two taking the product of these two expressions. Now these are the partition functions which are given by the p exponential factors here.

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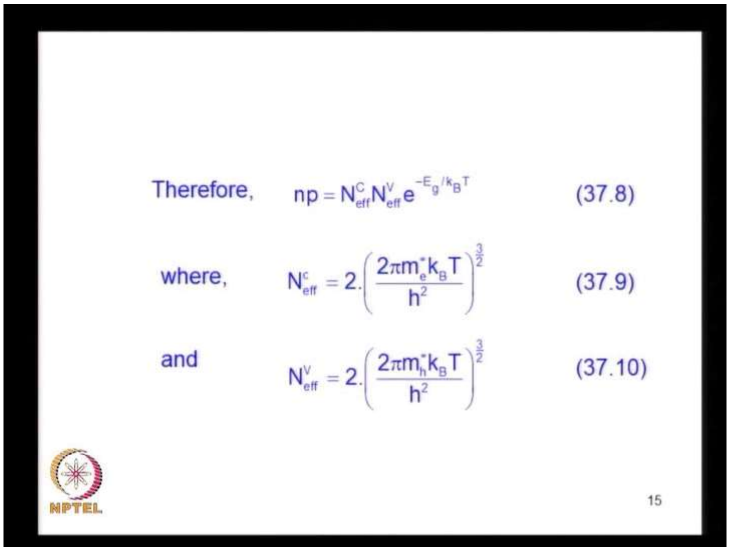

Therefore, $np = N_{eff}^{C} N_{eff}^{V} e^{-E_g/k_B T}$ (37.8)

where, $N_{eff}^{c} = 2.\left(\dfrac{2\pi m_e^* k_B T}{h^2}\right)^{\frac{3}{2}}$ (37.9)

and $N_{eff}^{v} = 2.\left(\dfrac{2\pi m_h^* k_B T}{h^2}\right)^{\frac{3}{2}}$ (37.10)

Now, the charge in locality requires that N plus N a minus equals p plus N d plus where N a is the acceptor atoms which are negatively ionized x N d is the donor atoms negatively ionized here whereas, the donor atoms you can positively ionized this is charge neutrality.

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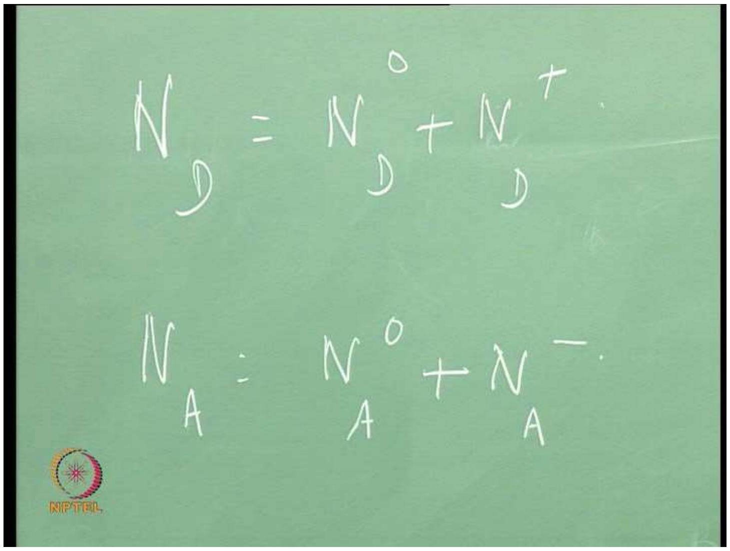

$$N_D = N_D^0 + N_D^+ .$$

$$N_A : N_A^0 + N_A^- .$$

Now N d concentration of donor atoms can be written as plus N D plus and similarly N A is N A 0 the neutral acceptor atoms plus N A minus. Now it is rather difficult to discuss the general case in the both donors and acceptors.

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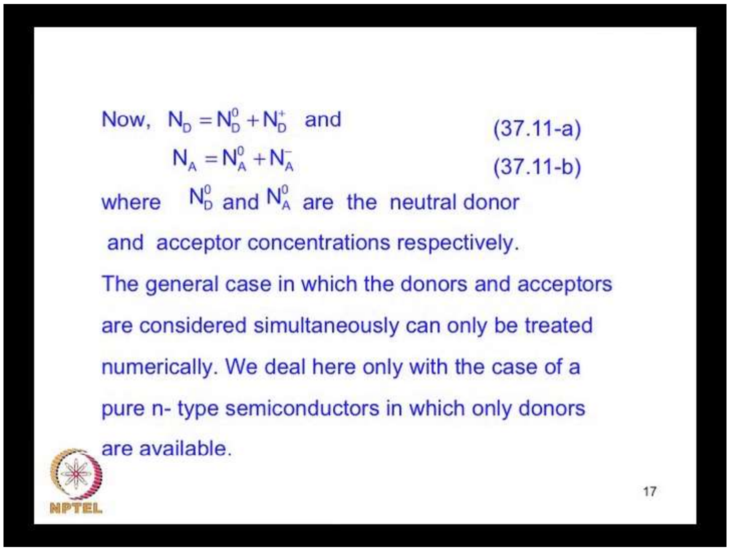

Now, $N_D = N_D^0 + N_D^+$ and (37.11-a)

$N_A = N_A^0 + N_A^-$ (37.11-b)

where N_D^0 and N_A^0 are the neutral donor and acceptor concentrations respectively.

The general case in which the donors and acceptors are considered simultaneously can only be treated numerically. We deal here only with the case of a pure n- type semiconductors in which only donors are available.

A simultaneous present is can be considered only numerically we do not want to do the here be deal with

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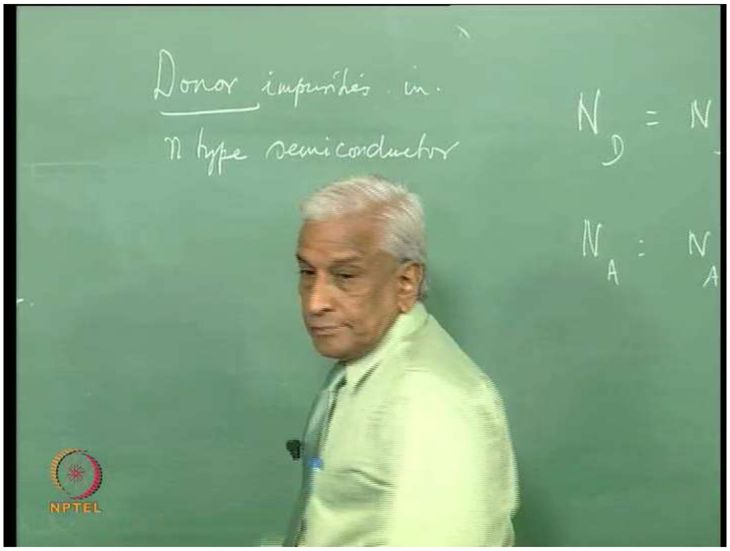

Only the case of a donor impurities, which is theoretically easier to deal with in an n types semiconductor.

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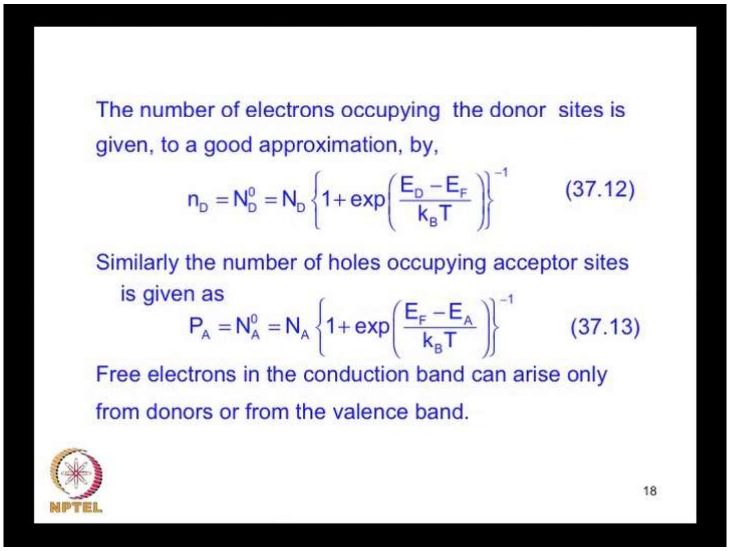

The number of electrons occupying the donor sites is given, to a good approximation, by,

$$n_D = N_D^0 = N_D \left\{ 1 + \exp\left(\frac{E_D - E_F}{k_B T} \right) \right\}^{-1} \qquad (37.12)$$

Similarly the number of holes occupying acceptor sites is given as

$$P_A = N_A^0 = N_A \left\{ 1 + \exp\left(\frac{E_F - E_A}{k_B T} \right) \right\}^{-1} \qquad (37.13)$$

Free electrons in the conduction band can arise only from donors or from the valence band.

The concentration of donor electrons is N D 0 substituting for and the plus this is N D by one plus exponential E f minus. Similarly, we can write P A a similar expression at P A 0 we are talking about the ionized impurities which involve only the spacing between the donor level and the bottom of the conduction band and the acceptor level at the top of the valance band.

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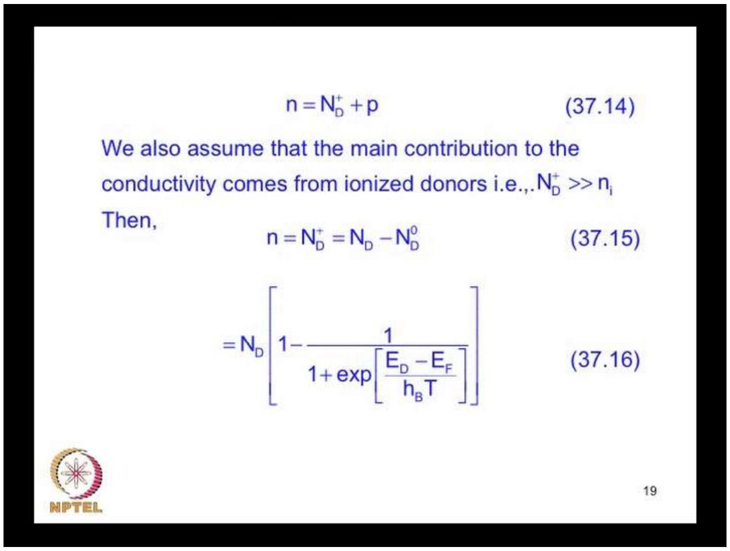

$$n = N_D^+ + p \qquad (37.14)$$

We also assume that the main contribution to the conductivity comes from ionized donors i.e.,.$N_D^+ >> n_i$

Then,

$$n = N_D^+ = N_D - N_D^0 \qquad (37.15)$$

$$= N_D \left[1 - \frac{1}{1 + \exp\left[\frac{E_D - E_F}{h_B T} \right]} \right] \qquad (37.16)$$

So, with this we can also say that can be is in gender very large compare to m that is the ionized impurity atom concentration is large the main contribution to conduct to becomes only from this with that we can an expression for n which is the difference between N D 0 and N D minus.

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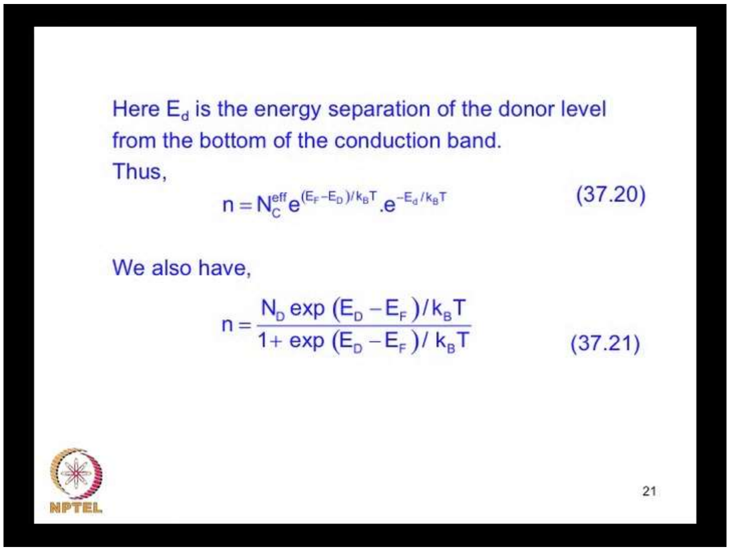

Here E_d is the energy separation of the donor level from the bottom of the conduction band.

Thus,

$$n = N_C^{eff} e^{(E_F - E_D)/k_B T} . e^{-E_d/k_B T} \qquad (37.20)$$

We also have,

$$n = \frac{N_D \exp\left(E_D - E_F\right)/k_B T}{1 + \exp\left(E_D - E_F\right)/k_B T} \qquad (37.21)$$

And therefore, we can do a little algebraic manipulation to get a closed expression in terms of.

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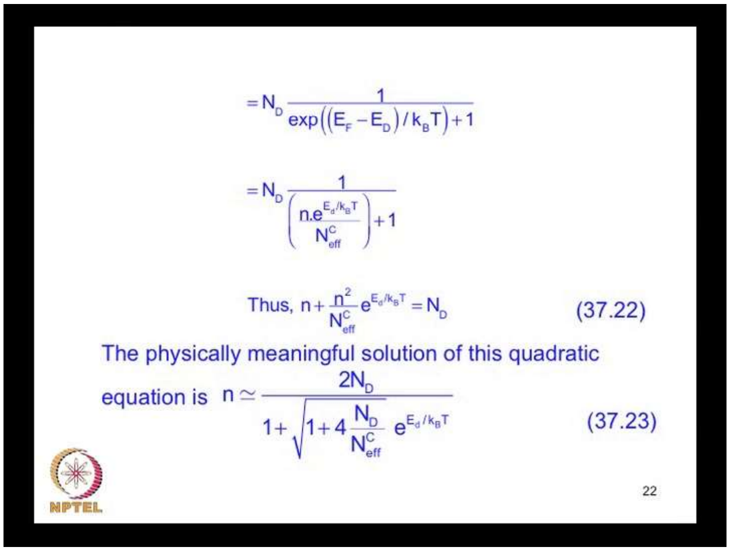

$$= N_D \frac{1}{\exp\left(\left(E_F - E_D\right)/k_BT\right)+1}$$

$$= N_D \frac{1}{\left(\frac{n.e^{E_d/k_BT}}{N_{eff}^C}\right)+1}$$

$$\text{Thus, } n + \frac{n^2}{N_{eff}^C} e^{E_d/k_BT} = N_D \qquad (37.22)$$

The physically meaningful solution of this quadratic equation is

$$n \simeq \frac{2N_D}{1+\sqrt{1+4\frac{N_D}{N_{eff}^C}e^{E_d/k_BT}}} \qquad (37.23)$$

So, that gives the concentration and which with a little bit of manipulation again as you break a manipulation lives to a simple quadratic equation for the concentration this quadratic equation has you form.

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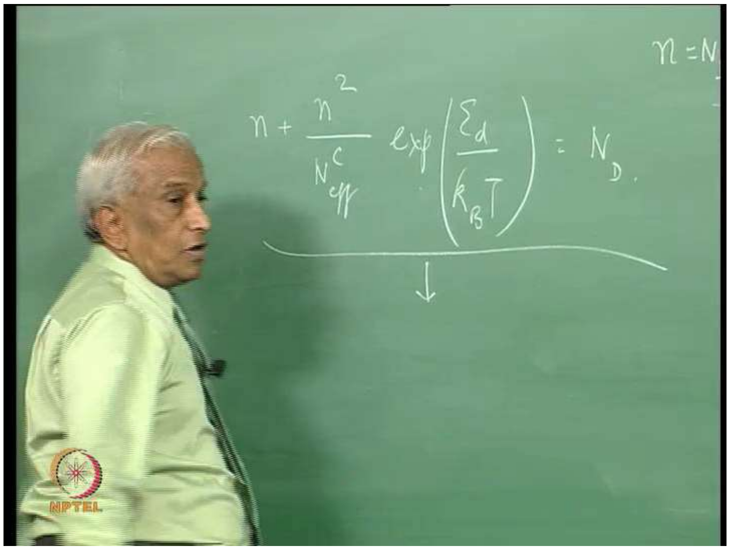

So, for which this quadratic equation can be solved to get a solution for N which has this form so that gives the concentration.

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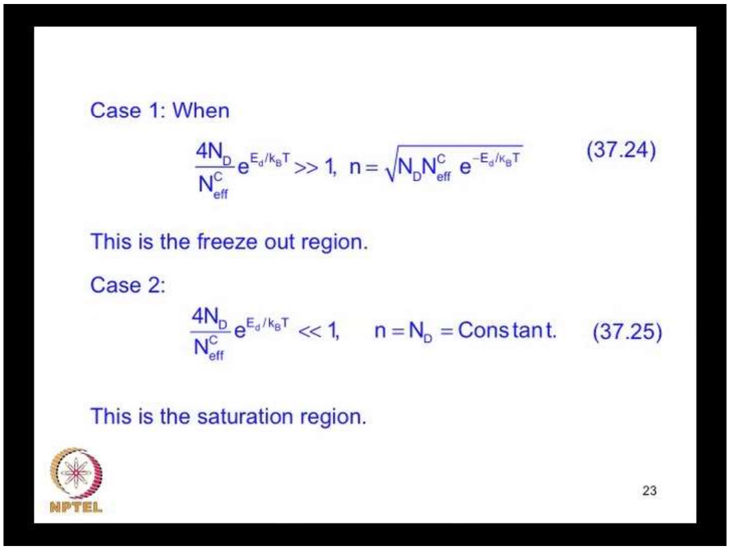

Case 1: When

$$\frac{4N_D}{N_{eff}^C} e^{E_d/k_BT} >> 1, \; n = \sqrt{N_D N_{eff}^C \, e^{-E_d/k_BT}} \qquad (37.24)$$

This is the freeze out region.

Case 2:

$$\frac{4N_D}{N_{eff}^C} e^{E_d/k_BT} << 1, \qquad n = N_D = \text{Constant}. \qquad (37.25)$$

This is the saturation region.

And we can discuss in particular three main cases is one when this quantity under the square root sign is such that.

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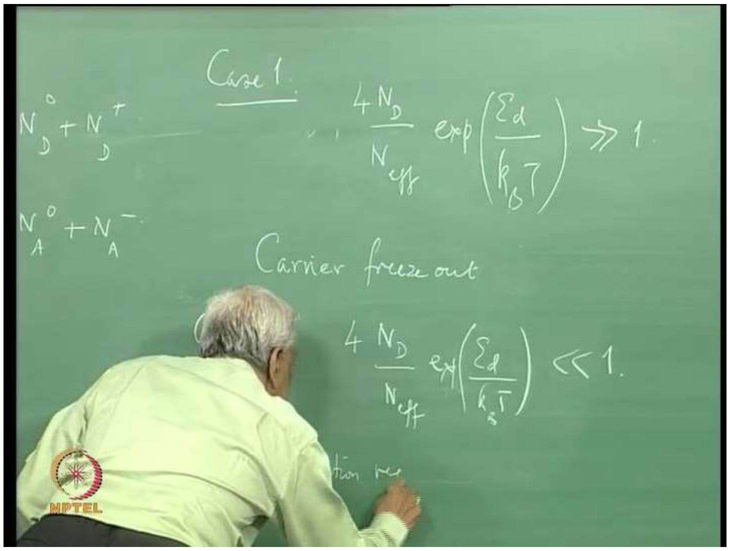

Case 1.

$N_D^0 + N_D^+$

$N_A^0 + N_A^-$

$$\frac{4N_D}{N_{eff}} \exp\left(\frac{\mathcal{E}_d}{k_B T}\right) \gg 1.$$

Carrier freeze out

$$4\frac{N_D}{N_{eff}} \exp\left(\frac{\mathcal{E}_d}{k_B T}\right) \ll 1.$$

tion re

Four N D by N effective exponential E d by k B T, this quantity is very large is comparison to one when I can ignore this and write this in terms of this is the so called carrier freeze out region. Whereas, the second case is when this factor is small in comparison to one, so that this can be neglected and we have a constant concentration. So, this is the saturation region and then third case.

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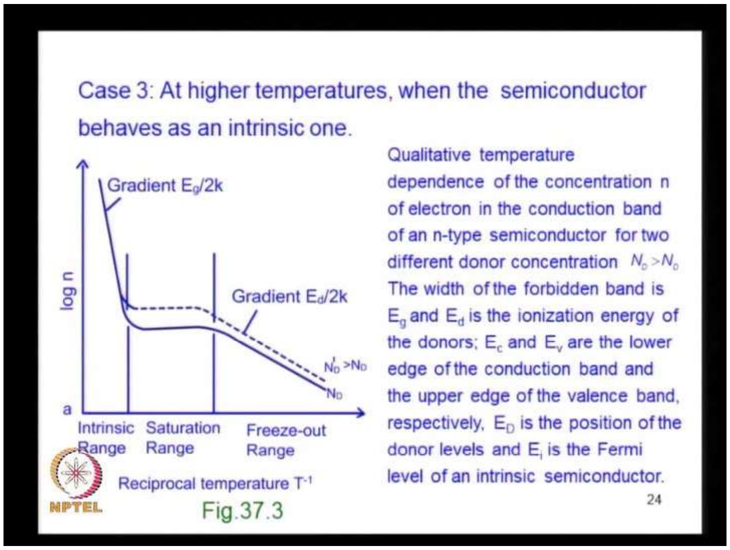

Case 3: At higher temperatures, when the semiconductor behaves as an intrinsic one.

Fig.37.3

Qualitative temperature dependence of the concentration n of electron in the conduction band of an n-type semiconductor for two different donor concentration $N_D' > N_D$ The width of the forbidden band is E_g and E_d is the ionization energy of the donors; E_c and E_v are the lower edge of the conduction band and the upper edge of the valence band, respectively, E_D is the position of the donor levels and E_i is the Fermi level of an intrinsic semiconductor.

Case 3 is at still higher temperatures the factor T enters here the conduction becomes intrinsic. So, the figure show the three regions one is the intrinsic range as a function of one by T logarithm of the concentration is plotted and you have an intrinsic range then this saturation range where the concentration is constant then a fees outrange.

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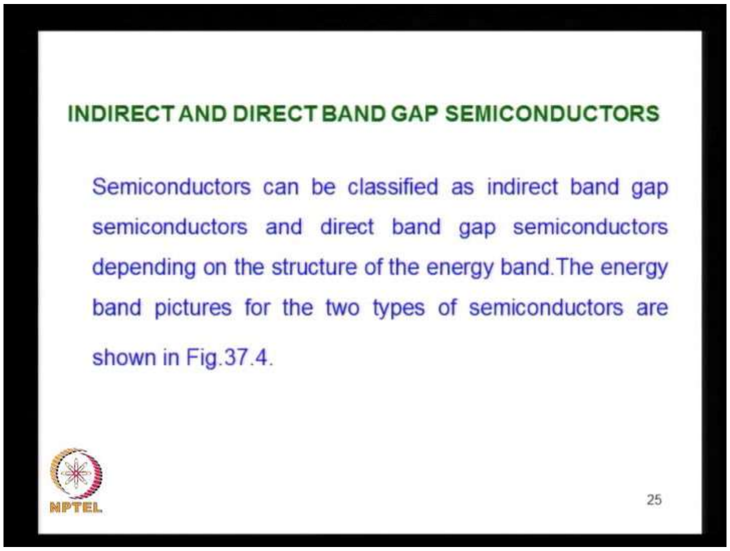

INDIRECT AND DIRECT BAND GAP SEMICONDUCTORS

Semiconductors can be classified as indirect band gap semiconductors and direct band gap semiconductors depending on the structure of the energy band. The energy band pictures for the two types of semiconductors are shown in Fig.37.4.

So, this gives the basic mechanism and basic results of carrier transport in a pure n type of semiconductors this can be treated analytically similarly f b type semiconductor also can be treated analytically, but as I already said and both are present then this cannot be treated analytically, but it has to be done only numerically.

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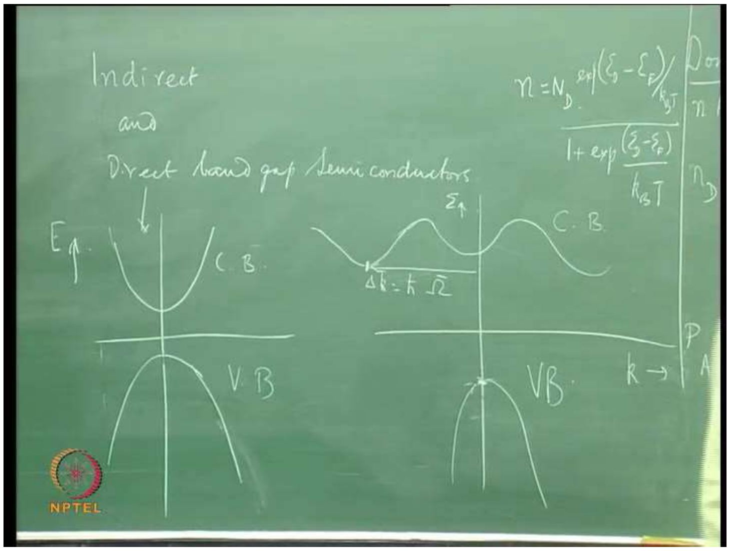

You know paws on to consider an important distinction between indirect and direct band gap semiconductors.

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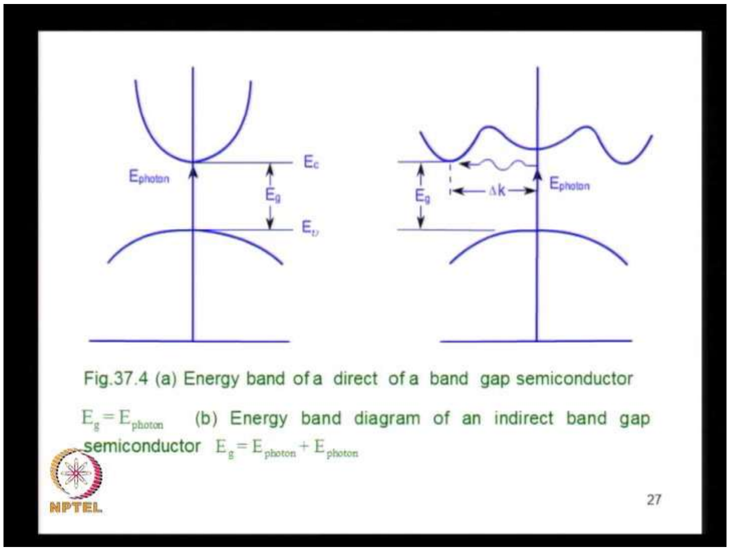

Fig.37.4 (a) Energy band of a direct of a band gap semiconductor $E_g = E_{photon}$ (b) Energy band diagram of an indirect band gap semiconductor $E_g = E_{photon} + E_{photon}$

These are illustrated in the next figure in the direct band gap semiconductor the the conduction band the bottom to the conduction band. So, this is the conduction band this is the valance band. So, this bottom of the conduction band lies energetically at the same value as the top of the valance band, so that the band gap is all the energy needed to promote a carrier from the valance band into the conduction band. Whereas, an indirect band gap is one in which and you have a slightly lower structure here and whereas, we have the valance band here the conduction band energy structure like this. So, the bottom of the conduction band lies here while the top of the valance band likes here there do not occur at the same k value. So, one needs to promote the carrier from here to this and then translate it to this by an amount delta k or h cross omega.

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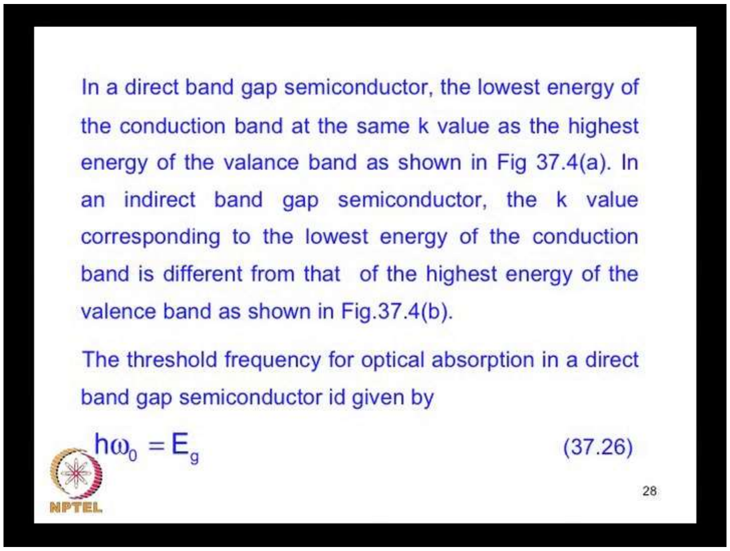

In a direct band gap semiconductor, the lowest energy of the conduction band at the same k value as the highest energy of the valance band as shown in Fig 37.4(a). In an indirect band gap semiconductor, the k value corresponding to the lowest energy of the conduction band is different from that of the highest energy of the valence band as shown in Fig.37.4(b).

The threshold frequency for optical absorption in a direct band gap semiconductor id given by

$$h\omega_0 = E_g \qquad (37.26)$$

So, for conduction one has to get a threshold frequency for conduction is just the energy gap for a direct band gap for a direct band gap semiconductor, for example, gallium arsenide you such a material.

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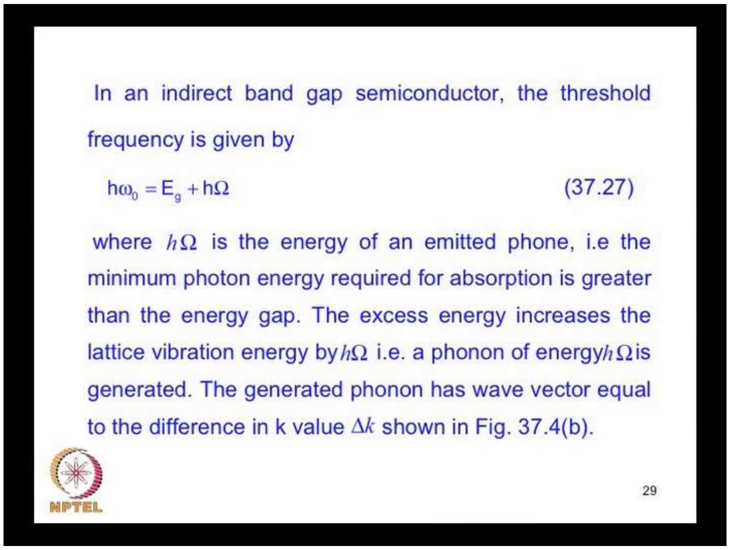

In an indirect band gap semiconductor, the threshold frequency is given by

$$h\omega_0 = E_g + h\Omega \qquad (37.27)$$

where $h\Omega$ is the energy of an emitted phone, i.e the minimum photon energy required for absorption is greater than the energy gap. The excess energy increases the lattice vibration energy by $h\Omega$ i.e. a phonon of energy $h\Omega$ is generated. The generated phonon has wave vector equal to the difference in k value Δk shown in Fig. 37.4(b).

Whereas in the case of an indirect band gap we have to have in an indirect band gap.

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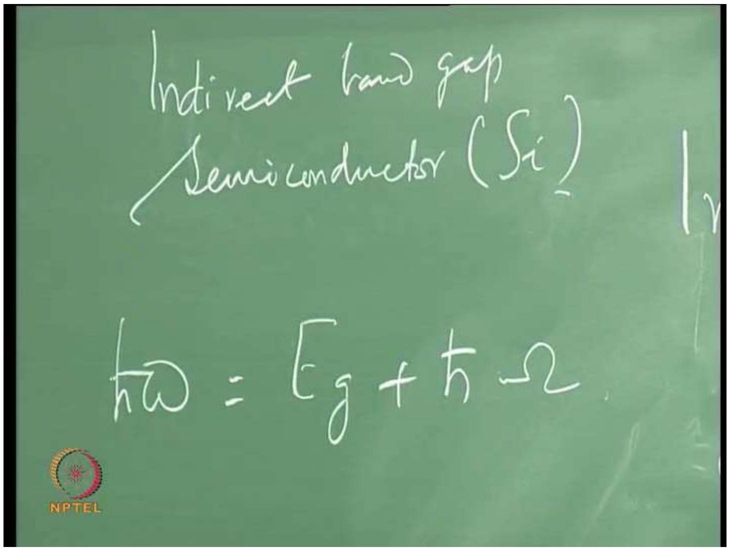

Indirect band gap
Semiconductor (Si)

$$\hbar\omega = E_g + \hbar\Omega$$

Semiconductor such as silicon one has to have their omega is given by the condition for the wave vector.

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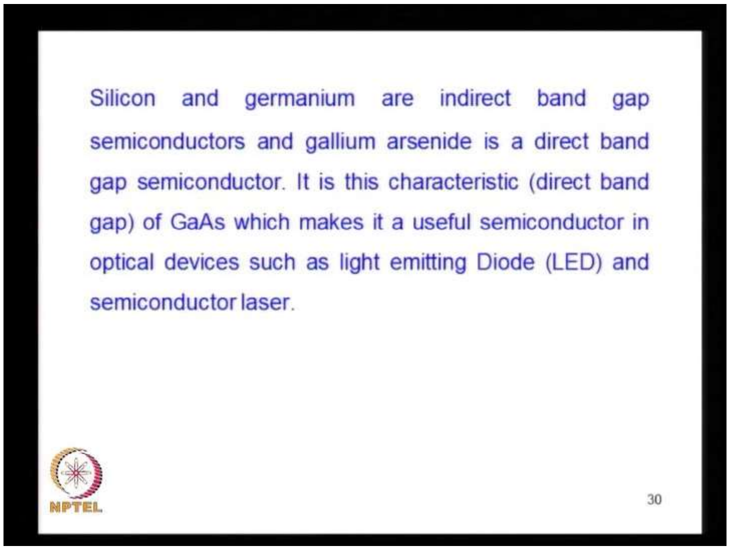

Silicon and germanium are indirect band gap semiconductors and gallium arsenide is a direct band gap semiconductor. It is this characteristic (direct band gap) of GaAs which makes it a useful semiconductor in optical devices such as light emitting Diode (LED) and semiconductor laser.

So, it is because of these the gallium arsenide is a useful conductor and for example, optoelectronic devices led's semiconductor lasers and so on.

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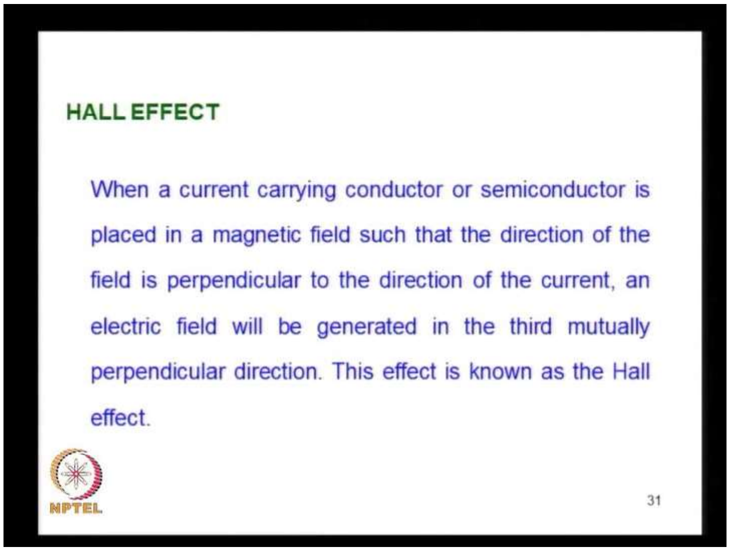

HALL EFFECT

When a current carrying conductor or semiconductor is placed in a magnetic field such that the direction of the field is perpendicular to the direction of the current, an electric field will be generated in the third mutually perpendicular direction. This effect is known as the Hall effect.

Next we pass on to a consideration of hole effect hall effect is a very well known phenomenon especially in semiconductor.

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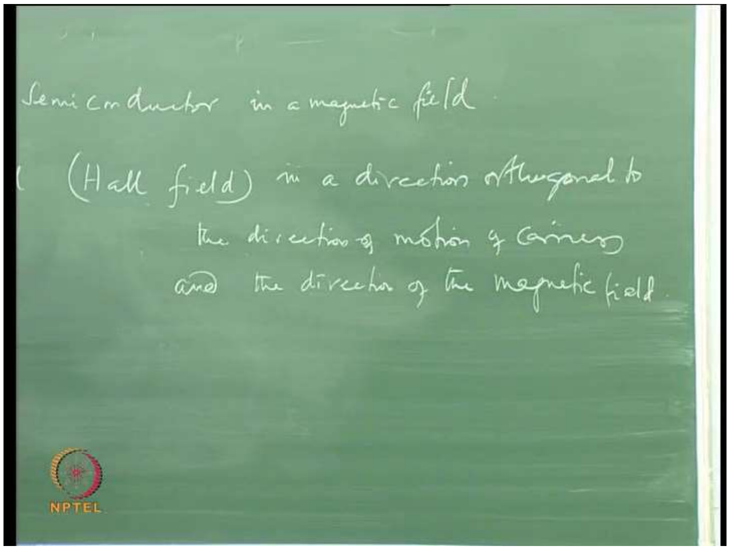

Semiconductor in a magnetic field.

(Hall field) in a direction orthogonal to
the direction of motion of carriers
and the direction of the magnetic field.

So, then a current carrying conductor or semiconductor is placed a magnetic field let us discuss a semiconductor placed a magnetic field. So, because of the Lorentz force acting on a moving charge practically magnetic field you get a lateral displacement of the carriers and therefore, there is a its field which is set up in the direction perpendicularly directional motion of the charge carriers and the direction of the magnetic field. So, this field is known as the hall field and the setting up of this is known as the Hall Effect. So, this is in a direction orthogonal to the direction of the motion of the carriers and the direction of the magnetic field. So, that is the effect which is known as the classical Hall Effect.

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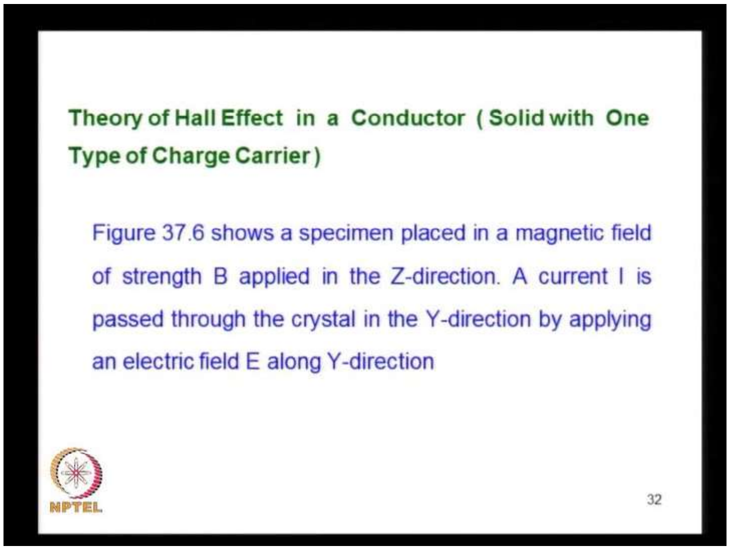

Theory of Hall Effect in a Conductor (Solid with One Type of Charge Carrier)

Figure 37.6 shows a specimen placed in a magnetic field of strength B applied in the Z-direction. A current I is passed through the crystal in the Y-direction by applying an electric field E along Y-direction

If you have a conductor with one type of charge carriers the situation is extremely simple to deal with

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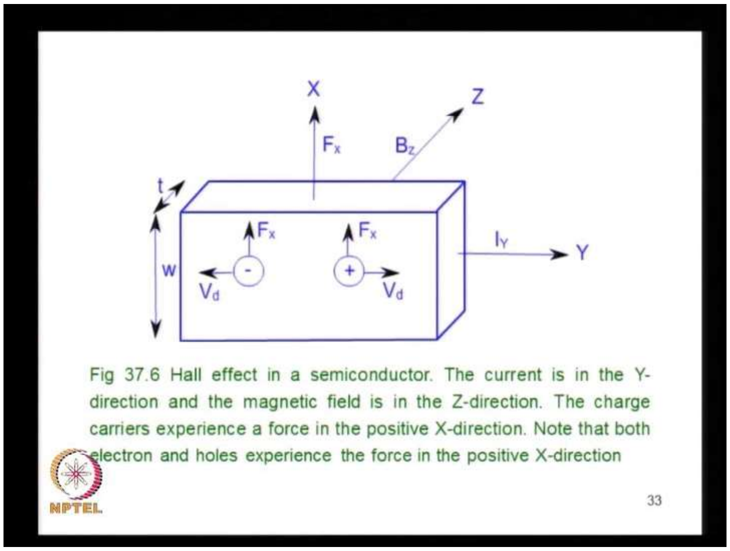

Fig 37.6 Hall effect in a semiconductor. The current is in the Y-direction and the magnetic field is in the Z-direction. The charge carriers experience a force in the positive X-direction. Note that both electron and holes experience the force in the positive X-direction

Let us say consider a configuration which you shown in the figure here where the field and the current configuration are shown.

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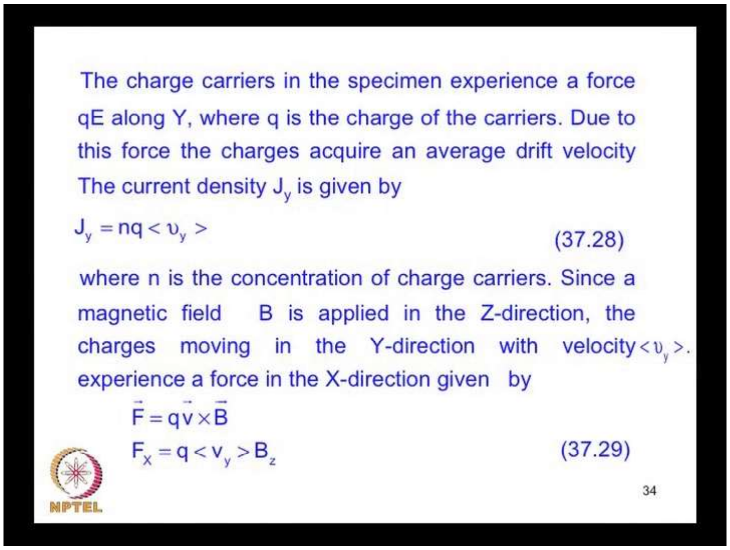

The charge carriers in the specimen experience a force qE along Y, where q is the charge of the carriers. Due to this force the charges acquire an average drift velocity The current density J_y is given by

$$J_y = nq < \upsilon_y > \qquad (37.28)$$

where n is the concentration of charge carriers. Since a magnetic field B is applied in the Z-direction, the charges moving in the Y-direction with velocity $< \upsilon_y >$. experience a force in the X-direction given by

$$\vec{F} = q\vec{v} \times \vec{B}$$

$$F_X = q < v_y > B_z \qquad (37.29)$$

And one can straight away using the Lorentz source law f equals q v cross b where b is that of the current and you have a b direction. So, the force the lateral force can be readily calculated.

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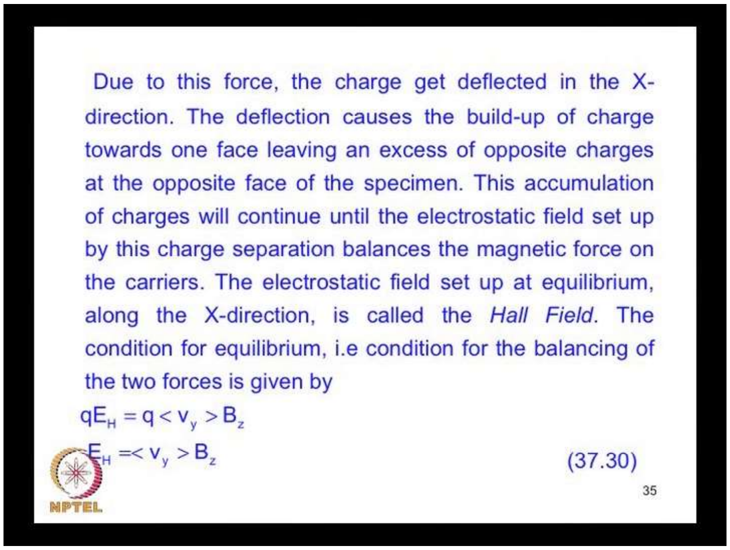

Due to this force, the charge get deflected in the X-direction. The deflection causes the build-up of charge towards one face leaving an excess of opposite charges at the opposite face of the specimen. This accumulation of charges will continue until the electrostatic field set up by this charge separation balances the magnetic force on the carriers. The electrostatic field set up at equilibrium, along the X-direction, is called the *Hall Field*. The condition for equilibrium, i.e condition for the balancing of the two forces is given by

$$qE_H = q < v_y > B_z$$

$$E_H = < v_y > B_z \qquad (37.30)$$

And therefore, the Hall field can be calculated also, the hall field is given is if the direction of motion X…

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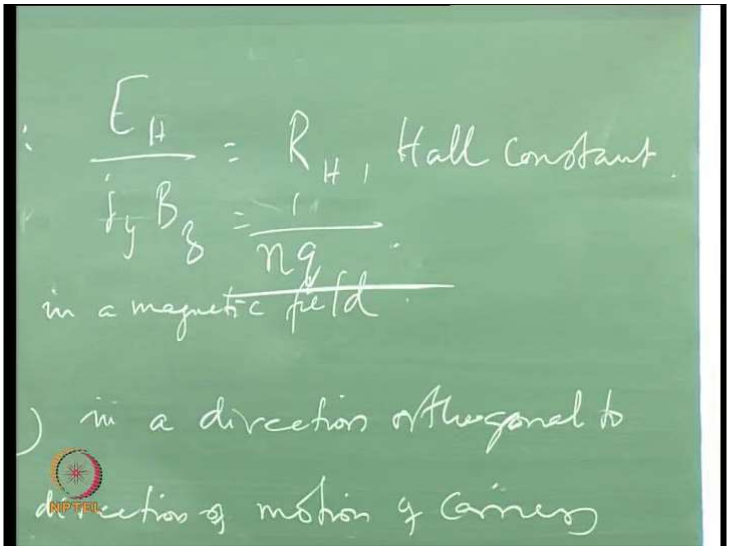

$$\frac{E_H}{j_y B_z} = R_H, \text{ Hall constant} = \frac{1}{nq}.$$

in a magnetic field.

) in a direction orthogonal to

direction of motion of carriers

The B field is along the z direction the hall field is directed along the y direction. So, this will be j y B z by n. Let us write q here to denote the charge in a general way. So, this E h by j y b z is known as Hall constant and that readily seen to be just 1 by n q.

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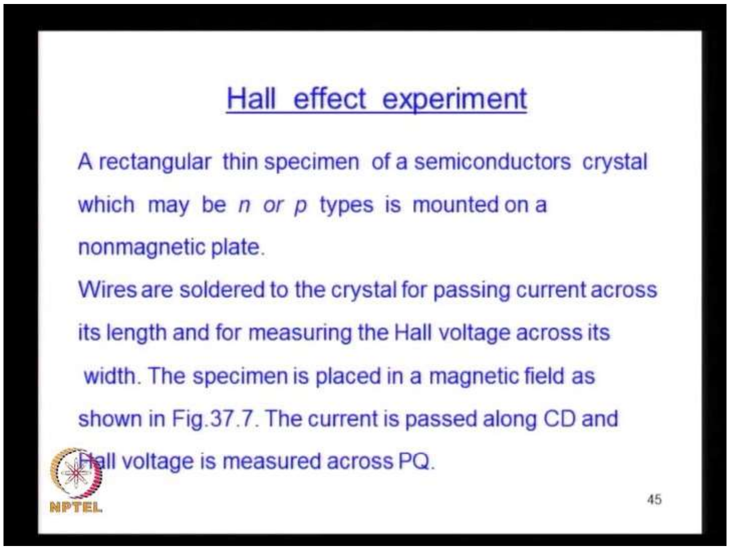

Hall effect experiment

A rectangular thin specimen of a semiconductors crystal which may be *n or p* types is mounted on a nonmagnetic plate.

Wires are soldered to the crystal for passing current across its length and for measuring the Hall voltage across its width. The specimen is placed in a magnetic field as shown in Fig.37.7. The current is passed along CD and Hall voltage is measured across PQ.

So, this proportionally constant is what is seen here and therefore, the Hall voltage can straight away be calculated.

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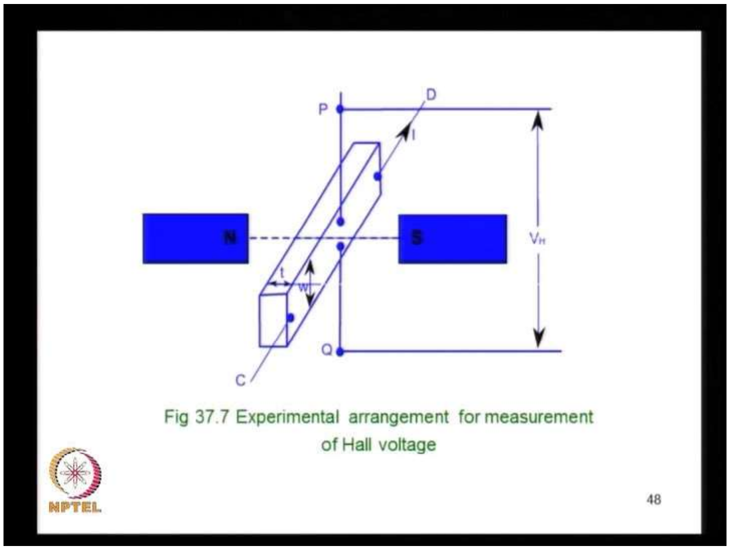

Fig 37.7 Experimental arrangement for measurement of Hall voltage

So, this is the typical experimental configuration for measuring the Hall co efficient and contacts made along to pass the current.

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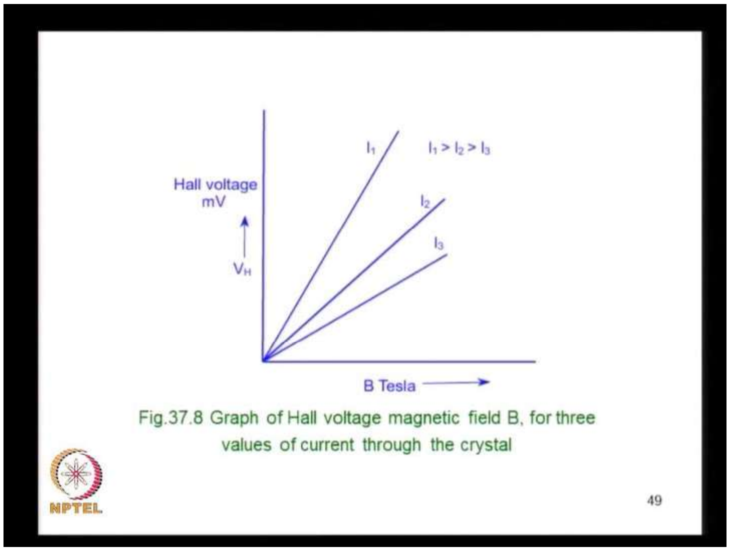

Fig.37.8 Graph of Hall voltage magnetic field B, for three values of current through the crystal

And a magnetic field is supplied perpendicular to the direction of flow the current, and then the contracture made also in the third direction to measure the Hall voltage, and this gives the Hall voltage as a function of the applied magnetic field, in different values of the magnetic field.

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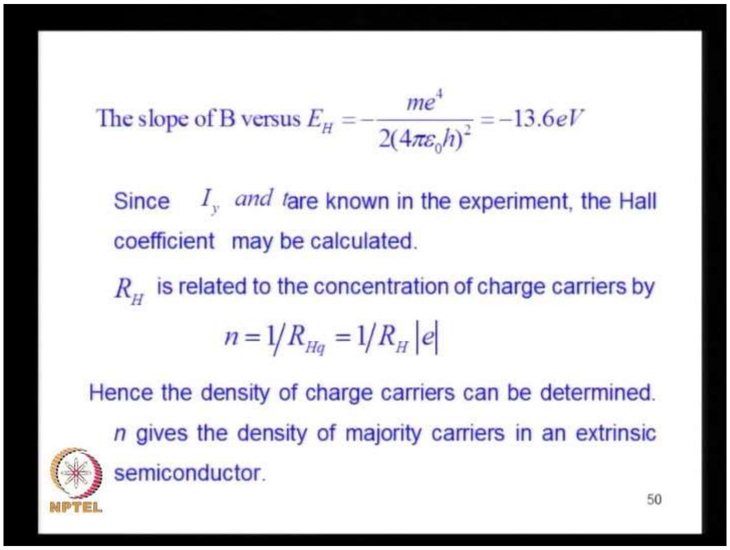

The slope of B versus $E_H = -\frac{me^4}{2(4\pi\varepsilon_0 h)^2} = -13.6eV$

Since I_y and t are known in the experiment, the Hall coefficient may be calculated.

R_H is related to the concentration of charge carriers by

$$n = 1/R_{Hq} = 1/R_H|e|$$

Hence the density of charge carriers can be determined.

n gives the density of majority carriers in an extrinsic semiconductor.

The hall constant is related to the carrier concentration, so 1 by R H and q magnitude of q.

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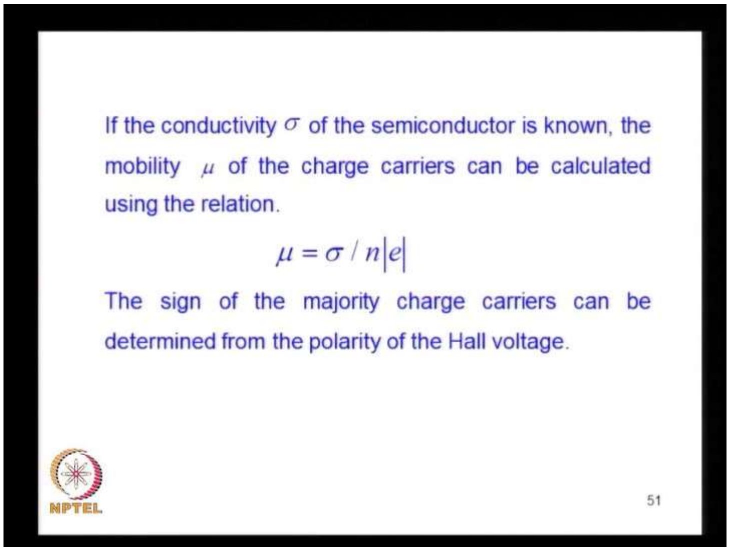

If the conductivity σ of the semiconductor is known, the mobility μ of the charge carriers can be calculated using the relation.

$$\mu = \sigma / n|e|$$

The sign of the majority charge carriers can be determined from the polarity of the Hall voltage.

So, one can straight away measure the carrier density by measuring the Hall constant. And since the mobility is just therefore, if we know the electrical conductivity and the concentration one can determine the mobility as well.

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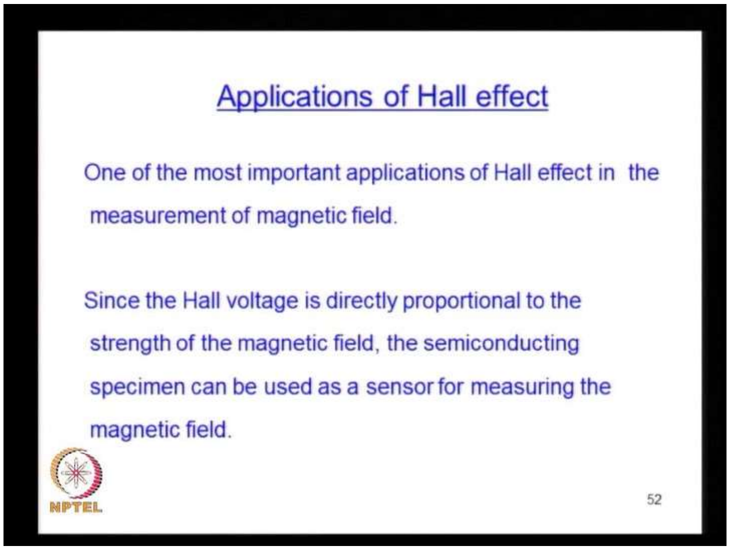

Applications of Hall effect

One of the most important applications of Hall effect in the measurement of magnetic field.

Since the Hall voltage is directly proportional to the strength of the magnetic field, the semiconducting specimen can be used as a sensor for measuring the magnetic field.

So, the Hall effect is used extensively in the measurement of the magnetic field, it is used as a magnetometer and to measure sign and concentration of charge carrier, and the mobility. These are the important applications of Hall Effect measurements.

Condensed Matter Physics
Prof. G. Rangarajan
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Indian Institute of Technology, Madras

Lecture - 37
Semiconductors - Worked Examples

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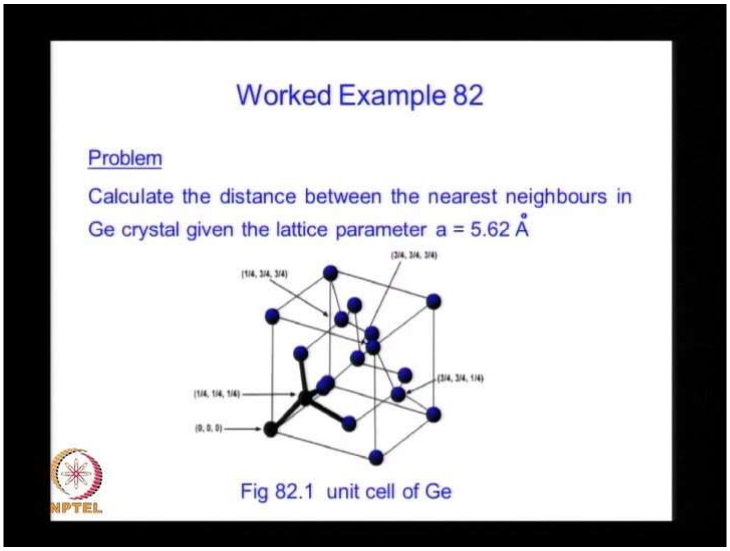

Worked Example 82

Problem

Calculate the distance between the nearest neighbours in Ge crystal given the lattice parameter a = 5.62 Å

Fig 82.1 unit cell of Ge

Today we will solve some problems on the topic of semiconductors, which we discussed the first problem concerns.

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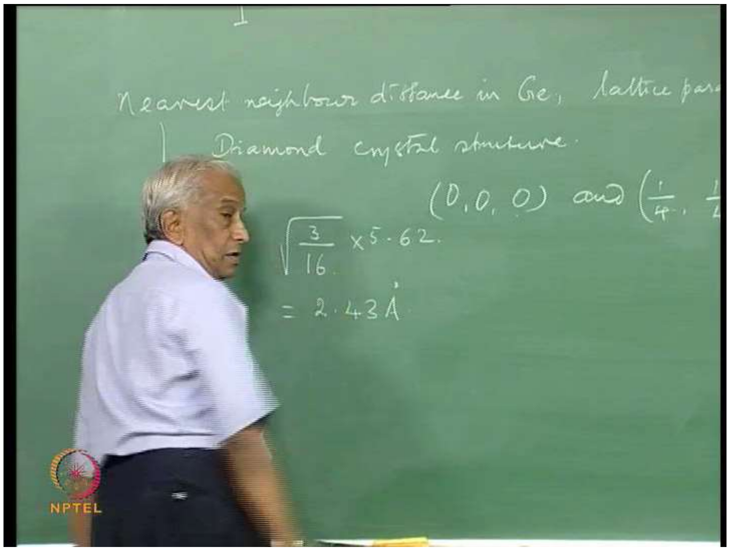

I

Nearest neighbour distance in Ge, lattice para

Diamond crystal structure.

(0, 0, 0) and $\left(\frac{1}{4}, \right.$

$$\sqrt{\frac{3}{16}} \times 5.62$$

$$= 2.43\,\text{Å}$$

The calculation as a distance between near neighbours in their germanium crystal whose lattice parameter is given noise 5.62 Armstrong's germanium. And silicon both have a cubic unit cell in which the structure is that of diamond, which is shown in the figure with the atoms at noise the origin which is at the vertex of a cube at one vertex of the cube 0 0 0. And then at a distance of one fourth one fourth one fourth along the body diagonal atoms are at these points noise this is the basic problem in the unit..

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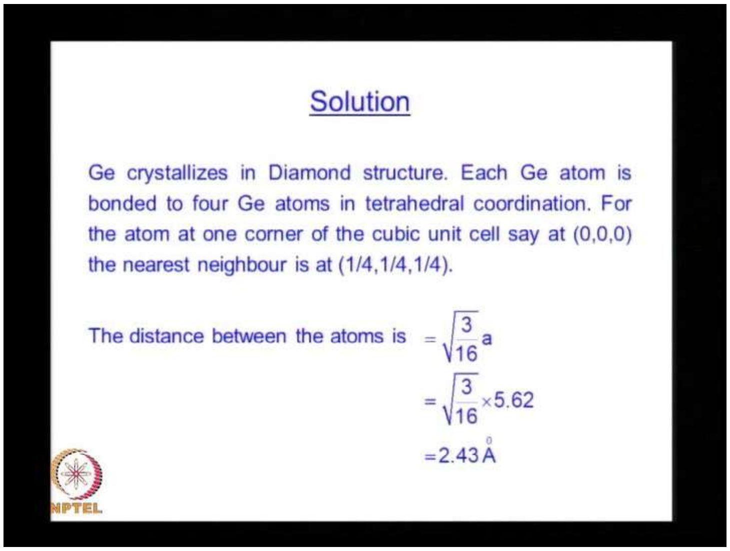


Solution

Ge crystallizes in Diamond structure. Each Ge atom is bonded to four Ge atoms in tetrahedral coordination. For the atom at one corner of the cubic unit cell say at (0,0,0) the nearest neighbour is at (1/4,1/4,1/4).

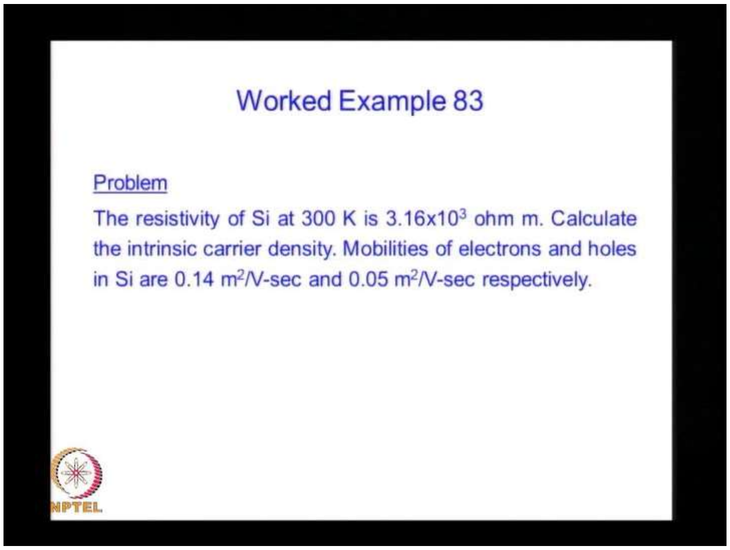
The distance between the atoms is $= \sqrt{\frac{3}{16}}a$

$$= \sqrt{\frac{3}{16}} \times 5.62$$

$$= 2.43 \overset{0}{A}$$

So, this is the unit cell which is shown in figure and we have to simply use geometry and distance which is asked is just root of three by root three by 4, which is root of 3 by 16 times 5.62. That is the distance required between the atom at 0 0 0 and the atom at one fourth one fourth one fourth, and that works out to be two point four three Armstrong's having done.

(Refer Slide Time: 02:50)



Worked Example 83

Problem

The resistivity of Si at 300 K is 3.16×10^3 ohm m. Calculate the intrinsic carrier density. Mobilities of electrons and holes in Si are 0.14 m^2/V-sec and 0.05 m^2/V-sec respectively.

The geometrical calculation the crystal structure calculation. We now pass on to the calculation of the intrinsic carrier density.

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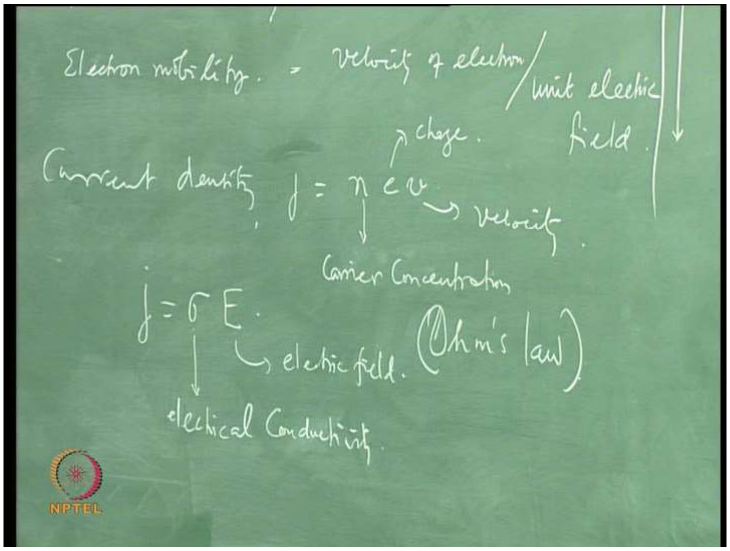

Electron mobility. = velocity of electron / unit electric field.

Current density $j = n e v$

charge.

velocity.

Carrier Concentration

$j = \sigma E$.

electric field. (Ohm's law)

electrical Conductivity.

In silicon which is another well-known semiconductor we are given that the intrinsic resistivity at three hundred k is given as 3.16 into ten to the power three ohm metre. So, we are also told that the electron mobility well I do not think we have discussed the concept of mobility. So, far let me introduce the definition of mobility is the velocity of electron per unit electric field, we all know that the current density is in general given as j is n e v, where n is the carrier concentration and e is the electronic charge v is the velocity. So, and we also know that this current density is related to the electric field via the conductivity this is the electric field, and sigma is the conductivity electrical as we all know this is just ohm's law.

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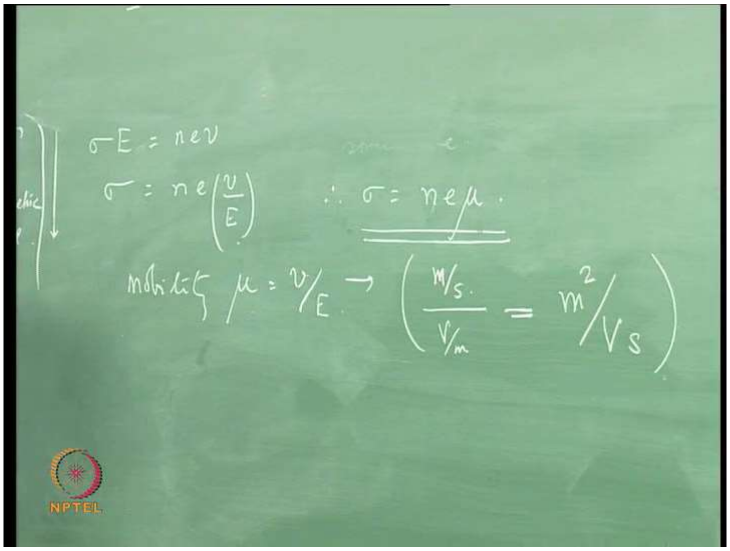

$$\sigma E = nev$$

$$\sigma = ne\left(\frac{v}{E}\right) \qquad \therefore \sigma = ne\mu$$

$$\text{mobility } \mu = v/E \rightarrow \left(\frac{m/s}{V/m} = m^2/Vs\right)$$

So, because of these we can write n e v is sigma e and therefore, sigma is n e v by e and it is this quantity which we have defined as the mobility. Therefore, sigma is n e mu this is a very basic relationship, which gives the electrical conductivity in terms of the carrier concentration the charge. And the electron mobility and in this problem we are given that the electron mobility in silicon at three hundred k is 0.14 metre square per volt second the unit of mobility is velocity is metre per second, and the electric field is volt per metre therefore, this is metre square per volt second.

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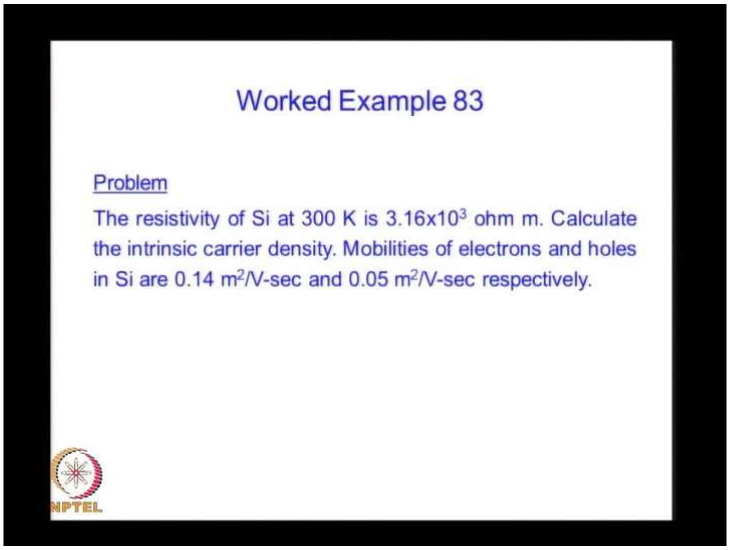

Worked Example 83

Problem

The resistivity of Si at 300 K is 3.16×10^3 ohm m. Calculate the intrinsic carrier density. Mobilities of electrons and holes in Si are 0.14 m^2/V-sec and 0.05 m^2/V-sec respectively.

So, that is given as 0.14 metre square per volt second, and the mobility of holes.

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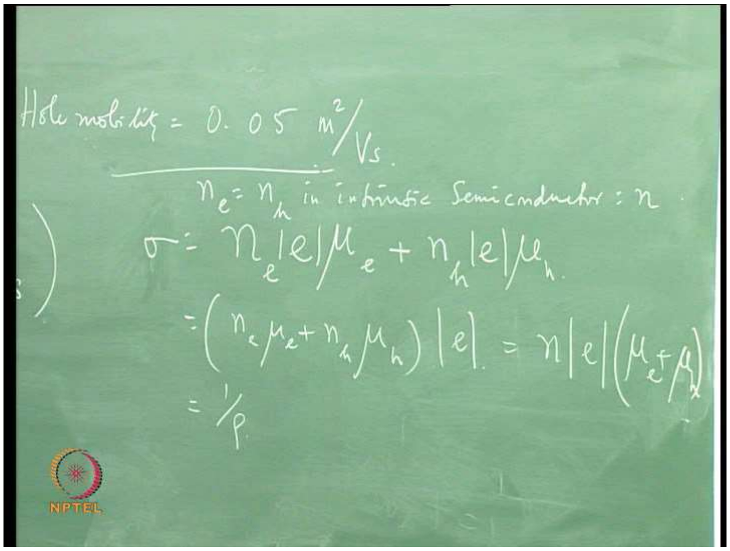

Hole mobility = $0.05\ m^2/Vs$.

$n_e = n_h$ in intrinsic Semiconductor : n

$$\sigma = n_e|e|\mu_e + n_h|e|\mu_h$$

$$= (n_e\mu_e + n_h\mu_h)|e| = n|e|(\mu_e + \mu_h)$$

$$= 1/\rho$$

Is given as naught 5 point naught 5 and the current density is due to the presence of both electrons and holes in the silicon. So, there is a contribution from the motion of electrons among states in the conduction band, and also the motion of holes in states in the balance band both contribute to the current density. And since the hole is positively charged and moves in the direction opposite to that of the electron in the given electric field, therefore the current density is due to both electrons and holes add up.

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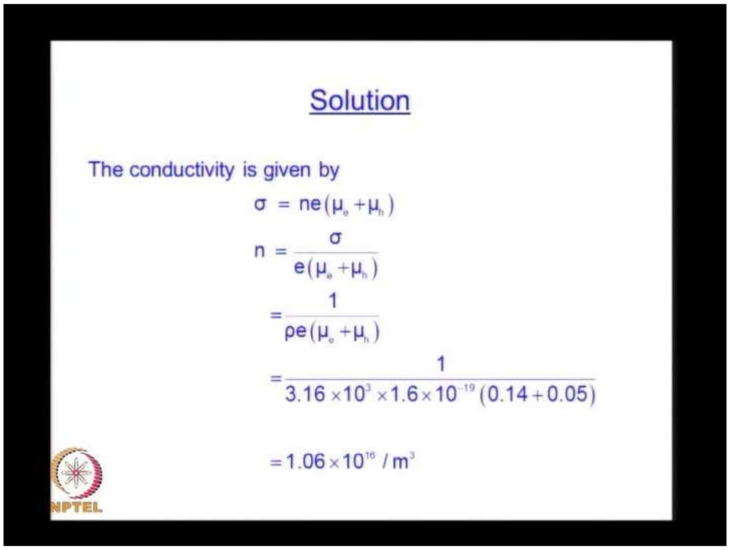

Solution

The conductivity is given by

$$\sigma = ne(\mu_e + \mu_h)$$

$$n = \frac{\sigma}{e(\mu_e + \mu_h)}$$

$$= \frac{1}{\rho e(\mu_e + \mu_h)}$$

$$= \frac{1}{3.16 \times 10^3 \times 1.6 \times 10^{-19} (0.14 + 0.05)}$$

$$= 1.06 \times 10^{16} / m^3$$

And therefore, we have a general relation using this using this fundamental relation. Now I can write n e e mu e plus n h e mu h where e is mod e the sign of the charge is included in the directions. Therefore, this is just n e mu e plus n h mu h times mod e and that is the general expression for j, and therefore sigma. And we also know that the resistivity rho is just one by sigma since it is a cubic material, we do not have to worry about anisotropic here sigma and rho are the same scalar quantities with just one value for the entire in all the directions inside the crystal. So, we are given the value the resistivity therefore, going back to this is equal to one by rho rho is given, and since it is intrinsic material the number of electrons is equal to the number of holes. So, let us write it together as n. So, that this becomes n e mu e plus mu h.

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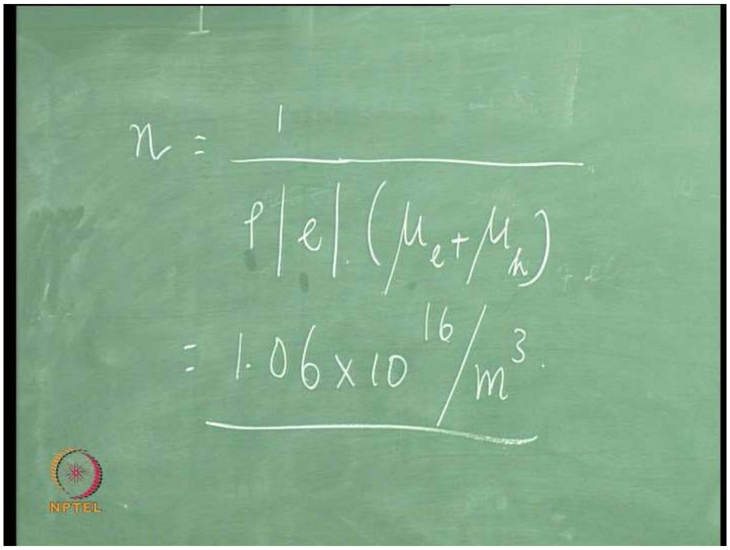

$$n = \frac{1}{\rho|e|.(\mu_e+\mu_h)}$$

$$= 1.06 \times 10^{16}/m^3.$$

So, we have this and we are asked to determine n the intrinsic carrier concentration n, which is asked which is required is just given by one by rho times mod e noise times mu e plus mu h. So, plugging in the values the given values for the resistivity the electronic charge is known as standard value and the values of the mobilities are given substituting all these we get the value the carrier concentration is 1.06 into 10 to the power 16 per metre cube.

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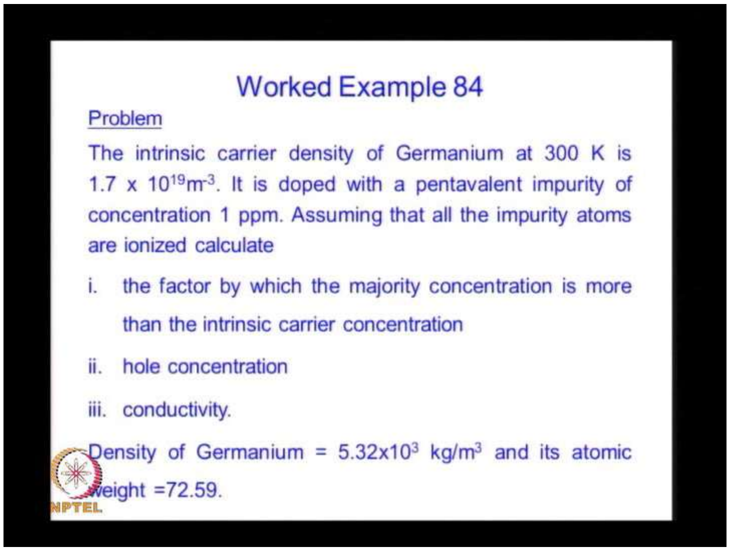

Worked Example 84

Problem

The intrinsic carrier density of Germanium at 300 K is 1.7 x $10^{19}m^{-3}$. It is doped with a pentavalent impurity of concentration 1 ppm. Assuming that all the impurity atoms are ionized calculate

i. the factor by which the majority concentration is more than the intrinsic carrier concentration

ii. hole concentration

iii. conductivity.

Density of Germanium = 5.32×10^3 kg/m^3 and its atomic weight =72.59.

Next, we pass on to a case of intrinsic germanium .

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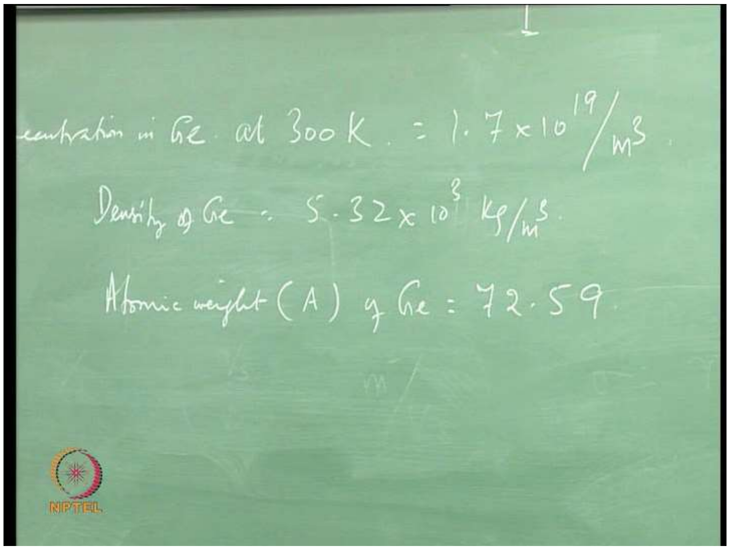

centration in Ge at 300 K $= 1.7 \times 10^{19}/m^3$

Density of Ge $= 5.32 \times 10^3$ kg/m^3

Atomic weight (A) of Ge : 72.59

We are given the intrinsic carrier concentration in germanium at 300 k, and that is given as 1.7 into 10 to the power nineteen per metre cube. We are also given the value of the density bulk density of germanium as 5.32 into ten to the power three kilograms per metre cube, and the atomic weight of germanium is given as seventy 2.59 noise.

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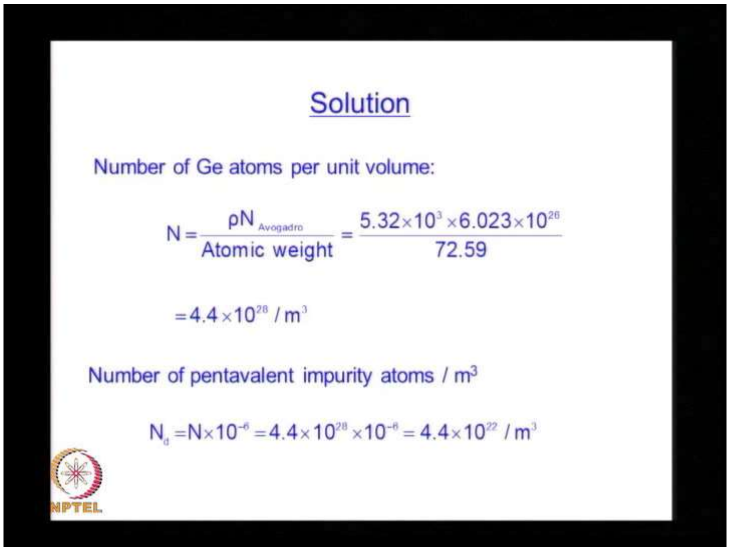

Solution

Number of Ge atoms per unit volume:

$$N = \frac{\rho N_{\text{Avogadro}}}{\text{Atomic weight}} = \frac{5.32 \times 10^3 \times 6.023 \times 10^{26}}{72.59}$$

$$= 4.4 \times 10^{28} / m^3$$

Number of pentavalent impurity atoms / m^3

$$N_d = N \times 10^{-6} = 4.4 \times 10^{28} \times 10^{-6} = 4.4 \times 10^{22} / m^3$$

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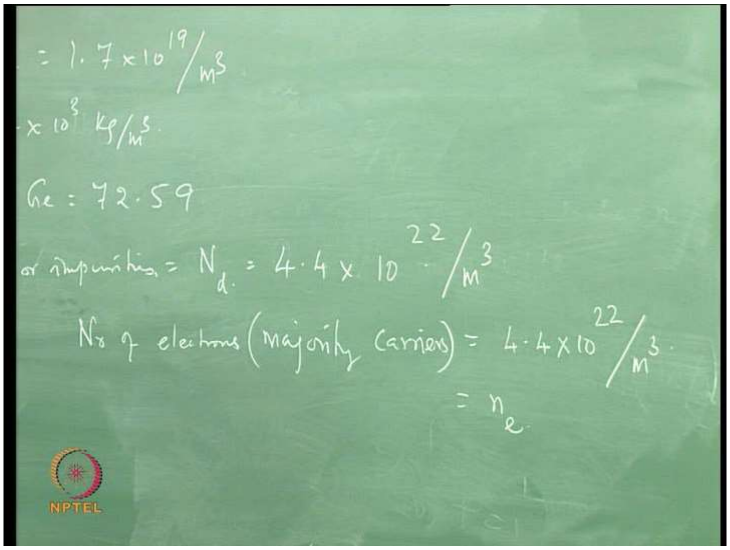


$= 1.7 \times 10^{19} / m^3$

$\times 10^3 \ kg/m^3$

Ge : 72.59

or impurities = $N_d = 4.4 \times 10^{22} / m^3$

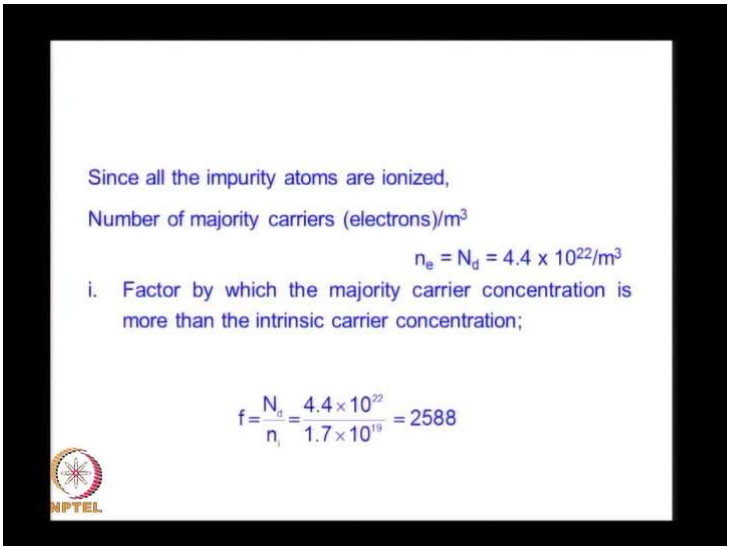
Nr of electrons (majority carriers) = $4.4 \times 10^{22} / m^3$

$= n_e$

So, the number of germanium atoms per unit volume can be calculated using allocator number the density. And their atomic weight as 4.4 into 10 to the power twenty eight we are asked to assume; that the this germanium is doped with pentavalent impurity atoms at doped with and the doping concentration is one part per million which is ten to the power minus 6.

So, this is the number of germanium atoms and the number of impurities. These are donor impurities, they donate electrons the number of donors impurities is standard notation is n d and that is taking this number 4.4 into 10 to the power 28 and 10 to the power minus 6, and 10 to the power 22 per metre cube. And we assume that all of them are ionised all the impurities atoms are ionised. So, the number of electrons donated which are the majority carriers this the same number each impurity atom donates an electron. So, that is what we call usually n with a subscript e.

(Refer Slide Time: 15:09)



Since all the impurity atoms are ionized,

Number of majority carriers (electrons)/m^3

$$n_e = N_d = 4.4 \times 10^{22}/m^3$$

i. Factor by which the majority carrier concentration is more than the intrinsic carrier concentration;

$$f = \frac{N_d}{n_i} = \frac{4.4 \times 10^{22}}{1.7 \times 10^{19}} = 2588$$

So, we were asked to calculate several quantities; for example the factor by which by what factor noise.

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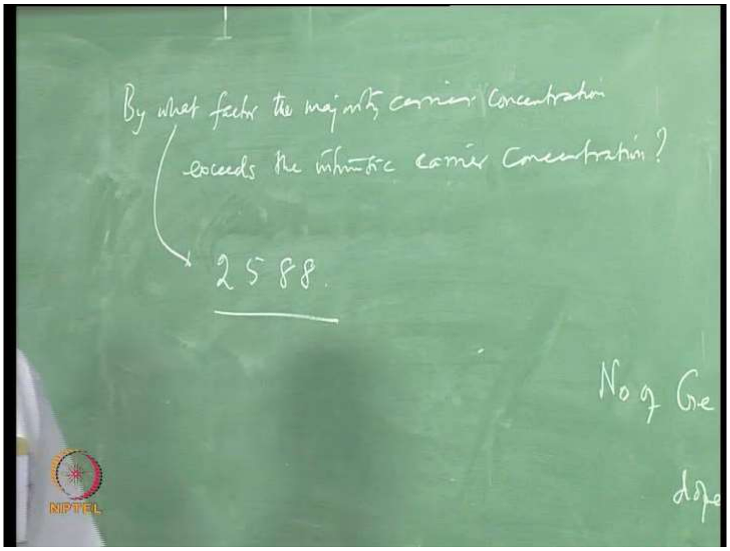


By what factor the majority carrier concentration exceeds the intrinsic carrier concentration?

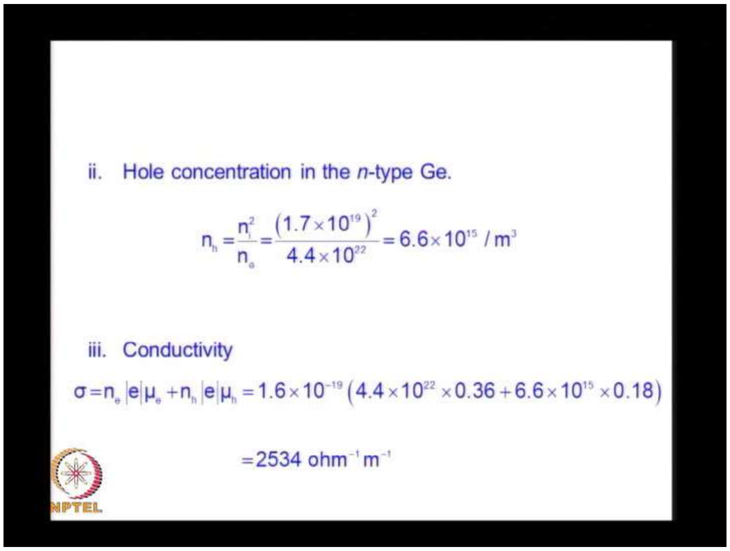
2588.

No of Ge

dope

The majority carriers exceed carrier concentration exceeds the intrinsic carrier concentration. So, all we have to do is we are given the intrinsic carrier concentration, and we have determined the number of the majority carrier concentration namely that of electrons. So, we divide one by the other and get the factor as the answer is two thousand five hundred and eighty eight noise there are 2588 majority carriers for each intrinsic carrier. And since we know the number of this is what we know as n i intrinsic concentration.

(Refer Slide Time: 16:23)



ii. Hole concentration in the *n*-type Ge.

$$n_h = \frac{n_i^2}{n_e} = \frac{(1.7\times10^{19})^2}{4.4\times10^{22}} = 6.6\times10^{15}\ /\mathrm{m}^3$$

iii. Conductivity

$$\sigma = n_e|e|\mu_e + n_h|e|\mu_h = 1.6\times10^{-19}\left(4.4\times10^{22}\times0.36 + 6.6\times10^{15}\times0.18\right)$$

$$= 2534\ \mathrm{ohm}^{-1}\mathrm{m}^{-1}$$

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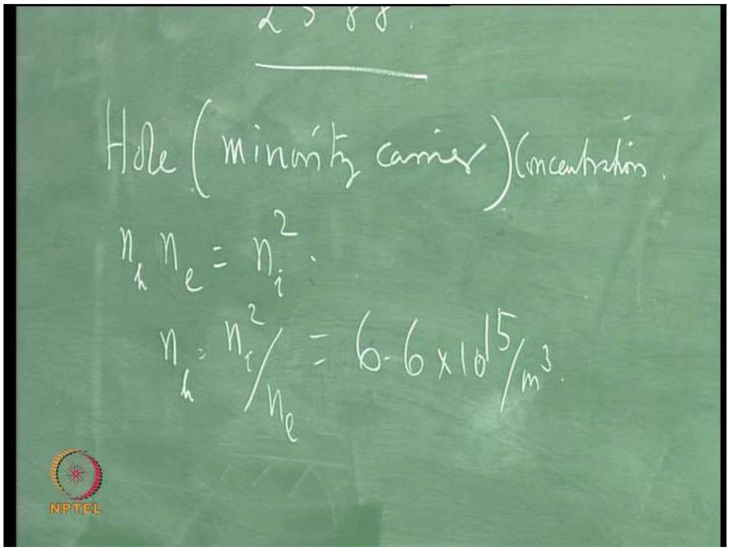

2588.

Hole (minority carrier) Concentration.

$$n_h n_e = n_i^2.$$

$$n_h = n_i^2/n_e = 6.6\times10^{15}/m^3.$$

And therefore, the hole concentration hole, which is the minority carrier concentration is given by n h equals is such that n h times n e is n i square. So, we know n h is n i square by n e. So, substituting n i and n e we get the value of n h as 6.6 into 10 to the power fifteen per metre cube, because we know the majority and minority carrier concentrations. And we have been given the mobilities of the electrons, and holes we are now in a position to calculate the conductivity contributed by the electrons and holes.

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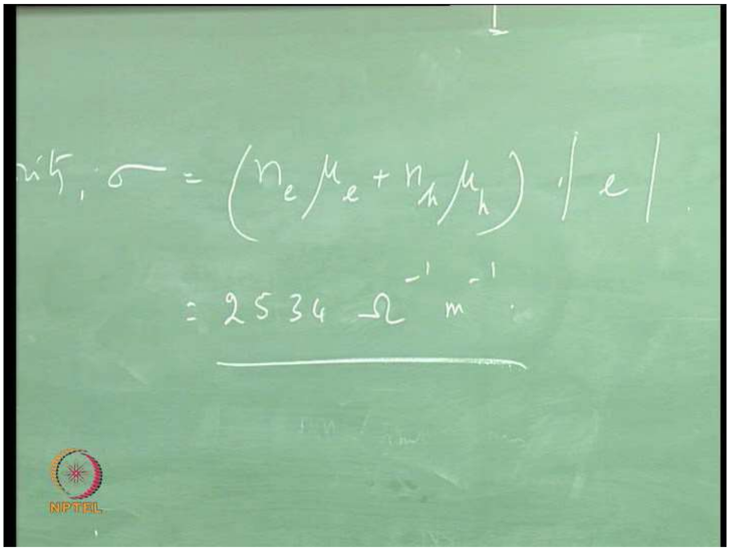

$$\sigma = (n_e\mu_e + n_h\mu_h)\,|e|$$

$$= 2534\ \Omega^{-1}\,m^{-1}$$

And hence the total conductivity noise sigma, which as we have seen n e mu e n h mu h times mod e. So, n e is known n h is known and therefore, we can calculate the conductivity and this turns out to be that is the value for the conductivity with the given mobility values.

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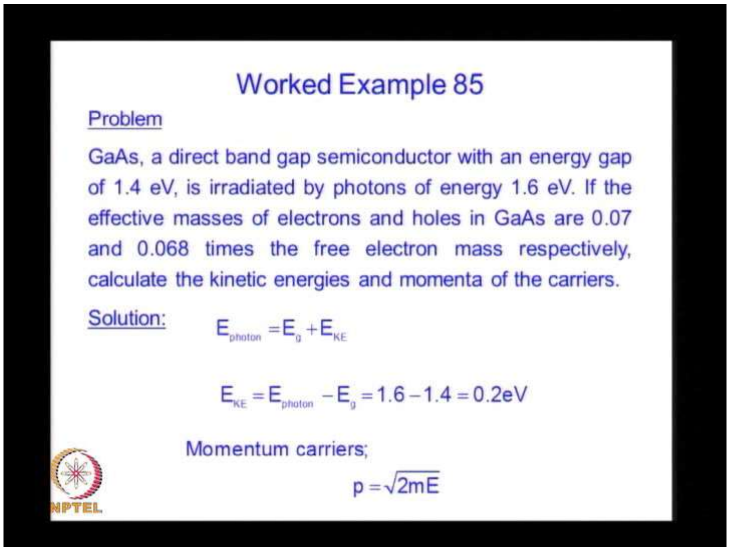

Worked Example 85

Problem

GaAs, a direct band gap semiconductor with an energy gap of 1.4 eV, is irradiated by photons of energy 1.6 eV. If the effective masses of electrons and holes in GaAs are 0.07 and 0.068 times the free electron mass respectively, calculate the kinetic energies and momenta of the carriers.

Solution:

$$E_{photon} = E_g + E_{KE}$$

$$E_{KE} = E_{photon} - E_g = 1.6 - 1.4 = 0.2\text{eV}$$

Momentum carriers;

$$p = \sqrt{2mE}$$

Next, we pass on to the case of gallium arsenide as we have already seen gallium arsenide is a compound semiconductor.

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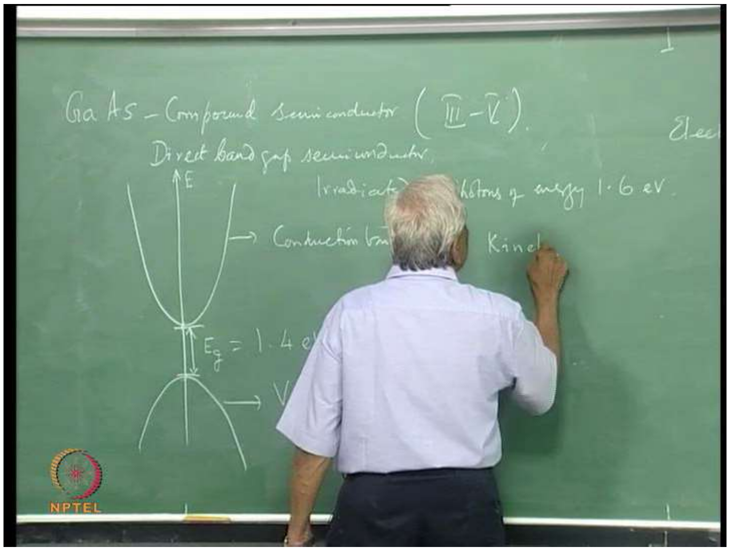

The gallium and arsenic gallium for the group three and arsenic from group five in the periodic table. So, it is a three to 535 compound. And we already saw in the lecture that it is a direct band gap semiconductor which means that the bottom of the conduction band and the top of the valence band lie exactly one above the other. So, these two are just above each other, and this difference in energy is the energy gap whose value is given in the case of gallium arsenide as 1.4 electron volts we are also told that this sample is evaluated with photons of energy 1.6 electron volts.

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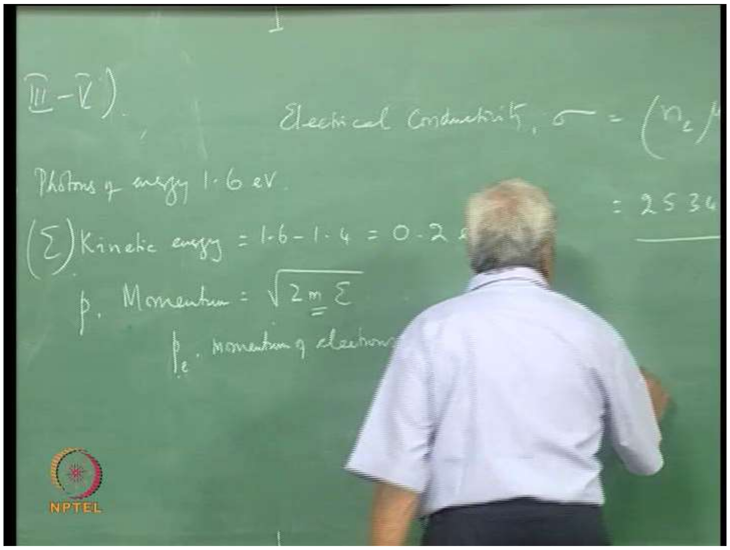

III – V)

Electrical Conductivity, $\sigma = (n_e \mu$

Photons of energy 1.6 eV.

$= 2534$

(Σ) Kinetic energy $= 1.6 - 1.4 = 0.2$

p. Momentum $= \sqrt{2 \underline{\underline{m}} \Sigma}$

p_e : momentum of electrons

So, the difference in energy one point six and one point four gives you the kinetic energy of carriers that is the kinetic energy, and the carriers and since this is say e and therefore, the momentum is just root two m e p, therefore the momentum.

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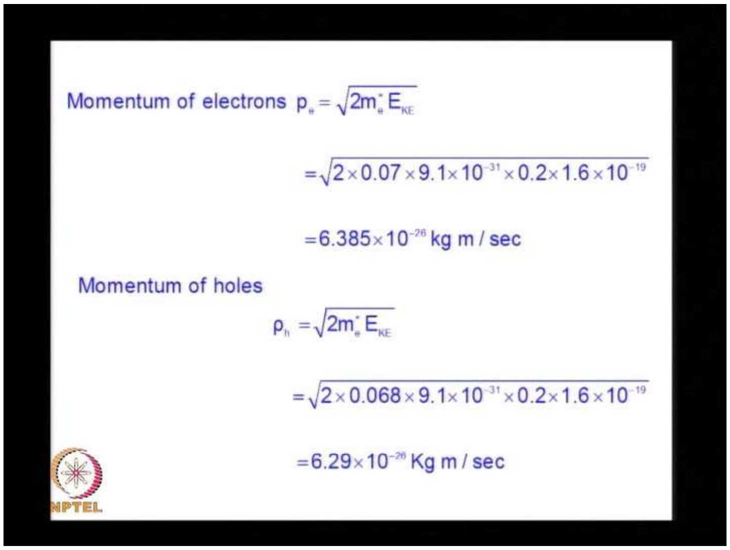

Momentum of electrons $p_e = \sqrt{2m_e^* E_{KE}}$

$$= \sqrt{2 \times 0.07 \times 9.1 \times 10^{-31} \times 0.2 \times 1.6 \times 10^{-19}}$$

$$= 6.385 \times 10^{-26} \text{ kg m / sec}$$

Momentum of holes

$$p_h = \sqrt{2m_e^* E_{KE}}$$

$$= \sqrt{2 \times 0.068 \times 9.1 \times 10^{-31} \times 0.2 \times 1.6 \times 10^{-19}}$$

$$= 6.29 \times 10^{-26} \text{ Kg m / sec}$$

Of course in this case the mass is involved. So, the momentum will be different for the electrons and holes because the effective masses are different. So, the momentum of electron is root 2 m e star e. So, substituting the effective mass of electron which is given as point naught seven times that of the electron free electron therefore, substituting that they get at the momentum as 6.835 into 10 to the power of minus 26 momentum kilogram meters per second proceeding the same way.

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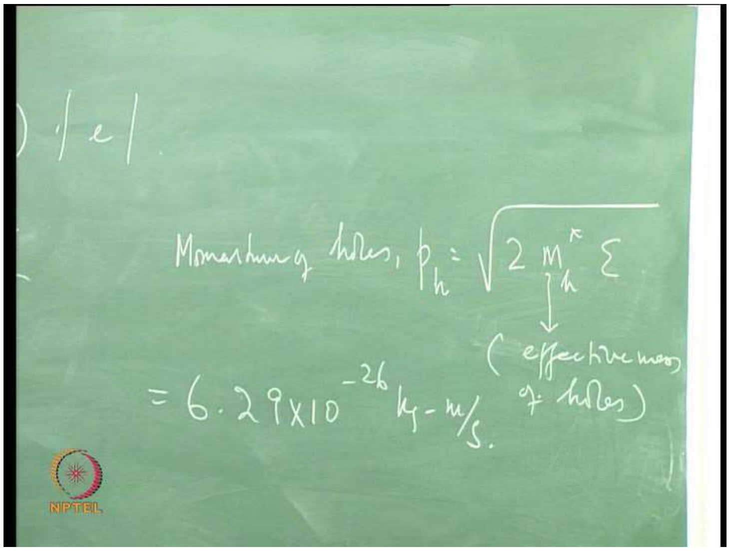

) /e/ .

Momentum of holes, $p_h = \sqrt{2 m_h^* E}$

$\downarrow$ (effective mass of holes)

$= 6.29 \times 10^{-26}$ kg-m/s.

We get the momentum of holes two m h star e where this is effective mass of the... So, that is again given to be 0.68 times that of the free electron. So, substituting this value, we get the momentum as 6.29 into 10 to the power minus twenty six kilogram metre per second

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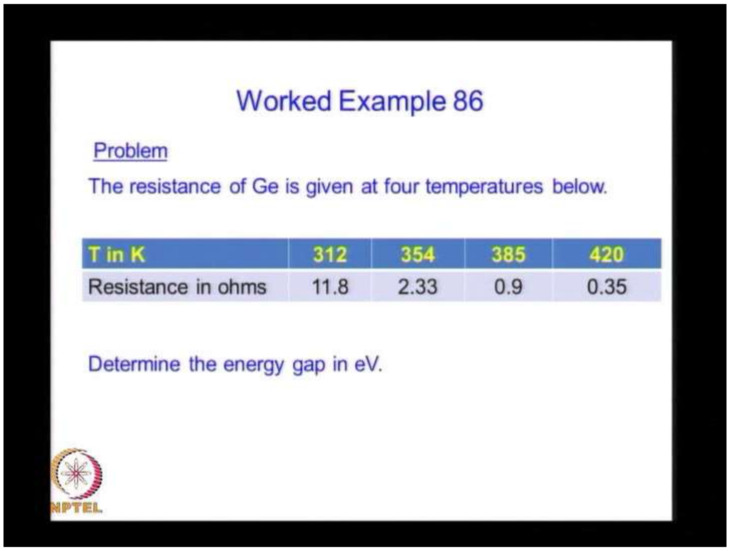

Worked Example 86

Problem

The resistance of Ge is given at four temperatures below.

T in K	312	354	385	420
Resistance in ohms	11.8	2.33	0.9	0.35

Determine the energy gap in eV.

In the next problem, we are given data in the tabular form for the resistance of germanium.

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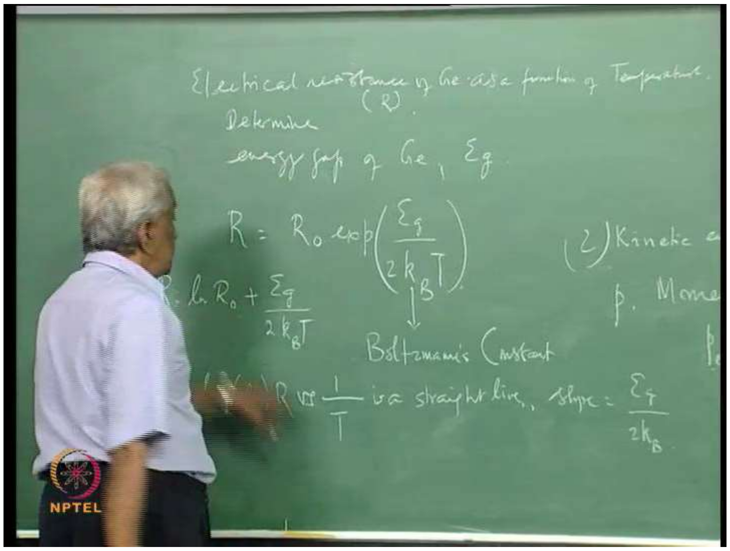

The electrical resistance of germanium is given as a function of temperature. So, we are given the values in ohm's of the resistance at 300, and 12 k, 354 k, 385 k, and 420 k.

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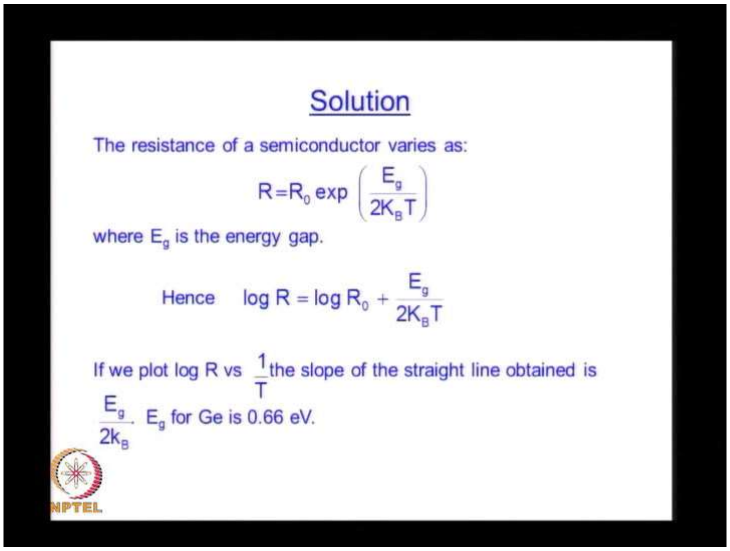

Solution

The resistance of a semiconductor varies as:

$$R = R_0 \exp\left(\frac{E_g}{2K_BT}\right)$$

where E_g is the energy gap.

Hence $$\log R = \log R_0 + \frac{E_g}{2K_BT}$$

If we plot log R vs $\frac{1}{T}$ the slope of the straight line obtained is $\frac{E_g}{2k_B}$. E_g for Ge is 0.66 eV.

And we are asked to determine the energy gap at as a function of temperature resistance r. So, determine energy gap of germanium that is the question and for this. We know that the resistance as the temperature dependence, which has the form where e g is energy gap and kb is the Boltzmann's constant therefore, we take logarithms . So, a plot of log r r log also versus one by t is a straight line whose slope is e g by 2 k b. So, plotting this graph of log r versus 1 by t from the given values we get a straight line and the slope gives the energy gap in terms of twice the Boltzmann constant. And so we can determine the energy gap the energy gap turns out to be point six electron volts from the given data.

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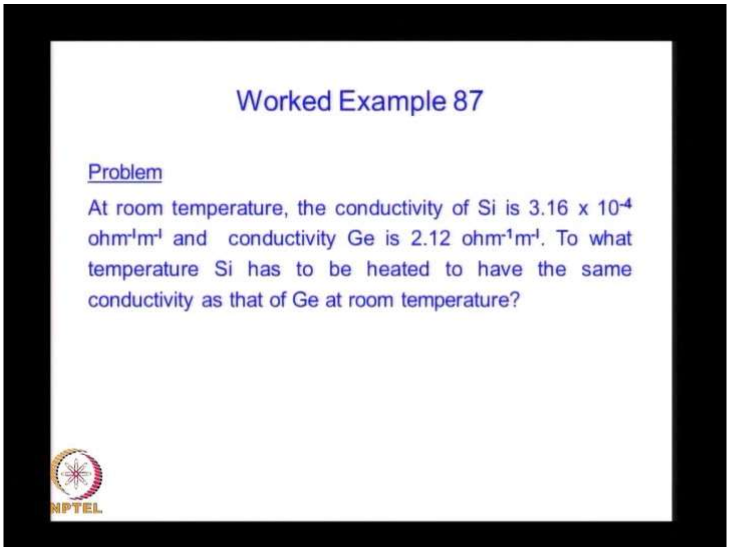

Worked Example 87

Problem

At room temperature, the conductivity of Si is 3.16 x 10^{-4} $ohm^{-1}m^{-1}$ and conductivity Ge is 2.12 $ohm^{-1}m^{-1}$. To what temperature Si has to be heated to have the same conductivity as that of Ge at room temperature?

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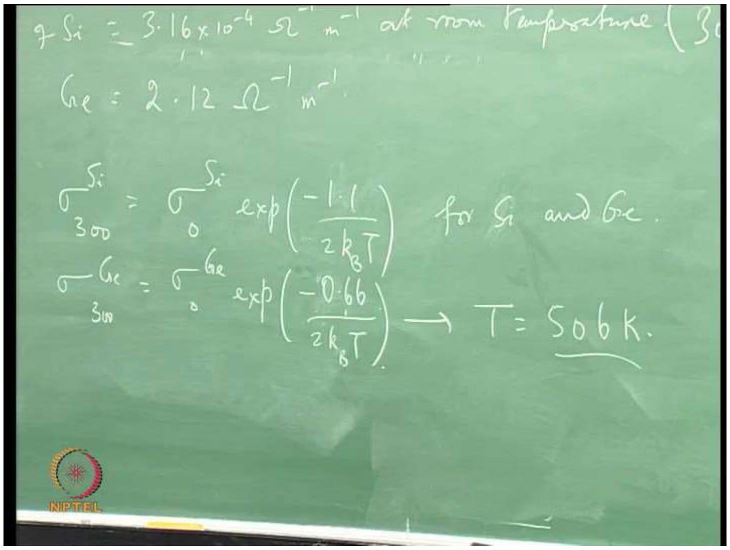

$\sigma_{Si} = 3.16 \times 10^{-4}\ \Omega^{-1} m^{-1}$ at room temperature (3

$Ge = 2.12\ \Omega^{-1} m^{-1}$

$$\sigma^{Si}_{300} = \sigma^{Si}_{0} \exp\left(\frac{-1.1}{2k_BT}\right)$$ for Si and Ge.

$$\sigma^{Ge}_{300} = \sigma^{Ge}_{0} \exp\left(\frac{-0.66}{2k_BT}\right) \longrightarrow T = \underline{506\,K}.$$

Next, question concerns the comparison of the conductivity of silicon conductivity means always electrical conductivity, in this case silicon is 3.16 into 10 to the power minus four at room temperature, and that of germanium is also given at room temperature as 2.12 ohm minus one metre minus one four orders higher.

So, we are asked to what temperature; obviously, if silicon is heated the conductivity increases if it has to have the same conductivity as germanium to what temperature should silicon be heated. So, that is the question. So, we have sigma three hundred we take this has three hundred k

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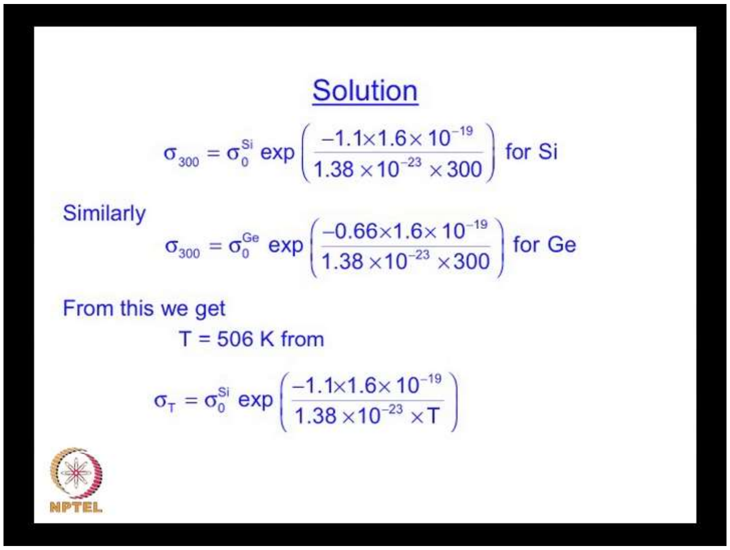

Solution

$$\sigma_{300} = \sigma_0^{Si} \exp\left(\frac{-1.1\times1.6\times10^{-19}}{1.38\times10^{-23}\times300}\right) \text{ for Si}$$

Similarly

$$\sigma_{300} = \sigma_0^{Ge} \exp\left(\frac{-0.66\times1.6\times10^{-19}}{1.38\times10^{-23}\times300}\right) \text{ for Ge}$$

From this we get

T = 506 K from

$$\sigma_T = \sigma_0^{Si} \exp\left(\frac{-1.1\times1.6\times10^{-19}}{1.38\times10^{-23}\times T}\right)$$

Is for sigma naught exponential minus e g by two kb t for both for silicon as well as Germanium. So, we can write it separately for the two of course, the energy gap values are different. So, the energy gap in this case is one point one electron volt and in this case it is 0.66 as we just know saw. So, we get using this eliminating sigma zero we get t s pi 06 kelvin. So, we have to heat silicon to 230 degrees celsius for it to get the same conductivity as germanium at room temperature.

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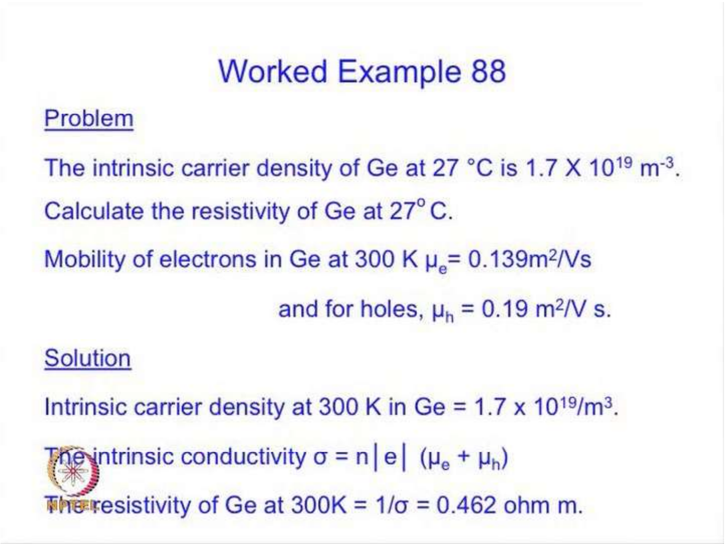

Worked Example 88

Problem

The intrinsic carrier density of Ge at 27 °C is 1.7 X 10^{19} m^{-3}.

Calculate the resistivity of Ge at 27° C.

Mobility of electrons in Ge at 300 K μ_e= 0.139m^2/Vs

and for holes, μ_h = 0.19 m^2/V s.

Solution

Intrinsic carrier density at 300 K in Ge = 1.7 x 10^{19}/m^3.

The intrinsic conductivity $\sigma = n|e|\ (\mu_e + \mu_h)$

The resistivity of Ge at 300K = 1/σ = 0.462 ohm m.

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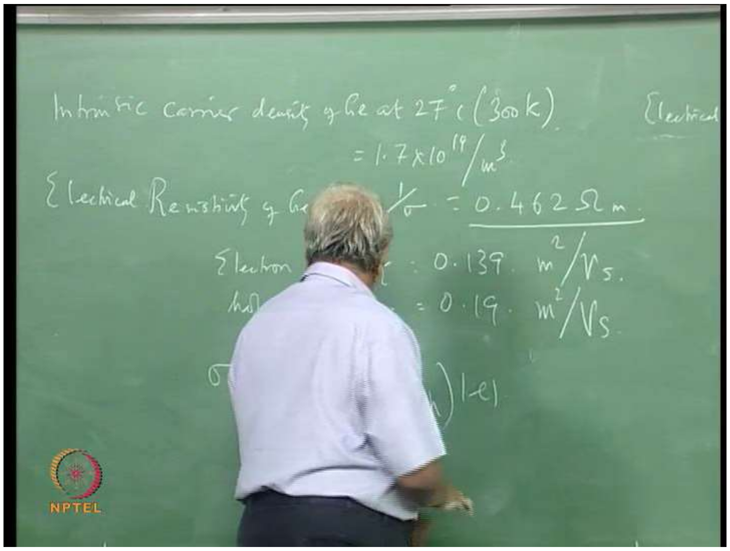

Next, we are given the intrinsic carrier density of germanium as 1.7 at 27celsius, which is the same as 300 k as 1.7 into ten to the power 19 per metre cube. So, we are asked to calculate the resistivity of course, electrical resistivity we have given electron and hole mobilities for germanium they are given at this temperature as point one three nine ten point one nine metre square per volt second. Therefore, with this we can write the usual conductivity formula where of course n e and n h are the same, therefore we need even write this like this where n is the common concentration.

So, the resistivity is one by sigma. So, this is one by sigma, and therefore we can calculate from these substituting finding sigma from here and then taking the reciprocal we get the value as naught 0.452 ohm metre, which is the answer we have done given a problem on silicon

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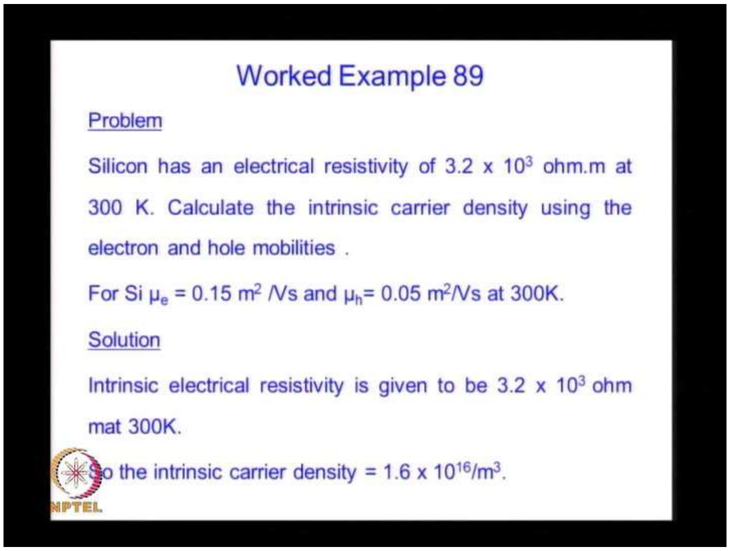

Worked Example 89

Problem

Silicon has an electrical resistivity of 3.2×10^3 ohm.m at 300 K. Calculate the intrinsic carrier density using the electron and hole mobilities .

For Si $\mu_e = 0.15\ m^2/Vs$ and $\mu_h = 0.05\ m^2/Vs$ at 300K.

Solution

Intrinsic electrical resistivity is given to be 3.2×10^3 ohm mat 300K.

So the intrinsic carrier density = $1.6 \times 10^{16}/m^3$.

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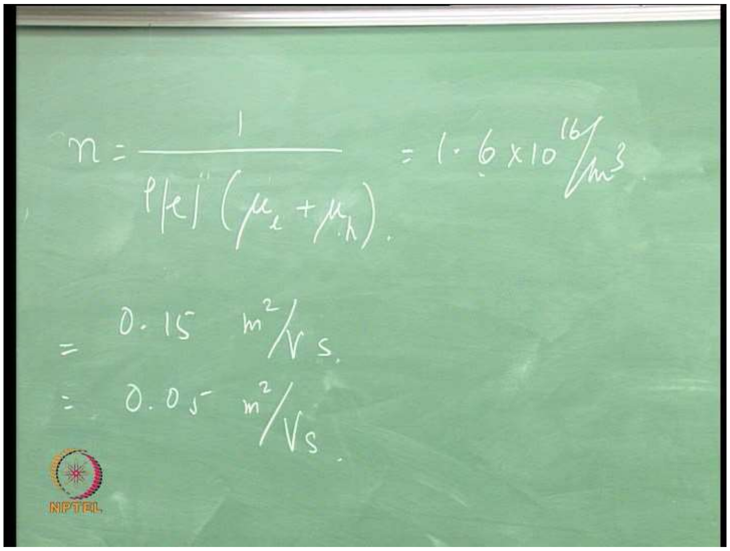

$$n = \frac{1}{\rho |e| (\mu_e + \mu_h)} = 1.6 \times 10^{16}/m^3$$

$$= 0.15\ m^2/Vs$$

$$= 0.05\ m^2/Vs$$

Here it is the inverse problem the resistivity is given no it was three resistivity at three hundred k. So, we are asked to calculate intrinsic carrier density with the data on electron and hole mobility in silicon. So, this is given as point one five and point zero five metre square per volt second. So, this is mu e this is mu h noise. So, we have to calculate the intrinsic current density which is straightaway given by and... So, substituting all this values we get one point six into ten to the power 16.

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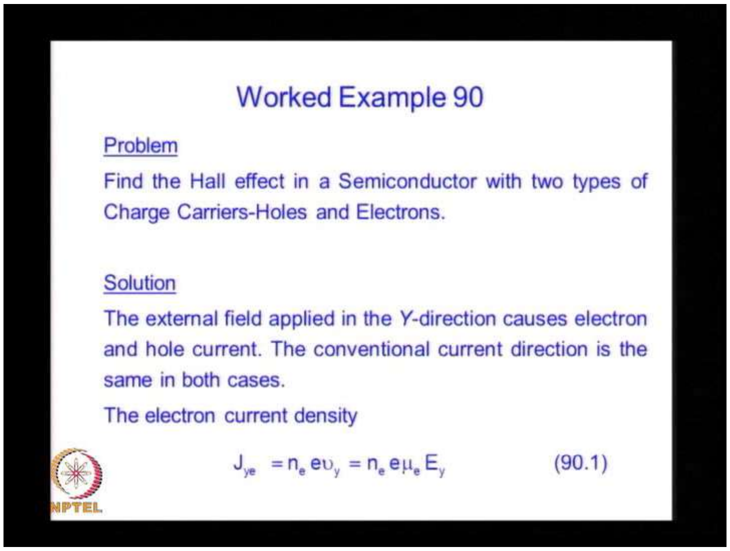

Worked Example 90

Problem

Find the Hall effect in a Semiconductor with two types of Charge Carriers-Holes and Electrons.

Solution

The external field applied in the *Y*-direction causes electron and hole current. The conventional current direction is the same in both cases.

The electron current density

$$J_{ye} = n_e e \upsilon_y = n_e e \mu_e E_y \qquad (90.1)$$

The last question concerns the hall effect in a semiconductor with two types of carriers the electrons and holes.

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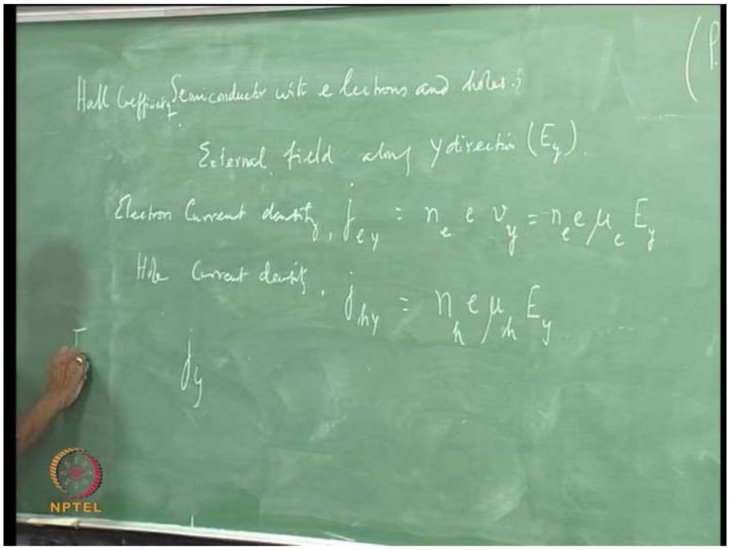

Hall Coefficient Semiconductor with electrons and holes:

External field along y direction (E_y).

Electron Current density, $j_{ey} = n_e e v_y = n_e e \mu_e E_y$

Hole Current density, $j_{hy} = n_h e \mu_h E_y$

j_y

So, we discussed in the lecture the hall effect for a semiconductor with one type of carriers now hall coefficient. So, that is what we are asked to determine. So, suppose we have an external field, hall effect is an effect which is produced then there is an external field applied at right angles to the direction of motion of the carrier in a current carrying semiconductor. So, external field is taken along y. So, let us call it e y. So, the electron current density will be will be j e y, which will be carrier concentration electron concentration times the electron charge times the speed of the electron along the y direction. And this in terms as the mobility, it is mu e mobility as electron times the field e y similarly for the hole current density h y that would be by the same token it will be n h e mu h e y. And therefore, the total current as we already discussed the holes will move in the direction opposite to that of the electrons they will move along the electric field direction. And these electrons will move opposite to the electric field direction, but since they are of opposite charges the current densities will be added. So, this will be n e mu e plus n h mu h times e e y now because of this current.

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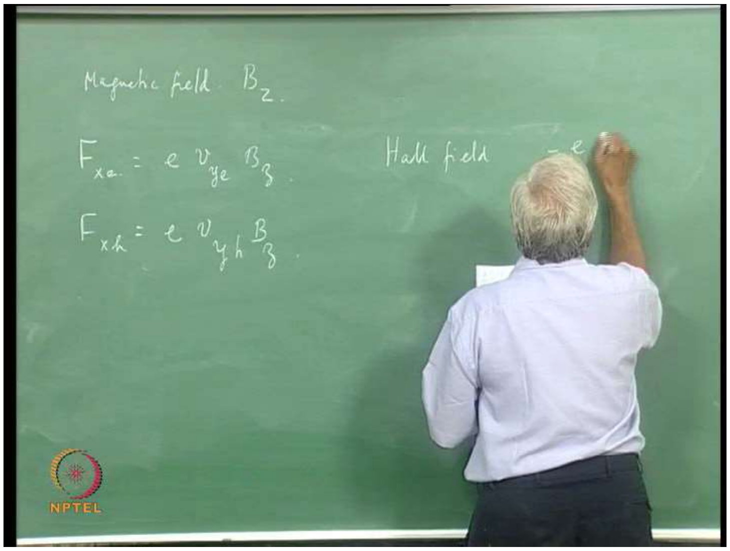

Magnetic field B_z.

$F_{xe} = e\, v_{ye} B_z$.

$F_{xh} = e\, v_{yh} B_z$.

Hall field = e

And because of the magnetic field is taken it should be at right angles the electric field y direction as well as the initial current density. So, we take it along the z direction. So, the force the Lawrence force on the electron which will be in the direction perpendicular to y and z namely x direction. So, we write it as f x e will be e v ye b z the force acting on the hole is e v y h b z.

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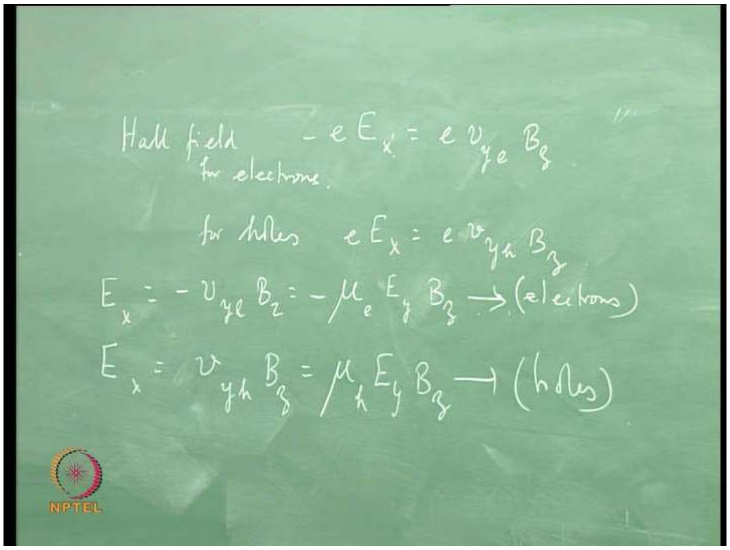

Hall field for electrons. $-eE_x = e v_{ye} B_z$

for holes $eE_x = e v_{yh} B_z$

$E_x = -v_{ye} B_z = -\mu_e E_y B_z \rightarrow$ (electrons)

$E_x = v_{yh} B_z = \mu_h E_y B_z \rightarrow$ (holes)

So, the hall field because of the lateral moment of the electrons and holes there will be a hall fields which in the case of the electrons it is directed along the x direction. Therefore this is e v y e b z, and for electrons due to motion of electrons in the x direction and for holes similarly it will be e ex equals e v y h b z noise. Therefore, ex in these two cases will be minus v ye b z, which in terms of the mobility it is mu e times e y b z and for this is for the electrons. And similarly ex will be e v y h b z which in terms of the mobility is mu h e y b z this is for the holes. So, since there is a hall field in the lateral direction given by the sum of these two there will be a current density the motion of carriers.

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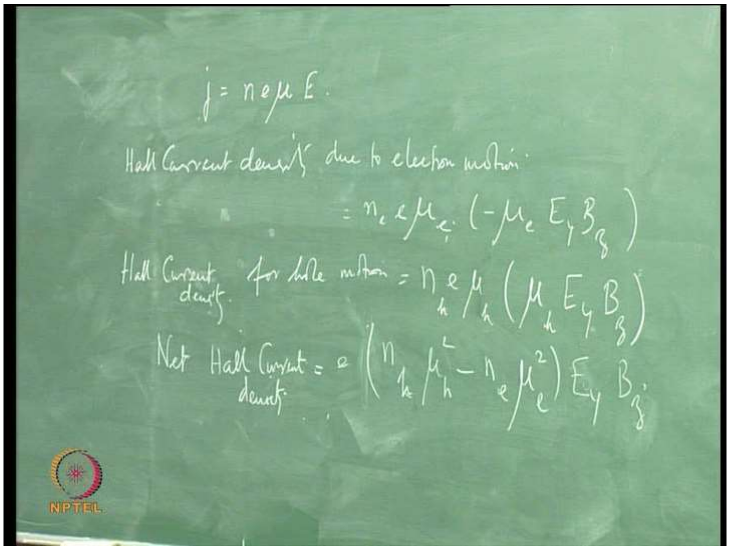

$j = ne\mu E$.

Hall Current density due to electron motion

$= n_e e \mu_e (-\mu_e E_y B_z)$

Hall Current density for hole motion $= n_h e \mu_h (\mu_h E_y B_z)$

Net Hall Current density $= e(n_h \mu_h^2 - n_e \mu_e^2) E_y B_z$

And there will be a current density contributed from both which is given by the standard relation n e mu e. Therefore, the hall current densities due to electrons electron motion and that will be n e e mu e using this times that electric field. So, that will be minus mu e e y b z and for the holes. Similarly for hole motion this will be n h e mu h into mu h e y b z noise. So, the total current a net hall current will be e times n h taking these two n h mu h square minus ne mu e square times e y b z. So, this will be the hall current density.

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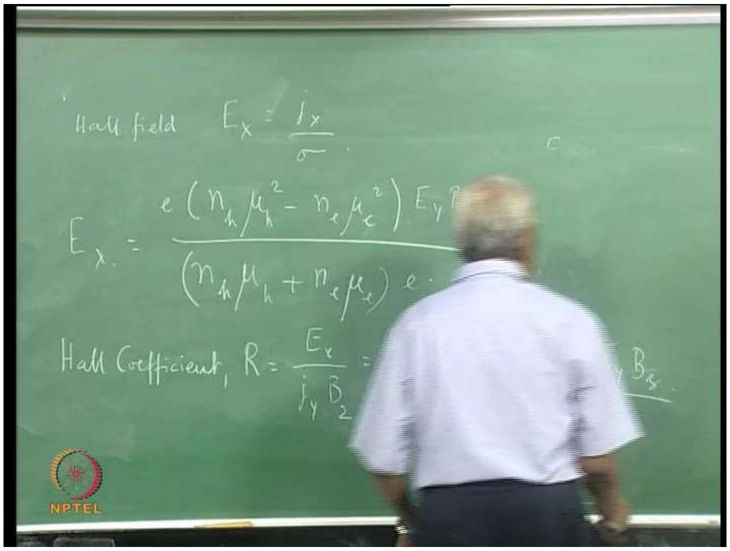

Hall field $E_x = \frac{j_x}{\sigma}$.

$$E_x = \frac{e\left(n_h\mu_h^2 - n_e\mu_e^2\right)E_y B}{\left(n_h\mu_h + n_e\mu_e\right)e}$$

Hall Coefficient, $R = \frac{E_x}{j_y B_z} =$

So, this hall current density will be result in a hall field due to this current density and that is e x is j x by sigma by ohm's law again therefore, this will be e times borrowing this expression n h mu h square minus n e mu e square into e y b z by the conductivity which is n h mu h plus n e mu e times e noise. So, and the hall coefficient r is just ex by j y b z and that will be borrowing, this expression n h mu h square minus n e mu e square times e y b z by n h mu h plus n e mu e here times j y b z, and this is nothing but sigma e y b z. So, this will give me simplifying substituting for sigma again that will be the hall coefficient in a semiconductor containing two carriers. And it is a simple matter to go from here, and show that this will lead to the standard expression r equal to one by n e in the case of a semiconductor with just one type of carriers.

Condensed Matter Physics

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Lecture - 19
Dia- and Paramagnetism

Today we will start an important section of Condensed Matter meant physics namely magnetism. We have just finished discussing the mechanism of dielectric polarization in dielectric materials, how an applied electric field polarizes a dielectric medium and produces a polarization with various effects such as dispersion, phase transition into the ferroelectric field and things like that. We will, now go on a very similar process which takes place in magnetic materials. In the case of magnetism instead of a dielectric or electric polarization, we will have a magnetization, which is caused by an applied magnetic field. So, the analogy is very clear just as the dielectric polarization is established by an applied electric field a magnetization is produced in a magnetic material by an applied magnetic field. The process by which this magnetization is established goes on lines, which is very similar to that of electric polarization. Of course, there are very significant and important fundamental differences also.

So, in the course of this lecture, and in few subsequent lectures, we will be discussing some these processes and mechanisms. We start with magnetism is a well-known phenomenon of nature which has attracted the attention of people from time immemorial, immemorial. We know that people have talked about load stones in Sanskrit, people have talk quietly they have talked about [FL], so they have talked about how a magnate attracts iron. Similarly, people talked about lodestone, mariners people who go voyages in the sea have uses the magnetic compass to know the direction in the sea. So, these are all known for a very, very long time since ancient times.

So, magnetism is a phenomenon which is very well known even Aryabhata has talked about magnetism. So, the phenomenon of magnetism occupies a central position in condensed matter physics. There are reasons for this, not because magnetism in particular is a special topic. It is similar to many other topics, but the entities which produce magnetization which magnetize a material namely we are known as spins, magnetic spins, spin angular momentum, it is something which is new to classical physics. It is a totally a new degree of freedom in the case of electronic atomic and molecular system. But the spins are probably the cleanness to physical entity treat theoretically as well as experimentally. The spins give rise to magnetic effects and can be studied by a variety of techniques and can be described theoretically we have very considerably extends with great success. Now all magnetism mainly arises from the electrons of the atoms and molecules; of course, the nuclei also produce magnetic effects, we will discuss this later. But for recent which will become clear later on magnetism as a phenomenon is mainly due to the electrons in atoms and molecules.

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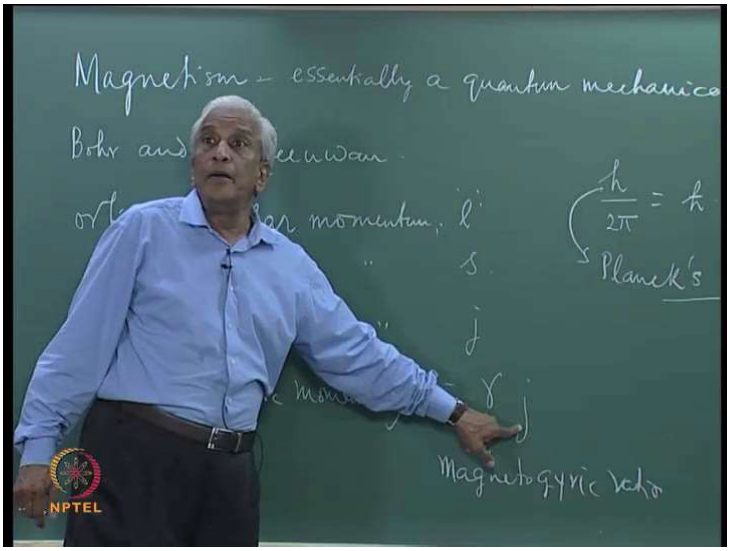

There is no classical way of describing magnetism. In fact, there is a theorem by there is theorem due to Bohr and von Leeuwen if states that if you applied classical statistical mechanical considerations to an assembly of electrons which produces magnetism you will find that the average magnetization vanishes. So, you cannot account for any magnetism using classical theories. Magnetism is essentially a quantum mechanical phenomenon. So, this is the first point to be understood that in order to understand magnetism, we have to learn quantum mechanics or at least be familiar with the fundamental principles of quantum physics, because we are talking about the orbital motion of electrons as well as spin of electrons.

Spin is a completely quantum mechanical effect, relativistic quantum mechanical effect. Even the orbital motion in a finite sample the macroscopic magnetic moment produced by the orbital angular moment of electrons vanishes identically by Bohr and von leeuwan theorem. Therefore, in order know how this magnetism arises and in order to quantitatively, describe the behavior of this magnetic moment one has to apply quantum mechanics and quantum statistical physical concepts. So, this is the first point be realized next we will ask how there is the magnetic moment is produced for an electron. In the case of an electron, we all know that the electron orbiting around the nucleus of an atom and similarly in the case of a molecule there are molecular orbital's in which the electron is oppose to the moving.

So, the cause of this motion this orbit to the motion whenever the charge is moving a current is produced in that loopso this orbit is like a current carry in loop and the current carry in loop always produces a magnetic moment as orsted describe first discovered. So, we know that the orbital motion it is very easy to see that the orbital motion of an electron will produced magnetic field because the orbit of an electron around the nucleus serves as a closed current loop in which the current don not vanish.

So, this is theoretically described by saying that the orbiting electron has an orbital angular momentum which is usually denoted by the letter l in books on quantum mechanics or j this is orbital, but usually there is also a spin angle of momentum which we will discuss later and that is represented by the letter s and. So, there is a total angle of momentum disguise as by the letter represented by the letter j. So, all these angular momentum are quantized according to the rules of quantum mechanics in other words the orbital angle of momentum can only be in units an integral multiples of a fundamental unit which is you fundamental usually the fundamental unit of angle of momentum is h by two pi or h cross where h is the Planck's constant.

So, the angle of momentum is measure as j h cross when we say that the angular momentum is j what we mean is the angular momentum is j h by two pi if this is. So, then quantum mechanics cause or tell us that there is a corresponding magnetic moment due to this angular momentum which is represented usually by the letter mu and that is proportional to this angular momentum orbital angular momentum. So, mu equal to gamma j where gamma is known as the magneto gyric ratio. In other words, it is the ratio of the magnetic moment to the gyro or angular momentum in world or books this should have been written as gyro magnetic ratio gamma is the magneto gyric ratio. So, this only means that the magnetic moment vector both mu and j are vector quantities.

So, the magnetic moment is parallel to the orbital angular momentum or the total angular momentum. So, this is what this expression says you would like to understand how this magnetic moment arises as I said this has been to be done in the framework of quantum mechanics.

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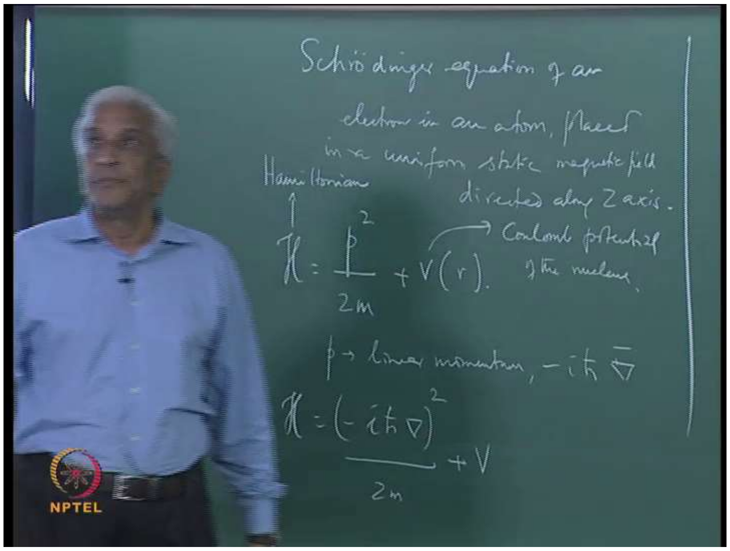

Schrödinger equation of an electron in an atom, placed in a uniform static magnetic field directed along Z axis.

Hamiltonian

$$\mathcal{H} = \frac{p^2}{2m} + V(r).$$

Coulomb potential of the nucleus.

$p \rightarrow$ linear momentum, $-i\hbar\nabla$

$$\mathcal{H} = \frac{(-i\hbar\nabla)^2}{2m} + V$$

So, let us do some basic quantum mechanics by writing the Schrodinger equation of an electron in an atom placed the magnetic field in a uniform magnetic field uniform static magnetic field whose direction is taken as the z direction. So, how do we write the equation the Schrodinger equation for such an electron we know that this electron is in the potential of the nucleus. So, we have the standard way in the absence of an applied magnetic field the electron Hamiltonian this is the Hamiltonian which is the starting point of writing the Schrodinger equation is just equal to p square by two m plus b f I where p is the linear momentum.

And in quantum mechanics p is an operator which is represented by minus I h cross tell m is the mass of the electron b f r is the coulomb potential of the nucleus it is written as b f for because we know that the nucleus exerts a centre central coulomb potential. And therefore, it is function only the distance between the electron and the nucleus.

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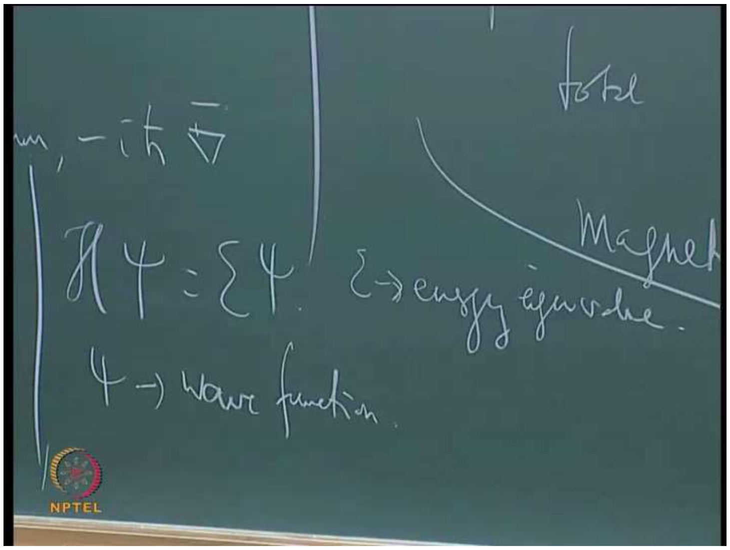

So, this gives me the Hamiltonian has minus I h cross del square by two m plus b and the Schrodinger equation h psi is just h psi equal e psi where psi is the wave function and e is the energy eigen value this Hamiltonian gets modified when an magnetic field is applied again quantum theory tells us that.

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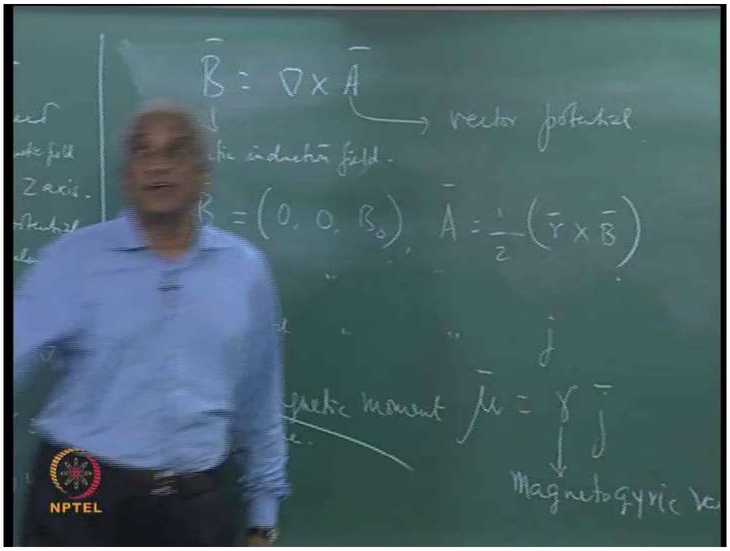

In fact, these an electro dynamic result that when there is an applied magnetic field this magnetic field has an induction which is given by a vector potential a. So, this is the magnetic induction field and a is the vector potential and b o and a are related in this form, so if b is constant and uniform directed along is that direction we can write between this form and if this is. So, we can choose the the form of the vector potential which will give you a b like this can be chosen as half r cross b this is the standard result from electro dynamics which can be written in the form.

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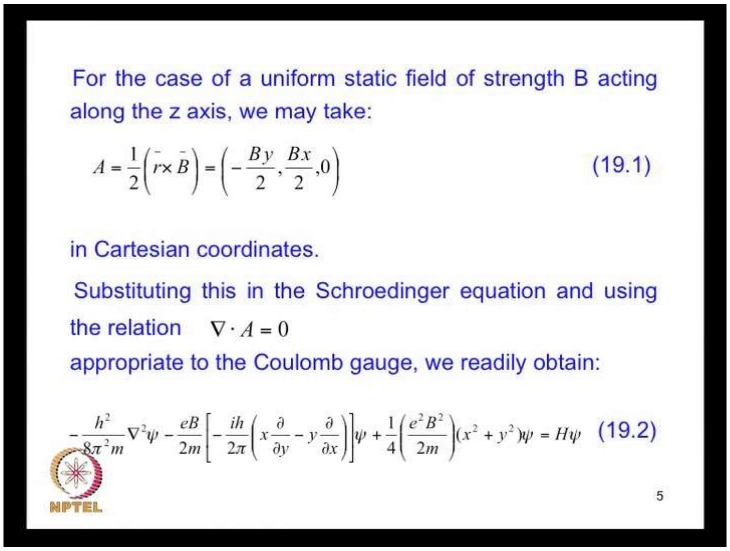

For the case of a uniform static field of strength B acting along the z axis, we may take:

$$A = \frac{1}{2}\left(\bar{r} \times \bar{B}\right) = \left(-\frac{By}{2}, \frac{Bx}{2}, 0\right) \qquad (19.1)$$

in Cartesian coordinates.

Substituting this in the Schroedinger equation and using the relation $\nabla \cdot A = 0$
appropriate to the Coulomb gauge, we readily obtain:

$$-\frac{h^2}{8\pi^2 m}\nabla^2\psi - \frac{eB}{2m}\left[-\frac{ih}{2\pi}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\right]\psi + \frac{1}{4}\left(\frac{e^2B^2}{2m}\right)(x^2+y^2)\psi = H\psi \qquad (19.2)$$

So, these are the components of the vector potential in Cartesian coordinates, now when such a magnetic field is applied the Hamiltonian gets modified in the following manner.

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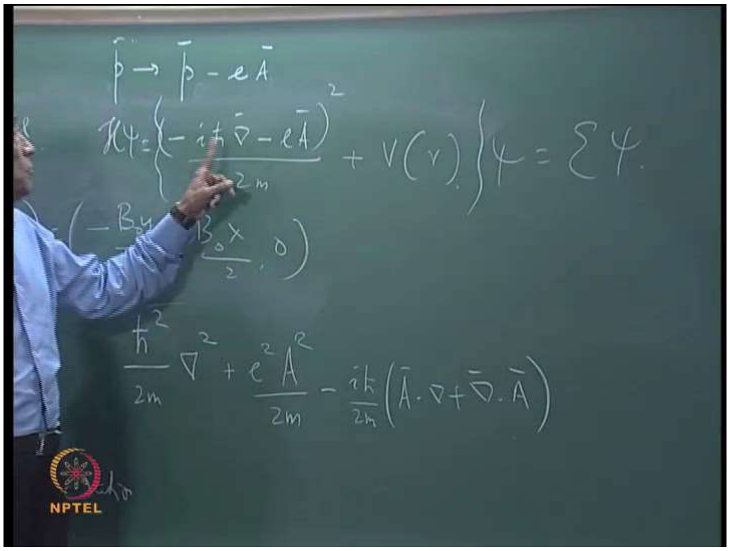

$$\bar{p} \to \bar{p} - e\bar{A}$$

$$\mathcal{H}\psi = \left\{\frac{\left(-i\hbar\bar{\nabla} - e\bar{A}\right)^2}{2m} + V(r)\right\}\psi = \mathcal{E}\psi.$$

$$\left(-\frac{B_0 y}{2}, \frac{B_0 x}{2}, 0\right)$$

$$\frac{\hbar^2}{2m}\nabla^2 + \frac{e^2A^2}{2m} - \frac{i\hbar}{2m}\left(\bar{A}\cdot\nabla + \bar{\nabla}\cdot\bar{A}\right)$$

If p is the operator p is replaced by the operator p minus e A. So, that is the result of classical physics. So, p goes to p minus e A and therefore, the Hamiltonian in a magnetic field is written as minus i h cross del minus e A by whole square by two m plus v of r. So, this is the Hamiltonian and therefore, h psi equals and this is the equal to e psi that is the Schrodinger equation. And we can now replace A by these component, and rewrite this. When we do this do this we get h cross square by two m del square, that is the first term from squaring this. And then we have another term plus e square A square by two m and then we have cross term minus i h cross by two m into a dot del plus del dot A. We cannot just write two del dot A, we have keep the sequences separate.

So, we have two such term one from this del dot A, another from A dot del. Then we have v of r. So, i z equals psi where we can now substitute for A square and A. So, that is the Schrodinger equation which as to be solve in order to find the eigen values of energy and that is how we can find the magnetic moment. So, if we do this arrive at this result we arrive at this result we have the minus h cross to a del square by two m which is the kinetic energy term that is the kinetic energy term of the electron. Then we have minus i h cross by two m and then we have a dot del plus del dot a in order to a go further we choose the gauge we has the freedom to choose the gauge in which we work and we choose the coulomb gauge in which del dot a equal zero. If we apply this condition, we can show the a dot del and del dot a become the same.

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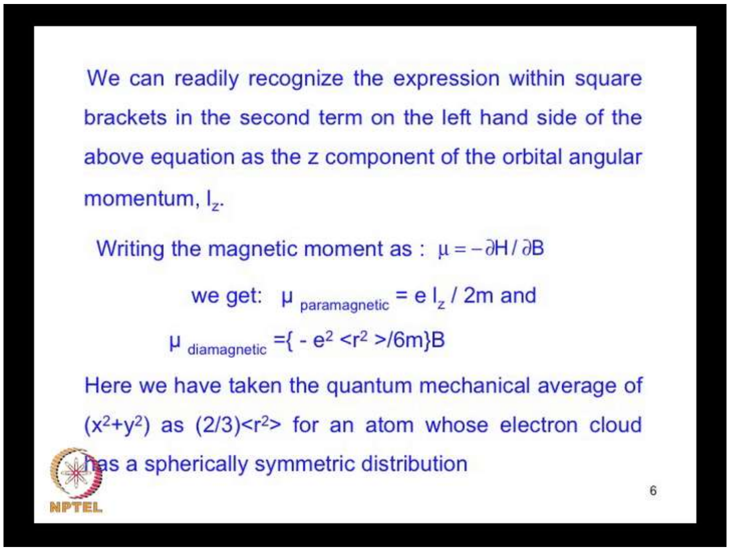

We can readily recognize the expression within square brackets in the second term on the left hand side of the above equation as the z component of the orbital angular momentum, l_z.

Writing the magnetic moment as : $\mu = -\partial H / \partial B$

we get: $\mu_{\text{paramagnetic}} = e\, l_z / 2m$ and

$\mu_{\text{diamagnetic}} = \{ -e^2 <r^2>/6m\}B$

Here we have taken the quantum mechanical average of (x^2+y^2) as $(2/3)<r^2>$ for an atom whose electron cloud has a spherically symmetric distribution

So, that this becomes then we have well this becomes plus and then this because has a minus sign, where we can now replace a square a square is nothing, but we have there b naught square by four into x square plus y square is a square. And similarly for A, we have those results there. So, A dot del will simply become minus b naught by two into minus y d by d x plus x d by d y and remembering that minus I h cross del is the moment operator this can be written as where p x p y are the components of p x and y components. So, this is nothing, but the z component of the orbital angular momentum l z if l is r cross p which is the definition of arbitral angular momentum l z will be plus x p y minus y p x therefore, the Schrodinger equation can now b rewritten a very simple form.

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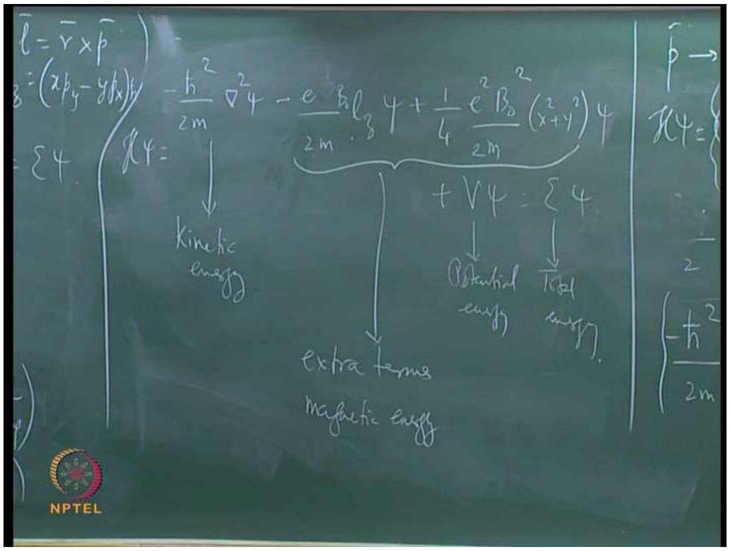

$$\mathcal{H}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi - \frac{e}{2m}B_0 l_z\psi + \frac{1}{4}\frac{e^2B_0^2}{2m}(x^2+y^2)\psi + V\psi = \varepsilon\psi$$

I have forgotten e here. So, e h cross by m into l z psi plus one four e square b naught square by m two m into x square plus y square psi plus b psi equals psi. Now in we cannot need not a and solve this Schrodinger equation to understand what this mean we can just look at it by inspection we can interpret the various terms in this energy Hamiltonian is nothing, but the energy. So, what is the Hamiltonian operator this term is the kinetic energy and this is the potential energy and the Schrodinger equation simply says this plus this plus these term is equal to the total energy. Obviously, these are the two-terms which arise which contribute to the energy on account of the application of the static magnetic field study magnetic field.

So, this means we have forgotten b naught by two right. So, this h cross is observed in a l zl z is really h cross, because l z is measured in units of h cross. So, this is these are the two terms extra terms which represent a magnetic energy the additional contribution to energy from the application of the magnetic field one of them is negative, another is positive. That is the really reveals what do you mean by a negative energy and a positive energy for this we have to just go back to classical electro dynamics.

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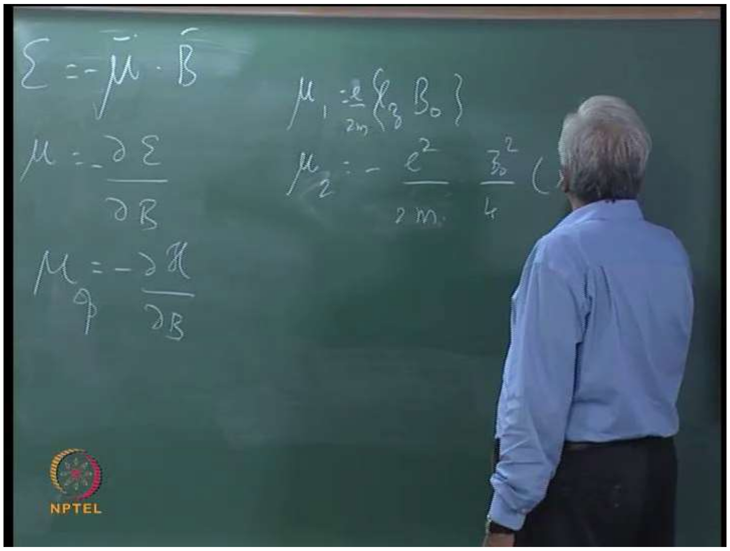

And see what happens when a dipole of magnetic moment mu displays at an applied magnetic field then the energy is just therefore, we know that the magnetic movement is just nothing, but b e minus b e by e b where. So, by looking at the Hamiltonian operator if you write it in a and operator form this is just mu operator this minus b h by d b. So, if you look at these two terms in the Hamiltonian that has looked what we get the negative term gives me mu one is l z b naught that is the contribution. Now similarly the other terms is going to give me this is going to give me minus e square del there is A one by two m and e by two m. And here it is e square by four into well it should be to have square right as we will see about that this square by two m into one by four b naught square into h square plus y square.

So, these are negative term a negative magnetic moment whereas, this is a positive moment and what is interpretation of this, whenever we have a magnetic field magnetizing a material. If you get a magnetic moment which is parallel are in the same direction as the applied magnetic field we say that the material is paramagnetic a paramagnetic material is only one in which the magnetic movement is parallel to magnetic field whereas, the magnetic moment is anti parallel then we call it a diamagnetic material. So, we have two cases here one giving a magnetic moment is parallel to the applied magnetic field which is also directed along the z direction. And the other gives a term which contributes to a magnetic moment which is anti parallel to the magnetic field because this is a positive definite everything is a square and therefore, you have a negative sign.

So, it gives a negative magnetic moment which indicates that the magnetic moment is anti parallel to the applied magnetic field. So, this is a paramagnetic term this is a diamagnetic term. So, by simply looking at the Hamiltonian of the electron an a applied magnetic field and looking at the various terms in the presence of the field here in a position to say that there are two new contributions to the energy arising from the application of the magnetic field one of these contributions is a paramagnetic contribution. And the other one is a diamagnetic contribution the paramagnetic contribution comes from the alignment of the angular momentum vector in the direction of the applied magnetic field.

So, just like in the case of the dielectric polarization these are that there was an electric dipole which gets lined up in the direction of the applied electric field creating dielectric polarization. In the same way, here we have an electron magnetic moment which is like a dipolar magnetic moment, there is no monopole in nature this lowest order magnetic moment is that of a dipole. Therefore, the electronic dipole lines itself in the direction of the applied magnetic field and gives rise a paramagnetic contribution which as this form and this is the gyro magneto gyric ratio e by m is the magneto gyric ratio.

So, this is equal to gamma and in addition the orbital motion of the electron because the electron is orbiting round this as a classical explanation. So, if you have an orbiting current loop a close current loop in which as charge is circulating this current loop when an applied magnetic field is produced A by lends as law there is a back e m f induced when therefore, there is a resistance to this motion. And this change is changes the acceleration this entry plate is the acceleration of the electron in its orbital motion and therefore, this produces the change in the angular momentum. And therefore, induces a magnetic moment which is of diamagnetic now this is of course, for an individual electron if you have a macro scope example in which there are a large number of ten to the twenty three are. So, of atoms are molecule each have which contain several electron then the makeup quantum mechanical and statistical average now for this the average is x square plus y square average. So, the average magnetic moment quantum mechanical average is just this this these bracket represent average. So, the quantum-mechanical average can be easily figured out.

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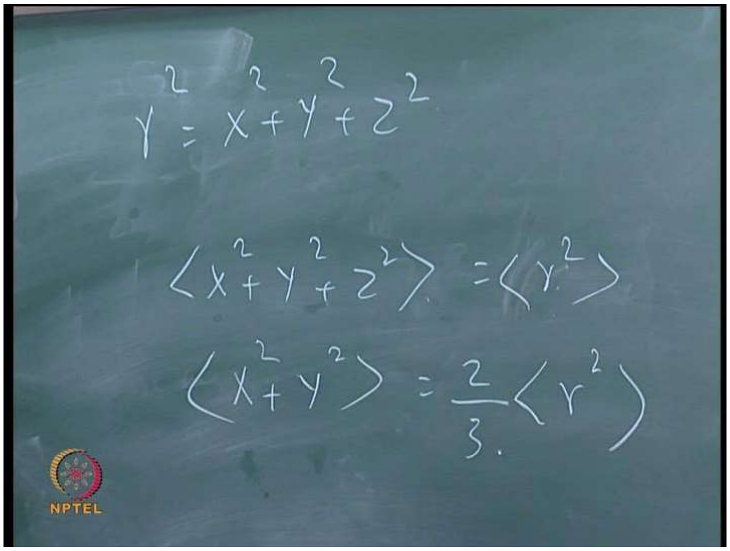

$$r^2 = x^2 + y^2 + z^2$$

$$\langle x^2 + y^2 + z^2 \rangle = \langle r^2 \rangle$$

$$\langle x^2 + y^2 \rangle = \frac{2}{3} \langle r^2)$$

Because we known that in Cartesian coordinates r square is x square plus y square plus z square, where x y z are the compliments of r for any general direction position vector r. Therefore, if you take the average with all three directions x y z are equally probable the quantum mechanical average of this x square plus y square plus z square is. So, substituting this we can calculate the diamagnetic moment using this result.

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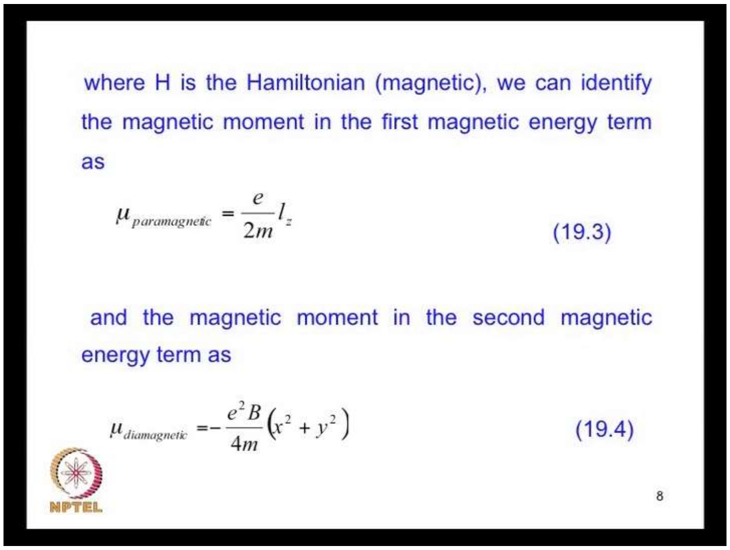

where H is the Hamiltonian (magnetic), we can identify the magnetic moment in the first magnetic energy term as

$$\mu_{paramagnetic} = \frac{e}{2m} l_z \qquad (19.3)$$

and the magnetic moment in the second magnetic energy term as

$$\mu_{diamagnetic} = -\frac{e^2 B}{4m}\left(x^2 + y^2\right) \qquad (19.4)$$

So, now we go to the magnetic moment terms and look at them closely. So, we have the paramagnetic moment.

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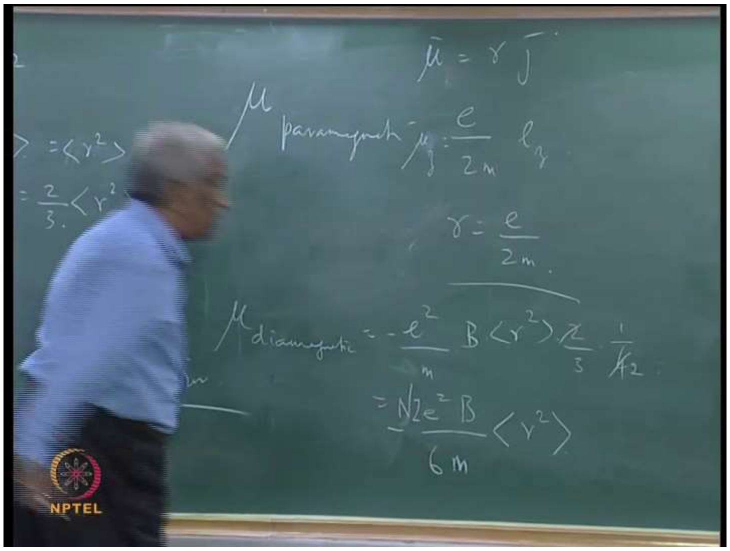

This is the paramagnetic energy the energy due to this because this is the Hamiltonian operator. So, the magnetic moment is just got by differentiating and this will will remove this because they are differentiated the linear term in the Hamiltonian. So, the b goes off. So, we simply have paramagnetic moment is e by two m into l z. So, that is mu z since it is directed along is that direction. So, this is the z component on the paramagnetic moment and that is why comparing it with our earlier equation mu equal to gamma j. We arrive at the result that gamma the magneto gyric ratio is just e by two m and the case as the diamagnetic term the result the corresponding result is e square by two m into b square will give you another two to be. So, b times r square into two by three into one by four which is one by six. So, this will give me minus e square b bb by six m times r square where r square is the quantum-mechanical average of the square o f the orbital radios of the electron since this is if the electron cloud spherically symmetric. So, this is the basic theory due to Langevin theory and this gives you the diamagnetic moment this is the contribution to the diamagnetic moment give to one orbiting electron if there are z orbiting electron this as to be multiplied by z if there are n atoms are molecule then it has to be further multiplied by n.

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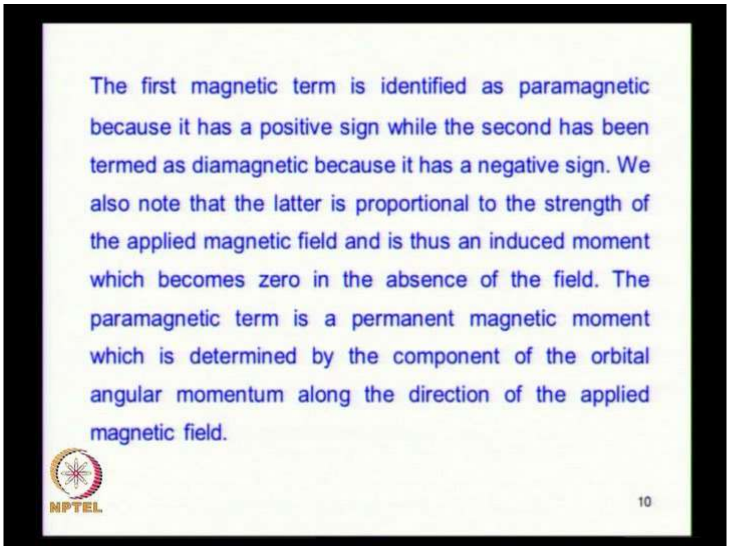

The first magnetic term is identified as paramagnetic because it has a positive sign while the second has been termed as diamagnetic because it has a negative sign. We also note that the latter is proportional to the strength of the applied magnetic field and is thus an induced moment which becomes zero in the absence of the field. The paramagnetic term is a permanent magnetic moment which is determined by the component of the orbital angular momentum along the direction of the applied magnetic field.

So, will give you the total diamagnetic moment in an assembly n atom each containing z electrons, so this is the basic theory due to langevin, which explains the diamagnetic moment which as a negative sign. The all matter which contain atoms are molecules and therefore, orbiting electrons around nuclei or molecular centers because of that every material is basically diamagnetic. There is a diamagnetism associated with every atom for molecule in nature there is no material which is not diamagnetic this diamagnetism is present only when there is a field if the field is removed it vanishes.

So, this is an induce effect diamagnetism is induced and is a reaction to the the applied magnetic field which states only as long as the applied magnetic field exists. So, the diamagnetic moment vanishes when up field is removed whereas, the paramagnetic term is a permanent magnetic moment which is determined by the component of the orbital angle of momentum along the direction of the applied field.

So, this situation is very similar to the polarizability of an atom in the presence of an applied electric field in the case of dielectric polarization this polarizability is zero once the field is applied electric field become is removed. Similarly, the polarizability as well as the diamagnetic moment are induced effects whereas, there are permanent dipoles electric dipole like water in the case of dielectric polarization. These dipoles get aligned along the electric field giving rise to a polar depolarization polarization associated with a polar nature of such a dielectric. In the same way, we have materials, which can become paramagnetic because there is there are there is an angle of momentum, and associated with this angle momentum there is a dipole magnetic magnet and these dipole lines up in the direction of the magnetic field. And therefore, this is parallel to the applied magnetic field the energy proper contribution is negative because the energy is minus mu dot b the paramagnetic moment is present all the time for a material and this will be their only if the orbital angular momentum is not zero. So, these are the main difference.

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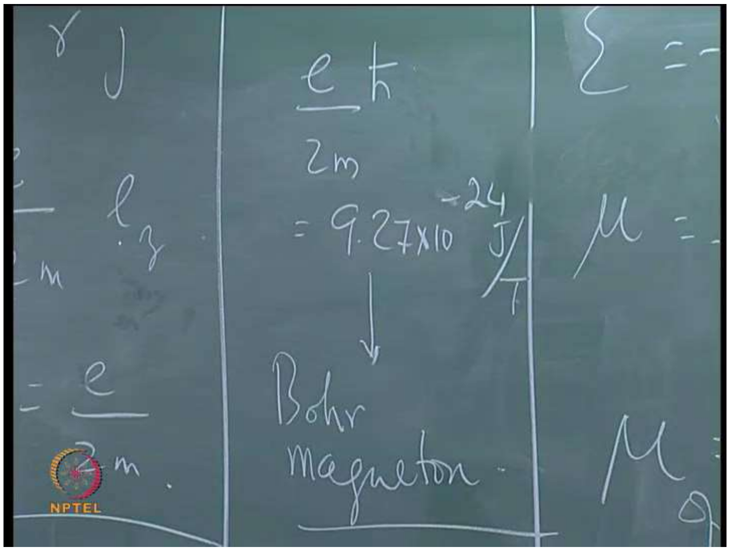

Now, this e by two m e by two m and as I already told you told you l z is an integer times h cross. So, e h cross by two m this as a value 9.27 into 10 to the power minus 24 joules per tesla. So, this has a special name that is the unit of magnetic moment in quantum mechanics in all electronic material. Therefore, this as a special name it is called the Bohr magnetron. So, we measure magnetic moments of electron in units of the Bohr magnetron. Now this immediately tells us why the the nuclear contribution is not very important in the case of magnetism, because of the presence of the mass term here. So, the nuclear mass is 2000 times more when that of the electron. So, the nuclear magnetic moment is going to be weaker by that factor. So, it is three orders weaker therefore, the nuclear magnetism is not seen easily. The thing that is seen generally is the electronic magnetic moment. We will stop at this point, and continue next time.

Condensed Matter Physics
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Magnetism-Worked Examples (Continued)

Today, we continue to do few more examples on magnetism.

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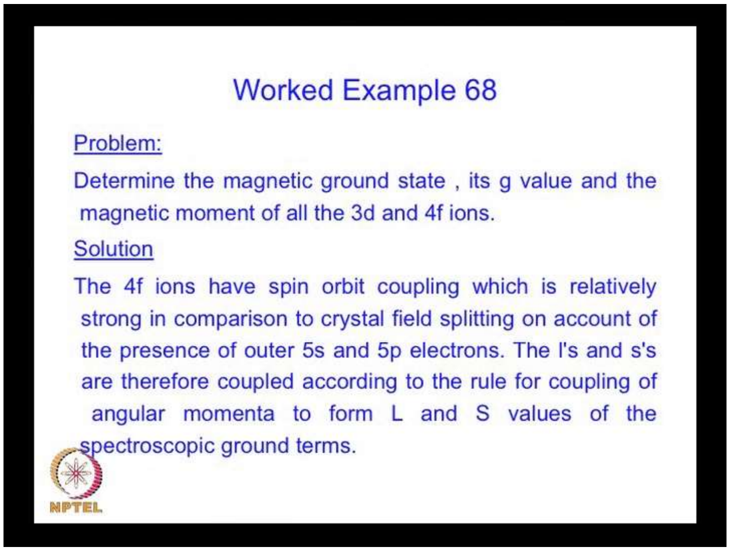

Worked Example 68

Problem:

Determine the magnetic ground state , its g value and the magnetic moment of all the 3d and 4f ions.

Solution

The 4f ions have spin orbit coupling which is relatively strong in comparison to crystal field splitting on account of the presence of outer 5s and 5p electrons. The l's and s's are therefore coupled according to the rule for coupling of angular momenta to form L and S values of the spectroscopic ground terms.

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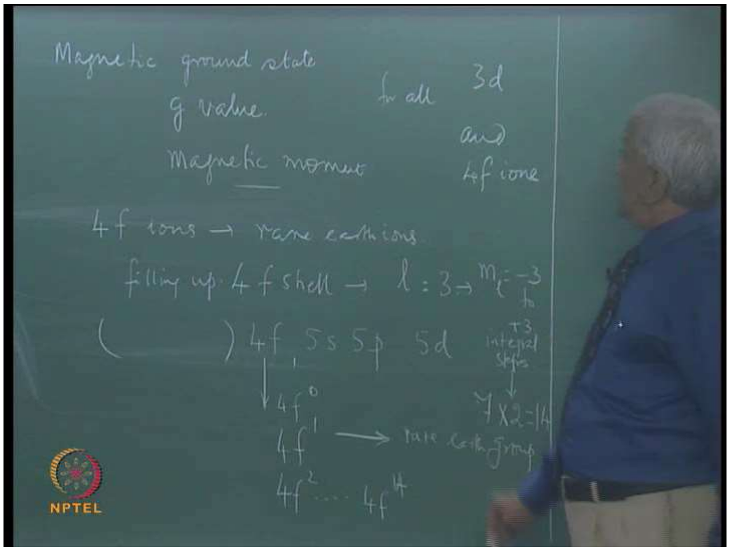

Magnetic ground state
g value
Magnetic moment
for all 3d and 4f ions

4f ions → rare earth ions

filling up 4f shell → $l : 3 \rightarrow m_l = -3$ to $+3$ integral steps → $7 \times 2 = 14$

( ) 4f 5s 5p 5d

$4f^0$

$4f^1$ → rare earth group

$4f^2 \ldots 4f^{14}$

This is an important question, in which we are asked, determine the magnetic ground state, its g value of this ground state and the corresponding magnetic moment for all 3d and 4f ions. Some of these results, we have already used in our discussion of the basic ideas of magnetism in solids, but today we will work out the magnetic ground state, the corresponding g value and the magnetic moment.

In the case all the members of the 3d and 4f groups in the periodic table. We will consider the 4f first for reasons, which will become obvious very soon. 4 f ions, which are better known as more commonly known as rare earth ions.

The rare earth ions are a group of elements in the periodic table, which correspond to the successive filling up of the 4f shell. The 4f shell corresponds to an angular momentum of 3.

So, the electronic configuration is such that the outermost shell is or the 4f and then 5s, 5p and in some cases 5d shells. So, these are the outer electron configurations.

There are of course, close shells inside, which do not contribute anything to the magnetic moment. It is only the unpaired electrons in the unfilled shell, which give rise to magnetic moment. So, we have the possibility since l is 3, we have m l going from minus 3 to plus 3 in integral steps.

So, this corresponds to 7 and then there is a spin which can be plus or minus. So, there are 2 orientations. So, there are 14 electronic states, 14 electrons can occupy the 4f shell. So, corresponding to 4f 0, where there is no electrons in the 4f shell and then 4f 1, 4f 2 etcetera 4f 14, all the elements corresponding to these different values of the electron in the 4f shell form these are called rare earth group.

We will consider one by one. These elements and the reason why, we consider this first rather than the 3d is, because in the 4f group there are outer electrons in the 5s, 5p and 5d shells, which start of shield the inner 4f electron.

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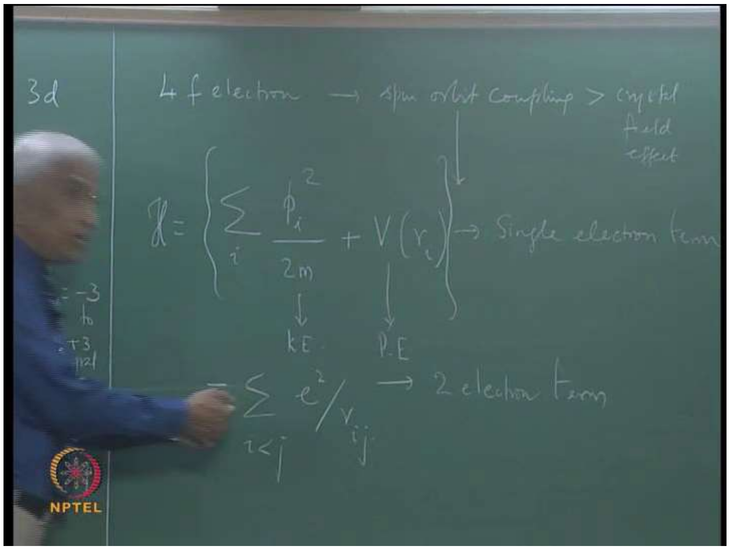

3d

4 f electron → spin orbit coupling > crystal field effect

$$\mathcal{H} = \left\{ \sum_i \frac{p_i^2}{2m} + V(r_i) \right\} \rightarrow \text{Single electron term}$$

$\frac{p_i^2}{2m}$ ↓ K.E. ; $V(r_i)$ ↓ P.E.

$$- \sum_{i<j} e^2/r_{ij} \rightarrow \text{2 electron term}$$

The spin orbit coupling is relatively strong in comparison to the crystal field effect. So, the spin orbit coupling is rather strong and therefore, if we wrote the free electron Hamiltonian. We have the single electrons states corresponding to the kinetic energy, there i, is going from one to the total number plus V of r i this is the kinetic energy, this is the potential energy the coulomb interaction energy between the ith electron and the nucleus.

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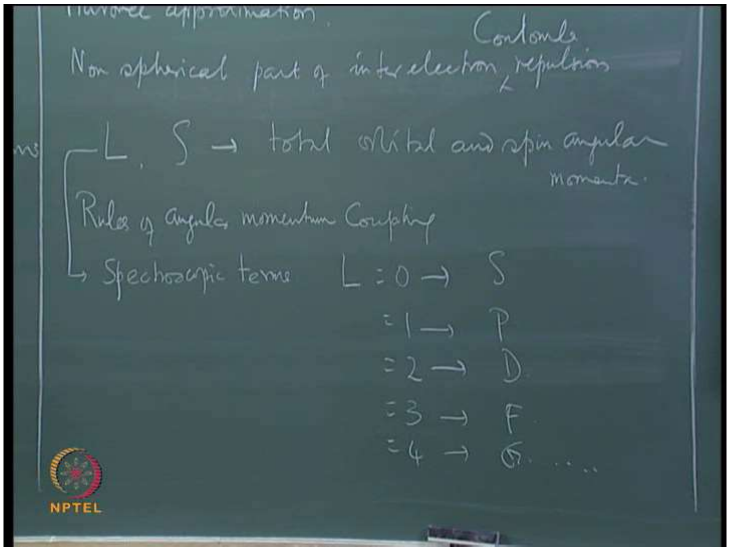

Hartree approximation.

Non spherical part of inter electron Coulomb repulsion

L, S → total orbital and spin angular momenta.

Rules of angular momentum Coupling

→ Spectroscopic terms L = 0 → S

= 1 → P

= 2 → D

= 3 → F

= 4 → G . . . .

So, this is all single electron terms. These define the angular momentum and spin of every individual electron. In addition next in descending order of strength, we have the inter electron coulomb repulsion. This is a two electron term so, this couples the individual electrons ((Refer Time: 06.55)) and in the Hartree approximation.

Considers this spherical part of this inter electron repulsion and adds this on to the single electron potential energy. So, that we get hydrogen like ground state, but there will be a non spherical part coulomb repulsion. This non spherical part of the coulomb repulsive potential couples the individual l s and s s of the single electron and produces a total angular momentum orbital angular momentum L and the total spin angular momentum S. According to the rules of angular momentum coupling in quantum mechanics, it is these l s and s s which define is so, called the spectroscopic terms.

So, these spectroscopic terms are identified by the total value of the orbital angular momentum, if L is 0, we call it an S term, if L is 1, it is a P term, if L is 2, it is a D term, if L is 3, it is a F term and then 4, 5, etcetera, it is in alphabetical order G etcetera and so on. So, these are the terms symbols corresponding to the different angular momentum values, orbital angular momentum values.

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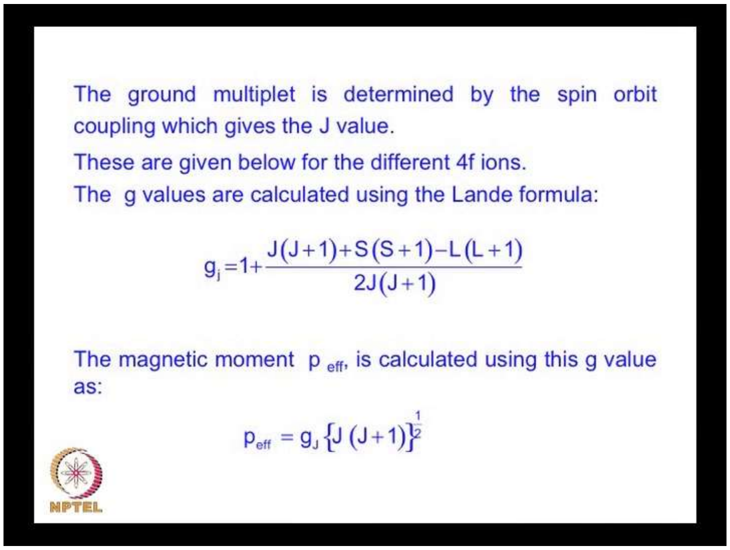

The ground multiplet is determined by the spin orbit coupling which gives the J value.

These are given below for the different 4f ions.

The g values are calculated using the Lande formula:

$$g_j = 1 + \frac{J(J+1)+S(S+1)-L(L+1)}{2J(J+1)}$$

The magnetic moment p_{eff}, is calculated using this g value as:

$$p_{eff} = g_J \{J(J+1)\}^{\frac{1}{2}}$$

Once we know the individual total orbital and spin angular momentum corresponding to the ground term. It is the ground stage which matters in magnetic properties and therefore, we are interested in the ground term.

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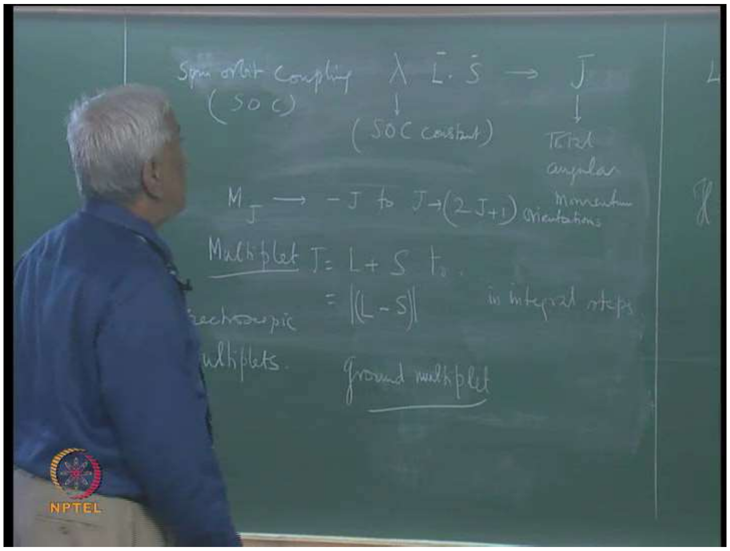

And this term now, is acted on by the spin orbit coupling, which is usually represented in the form lambda L dot S, where lambda is the spin orbit coupling constant. And this produces a coupling between these orbital and spin angular momenta to produce a total angular momentum which is usually represented by the symbol J.

Corresponding to a given value of J, you can have different values of M J, the magnetic quantum number which goes from minus J to plus J. There are 2 J plus 1 value, corresponding to different orientations of the spins magnetic moment of the ions with respect to an applied magnetic field. So, now, these correspond to so, called multiplet different J values correspond to different multiplet, when L and S are coupled. According to the rules of angular momentum coupling it can be coupled and the resultant angular momentum goes from J equal to L plus S to mod L minus S or S minus L depending on which is greater in integral steps that is all we get 2 J plus 1 values. Each of these J value corresponds to a different multiplet. So, this gives me the multiplet states, spectroscopic multiplet there are different multiplet corresponding to different values of J of which the ground multiplet is what matters for magnetic behaviour.

So, the magnetic ground state is determined by the multiplet which lies lowest on account of the fact that the excited states are normally not appreciably populated and are ordinary conditions of temperature and magnetic field. So, it is only the ground multiplet which determines the magnetic ground state and hence the magnetic behaviour.

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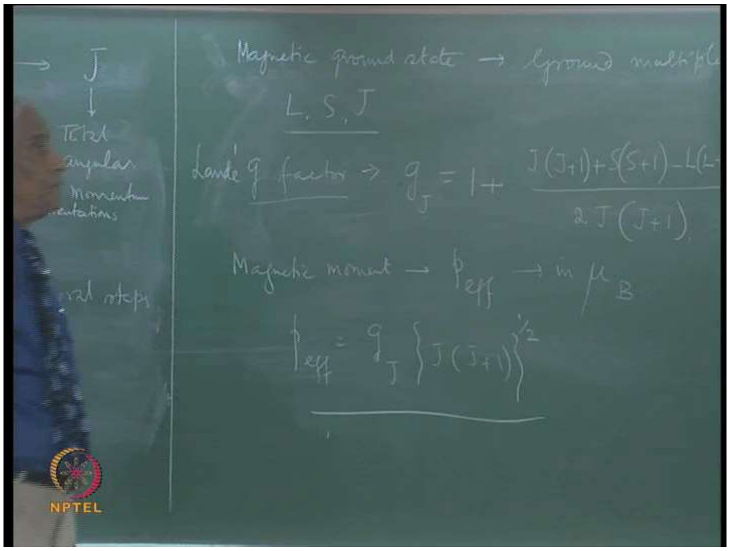

→ J ↓ Total angular momentum

Magnetic ground state → ground multipl

L, S, J

Lande g factor → $g_J = 1 + \frac{J(J+1)+S(S+1)-L(L}{2J(J+1)}$

Magnetic moment → p_{eff} → in μ_B

$p_{eff} = g_J \{J(J+1)\}^{1/2}$

So, the magnetic ground state which we have been asked to determine corresponds to the ground multiplet state. This is what we have to determine now in the case of the different ions. Once we know the multiplet ground state and the corresponding J value. So, we now, know the L S and J values for a given multiplet. A given multiplet is characterised by different values of L S and J and then the g factor which is known as the Lande g factor is given by corresponding to a given multiplet state with a given J value is given by the Lande expression.

So, since we know L S and J for a given multiplet charactered by a particular value of J. We can immediately find the corresponding g value is also what we have to find out. Once we know g J the magnetic moment of corresponding to this ground state it is usually represented by the symbol P effective which is in Bhor magnetrons. So, this P effective is given by g J into J into J plus 1 to the power half. So, this gives the magnetic moment in units of the Bhor magnetron.

So, this is the procedure which we will adopt, in the case of all the 14 rare earth ions, belonging to the progressive filling up of the 4 f shells. Well if there are no electrons in the 4 f shell there is no magnetic moment; obviously, because the shell is not occupied by any electron and therefore, the unpaired electron is necessary for it.

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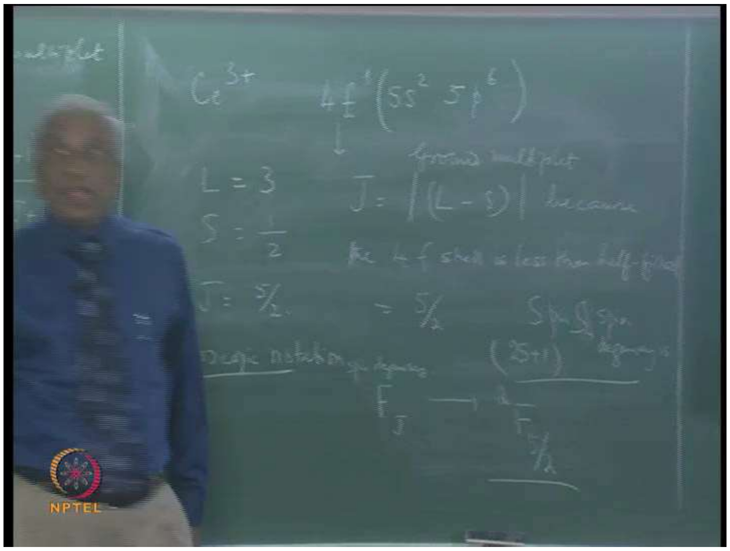

So, let us start from the first case, first rare earth ion, which is cerium 3 plus, which are the outer electron configuration of 4f 1 5s 2 and 5p 6. So, there are two electrons in the outer 5s shell and six electrons in the outer 5p shell and there is one unpaired electron in the 4f shell.

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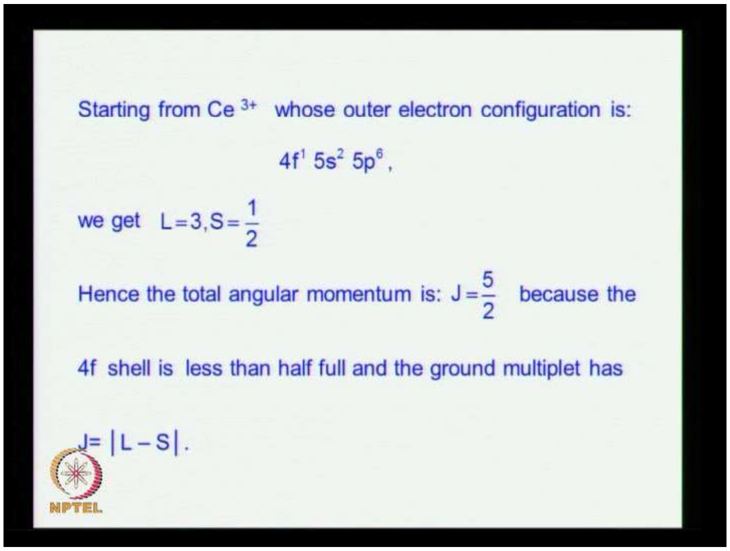

Starting from Ce^{3+} whose outer electron configuration is:

$4f^1\ 5s^2\ 5p^6$,

we get $L=3, S=\frac{1}{2}$

Hence the total angular momentum is: $J=\frac{5}{2}$ because the

4f shell is less than half full and the ground multiplet has

$J=|L-S|$.

So, it is this which gives the magnetic behaviour. So, since there we have only one electron, the L value is since it is an electron in the f shell, L is 3. And since there is only one electron the spin value is also the total spin angular momentum is just that of one electron so, S is half. So, you have J which in this case big low lying multiplet corresponds to L minus S rather than L plus S because, the 4f shell is less than half filled.

So, this is the ground multiplet. So, in this case since L is 3 and S is half this will give you 5 by 2. So, the ground multiplet has L equal to 3, S equal to half and J is 5 by 2. There is a way of denoting this ground multiplet the spectroscopic notation for this ground multiplet. The spectroscopic notation usually proceeds by giving the ground term symbol which we already saw in this case since L is three it is an f term and it has a superscript which has these spin degeneracy and the subscript which gives the J value.

So, that is the standard notation for the ground multiplet. In this case the spin degeneracy is for a spin of S spin degeneracy is 2 S plus 1; obviously. So, we will have in this case S is half so, 2 S plus 1 is so, it is 2 f and the J value is 5 by 2. So, that is the notation for the ground multiplet for the cerium 3 plus ion, which is the first member in the rare earth group with unpaired electron.

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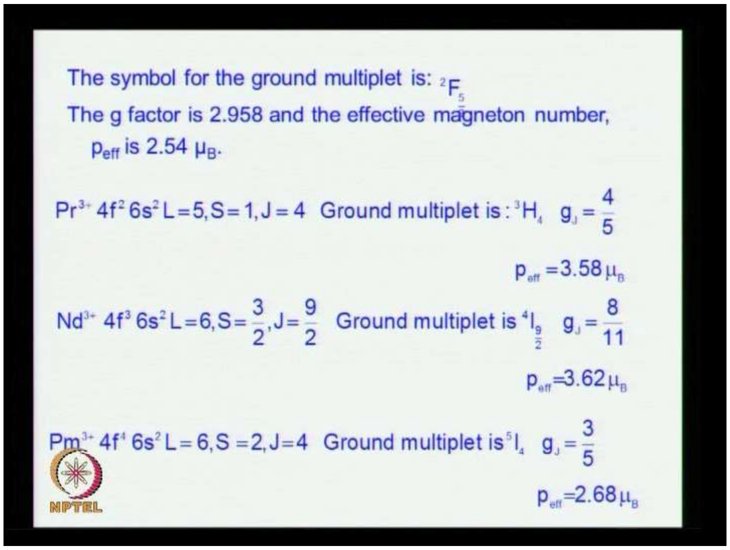

The symbol for the ground multiplet is: ${}^2F_5$

The g factor is 2.958 and the effective magneton number, p_{eff} is 2.54 μ_B.

Pr^{3+} $4f^2 6s^2 L=5, S=1, J=4$ Ground multiplet is : ${}^3H_4$ $g_J=\frac{4}{5}$

$p_{eff}=3.58\mu_B$

Nd^{3+} $4f^3 6s^2 L=6, S=\frac{3}{2}, J=\frac{9}{2}$ Ground multiplet is ${}^4I_{\frac{9}{2}}$ $g_J=\frac{8}{11}$

$p_{eff}=3.62\mu_B$

Pm^{3+} $4f^4 6s^2 L=6, S=2, J=4$ Ground multiplet is ${}^5I_4$ $g_J=\frac{3}{5}$

$p_{eff}=2.68\mu_B$

So, having found the ground multiplet, we use the expression for the Lande g factor to find g J, the g factor corresponding to this multiplet.

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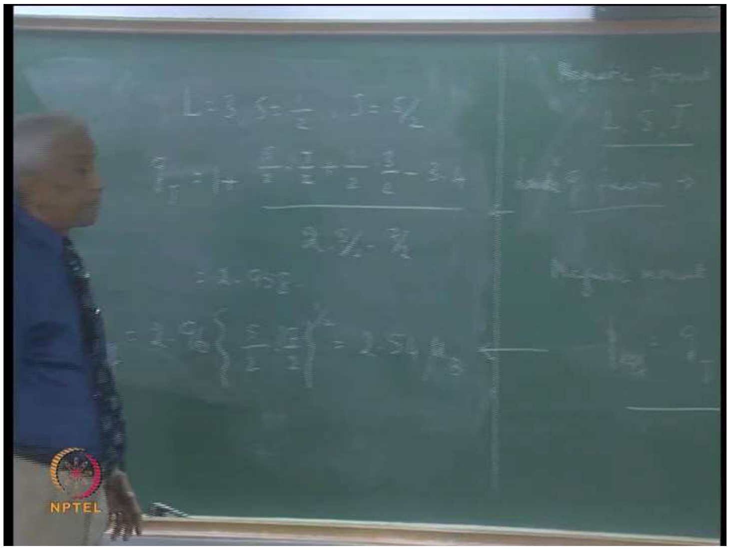

So, this has L equal to 3, S equal to half and J is 5 by 2. So, the Lande expression is for g J is 1 plus J into J plus 1, which is 5 by 2 into 7 by 2 plus S into S plus 1, which is half into 3 by 2 minus L into L plus 1, which is 3 into 4 divided by 2 J into J plus 1. This turns out to be 2.958 on simplification. The corresponding magnetic moment is given by this formula. So, we write P effective is this value for g J times 5 by 2 J into J plus 1 to the power half. So, this turns out to be 2.54 Bhor magnetron.

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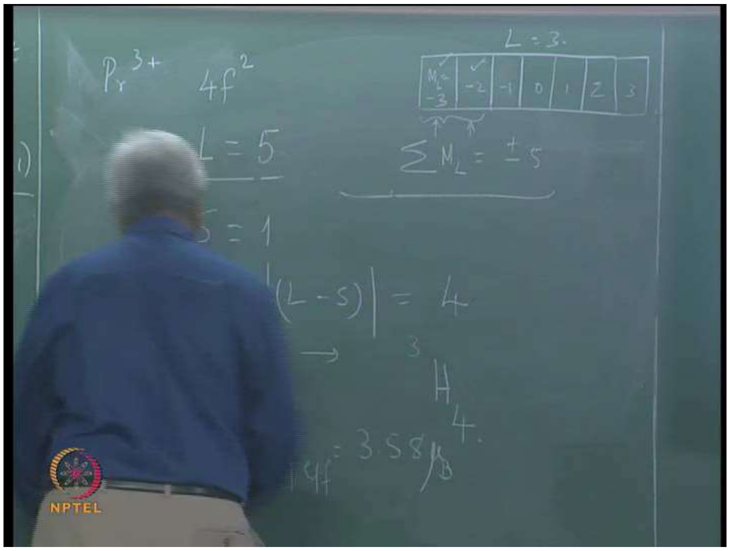

So, following the same procedure for the other ions, let us move on to the next ion in the rare earth group which has two electrons in the 4f shell this ion is praseodymium 3 plus. So, it has 4f 2 therefore, the corresponding L value is there are two electrons the Hunts rules tells you, if I have different values of a mell which I represent here. So, this is M L equal to minus 3, minus 2, minus 1, 0, 1, 2 and 3 corresponding to L equal to 3.

So, the Hunts rules tells us that the electrons will have a total M L value and hence a total L value due to the coupling, which will be correspond to the sum of the two stage which the electron occupies the corresponding M L values sigma M L corresponding to the two states such that this spin multiplicity is maximum. In other words the two electrons has spins parallel. So, these are the two states and therefore, we get minus 5 or it can also be here. So, it is plus or minus 5 and therefore, the corresponding L value is 5 since this summation is gives you M L as plus or minus 5, the only possibility for this is with L equal to 5.

So, that is the total orbital angular momentum of these two electrons and since there are two electrons the spins are parallel and therefore, S is 1 and J which is mod of L minus S because, it is still less than half filled. So, this will be 5 minus 1, 4. So, the ground multiplet in the case of the praseodymium 3 plus ion is has the L value 5, which means it is an H in the term and the spin multiplicity is 2S plus 1 for S equal to 1 is 3 and the J value is 4.

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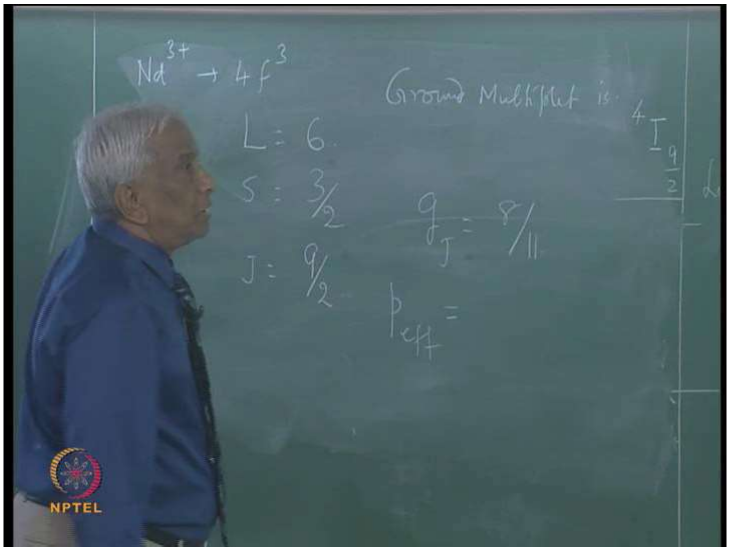

And if we substitute in the Lande g factor expression for this, the g J turns out to be 4 by 5 by substitution. And the corresponding effective magnetic moment is 3.58 Bhor magnetron. Adapting the same procedure for the next ion in the series, which is neodymium 3 plus, which has three electrons in the 4f shell and therefore following the same procedure sigma M L will be minus 3, minus 2 and minus 1. So, this will be minus 6.

So, L will be 6 and the S since there are three electrons all with spin parallel in order to maximise the spin. So, this will be 3 by 2 and therefore, J will be L minus S which is 9 by 2. So, the ground multiplet for neodymium 3 plus is, L equal to 6 which is an I term, 2 S plus 1 is 4 for S equal to 3 by 2 and the J is 9 by 2. So, this is the ground multiplet. All the rare earth ions have the valance is 3 plus the corresponding g J value in the Lande g factor expression works out to be 8 by 11. And the effective magnetic moment P effective is 3.62 Bhor magnetron.

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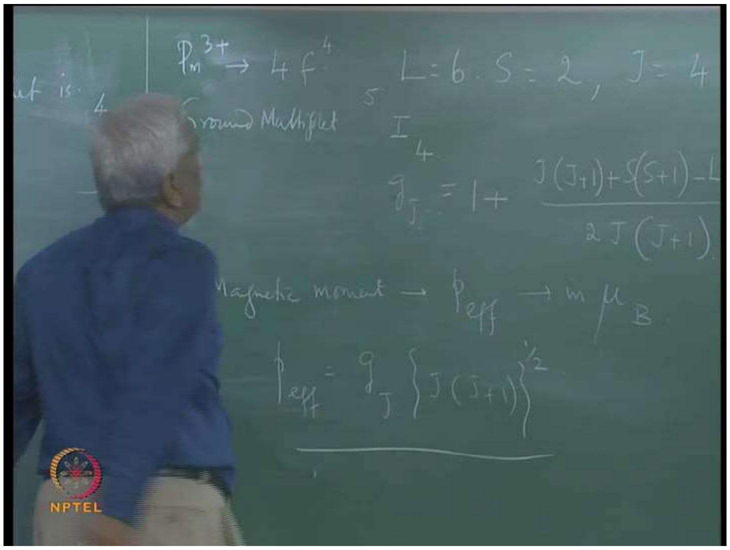

We then move on to promethium 3 plus, which is a short lived isotope. Still it is one with four electrons in the 4f shell. So, the corresponding L values since this would be four electron this would add zero to this. So, the L remains 6 and the S of course, becomes 2 since there are four electrons with parallel spins therefore, the J is 4.

So, the ground multiplet is again an I term, but with spin multiplicity 5, 2 S plus 1, 5 S equal to 2 and the J value is 4.

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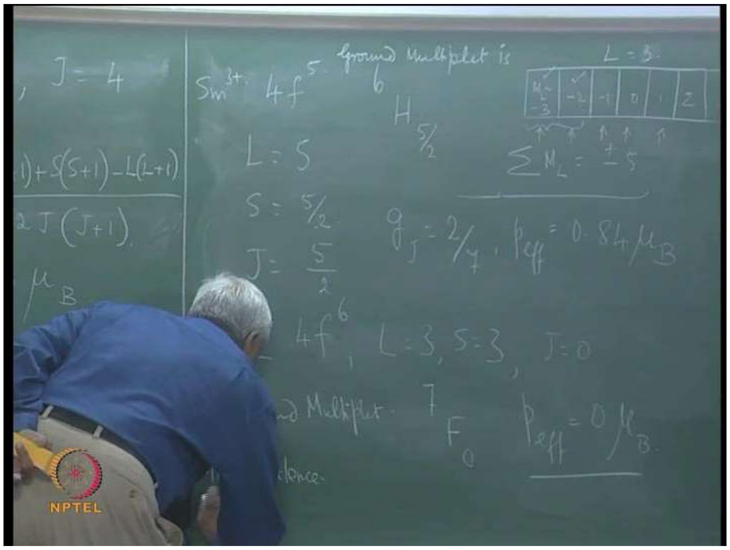

Next, we consider samarium 3 plus, which has a 4f 5 configuration therefore, the L now, there are five electrons so, the minus 1 and plus 1 will neutralise each other, leaving us with sigma M L equal to minus 5. So, that L is 5 and S for five electrons is still 5 by 2 because, all the electrons have parallel spins therefore, the J value is L minus S which is 5 by 2 and the g J has the value if ground multiplet is represented by L equal to 5.

So, it is again an H term with a spin multiplicity 6 corresponding to a spin of 5 by 2 and a J value of 5 by 2 this is the ground multiplet. And the corresponding g J value is 2 by 7 and the magnetic moment is having the value 0.84 Bhor magnetrons.

You go to europium 3 plus, which has 6 electrons in 4f shell. So, L is 3 by the same procedure S is also 3 because, six electrons with parallel spins. And So, J is 0. So, the ground multiplet is an F term with spin multiplicity 7 and a J value of 0. So, since this has J 0. So, the g value is 0 and the magnetic moment corresponding to that is also 0. Of course, europium 3 plus is nonmagnetic because, of this, but usually europium 3 plus also there is frequently you have a mixed valance with europium 2 plus, which contributes to some non zero magnetism, when europium 2 plus is present.

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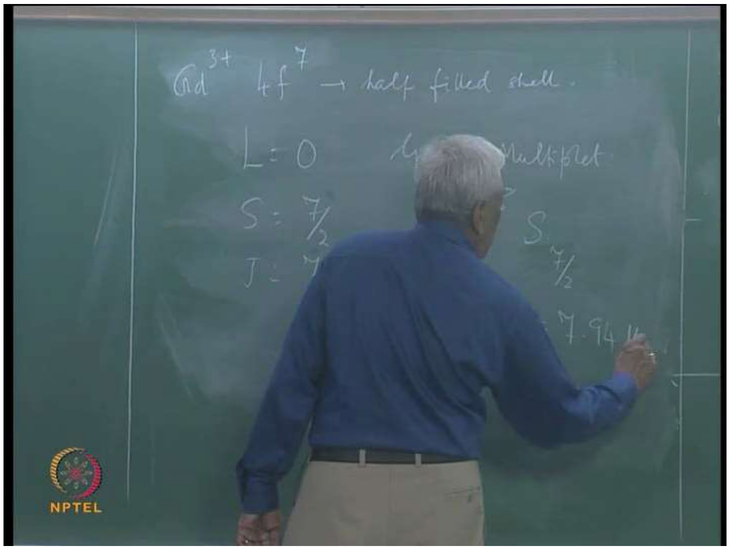

Next, we have gadolinium 3 plus which has seven electrons in the 4f shell, which can accommodate a total of fourteen electrons.

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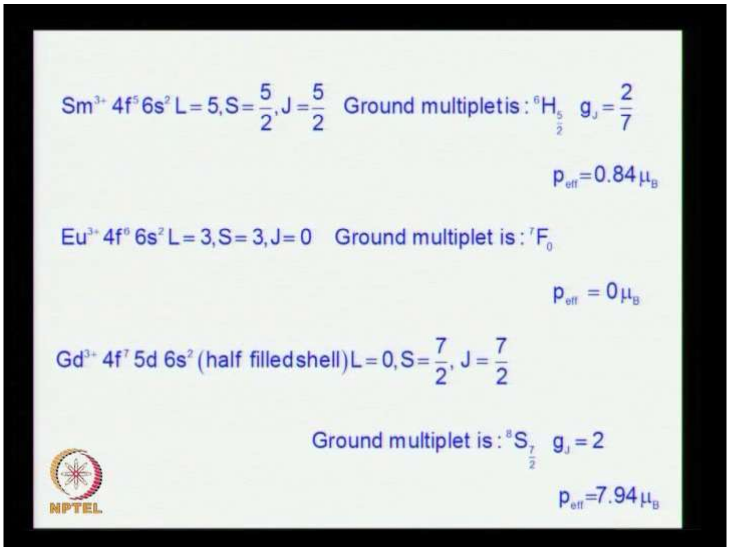

Sm^{3+} $4f^5 6s^2$ $L = 5, S = \frac{5}{2}, J = \frac{5}{2}$ Ground multiplet is : ${}^6H_{\frac{5}{2}}$ $g_J = \frac{2}{7}$

$p_{eff} = 0.84\,\mu_B$

Eu^{3+} $4f^6 6s^2$ $L = 3, S = 3, J = 0$ Ground multiplet is : ${}^7F_0$

$p_{eff} = 0\,\mu_B$

Gd^{3+} $4f^7 5d\, 6s^2$ (half filled shell) $L = 0, S = \frac{7}{2}, J = \frac{7}{2}$

Ground multiplet is : ${}^8S_{\frac{7}{2}}$ $g_J = 2$

$p_{eff} = 7.94\,\mu_B$

So, this is a half filled shell, the corresponding L value turns out to be 0, S is 7 by 2 and J is also 7 by 2. Since L is 0, the ground multiplet has a term symbol, which is that of an S term and therefore, this will be 8 S 7 by 2.

So, substituting these values of L S and J we get g J for gadolinium 3 plus as to we just this spin only value. Since it has only spin contribution, the orbital angular momentum is

0. So, it has a spin only g factor. And the corresponding magnetic moment has value of 7.94 Bhor magnetrons, in the same way we can work out the values for the other seven electrons.

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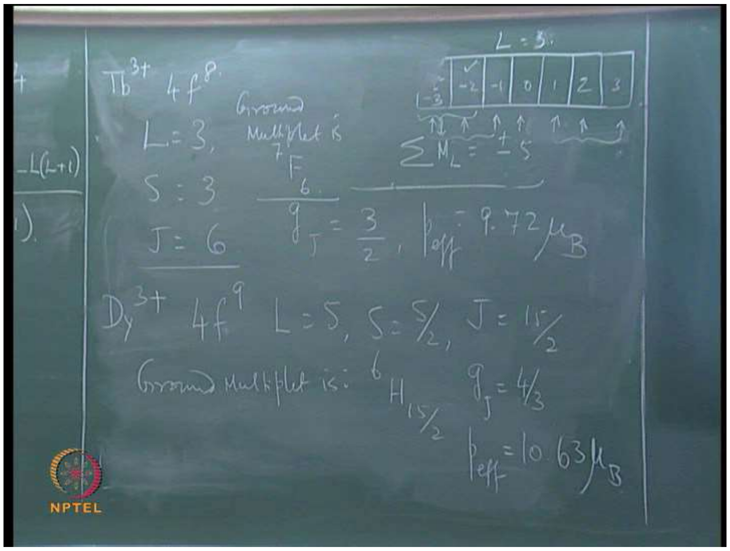

Tb^{3+} $4f^8$.
$L = 3$,
$S = 3$
$J = 6$

Ground Multiplet is $^7F_6$.

$L = 3$.

-3	-2	-1	0	1	2	3

$\sum M_L = \pm 5$

$g_J = \frac{3}{2}$, $p_{eff} = 9.72\mu_B$

Dy^{3+} $4f^9$ $L = 5$, $S = 5/2$, $J = 15/2$

Ground Multiplet is: $^6H_{15/2}$ $g_J = 4/3$

$p_{eff} = 10.63\mu_B$

So, terbium 3 plus, which has eight electrons in the 4 f shell. So, L is 3, S is 3, J is 6.

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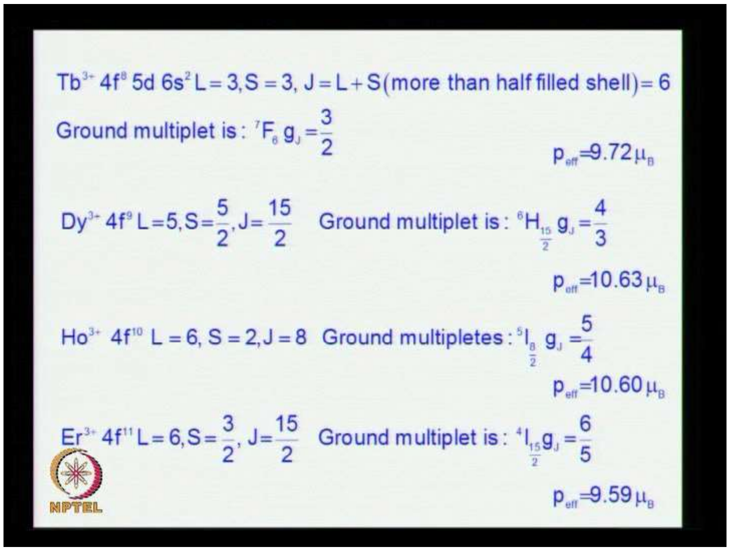

Tb^{3+} $4f^8\,5d\,6s^2$ $L = 3, S = 3, J = L + S$(more than half filled shell)$= 6$

Ground multiplet is : $^7F_6$ $g_J = \frac{3}{2}$

$p_{eff} = 9.72\,\mu_B$

Dy^{3+} $4f^9$ $L = 5, S = \frac{5}{2}, J = \frac{15}{2}$ Ground multiplet is : $^6H_{\frac{15}{2}}$ $g_J = \frac{4}{3}$

$p_{eff} = 10.63\,\mu_B$

Ho^{3+} $4f^{10}$ $L = 6, S = 2, J = 8$ Ground multipletes : $^5I_{\frac{8}{2}}$ $g_J = \frac{5}{4}$

$p_{eff} = 10.60\,\mu_B$

Er^{3+} $4f^{11}$ $L = 6, S = \frac{3}{2}, J = \frac{15}{2}$ Ground multiplet is : $^4I_{\frac{15}{2}} g_J = \frac{6}{5}$

$p_{eff} = 9.59\,\mu_B$

This case the S is 3 because, there are seven electrons with parallel spin and then the eighth electron goes to this. So, that we have plus 3 and minus 3 cancelling out leaving L equal to 3. The corresponding g J value since it is more than half L shell the ground multiplet is corresponding to L equal to 3 it is an F term with the spin multiplicity of 7 and the J value of 6, the g J value is 3 by 2 and the effective magnetic moment is 9.72 Bhor magnetrons.

Similarly, we consider dysprosium 3 plus, which has 4f 9 configuration. The corresponding values are L equal to 5, S equal to 5 by 2 and J is 15 by 2. So, the ground multiplet is 6 H 15 by 2 and the g J value is 4 by 3. The magnetic moment is 10.63 Bhor magnetrons.

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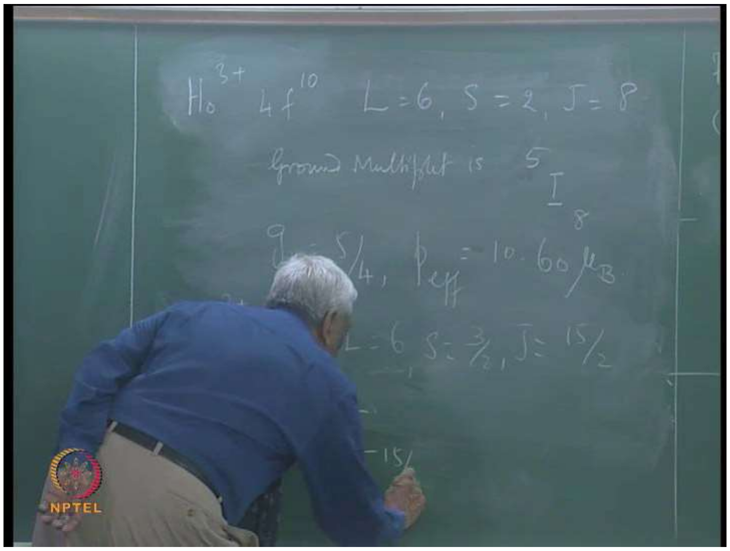

In the same way one can verify the cases of holmium 3 plus, which have 4 f 10 and the L value is 6, S value is 2, J value is 8. So, the ground multiplet is 6. So, it is an I term with the 3 no 5 8. So, the g J value is 5 by 4 in this case and the magnetic moment is 10.6 Bhor magnetrons.

Than we have erbium 3 plus, which has 4 f 11 and the corresponding L value is 6, S is 3 by 2 and J is 15 by 2. So, the ground multiplet is again an I term with 4 15 by 2, leading to a g J value of 6 by 5 and a P effective of 9.59 Bhor magnetrons.

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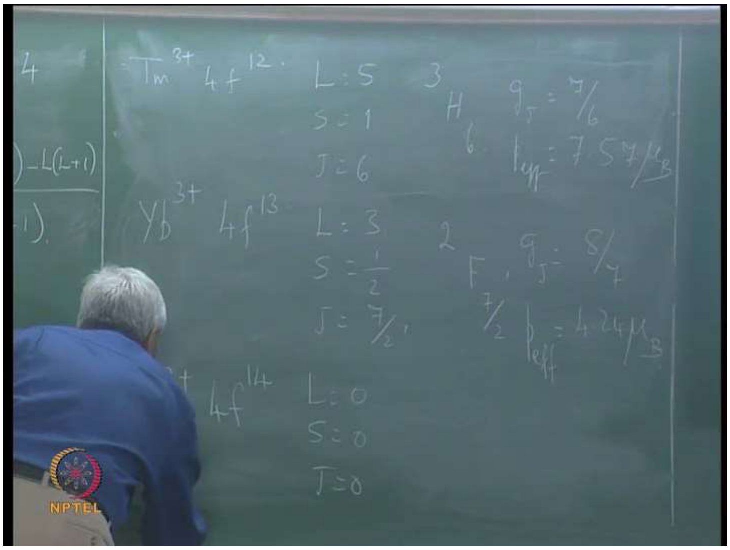

We next come to the case of thulium, which has 4 f 12. So, the L value is 5, S value is 1, J value is 6 and the ground multiplet is an H term with spin multiplicity 3, J equal to 6. So, the g J is 7 by 6 and the P effective is just 7.57 Bhor magnetrons. Lastly we have ytterbium 3 plus, which has thirteen electrons in the 4f shell and the corresponding values of L S J are, L equal to 3, S equal to half, J equal to 7 by 2 and the ground multiplet is F term because, L is 3 2 7 by 2. So, g J is 8 by 7 and P effective is 4.24 Bhor magnetrons. We of course, have the final case of lutetium which has the full shell filled with all the fourteen electrons.

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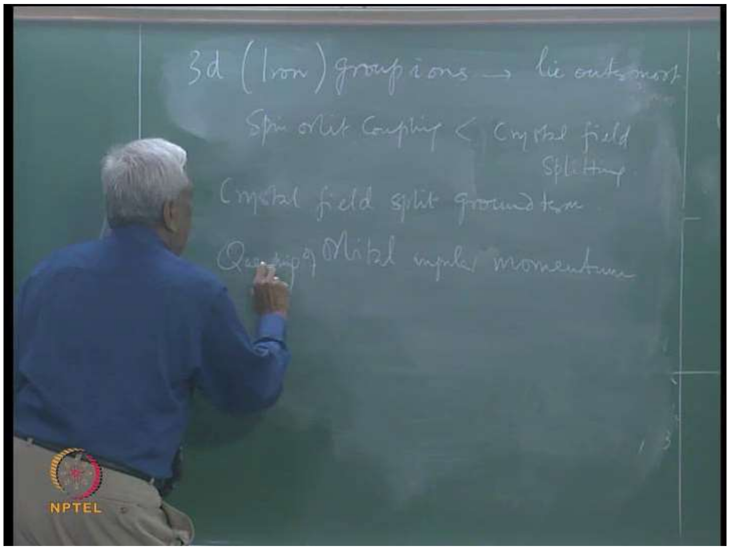

So, this corresponds to L equal to 0, S equal to 0, J equal to 0 because, it is a closed shell. And therefore, it is diamagnetic no Para magnetism no unpaired electrons. So, that completes the story about the rare earth ions. We now, move on to the iron group of 3 d group ions. The iron group corresponding to the progressive filling up of the 3 d shell.

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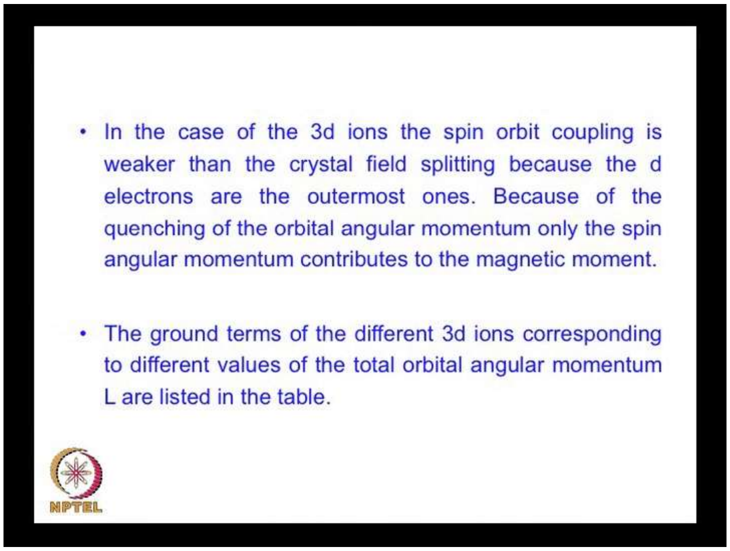

- In the case of the 3d ions the spin orbit coupling is weaker than the crystal field splitting because the d electrons are the outermost ones. Because of the quenching of the orbital angular momentum only the spin angular momentum contributes to the magnetic moment.
- The ground terms of the different 3d ions corresponding to different values of the total orbital angular momentum L are listed in the table.

In this case the spin orbit coupling is weaker when crystal field splitting because; there is a crystalline electric field and the 3 d ions, which lie outer most there are no outer electron shielding them. So, they lie outermost and therefore, they experience the effect of the crystal field and therefore, the crystal field splitting is much stronger than the spin orbit coupling.

So, one has to determine the crystal field split ground term. Usually the crystal field is so; strong that the orbital angular momentum is completely quenched therefore, the only angular momentum which contributes to magnetism is the spin angular momentum. So, it is spin only magnetism. So, the g factor is that of the spin value.

Pure spin value two close to two and the corresponding magnetic moment is 2S into S plus 1 to the power half, where S is the spin angular momentum. So, with this prescription let us look at the ions in the 3 d shell.

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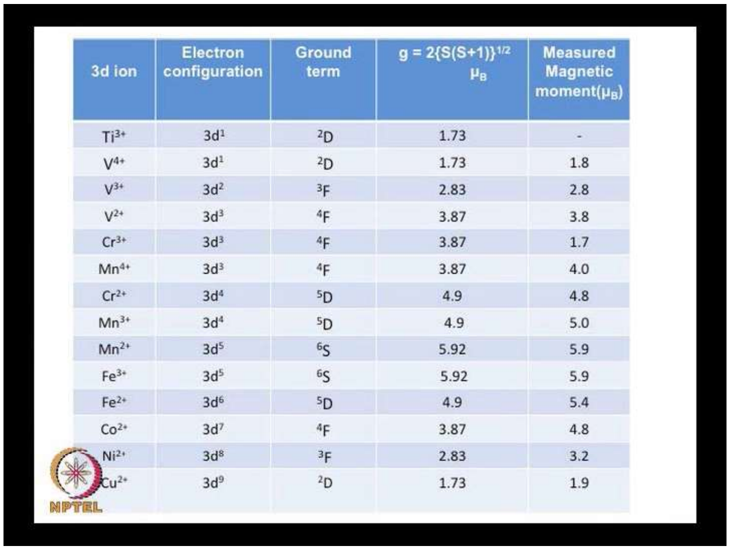

3d ion	Electron configuration	Ground term	$g = 2\{S(S+1)\}^{1/2}$ μ_B	Measured Magnetic moment(μ_B)
Ti^{3+}	$3d^1$	^2D	1.73	-
V^{4+}	$3d^1$	^2D	1.73	1.8
V^{3+}	$3d^2$	^3F	2.83	2.8
V^{2+}	$3d^3$	^4F	3.87	3.8
Cr^{3+}	$3d^3$	^4F	3.87	1.7
Mn^{4+}	$3d^3$	^4F	3.87	4.0
Cr^{2+}	$3d^4$	^5D	4.9	4.8
Mn^{3+}	$3d^4$	^5D	4.9	5.0
Mn^{2+}	$3d^5$	^6S	5.92	5.9
Fe^{3+}	$3d^5$	^6S	5.92	5.9
Fe^{2+}	$3d^6$	^5D	4.9	5.4
Co^{2+}	$3d^7$	^4F	3.87	4.8
Ni^{2+}	$3d^8$	^3F	2.83	3.2
Cu^{2+}	$3d^9$	^2D	1.73	1.9

So, we start with titanium 3 plus which has 3 d 1, one electron.

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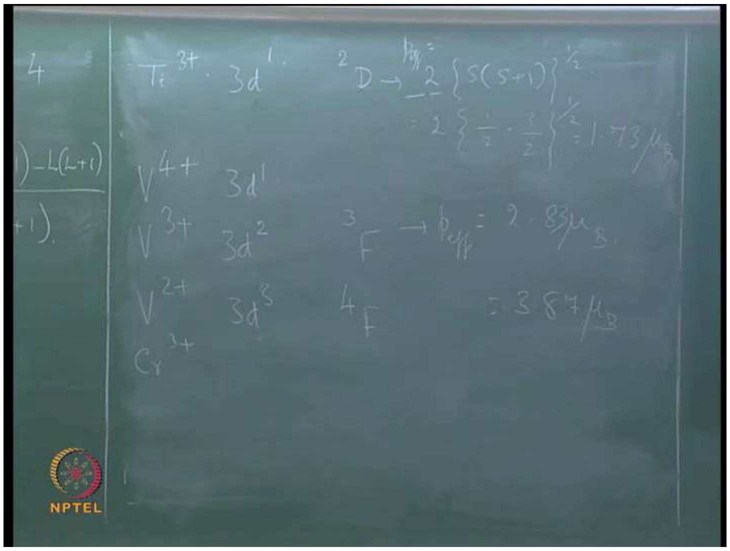

$Ti^{3+} \cdot 3d^1 \quad {}^2D \rightarrow \mu_{eff} = 2\{S(S+1)\}^{1/2}$

$= 2\{\frac{1}{2} \cdot \frac{3}{2}\}^{1/2} = 1.73\mu_B$

$V^{4+} \quad 3d^1$

$V^{3+} \quad 3d^2 \quad {}^3F \rightarrow \mu_{eff} = 2.83\mu_B$

$V^{2+} \quad 3d^3 \quad {}^4F \quad = 3.87\mu_B$

Cr^{3+}

So, it has since it is a D electron the ground term is has the symbol D and it is a 2 D term, which is the ground term therefore, 2S into S plus 1 to the power half. In this case is 2 into half into 3 by 2 to the power half. This is value of the effective magnetic moment, this is g value.

So, this works out to be 1.73 then we have V 4 plus vanadium, which has also 3 d 1. So, its behaviour is similar then vanadium 3 plus has two electrons 3 d 2 and that corresponds to a 3 F by the same reasoning as we did for the rare earth ions and the P effective in this case is 2.8. We can also have vanadium 2 plus, which is 3 d 3 and the spectroscopic ground term is 4 F and the P effective will be 3.87, 2.83 here.

Vanadium 2 plus as well as chromium 3 plus and manganese 4 plus all have the same electronic configuration of 3 d 3. And so, they have similar magnetic behaviour.

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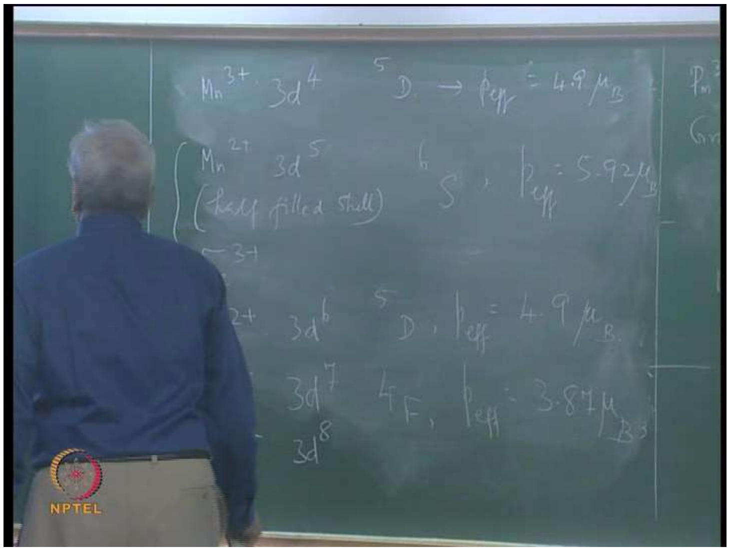

Then we move on to manganese 3 plus, which has four electrons in the 3 d shell and therefore, it has a 5 D term giving a magnetic moment of 4.9 Bhor magnet. Then Mn 2 plus which has five electrons. So, it is a half filled shell with a spectroscopic ground term of 6 S, it is an S state and so, the P effective since it is an s state. So, it will be 5.92 is also the case with iron 3 plus is identical isoelectronic. Then we go on to for s ion which has 3 d 6 configuration and again a 5 D ground term with a magnetic moment calculated magnetic moment of 4.9 as before. Then we have cobalt 2 plus, which is 3 d 7 and 4 F ground term P effective of 3.87. Then we have nickel 2 plus, which is 3 d 8 and so, a 3 F ground term and a magnetic moment of 2.83.

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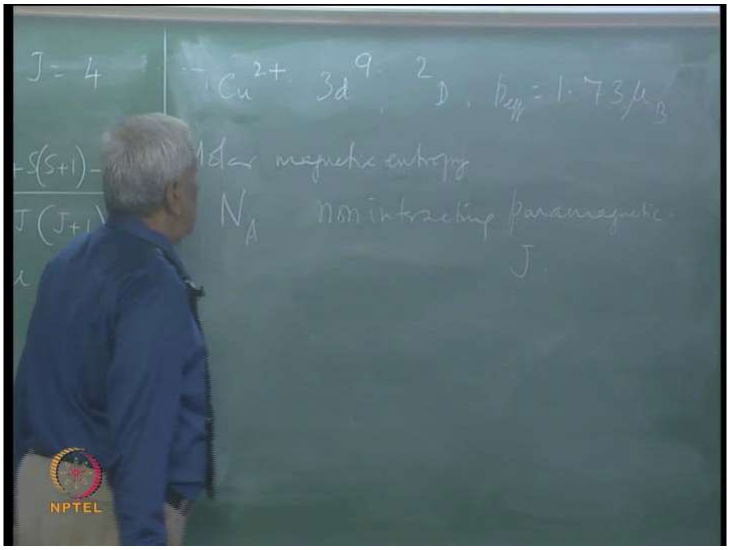

Finally, we come to copper 2 plus, cuprous ion which has a 3 d 9 configuration. So, it has a 2 D ground term with a P effective of 1.73 Bhor magnetrons. So, the experimental measured magnetic moments are given the last column in this table. So, you can see that the agreement with the spin only magnetic moment is fairly good.

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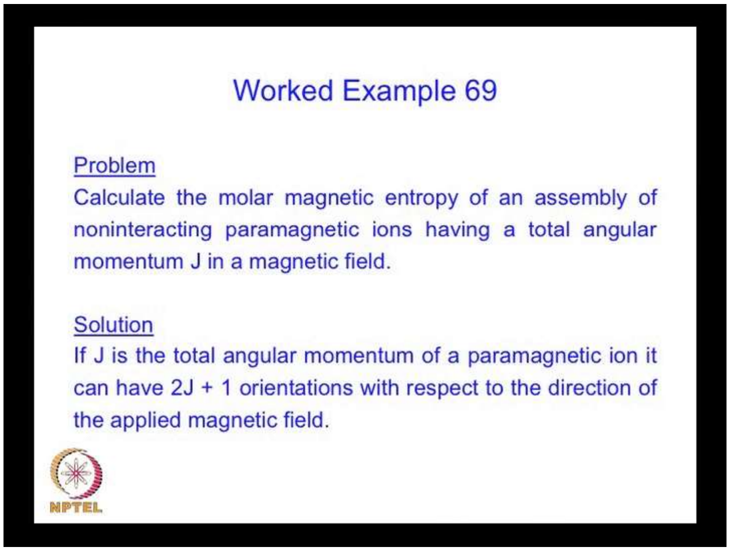

Worked Example 69

Problem

Calculate the molar magnetic entropy of an assembly of noninteracting paramagnetic ions having a total angular momentum J in a magnetic field.

Solution

If J is the total angular momentum of a paramagnetic ion it can have 2J + 1 orientations with respect to the direction of the applied magnetic field.

Next you are asked to calculate the molar magnetic entropy, of an assembly of non interacting paramagnetic ions. Molar means the number of spins is the Avogadro number. Each of these has a total angular momentum of J and a magnetic field is applied.

So, if you have a total angular momentum of J, there are 2 J plus 1 orientation possible for each ion with respect to the direction of the applied magnetic field.

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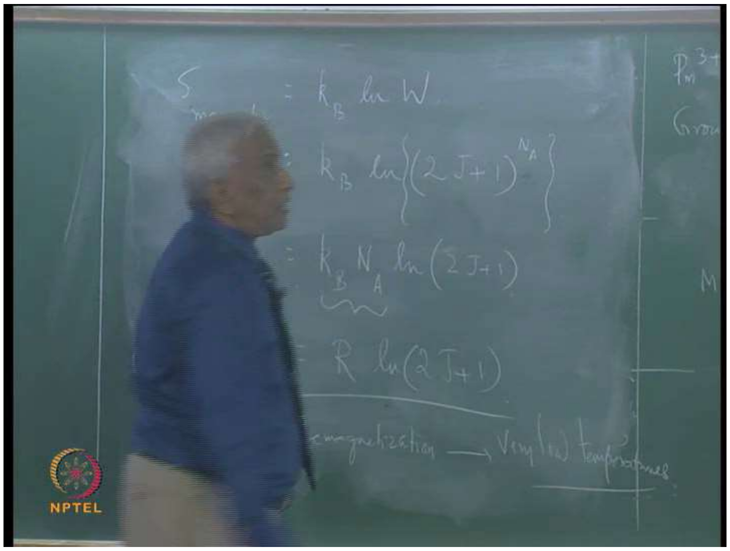

Therefore, the magnetic entropy can be calculated readily from the Boltzmann formula, which gives the magnetic entropy as K B log W, where K B is the Boltzmann constant and W is the number of different configurations.

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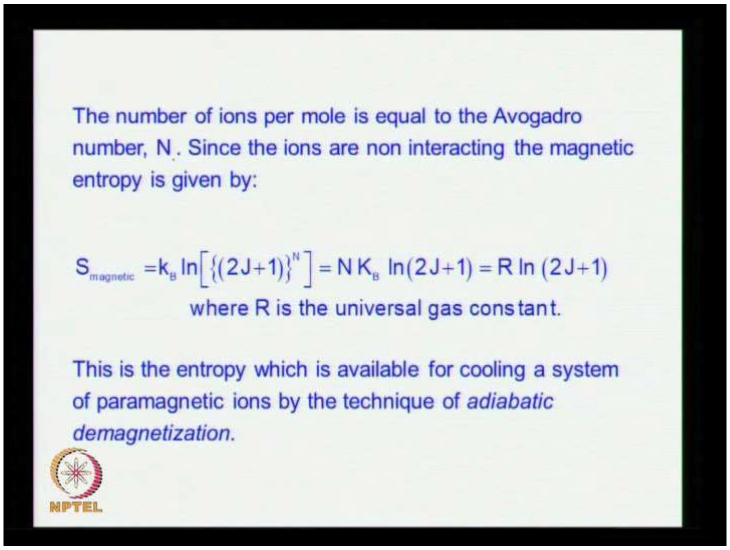

The number of ions per mole is equal to the Avogadro number, N. Since the ions are non interacting the magnetic entropy is given by:

$$S_{magnetic} = k_B \ln\left[\{(2J+1)\}^N\right] = N K_B \ln(2J+1) = R \ln(2J+1)$$

where R is the universal gas constant.

This is the entropy which is available for cooling a system of paramagnetic ions by the technique of *adiabatic demagnetization.*

So, this will be in this case, since there are N ions, N A where N A is the Avogadro number and therefore, the total probability is K B log 2 J plus 1 to the power N A therefore, since it is logarithm, it will be and we know that K B N A is just the universal gas constant R and therefore, it is R log 2 J plus 1.

So, this is the magnetic entropy that is available in a system of paramagnetic ions and in an applied magnetic field. So, you can have the technique of adiabatic de magnetisation by means of which we can remove the applied magnetic field suddenly keeping the spins in thermal isolation and this entropy causes a cooling of the spins or the paramagnetic ions by this technique, which takes these two very low temperatures. this technique has been used to achieve extremely low temperatures, it is a refrigeration technique.

Condensed Matter Physics
Prof. G. Rangarajan
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Lecture - 16
Dielectric (Insulating) Solids

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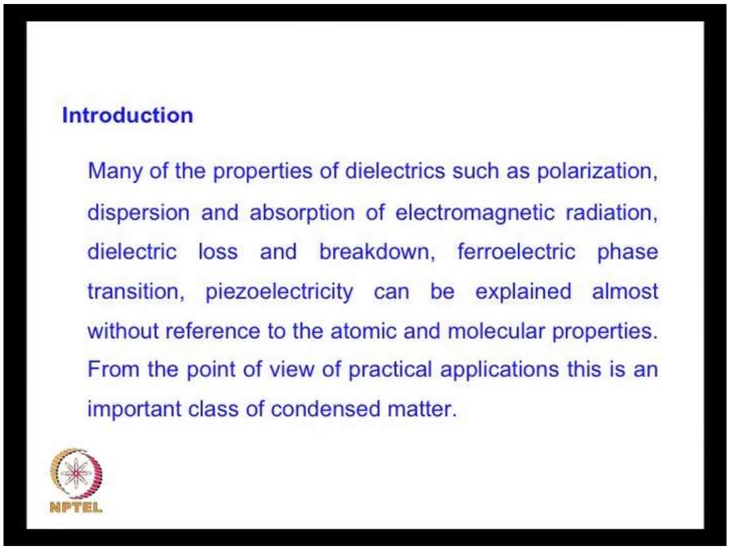

Introduction

Many of the properties of dielectrics such as polarization, dispersion and absorption of electromagnetic radiation, dielectric loss and breakdown, ferroelectric phase transition, piezoelectricity can be explained almost without reference to the atomic and molecular properties. From the point of view of practical applications this is an important class of condensed matter.

Today, we will to talk about insulators are dialectics now many of the properties have to dialectics such as electric polarization dispersion, and absorption of electromagnetic radiation by insulating materials dielectric loss dielectric break down, ferroelectric phase transition, piezoelectricity etcetera can be explained almost without reference to the atomic and molecular properties.

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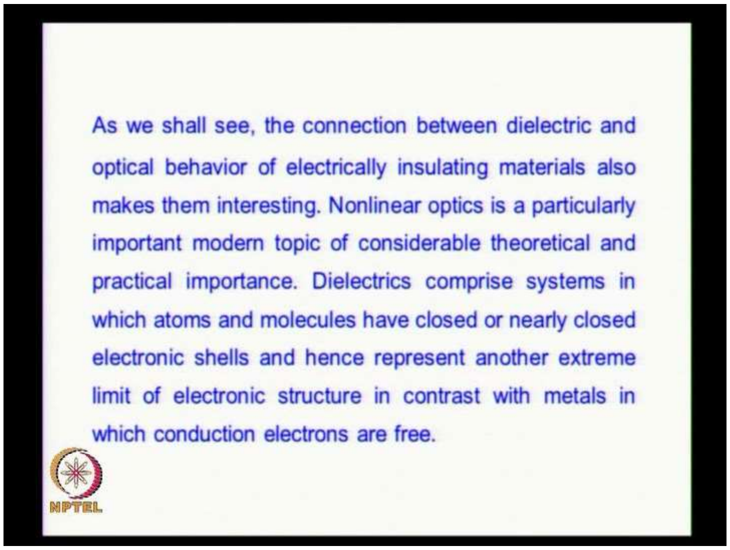

As we shall see, the connection between dielectric and optical behavior of electrically insulating materials also makes them interesting. Nonlinear optics is a particularly important modern topic of considerable theoretical and practical importance. Dielectrics comprise systems in which atoms and molecules have closed or nearly closed electronic shells and hence represent another extreme limit of electronic structure in contrast with metals in which conduction electrons are free.

And the point of view of practical applications, they insulators are dielectric constitute an important class of condensed matter. The connection between dielectric and optical behavior as we will see of such electrically insulating materials also makes them interesting from the point of view of modern areas such as non-linear optics which is a particularly important modern topic of considerable theoretical and practical importance dielectric comprise systems. In which atoms and molecules have closed on nearly closed shells structure for electrons. And therefore, they represent another extreme limit of electronics structure in contrast with metals in which conduction electrons are free.

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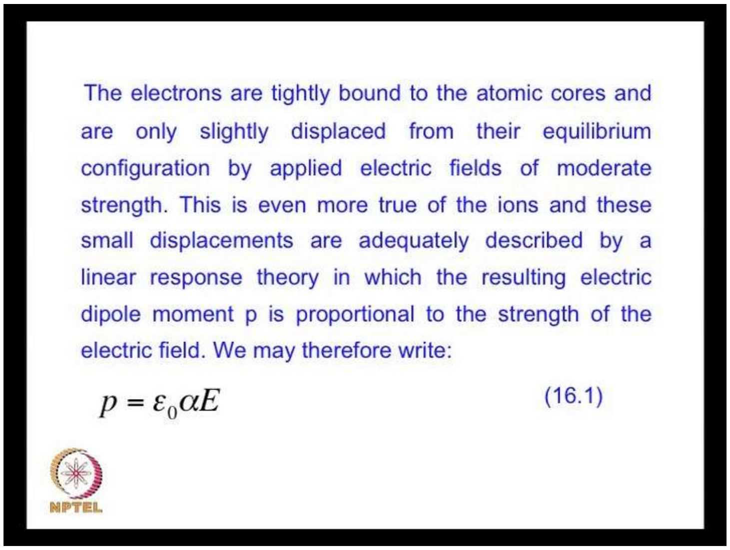

The electrons are tightly bound to the atomic cores and are only slightly displaced from their equilibrium configuration by applied electric fields of moderate strength. This is even more true of the ions and these small displacements are adequately described by a linear response theory in which the resulting electric dipole moment p is proportional to the strength of the electric field. We may therefore write:

$$p = \varepsilon_0 \alpha E \qquad (16.1)$$

The electrons in dielectric materials are tightly bound to the autonomic course and are only only slightly displays from that equilibrium configuration by applied electric fields of moderate strength, this is even more true of ions and these smaller displacement are adequately describe by a linear response theory.

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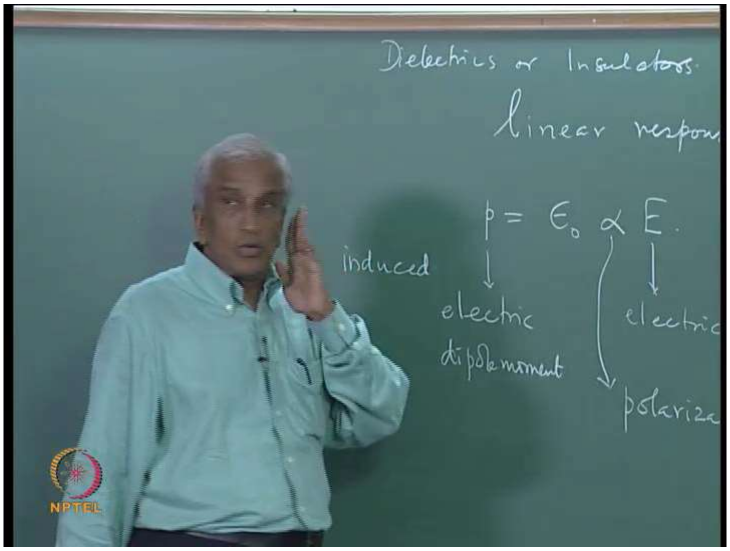

In which the linear response theory assumes that the electric de poll movement which results from the application of a in electric field of moderate strain it is proportional to this strength of the electric field therefore, if p is electric dipole moment. We can write p equals epsilon naught alpha e now here e is the electric field p is electric dipole moment and alpha is the constant of proportionality is known as polarizability. The atom are molecule that is a constant which is measured in units of epsilon naught the permittivity a free space. So, this p is the induced dipole e moment induced by he applied electric field. So, dielectric polarization this is the individual dipole moment induced per atom molecule.

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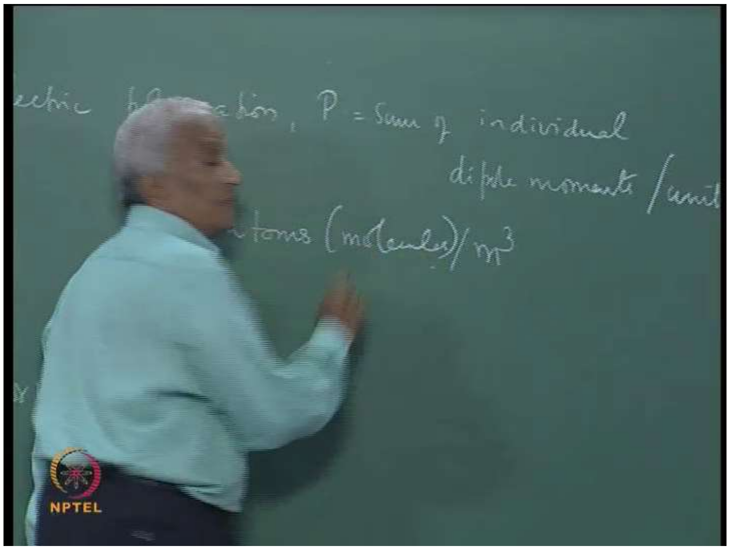

Dielectric polarization capital p is the vector sum of the individual dipole moments some of individual dipole moments and usually defined per unit volume of the material. So, if there are n such atoms are molecules n atoms or molecules per meter cube.

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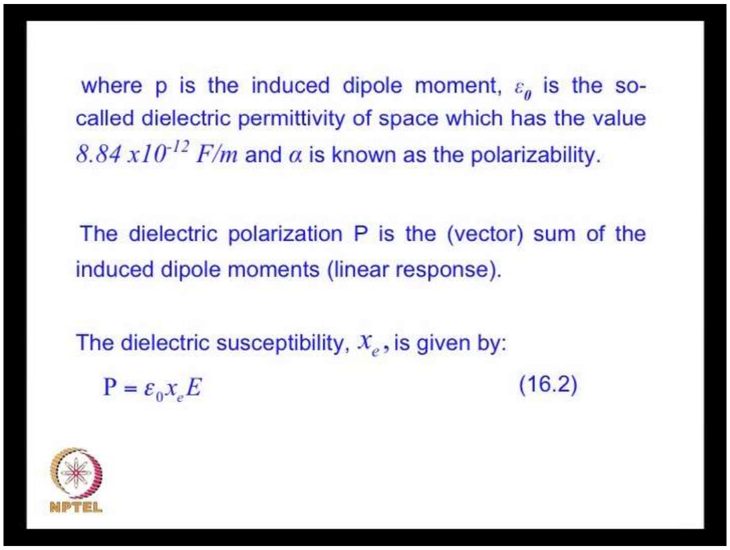

where p is the induced dipole moment, ε_0 is the so-called dielectric permittivity of space which has the value 8.84×10^{-12} F/m and α is known as the polarizability.

The dielectric polarization P is the (vector) sum of the induced dipole moments (linear response).

The dielectric susceptibility, x_e, is given by:

$$P = \varepsilon_0 x_e E \qquad (16.2)$$

So, and then polarization is also related to the applied electric field by the so-called electric susceptibility therefore, combining these relations we get immediately x i.

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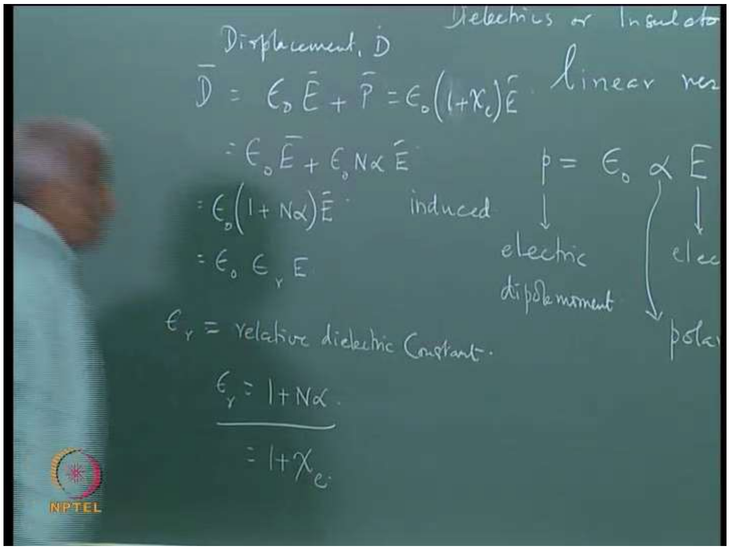

There is an important vector call the displacement D which is be defined by d equals epsilon naught e plus p. Therefore, plugging our epsilon naught e plus p is epsilon epsilon naught n alpha e therefore, I have epsilon naught times one plus n alpha times e and this is usually defined as epsilon naught epsilon naught e where epsilon r is the relating dielectric constant. So, that we arrive at epsilon r equal to one plus n alpha and and we also known that p is x I e epsilon naught x I e. Therefore, we can write here epsilon naught xi e one plus x I e times e. So, comparing this and this we also get one plus x I e.

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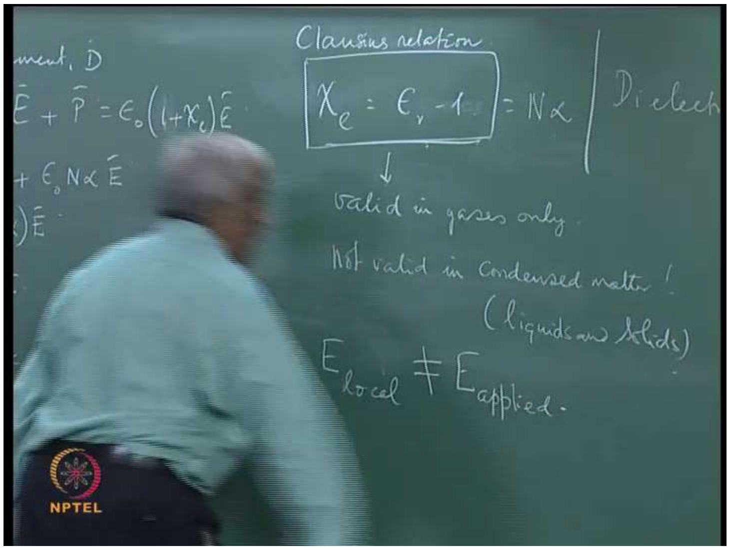

Therefore we get x e is equal to epsilon r minus one of course, this is relation which is valued only in gases. In this case, we as assume that will that we are applying here is the same as the field is seen by the atom or molecule this assumption is not valid not valid in condensed matter such as liquids and solids. So, this relationship between the electric ability and the dielectric constant, why are these so, x e also equal to n alpha. So, this has been verified a great extent many gas, but in a condensed material like a solid dielectric this assumption this relation is not valid this is known as the Clausius relation this is not valid because they dipoles which are present the atomic or molecular dipole interact themselves. There is dipole interaction, which produce internal electric fields. So, that local electric field seen by a solid at or liquid atom or molecule is different from the field which is actually apply, so these local field defers. So, e local is not equal to e applied that is the reason why this relationship is not valid how does it differ?

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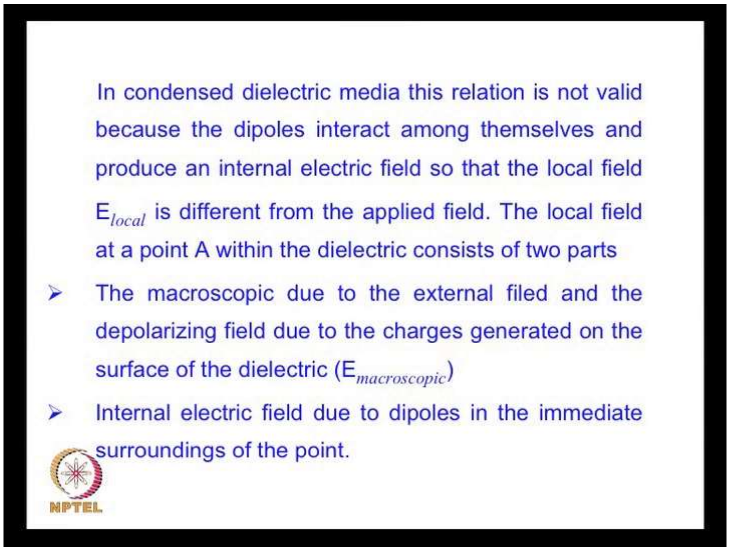

In condensed dielectric media this relation is not valid because the dipoles interact among themselves and produce an internal electric field so that the local field E_{local} is different from the applied field. The local field at a point A within the dielectric consists of two parts

- The macroscopic due to the external filed and the depolarizing field due to the charges generated on the surface of the dielectric ($E_{macroscopic}$)
- Internal electric field due to dipoles in the immediate surroundings of the point.

Now, the local the local electrical field as two contributions, let us look at the process of polarization carefully.

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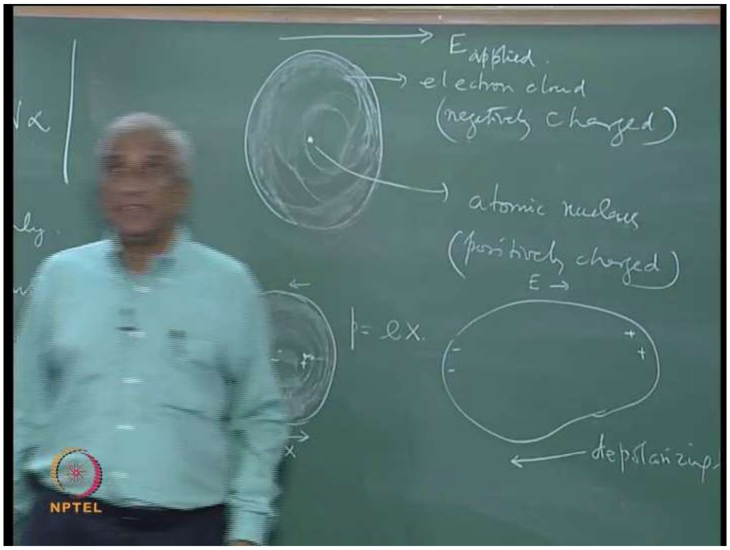

So, I have an atom in which there is an electronic clouds uniform charge density of electron and there is a central nucleus now this is a spiracle atom we are assuming it to spherical atom to keep the discussions simple such that centre's of positive and negative electric charge is the electron clouds negatively charged and this is the atomic nucleus which is positively charged and these two are equals wire. So, that is atom or molecule is electrically neutral to start with the centre of the negative charge distribution coincides with the central positive atomic charge.

Therefore, negative and positive charge that coincide and therefore, there is no dipole moment to start with, but when you apply electric field say this along this direction then the the nation electronic clouds moves away. So, this is the way the electronic clouds is displaced in this direction from the original position we assumed that it is a rigid displacement without any distortion. So, that this moves like this and the positive nucleus moves a little bit this is the nuclear charge.

So, this is displays to much smaller extent because the nucleus is much more massive therefore, it get displays to a much smaller extent, but still what is happening is the central of the negative charge and deposited charge here there is the relative displacement and this is what gives you a net dipole moment which is induced, and it is present only as long as the electric field this existing the moment you remove the electric field is dipole moment will also vanish because the everything will relax back to the original situation. So, this is really induced dipole moment. So, this is the mechanism of polarization. So, what really happened is that you have in a microscope dielectric you have positively charged going in one way and the negative charge is going in another way in the presence of an applied electric field. So, this is what gives you a net electric polarization, but because of this displacement there is also an electric field due to the presence or the positive and negative charges here. So, that gives you an internal electric field which depolarizes the original field because it is acting in the opposite direction from the positively the negative charge. So, this is the direction of the de polarizing field.

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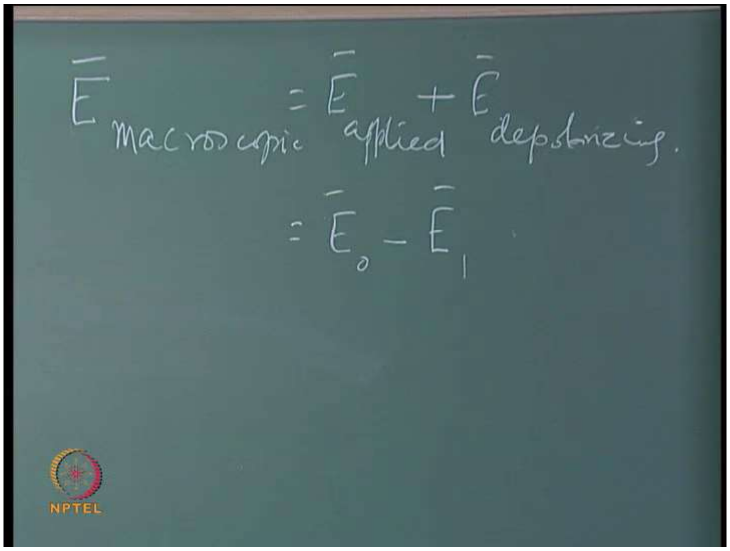

$$\bar{E}_{\text{macroscopic}} = \bar{E}_{\text{applied}} + \bar{E}_{\text{depolarizing}}.$$

$$= \bar{E}_0 - \bar{E}_1$$

So, the macroscopic electric field due to the applied field and de polarizing field duty the charges, which have been produced on the surface. And the dielectric that gives you a net macroscopic electric field which is the sum of the e applied vector sum and the de polarization, but in addition to that there is a interaction among the d I polls as I told you which produces another contribution to this internal local field. Now this therefore, let us called it e naught since this is opposing the applied field let us called it e 1. If you have an ellipse solid specimen, if you are dielectric is in the shape of an ellipse solid, this de polarizing field can be shown to vanish. But in all other geometries in the spicemen shape is different from a ellipse solid Debye de polarizing field is not vanishes, but even when it is not zero it can be determine for standard geometries such as medical specimen or a long thin brought and so on. So, we can find the de polarizing field and add iteratively to him apply a electric field to obtain the macro specific electric field.

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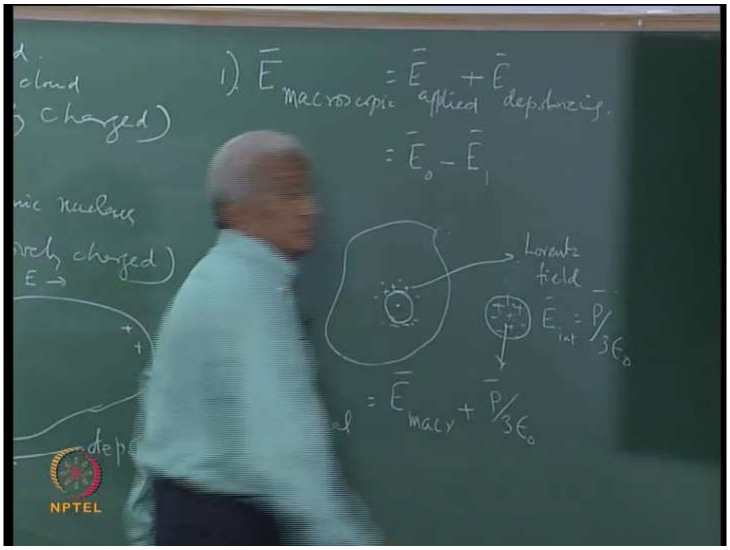

So, this is the first part the second part is due to the dipoles which are in the immediate neighborhood of suppose you have a dielectric and you have a given atomic dipoles sum were here it its immediate neighborhood there are other dipoles. So, these are all different dipoles. So, these dipoles interact with this dipoles and therefore, we have de pole de pole interaction which produce and internal electric fields this situation can be considered quantitatively by considering spherical cavity we assume that we scot out dielectric materially of course, a spherical plug and their four now you have charges on this surface this cavity.

So, these charges on the surfacewi9ll produce an electric field and then you have scooped out this material, but it within this cavity there are dipoles. So, these produced an internal electric field this electric field is known as the Lorentz field who calculated its value and it can be shown that this field is e internal is p by three epsilon naught for sphere and then this this is due to the surface charge. And in addition this, field due to the charges in this spherical cavity can be shown to be zero for a cubic material. So, we have all these various contribution and the macroscopic electric field e local the local electric field is e macroscopic p by three epsilon naught. So, it is this local electric field which is seen by the atom or molecule the dipole and therefore, this is what we have two here right here.

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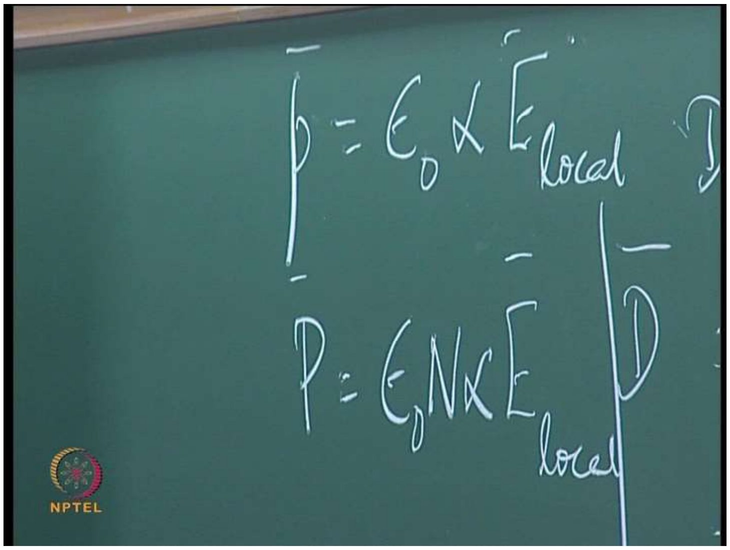

So, the individual dipole is now dipole moment is epsilon naught alpha e local where e local is given by this therefore, correspondingly p also will change accordingly. So, p is n n alpha e local. So, let the substitute this value of pin c what we get.

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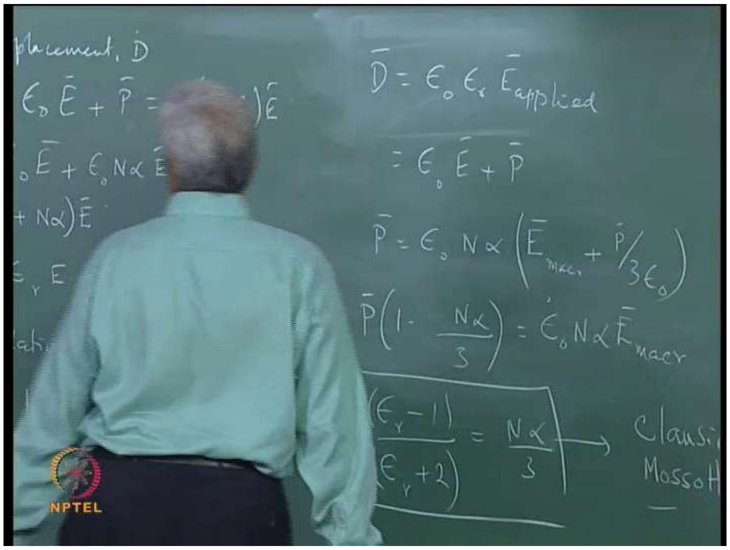

So, we will get d is epsilon naught epsilon r e applied and this is equal to epsilon naught e plus p. So, this will give me a relation p will be now epsilon naught n alpha into e local which is e macroscopic plus p three epsilon naught. So, collecting the p terms there is a together p times one minus epsilon naught n alpha by three epsilon naught cancels equals epsilon naught alpha e macroscopic. So, because of this we get a modification in the clauses relation between dielectric constant. All these are and the and this therefore, we can show straightforward to show that epsilon or minus one by epsilon on plus two equals n alpha by three this is the relation which replaces the Clausius relation for a gas the case of a solid or liquid dielectric this relation is known as the Clausius Mossotti equation. So, the presence of internal electric field produces this term in the denominator that is all this is change.

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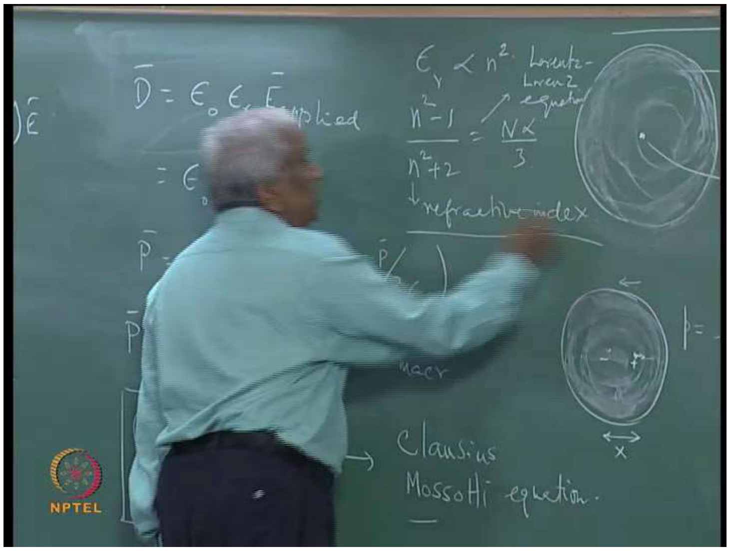

And since the relative dielectric constant is proportional to the squire or therefore, we can also write this relation the Clausius relation in this form where n is the refractive index say an optical frequencies. So, in this form this is known as the Lorentz equation. So, these are the basic equations which govern the relative dielectric constant in the refractive index in the case of condensed matter in the case of solids, so this situation.

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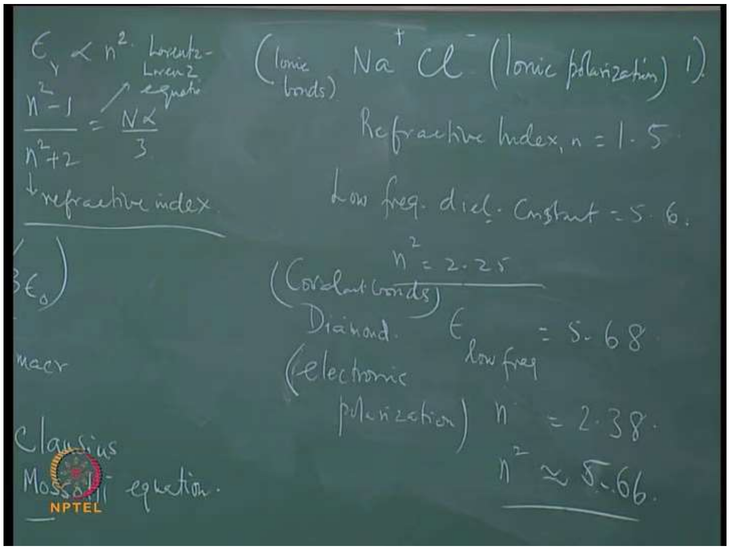

$\epsilon_r \propto n^2$ Lorentz-Lorenz equation

$$\frac{n^2-1}{n^2+2} = \frac{N\alpha}{3}$$

↓ refractive index

$3\epsilon_0)$

macr

Clausius Mossotti equation.

(Ionic bonds) $Na^+ Cl^-$ (Ionic polarization) !)

Refractive Index, n = 1.5

Low freq. diel. Constant = 5.6.

$n^2 = 2.25$

(Covalent bonds) Diamond. $\epsilon_{low\ freq} = 5.68$

(electronic polarization) $n = 2.38$

$n^2 \approx 5.66$

So, for example, if you take a material like sodium fluoride common salt, so this as a refractive index n which is one point five whereas, this low frequency dielectric constant are starting dielectric constant is 5.5, 5.6. So, if you squire the refractive index n squire it is only 2.25, so in going from low frequency career-high to a frequency the value of dielectric constant as comedown. Whereas, the case of material diamond in which the bonds are stronger therefore, the low frequency dielectric constant low frequency dielectric constant is five point six eight the refractive index at optical frequencies two point two three eight. So, squire is almost close to the epsilon. So, there is not. So, much difference n squire is 5.66. So, you can see that in the case of diamond polarization mechanism is entirely electronic the electrons contribute polarization whereas, in the case of sodium chloride you have sodium ions and clarian ions forming alternate alternatively occupying a cubic lattice. So, these ions also have dipole moments. So, there is an ionic polarization in addition to the electronic polarization only.

So, these are all readily how the electrons this start to produce give rise to here dipole moment that is the electron is polarization mechanism. So, we have two different polarization mechanism one of electron due to the displacement and the electronic cloud and the other it is due to displacement at the positive and negative ion as in allowing. So, when both are simultaneously present then the ions being massive are not able follow the frequency variations such as high frequencies therefore, ionic polarization drops of become decreases as the frequency increase.

So, hard high-frequency the electronic contribution alone remains whereas, at low frequencies both the ionic and electronic contribution give rise to a large dielectric constants static dielectric constant in the case of diamond it is exclusively electronic polarization there are no ions there is a covalent solid covalent bonds in the case of diamond whereas, here these are ionic bonds. So, when there are covalent bond it is only electronic polarization which contributes to the polarization, dielectric polarization and hence it is the dielectric constant when you consider material like water water as in addition to these the water molecule as a very large dipole moment ordinary water.

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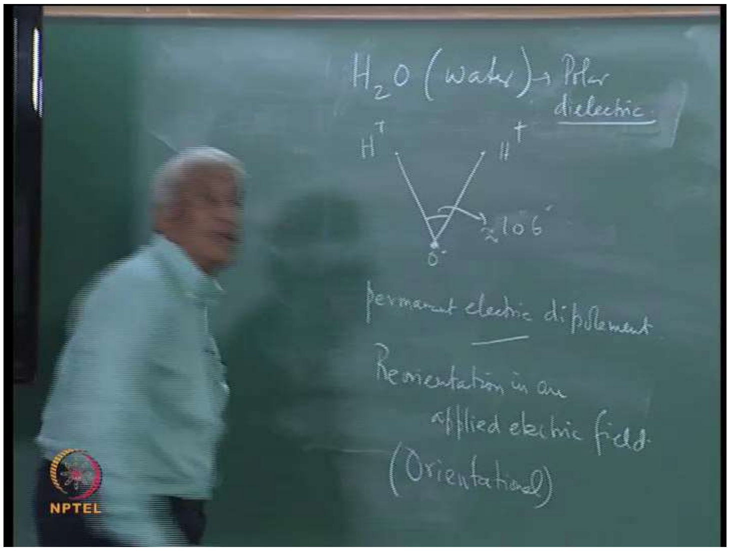

So, it has an oxygen and two hydrogen’s. So, this is the structure as the water molecule. So, the o h o bound angle is approximately tetrahedron something like hundred six degree approximately. So, this has a net permanent dipole moment it is because to have the positive and negative charges do not coincide and therefore, there is a net dipole moment even in the absence of an electric dipole electric field unlike the case of the spherical atoms which we saw in the case of electronic cloud.

So, this is known as the polar molecule poll dielectric which is an inherent non vanishing dipole moment and these dipoles due to the water molecules tend to reorient themselves in an applied field. So, reorientation in an applied electric field. So, this gives you in addition to the ionic and electronic contribution this gives us an additional orientation all contribution to the polarization and then and the dielectric constant.

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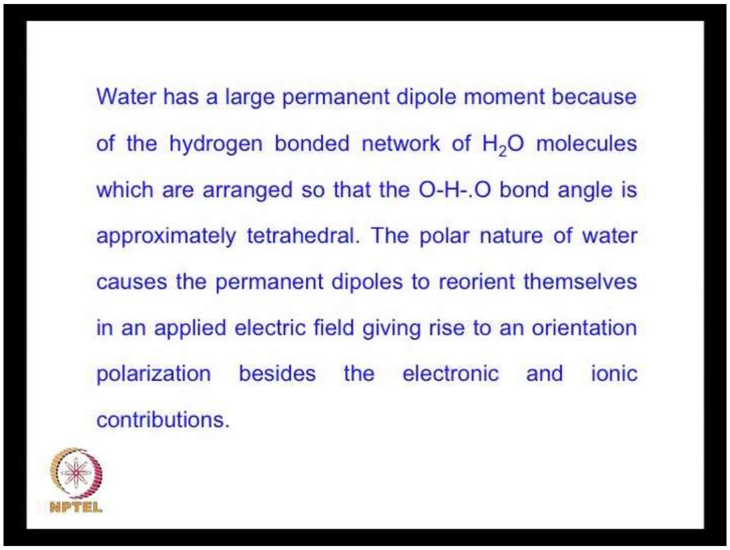

Water has a large permanent dipole moment because of the hydrogen bonded network of H_2O molecules which are arranged so that the O-H-.O bond angle is approximately tetrahedral. The polar nature of water causes the permanent dipoles to reorient themselves in an applied electric field giving rise to an orientation polarization besides the electronic and ionic contributions.

So, you have in all three contributions arising from different mechanism to the net direct polarization and Hensley dielectric constant.

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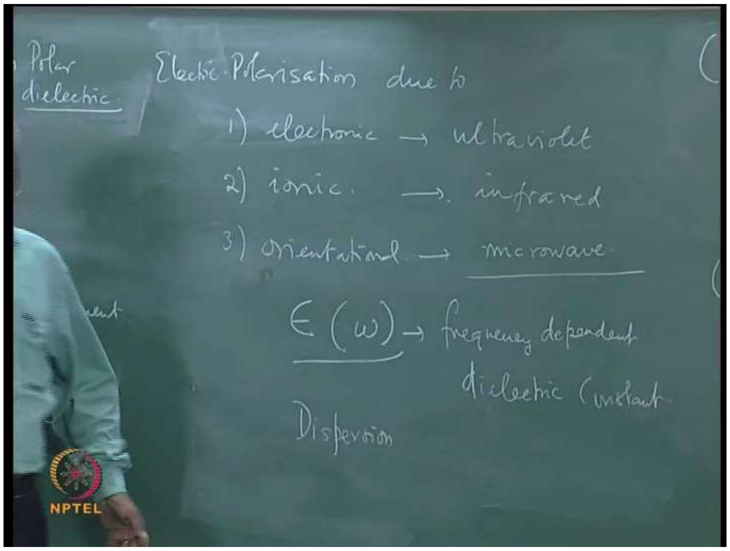

Polar dielectric.

Electric Polarisation due to

1) electronic → ultraviolet

2) ionic. →. infrared

3) orientational → microwave

$\epsilon(\omega)$ → frequency dependent dielectric Constant.

Dispersion

What are the polarization electric polarization due to one an electronic polarization two and ionic contribution and three orientation all contribution in general all three will be present for example, in the case of the water molecule, but when there are no permanent dipole moments the electric field induces only electronic ionic contributions the ionic contribution is there is only when there are ions which get displays and therefore, give you a polarization otherwise when there are no ions the structure like that of diamond the electric polarization mechanism is completely electronic.

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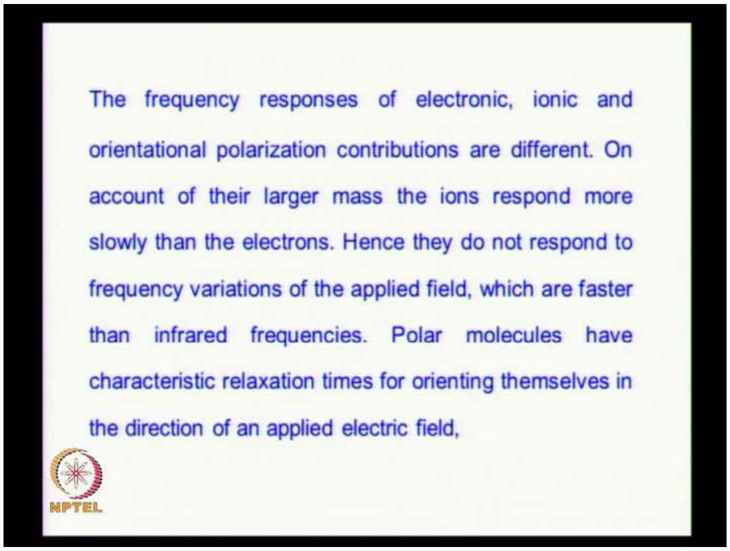

The frequency responses of electronic, ionic and orientational polarization contributions are different. On account of their larger mass the ions respond more slowly than the electrons. Hence they do not respond to frequency variations of the applied field, which are faster than infrared frequencies. Polar molecules have characteristic relaxation times for orienting themselves in the direction of an applied electric field,

So, these are even among dielectric there are different kinds of dielectric and since the electrons respond rapidly to even rapid frequency variation of the apply electric field the electronic contribution continues very high frequencies of the applied electric field. Therefore, ions being more massive they are unable to follow the rapid field variation of a certain frequency therefore, this ionic contributions are present only at will relatively low frequency similarly the orientation and the permanent dipole I gain happen at a relatively lower frequencies at the applied electric field.

So, the electronic contribution is usually the ultraviolet range ultraviolet frequencies the ionic contribution are in the infrared range and this is orientation contribution occurs the microwave frequency. So, as you change the frequency at the applied electric field and go through micro-wave infrared and ultraviolet ranges of frequencies these various contribution will give rise to polarization and n contribute to the dielectric constitute.

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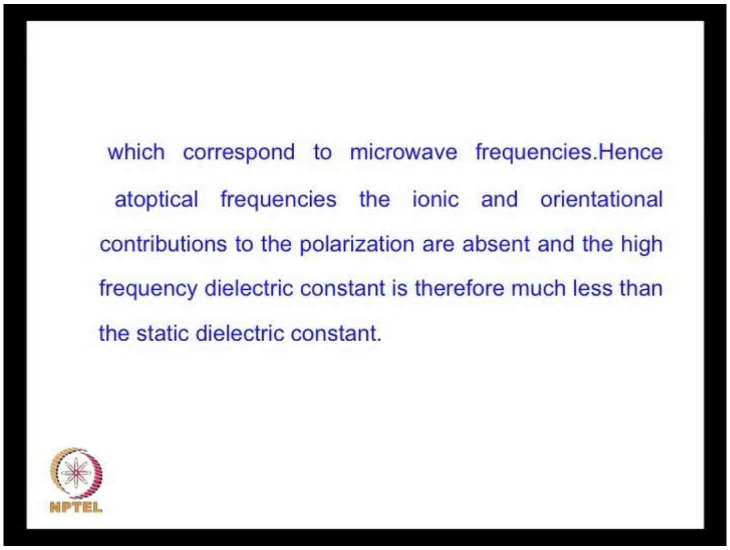

which correspond to microwave frequencies.Hence atoptical frequencies the ionic and orientational contributions to the polarization are absent and the high frequency dielectric constant is therefore much less than the static dielectric constant.

So, the dielectric constant is frequency dependent and it is frequency dependence which gave rise to a frequency dependent refractive index because epsilon disproportional to n squire and therefore, refractive index determines the phase velocity of electromagnetic wave in any given dielectric medium therefore, you can see that the phase velocity changes and this is what we know has dispersion. So, the phenomena of dispersion give rise to the arises from the frequency dependent of the dielectric constant.

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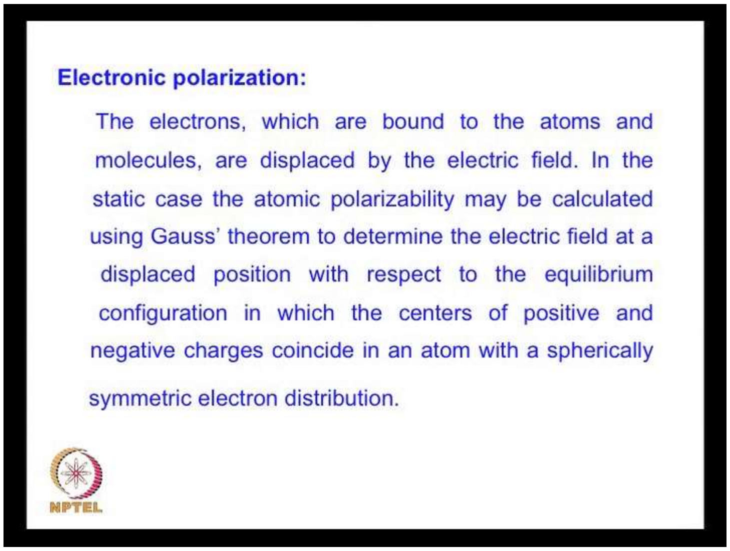

Electronic polarization:

The electrons, which are bound to the atoms and molecules, are displaced by the electric field. In the static case the atomic polarizability may be calculated using Gauss' theorem to determine the electric field at a displaced position with respect to the equilibrium configuration in which the centers of positive and negative charges coincide in an atom with a spherically symmetric electron distribution.

Now, let us consider this electronic polarization mechanism in a little detail when we already saw that the electrons in a dielectric material or bound to the parent atoms and molecules under displaced by the electric field. So, in the static limit when the electric field is a static electric field the atomic polarized ability can be calculated using cause theorem.

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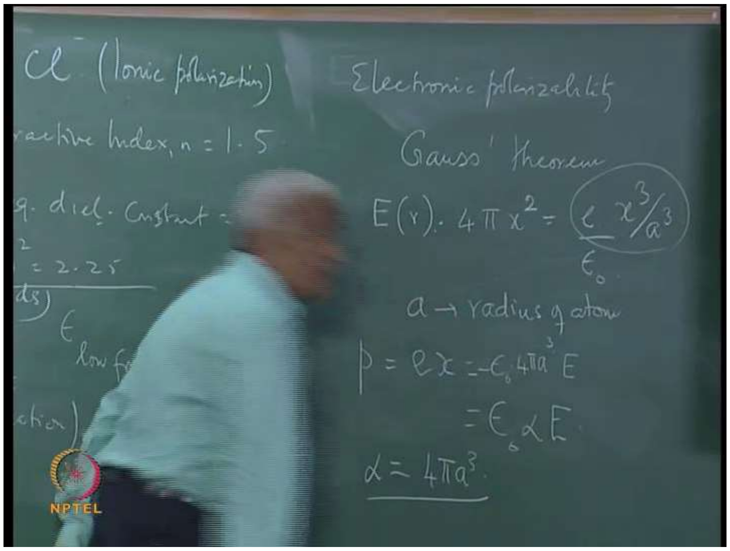

Cl⁻ (Ionic polarization)

ractive Index, n = 1.5

q. diel. Constant =

= 2.25

ds)

ϵ low f

ction)

Electronic polarizability

Gauss' theorem

$E(x) . 4\pi x^2 = \frac{e}{\epsilon_0} x^3/a^3$

$a \rightarrow$ radius of atom

$p = ex = -\epsilon_0 4\pi a^3 E$

$= \epsilon_0 \alpha E$

$\alpha = 4\pi a^3$

So, we assume a spherical atom and we apply cause theorem it is well-known in electro statics.

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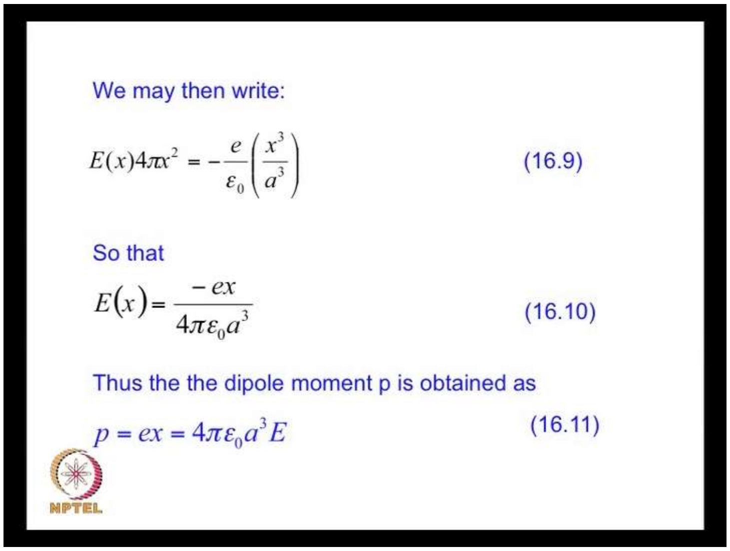


We may then write:

$$E(x)4\pi x^2 = -\frac{e}{\varepsilon_0}\left(\frac{x^3}{a^3}\right) \qquad (16.9)$$

So that

$$E(x) = \frac{-ex}{4\pi\varepsilon_0 a^3} \qquad (16.10)$$

Thus the the dipole moment p is obtained as

$$p = ex = 4\pi\varepsilon_0 a^3 E \qquad (16.11)$$

So, if we consider gauss theorem we can write e f r for a spherical atom the electric field is radically directed that is why I am writing times four pi x cube where x is the relating displacement between the electron and the nuclear charges. Therefore, this will be this will be the electric field and this is gauss theorem giving you the flux duty the electric field and this is given by the charge divided by epsilon naught. Now if the charge electronic charges is distributed over and atom of radius a a is the radius at the atom. Then the electronic charge is sphere over a volume four third pi cube of which we want to calculate be fraction of this charge intersected by spherical region of radius x therefore, this will be fourth third pi x cube.

Therefore, that is a how you get the fourth third pi cancels leaving you this fraction this is the fractional as the electronic charge which is closed. And therefore, this gives me the e x as e e times epsilon naught into for pi a cube with a minus sign in order to show the moment as the negative sign the charges negative. So, the dipole moment this is the induced dipole moment. So, this gives me comparing it with epsilon naught alpha e where alpha is polarized ability we arrive at polarized ability as four pi a cube. So, the polarized ability at the atom a spherical atom is simply four pi times the cube of the atomic radius the polarizability is proportional to the atomic volume let us now consider we will consider in the next discussion what happens when we go from a static field to be a frequency dependency in applied alternating field we will consider this.

UNIT-III-Dielectric and Magnetic properties of materials

Syllabus:

Dielectric constant and polarization of dielectric materials - Types of polarization – Equation for internal field in liquids and solids (one dimensional) – Clausius Mosotti equation – Ferro and Piezo electricity (qualitative) – Frequency dependence of dielectric constant- Important applications of dielectric materials.

Classification of dia, para and ferromagnetic materials. Curie Temperature Hysterisis in ferromagnetic materials. Soft and Hard magnetic materials. Applications.

Introduction

Dielectrics are insulating or non-conducting ceramic materials and are used in many applications such as capacitors, memories, sensors and actuators. Dielectrics are insulating materials that exhibit the property of electrical polarization, thereby they modify the dielectric function of the vacuum. A dielectric material is any material that supports charge without conducting it to a significant degree. In principle all insulators are dielectric, although the capacity to support charge varies greatly between different insulators. Although these materials do not conduct electrical current when an electric field is applied, they are not inert to the electric field. The field may cause a slight shift in the balance of charge within the material to form an electric dipole.

Thus the materials is called dielectric material.

Dielectric materials are used in many applications, from simple electrical insulation to sensors and circuit components.

Faraday was carried out the first numerical measurements on the properties of insulating materials when placed between the two parallel plates (capacitor), those materials, he called as dielectrics. He has found that the capacity of a condenser was dependent on the nature of the material separating the conducting surface. This discovery encouraged further empirical studies of insulating materials aiming at maximizing the amount of charge that can be stored by a capacitor. In search of suitable dielectric materials for specific applications, these materials have become increasingly concerned with the detailed physical mechanism governing the behavior of these materials.

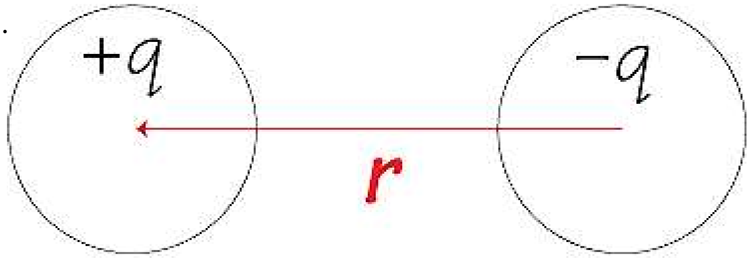
The difference between dielectric material and insulator depends on its application. Insulating materials are used to resist flow of current through it, on the other hand dielectric materials are used to store electrical energy. In contrast to the insulation aspect, the dielectric phenomena have become more general and fundamental, as it has the origin with the dielectric polarization.

Electric dipoles:

Upon application of a dc or static electric field, there is a long range migration of charges. However, there is a limited movement of charges leading to the formation of charge dipoles and the material, in this state, is considered as polarized. These dipoles are aligned in the direction of the applied field. The net effect is called Polarization of the material.

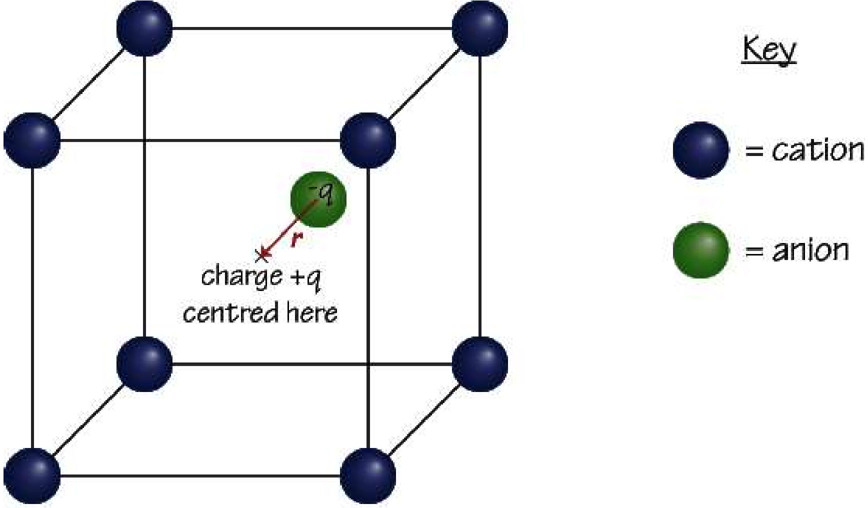
A dielectric supports charge by acquiring a polarisation in an electric field, whereby one surface develops a net positive charge while the opposite surface develops a net negative charge. This is made possible by the presence of electric dipoles – two opposite charges separated by a certain distance – on a microscopic scale.

1. If two discrete charged particles of opposite charges are separated by a certain distance, a dipole moment $\boldsymbol{\mu}$ arises.



$$\mu = q\mathbf{r}$$

2. If the centre of positive charge within a given region and the centre of negative charge within the same region are not in the same position, a dipole moment $\boldsymbol{\mu}$ arises. For example, in the diagram below the centre of positive charge from the 8 cations shown is at X, while the centre of negative charge is located some distance away on the anion.



$$\mu = q\mathbf{r}$$

The second view of dipole moment is more useful, since it can be applied over a large area containing many charges in order to find the net dipole moment of the material.

The dipoles can be aligned as well as be induced by the applied field.

Note that in the equation for dipole moment, ***r*** is a vector (the sign convention is that ***r*** points from negative to positive charge) therefore the dipole moment ***μ*** is also a vector

Electric field intensity or electric field strength (E)

The force experienced by a unit test charge is known as electric field strength E

$$E = \frac{Q}{4\pi\varepsilon r^2} \qquad \text{.....(1)}$$

where ε is the permittivity or dielectric constant of the medium in which electric charge is placed. For vacuum $\varepsilon = \varepsilon_o = 8.854 \text{ X}10^{-12}\text{Fm}^{-1}$

Electric flux density or electric displacement vector (D)

The electric flux density or electric displacement vector is the number of flux lines crossing normal to a unit surface area. The electric flux density at a distance from the point charge Q is

$$D = \frac{Q}{4\pi r^2} \qquad \text{.....(2)}$$

then from (1) and (2) $D = \varepsilon E$ ..... (3)

Dielectric constant (ε_r)

The dielectric constant of a material is defined as the ratio of the permittivity of the medium (ε) to the permittivity of free space (ε_o). It can also defined as the ratio of the capacitance with dielectric (C_d) and with air (C_A) between the plates.

$$\varepsilon_r = \frac{\varepsilon}{\varepsilon_o} = \frac{C_d}{C_A} \qquad \text{.....(4)}$$

Capacitance: The property of a conductor or system of conductor that describes its ability to store electric charge.

$C = q / V = A\,\varepsilon / d$ where

C is capacitance of capacitor
q is charge on the capacitor plate
V is potential difference between plates
A is area of capacitor plate
ε is permittivity of medium
d is distance between capacitor plates

Units: Farad .

Polarization

When an electric field is applied to a material with dielectrics, the positive charges are displaced opposite to the direction of the field and negative charges displaced in the direction of the field. The displacement of these two charges create a local dipole, creation of dipole by applying electric field is called as polarization.

Polarization is defined as induced dipole moment per unit volume.

$$P = \frac{\mu}{Volume} \qquad \ldots(5)$$

Polarisability

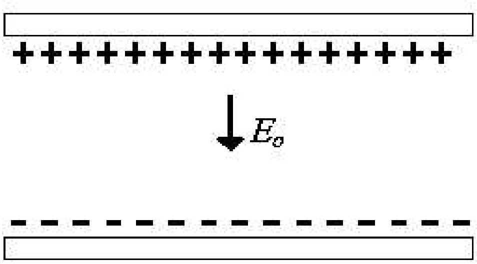
The polarization P is directly proportional to the electric field strength E

$$P \propto E$$
$$P = \alpha E \qquad \ldots(6)$$

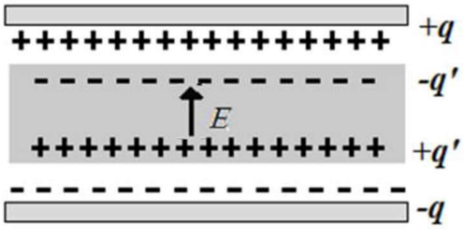
Where α proportionality is constant called as polarisability. The polarisability is defined as polarization per unit applied electric field. If the material contains N number of dipoles per unit volume then

$$P = N\alpha E \qquad \ldots.(7)$$

Relation between polarization and dielectric constant



Parallel plate condensor without dielectrics



Parallel plate condensor with dielectrics

Let us apply Gauss theorem for parallel plate condenser.

$$\int E_0 dA = \frac{q}{\varepsilon_0}$$

$$E_0 A = \frac{q}{\varepsilon_0}$$

$$E_0 = \frac{q}{A\varepsilon_0} = \frac{\sigma}{\varepsilon_0}. \qquad \ldots(1)$$

Where σ is the charge per unit area.

Let a dielectric slab placed between two plates. Due to polarization, charges appear on the two faces of the slab, and establish yet another field within the dielectric media. Let this field be E′. The direction of E′ will be opposite to that of E_0.

The resultant field E in the material can be written as,

$E = E_0 - E'$ ……………….(2)

If σ_p is the charge/unit area on the inserted dielectric slab surfaces, then by following equation (1), we write,

$$E' = \frac{q'}{A\varepsilon_0} = \frac{\sigma_p}{\varepsilon_0}. \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\mathbf{(3)}$$

From (1), (2) and (3),

$$E = \frac{\sigma}{\varepsilon_0} - \frac{\sigma_p}{\varepsilon_0}.$$

or

$$\varepsilon_0 E = \sigma - \sigma_p \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(4)$$

Since the magnitude of polarization P = dipole moment/ Unit Volume

But dipole moment = induced charge X distance

Therefore

P = induced charge/ Area= σ_p

We know that electric displacement fieldor electric flux density D is given by charge /unit area

D = q/A= σ

Therefore Equation 4 becomes

$$\varepsilon_0 E = D - P$$

$$P = D - E\varepsilon_0 \quad \ldots..(5)$$

in free space where there is no dielectric *P*=0

$$D = E\varepsilon_0$$

But in dielectric media the D changes. From electrostatics

$$D = \varepsilon_0 \varepsilon_r E$$

From (3)

$$P = E\varepsilon_o \varepsilon_r - E\varepsilon_0$$

$$\boxed{P = E\varepsilon_0(\varepsilon_r - 1)} \quad \ldots\ldots\ldots\ldots\ldots\ldots(6)$$

$$(\varepsilon_r - 1) = \frac{P}{E\varepsilon_0} = \chi$$

Where χ is electric susceptibility of the dielectric medium. It doesn't have any units.

Since P and E are vectors eqn (6) can be written as

$$\vec{P} = \vec{E}\varepsilon_0(\varepsilon_r - 1) \ldots (7)$$

This equation represents polarization vector.

Types of polarization

Dielectric polarization is the displacement of charge particles with the applied electric field. The displacement of electric charges results in formation of electric dipole moment in atoms, ions or molecules of the material. There are four different types of polarization, they are listed below.

1. Electric polarization,
2. Ionic polarization,
3. Orientation polarization
4. Space charge polarization

Electric polarization

The displacement of the positively charged nucleus and the negatively charged electrons of an atom in opposite directions, on application of an electric field, result in electronic polarization.

On applying a field, the electron cloud around the nucleus shifts towards the positive end of the field. As the nucleus and electron cloud are separated by a distance, dipole moment is created within each atom. The extent of this shift is proportional to the field strength.

Induced dipole moment

$$\mu_e \propto E$$

$$\mu_e = \alpha_e E$$

Where α_e is called electronic polarizability. The dipole moment per unit volume is called electronic polarization.

- It increases with increase of volume of the atom.
- This kind of polarization is mostly exhibited in monoatomic gases.(e.g. He, Ne, Ar, Kr, Xe etc..)

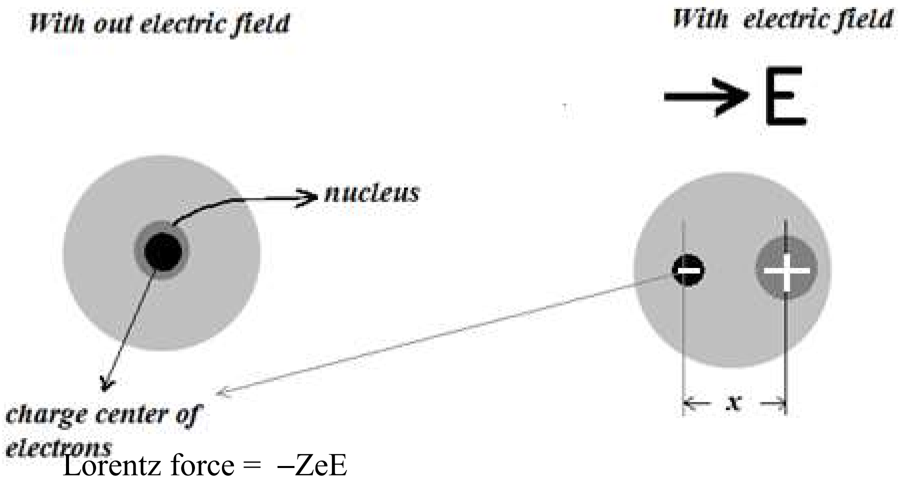
- It is independent of temperature.
- It occurs only at optical frequencies (10^{15}Hz)
- Vast fast process: 10^{-15}~10^{-16}s.

Calculation of electronic polarizability:

Electronic polarization can be explained by classical model of an atom in gasses. In gases the atoms are assumed that the interaction among the atoms is negligible. Here the nucleus of charge Ze is surrounded by an electron cloud of charge –Ze distributed in the sphere of radius R.

$$\text{Charge density,} \quad \rho = -\frac{Ze}{(4/3)\pi R^3} \qquad \ldots(1)$$

When an electric field E is applied, the nucleus and electrons experience Lorentz force of magnitude ZeE in opposite direction. Therefore the nucleus and electrons are pulled apart. As they are pulled apart a Coulomb force develops between them. At equilibrium these two forces are equal and nucleus and electron cloud are separated by a small distance x.



$$\text{Lorentz force} = -ZeE \qquad \ldots(2)$$

$$\text{Coulomb Force} = Ze \text{ X } \frac{\text{Charge enclosed in the sphere of radius } x}{4\pi\varepsilon_0 x^2}$$

$$\text{The charge enclosed} = \frac{4}{3}\pi x^3 \rho$$

$$\text{From equation (1)} \qquad = \frac{4}{3}\pi x^3\left[-\frac{3}{4}\left(\frac{Ze}{\pi R^3}\right)\right]$$

$$= -\frac{Zex^3}{R^3}$$

Hence Coulomb force is = $\frac{Ze}{4\pi\varepsilon_0 x^2}$ X $-\frac{Zex^3}{R^3} = -\frac{Z^2e^2x}{4\pi\varepsilon_0 R^3}$ …(3)

At equilibrium Lorentz force = Coulomb force (equation (2) equal to (3))

$$-ZeE = -\frac{Z^2e^2x}{4\pi\varepsilon_0 R^3}$$

$$x = -\frac{4\pi\varepsilon_0 R^3 E}{Ze} \qquad \ldots(4)$$

The displacement of the electron cloud is proportional to applied electric field.

The electric dipole moment $\mu_e = Zex = \frac{Ze4\pi\varepsilon_0 R^3 E}{Ze}$

$$\mu_e = 4\pi\varepsilon_0 R^3 E$$

$$\mu_e \propto E$$

$$\mu_e = \alpha_e E \qquad \ldots(5)$$

Where $\alpha_e = 4\pi\varepsilon_0 R^3$ is called electronic polarizability.

$P_e = N\mu_e = N\alpha_e E$

Where N is the number of atoms/m^3

But polarization $P = E\varepsilon_0(\varepsilon_r - 1) = N\alpha_e E$

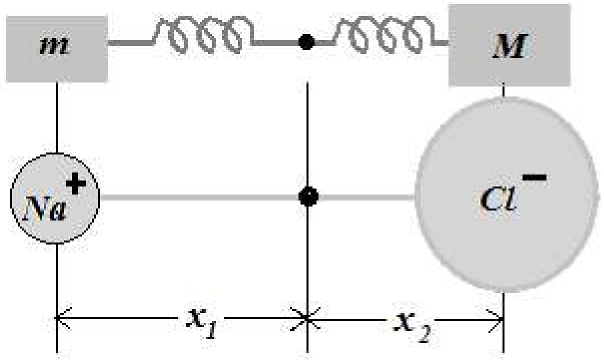
$$(\varepsilon_r - 1) = \frac{N\alpha_e}{\varepsilon_0} \quad \text{or} \quad \alpha_e = \frac{(\varepsilon_r - 1)\varepsilon_0}{N}$$

Ionic Polarization

Ionic polarization occurs in ionic solids such as NaCl, KBr, and LiBr. When an electric field is applied to an ionic solid the positive and negative ions displace to their respective polarities creating an electric dipole this is called as ionic polarization.

In the absence of an electric field there is no displacement of ions. When an electric field is applied an induced dipole moment μ_i is produced.

Let x_1 and x_2 be the displacement of positive and negative ion respectively. Then the induced dipole moment.



$$\mu_i = e(x_1 + x_2) \qquad \ldots(6)$$

Let F be restoring force F

$\propto x_1$

$\propto x_2$

$= \beta_1 x_1$

$= \beta_2 x_2$

From mechanics the spring constant of mass attached to a spring is given by $\beta = m\omega^2$

At equilibrium the Lorentz force = restoring force

$$eE = m\omega_0^2 x$$

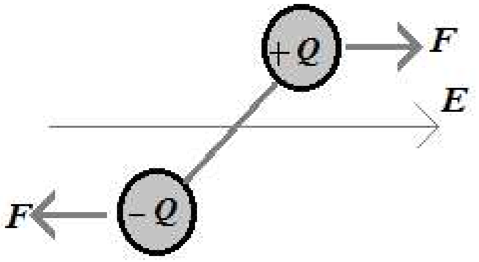
Therefore $x = \dfrac{eE}{m\omega_0^2}$ Then $x_1 = \dfrac{eE}{m\omega_0^2}$ $x_2 = \dfrac{eE}{M\omega_0^2}$

$$\mu = \frac{e^2}{\omega_0^2}\left[\frac{1}{m} + \frac{1}{M}\right]E = \alpha_i E \qquad \ldots(7)$$

Where $\alpha_i = \dfrac{e^2}{\omega_0^2}\left[\dfrac{1}{m} + \dfrac{1}{M}\right]$ is called as ionic polarisability …(8)

Orientation Polarization

Orientation polarization occurs only in polar molecules (the molecules which have permanent dipole moment eg H_2O, Phenol, etc.). When an electric field is applied to a polar molecule, the dipoles experience a torque and try to align parallel to the applied field.



Consider a polar molecule subjected to an electric field *E*. The alignment of electric dipole with the electric field is similar to the alignment of magnetic dipole with the applied magnetic field in paramagnetic material.

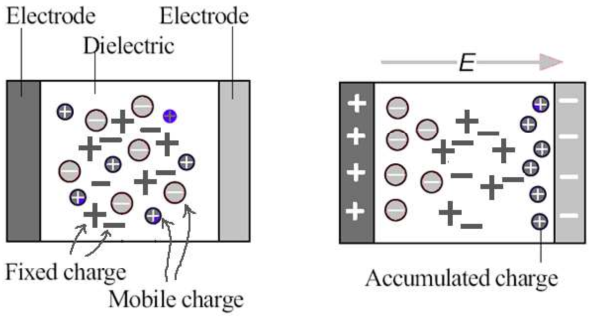
The expression for polarization can be obtained from the theory of paramagnetism.

The orientation polarization is given as

$$P_0 = \frac{N\mu_o^2 E}{3KT} = \alpha_o E \qquad \ldots(9)$$

Where $\alpha_0 = \dfrac{\mu_o^2}{3KT}$ is called as orientation polarisability …(10)

Space charge polarization



Space charge polarization occurs due to the accumulation of charges at the electrodes or at interfaces in a multiphase materials.

In the presence of an applied field, the mobile positive ions and negative ions migrate toward the negative electrode and positive electrode respectively to an appreciable distance giving rise to redistribution of charges , but they remain remains in the dielectric material (electrode is blocking). The space charge polarization can be defined as the redistribution of charges due to the applied electric field and the charges accumulate on the surface of the electrodes. It occurs when the rate of charge accumulation is different from rate of charge removal. Space charge polarization is not significant in most of the dielectric materials.

Internal field in liquids and solids (one dimensional)

In gases state the atoms are separated by large distances and the interaction between the atoms can be neglected. When an external electric field E is applied, the intensity of the electric field experienced by an atom in gases state will be equal to the applied electric field E.

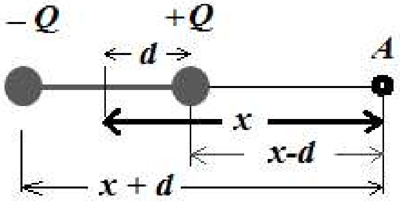
In solids and liquids, the atoms are close to each other leading to strong interaction between them. In solids and liquids the intensity of the electric field at a given point of the material is not equal to the applied electric field but equal to internal field which is the sum of applied electric field and field due to other dipoles present in the material.

$$\text{Internal field} \quad E_i = E + E` \qquad \ldots(1)$$

The internal field can be calculated by Epstein model in the case of one dimensional atomic array.

Electric field along the axis of an electric dipole

Consider an electric dipole of length ***2d*** and charge *Q,* the field along the axis of the dipole at point A is the sum of the electric field due to +Q and –Q.



The electric field due to +Q at point A is $E^+ = \dfrac{Q}{4\pi\varepsilon_o (x-d)^2}$

The electric field due to +Q at point A is $E^- = \dfrac{Q}{4\pi\varepsilon_o (x+d)^2}$

Electric field of dipole at A is $E_A = E^+ - E^- = \dfrac{Q}{4\pi\varepsilon_o}\left[\dfrac{1}{(x-d)^2} - \dfrac{1}{(x+d)^2}\right]$

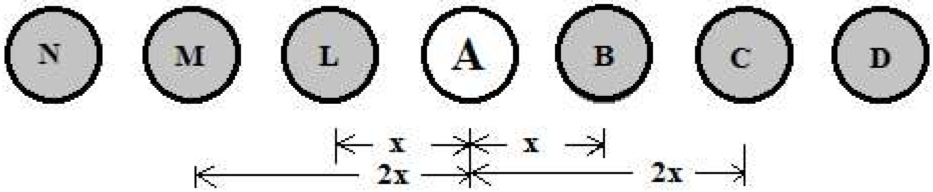
$$= \frac{2Q}{4\pi\varepsilon_o}\left[\frac{2dx}{(x-d)^2(x+d)^2}\right]$$

since $x >> d \quad (x\text{-}d)^2 \approx (x+d)^2 \approx x^2$ then

$$= \frac{2Q}{4\pi\varepsilon_o}\left[\frac{2dx}{x^4}\right] = \frac{4dQ}{4\pi\varepsilon_o x^3}$$

since $2dQ = \mu_i$ $$E_A = \frac{2\mu_i}{4\pi\varepsilon_o x^3} \qquad \ldots(2)$$

Consider an array of one dimensional atoms along x- axis. The all the atoms are similar, equally spaced and have induced electric dipole moment μ_i in an applied electric field *E*. The electric field experienced at the A is the sum of electric fields of other dipoles and applied electric field E.



The electric field at A due to the induced dipole B and L which are at a distance x is

$$E_B = E_L = \frac{2\mu_i}{4\pi\varepsilon_o x^3}$$

The electric field at A due to the induced dipole C and M which are at a distance 2x is

$$E_C = E_M = \frac{2\mu_i}{4\pi\varepsilon_o (2x)^3}$$

Therefore the field due to other dipoles is

$$E' = E_B + E_L + E_C + E_M + E_D + E_N + \ldots \qquad \ldots(3)$$

$$E' = \frac{2\mu_i}{4\pi\varepsilon_o x^3} + \frac{2\mu_i}{4\pi\varepsilon_o x^3} + \frac{2\mu_i}{4\pi\varepsilon_o (2x)^3} + \frac{2\mu_i}{4\pi\varepsilon_o (2x)^3} + \frac{2\mu_i}{4\pi\varepsilon_o (3x)^3} + \frac{2\mu_i}{4\pi\varepsilon_o (3x)^3} + \ldots$$

$$E' = \frac{4\mu_i}{4\pi\varepsilon_o x^3} + \frac{4\mu_i}{4\pi\varepsilon_o (2x)^3} + \frac{4\mu_i}{4\pi\varepsilon_o (3x)^3} + \ldots$$

$$E' = \frac{\mu_i}{\pi\varepsilon_o x^3}\left[1 + \frac{1}{2^3} + \frac{1}{3^3} + \frac{1}{4^3} + \frac{1}{5^3} + \ldots\right] \quad \text{where } 1 + \frac{1}{2^3} + \frac{1}{3^3} + \frac{1}{4^3} + \frac{1}{5^3} + \ldots = 1.2$$

$$E' = \frac{1.2\mu_i}{\pi\varepsilon_o x^3}$$

Therefore the internal field $$E_i = E + \frac{1.2\mu_i}{\pi\varepsilon_o x^3} \qquad \ldots(4)$$

The local field in a three dimensional solid is similar the above equation the number density N of atoms replaces $1/a^3$. Since $N\mu_i=P$ and $1.2/\pi$ is replaced by γ. Then the internal field is

$$E_i = E + \frac{1.2N\mu_i}{\pi\varepsilon_o} = E + \frac{1.2P}{\pi\varepsilon_o} = E + \frac{\gamma P}{\varepsilon_o}$$

γ depends on the internal structure For a cubic symmetry crystal γ value is1/3

$$\boxed{E_i = E + \frac{P}{3\varepsilon_o}} \quad \text{…(5)}$$

The field given by the above equation is called Lorentz field.

Clausius - Mosotti equation

Let us consider elemental solid dielectric which exhibits only electronic polarization. If α_e is the electronic polarisability per atom, it is related to the bulk polarization *P* through the relation

$$P = N\alpha_e E_i \quad \text{…(6)}$$

$$\alpha_e = \frac{P}{NE_i} \quad \text{…(7)}$$

Where *N* is the number of atoms per unit volume and E_i is the local field using the relation (5)

$$\alpha_e = \frac{P}{N\left[E + \frac{P}{3\varepsilon_o}\right]} \quad \text{…(8)}$$

By using the relation between the polarization and permittivity we have

$$P = E\varepsilon_0(\varepsilon_r - 1) \quad \text{…(9)}$$

$$E = \frac{P}{\varepsilon_0(\varepsilon_r - 1)} \quad \text{…(10)}$$

Substitute the value of *E* from (10) in (8)

$$\alpha_e = \frac{P}{N\left[\frac{P}{\varepsilon_0(\varepsilon_r - 1)} + \frac{P}{3\varepsilon_o}\right]}$$

$$\frac{N\alpha_e}{\varepsilon_0} = \frac{1}{\left[\frac{1}{(\varepsilon_r - 1)} + \frac{1}{3}\right]} = \frac{1}{\left[\frac{\varepsilon_r + 2}{3(\varepsilon_r - 1)}\right]}$$

$$\boxed{\frac{\varepsilon_r - 1}{\varepsilon_r + 2} = \frac{N\alpha_e}{3\varepsilon_0}} \quad \ldots(11)$$

The above equation is known as Clausius Mosotti equation which is valid for nonpolar solids

Dielectric loss:

Dielectric loss is the dissipation of energy through the movement of charges in an alternating electromagnetic field as polarisation switches direction.

An efficient dielectric supports a varying charge with minimal dissipation of energy in the form of heat is called dielectric loss. There are two main forms of loss that may dissipate energy within a dielectric. In conduction loss, a flow of charge through the material causes energy dissipation.

Dielectric loss is especially high around the relaxation or resonance frequencies of the polarisation mechanisms as the polarisation lags behind the applied field, causing an interaction between the field and the dielectric's polarisation that results in heating. This is illustrated by the diagram below (recall that the dielectric constant drops as each polarisation mechanism becomes unable to keep up with the switching electric field.)

Dielectric loss quantifies a dielectric material's inherent dissipation of electromagnetic energy into, e.g., heat.

It can be represented in terms loss tangent tan δ and is defined:

$$\tan \delta_\varepsilon = \frac{\epsilon''}{\epsilon'}$$

Dielectric Breakdown : The dielectric breakdown is the sudden change in state of a dielectric material subjected to a very high electric field , under the influence of which , the electrons are lifted into the conduction band causing a surge of current , and the ability of the material to resist the current flow suffers a breakdown .

Or

When a dielectric material loses its resistivity and permits very large current to flow through it, then the phenomenon is called dielectric breakdown

Or

At high electric fields, a material that is normally an electrical insulator may begin to conduct electricity – i.e. it ceases to act as a dielectric. This phenomenon is known as dielectric breakdown.

Frequency dependence of polarizability:

On application of an electric field, polarization process occurs as a function of time. The polarization P(t) as a function of time. The polarization P(t) as a function of time t is given by

$P(t) = P[\,1 - \exp(-t / t_r)]$

Where P – max. Polarization attained on prolonged application of static

field. t_r - relaxation time for particular polarization process

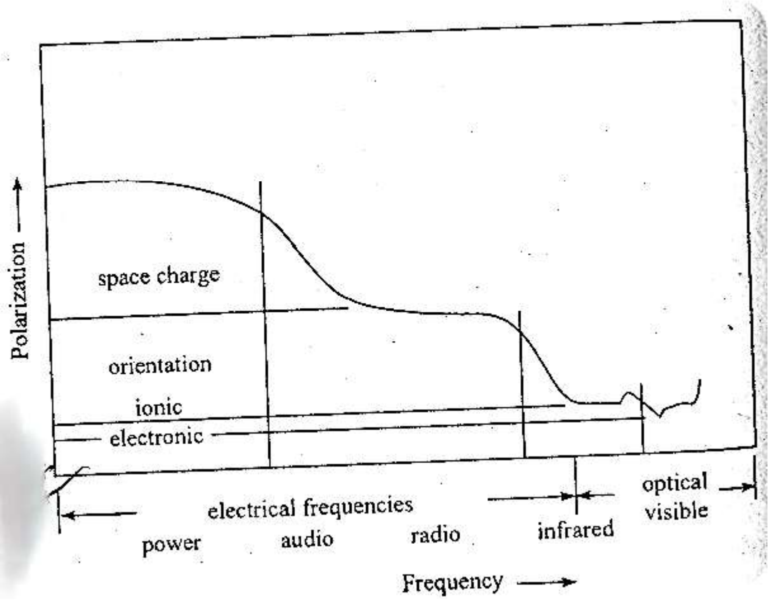
The relaxation time t_r is a measure of the time scale of polarization process. It is the time taken for a polarization process to reach 0.63 of the max. value.

Electronic polarization is extremely rapid. Even when the frequency of the applied voltage is very high in the optical range (≈10^{15} Hz), electronic polarization occurs during every cycle of the applied voltage.

Ionic polarization is due to displacement of ions over a small distance due to the applied field. Since ions are heavier than electron cloud, the time taken for displacement is larger. The frequency with which ions are displaced is of the same order as the lattice vibration frequency (≈1013Hz). Hence, at optical frequencies, there is no ionic polarization. If the frequency of the applied voltage is less than 1013 Hz, the ions respond.

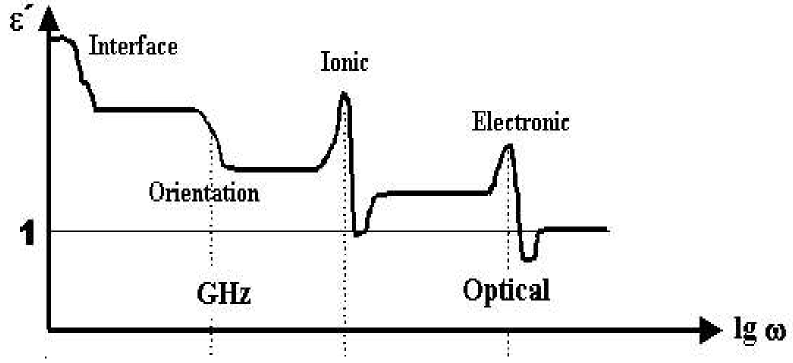
Orientation polarization is even slower than ionic polarization. The relaxation time for orientation polarization in a liquid is less than that in a solid. Orientation polarization occurs, when the frequency of applied voltage is in audio range (1010 Hz).

Space charge polarization is the slowest process, as it involves the diffusion of ions over several interatomic distances. The relaxation time for this process is related to frequency of ions under the influence of applied field. Space charge polarization occurs at power frequencies (50-60 Hz).



Frequency Dependence of dielectric constant

When a dielectric material is subjected to an alternating field, the polarization component required to follow the field in order to contribute to the total polarization of the dielectrics. The relative permittivity which is a measure of the polarization also depends on the frequency. The dependence of ε_r on frequency of the electric field is shown in the figure.



At very low frequency, the dipoles will get sufficient time to orient themselves completely with the field and all types of polarization exist. Since the dielectric is characterized by polarisability α ($\alpha = \alpha_e + \alpha_i + \alpha_o$) at low frequency i.e at radiofrequency region the dielectric constant will be due to all polarisability.

The orientation polarization, which is effective at low frequencies, is damped out for higher frequencies. In the microwave region the dipoles fail to follow the field and the polarisability reduces to ($\alpha = \alpha_e + \alpha_i$), as a result ε_r decreases to some amount.

In the IR region the ionic polarization fails to follow the field so the contribution of ionic polarization dies away. In this region only electronic polarization contributes to the total polarization. Therefore ($\alpha = \alpha_e$) the ε_r still decreases and only electronic polarization exist.

We know that $$P = N\alpha_e E = \varepsilon_o(\varepsilon_r - 1)E$$

Then the relative permittivity is $$\varepsilon_r = 1 + \frac{N\alpha_e}{\varepsilon_o} \qquad \ldots(1)$$

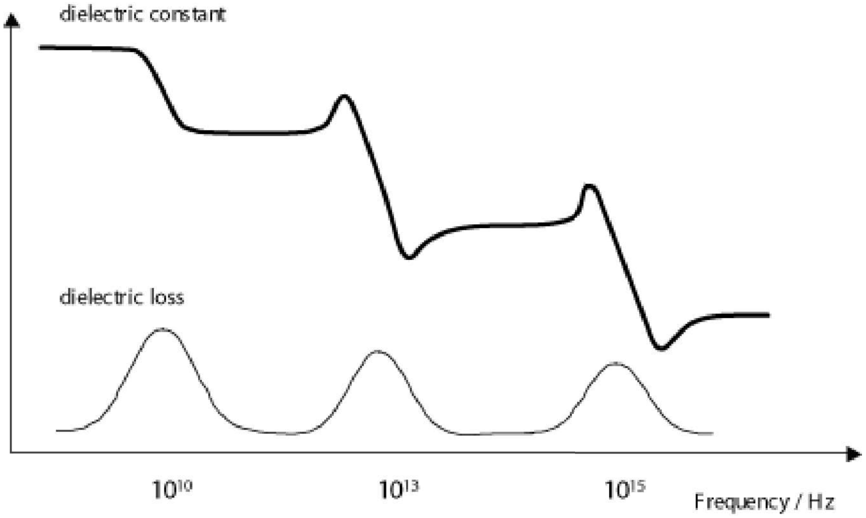
In the ultraviolet region even the electron cloud could not follow the field and electronic polarizability becomes almost zero and the permittivity becomes one.

$$[\varepsilon_r]_{X-ray} = 1$$

For example at low frequency the dielecric constant of water at room temperature is about 80, but it fall to about 1.8 in the optical region.

Frequency Dependence of dielectric loss:

Dielectric loss tends to be higher in materials with higher dielectric constants. This is the downside of using these materials in practical applications. Dielectric loss is utilised to heat food in a microwave oven: the frequency of the microwaves used is close to the relaxation frequency of the orientational polarisation mechanism in water, meaning that any water present absorbs a lot of energy that is then dissipated as heat. The exact frequency used is slightly away from the frequency at which maximum dielectric loss occurs in water to ensure that the microwaves are not all absorbed by the first layer of water they encounter, therefore allowing more even heating of the food.



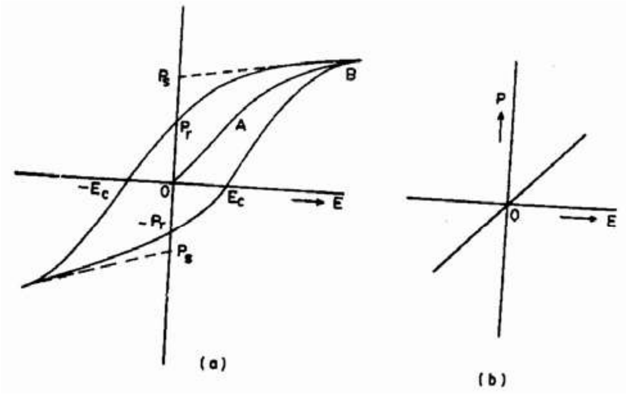
Ferroelectrics

Below certain temperature it is found that some materials spontaneously acquire an electric dipolemoment. These materials are called as ferroelectric materials or ferroelectrics.The temperature at which ferroelectric property of the material disappears is called as ferroelectric Curie temperature.

Ferroelectric materials are anisotropic crystals which exhibit a hysteresis curve P versus E which can be explained by domain hypothesis.

Ferro electricity: Ferro electric materials are an important group not only because of intrinsic Ferro electric property, but because many possess useful piezo electric, birefringent and electro optical properties.

The intrinsic Ferro electric property is the possibility of reversal or change of orientation of the polarization direction by an electric field. This leads to hysteresis in the polarization P, electric field E relation , similar to magnetic hysteresis. Above a critical temperature, the Curie point T_c, the spontaneous polarization is destroyed by thermal disorder. The permittivity shows a characteristic peak at T_c.



Piezo – Electric Materials and Their Applications: Single crystal of quartz is used for filter, resonator and delay line applications. Natural quartz is now being replaced by synthetic material.

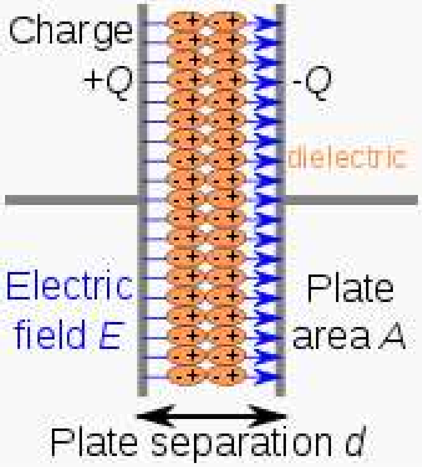
Rochelle salt is used as transducer in gramophone pickups, ear phones, hearing aids, microphones etc. the commercial ceramic materials are based on barium titanate, lead zirconate and lead titanate. They are used for high voltage generation (gas lighters), accelerometers, transducers etc. Piezo electric semiconductors such as GaS, ZnO & CdS are used as amplifiers of ultrasonic waves.

Applications of Dielectric Materials:

Almost any type of electrical equipment employs dielectric materials in some form or another. Wires and cables that carry electrical current, for example, are always coated or wrapped with some type of insulating (dielectric) material. Sophisticated electronic equipment such as rectifiers, semiconductors, transducers, and amplifiers contain or are fabricated from dielectric materials. The insulating material sandwiched between two conducting plates in a capacitor is also made of some dielectric substance.

Liquid dielectrics are also employed as electrical insulators. For example, transformer oil is a natural or synthetic substance (mineral oil, silicone oil, or organic esters, for example) that has the ability to insulate the coils of a transformer both electrically and thermally.

1. Capacitors



Charge separation in a parallel-plate capacitor causes an internal electric field. A dielectric (orange) reduces the field and increases the capacitance.

Commercially manufactured capacitors typically use a solid dielectric material with high permittivity as the intervening medium between the stored positive and negative charges. This material is often referred to in technical contexts as the *capacitor dielectric*.

The most obvious advantage to using such a dielectric material is that it prevents the conducting plates, on which the charges are stored, from coming into direct electrical contact. More significantly, however, a high permittivity allows a greater stored charge at a given voltage. This can be seen by treating the case of a linear dielectric with permittivity ε and thickness d between two conducting plates with uniform charge density σ_ε. In this case the charge density is given by

$$\sigma_\varepsilon = \varepsilon \frac{V}{d}$$

and the capacitance per unit area by

$$c = \frac{\sigma_\varepsilon}{V} = \frac{\varepsilon}{d}$$

From this, it can easily be seen that a larger ε leads to greater charge stored and thus greater capacitance.

Dielectric materials used for capacitors are also chosen such that they are resistant to ionization. This allows the capacitor to operate at higher voltages before the insulating dielectric ionizes and begins to allow undesirable current.

2. Dielectric resonator

A *dielectric resonator oscillator* (DRO) is an electronic component that exhibits resonance of the polarization response for a narrow range of frequencies, generally in the microwave band. It consists of a "puck" of ceramic that has a large dielectric constant and a low dissipation factor. Such resonators are often used to provide a frequency reference in an oscillator circuit. An unshielded dielectric resonator can be used as a Dielectric_Resonator Antenna (DRA).

3. **Insulators-**

   Required Qualities of Good Insulating Materials: The required qualities can be classified as under electrical, mechanical, thermal and chemical applications.

   i) Electrical: 1. electrically the insulating material should have high electrical resistivity and high dielectric strength to withstand high voltage.

   2 .The dielectric losses must be minimum.

   3. Liquid and gaseous insulators are used as coolants. For example transformer oil, hydrogen and helium are

   ii) Mechanical: 1. insulating materials should have certain mechanical properties depending on the use to which they are put.

   2. When used for electric machine insulation, the insulator should have sufficient mechanical strength to withstand vibration.

   iii) Thermal: Good heat conducting property is also desirable in such cases. The insulators should have small thermal expansion and it should be non-ignitable.

   iv) Chemical: 1. chemically, the insulators should be resistant to oils, liquids, gas fumes, acids and alkali's.

   2. The insulators should be water proof since water lowers the insulation resistance and the dielectric strength.

Other Applications:

Solid dielectrics are perhaps the most commonly used dielectrics in electrical engineering, as very good insulators. Some examples include porcelain, glass, and most plastics.
Air, nitrogen and sulfur hexafluoride are the three most commonly used gaseous dielectrics.

Industrial coatings such as parylene provide a dielectric barrier between the substrate and its environment.

Mineral oil is used extensively inside electrical transformers as a fluid dielectric and to assist in cooling. Dielectric fluids with higher dielectric constants, such as electrical grade castor oil, are often used in high voltage capacitors to help prevent corona discharge and increase capacitance.

Because dielectrics resist the flow of electricity, the surface of a dielectric may retain stranded excess electrical charges. This may occur accidentally when the dielectric is rubbed (the triboelectric effect). This can be useful, as in a Van de Graaff generator or electrophorus, or it can be potentially destructive as in the case of electrostatic discharge.

Piezoelectric materials are another class of very useful dielectrics which are used for transducers and sensors.

Ferroelectric materials often have very high dielectric constants, making them quite useful for capacitors.

Magnetic Materials

Classification of dia, para and ferromagnetic materials. Curie Temperature Hysterisis in ferromagnetic materials. Soft and Hard magnetic materials. Applications.

Introduction

The materials that can be magnetised are called as magnetic materials

Magnetic dipoles and magnetic dipole moment

Any two opposite poles separated by distance constitute an magnetic dipole. A magnet is a dipole which has north pole and south pole and the length of the magnet is the distance of separation.

Magnetic dipole moment is the product of magnetic pole strength (m) and length of the magnet(*l*)

$$\mu_m = m.l$$

Magnetic field intensity (H)

The force experienced by a unit north pole (of strength 1 Wb) placed at a point in a magnetic field is a measure of the` field intensity' or `field strength'

Magnetisation or Intensity of magnetisation (M)

Magnetization may be defined as the process of converting a non magnetic bar into a magnetic bar

Magnetic Induction Or Flux Density*(B)*

Magnetic induction or magnetic flux density in an any material is the number of lines of magnetic force passing through unit area perpendicular . Wb/m^2

$$B = \frac{\phi}{A} = \mu_0 (M + H)$$

Magnetic Susceptibility *(χ)*

The ratio of the magnetization to the field strength

$$\chi = \frac{M}{H}$$

Permeability *(μ)*

The ration of the amount of magnetic density B to the applied magnetic field . It is used to measure magnetic lines of forces passing through the material

$$\mu = \frac{B}{H}$$

Origin of Magnetic moment – Bohr Magneton

When ever a charged particle has an angular momentum , it contributes to permanent dipole moment. Consider an hydrogen atom, electron revolving around the nucleus is equal to a current loop. Orbital angular momentum arises due this current loop. The electron spin angular momentum and nuclear spin angular momentum arises due to spin of the electron and nucleus respectively.

There are three angular momentum of an atom

1. Orbital angular momentum of the electron
2. Electron spin angular momentum
3. Nuclear spin angular momentum

Total angular magnetic momentum

Bohr Magneton

The orbital angular momentum of an electron in an atom can be expressed in terms of atomic unit of magnetic moment called Bohr Magneton.

$$\mu_B = \frac{eh}{4\pi m}$$

Classification of the magnetic materials

The magnetic materials are broadly classified in to two types. They are 1. Those atoms or molecules do not have permanent dipole moments and 2. Those atoms or molecules have permanent dipole moments even in the absence of external magnetic field.

Based on the magnetic moments the materials are classified as

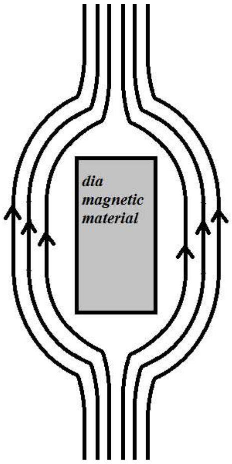
Diamagnetic materials
Paramagnetic materials
Ferromagnetic materials
Anti ferromagnetic materials
Ferri magnetic materials

Diamagnetic materials

Dia magnetic materials has completely filled sub shell electronic structure resultant magnetic moment is zero. There are no permanent dipoles and hence the magnetic effect are small. When a diamagnetic material is placed in a magnetic field, there will be a small induced magnetic moment which always oppose the applied field(accordance with Lenz`s Law). Due to this effect the magnetic lines of forces expelled from the materials.

Mostly the covalent and ionic crystals exhibits the diamagnetic properties. The magnetic susceptibility is small and negative and is independent of temperature.

The examples of diamagnetic materials are 1. Covalent materials such as Si,Ge, diamond, ii) some metals such as copper, silver, gold.

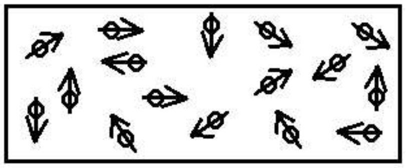


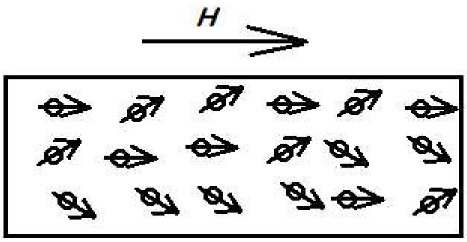
Para magnetic materials.

Atoms or molecules of paramagnetic materials have permanent magnetic moment oriented in random direction. The magnetic interaction between the dipoles try to align themselves but the thermal agitation disturb the alignment**.** In paramagnetic materials vector sum of magnetic moments is zero in the absence of field.

When an external magnetic field is applied the partial alignment of permanent atomic magnetic moments occur

When a magnetic field is applied , the individual magnetic moment takes the alignment along the applied field as shown in figure . The magnetization of a paramagnetic material increases with the increase in the applied field. Increase in temperature it reduces the magnetization and destroys the alignment of dipoles with applied field.





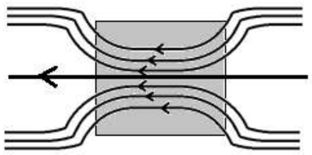
Consider a paramagnetic material placed in non-uniform magnetic field. The paramagnetic materials experience a net magnetic force towards the greater field. The magnetic susceptibility is small and positive and is dependent on temperature**.** The susceptibility of the magnetic field is given by

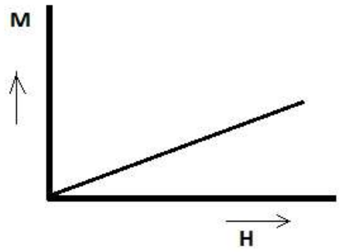
$$\chi = \frac{C}{T}$$

Where C is the curie temperature and T is the temperature in Kelvin scale.

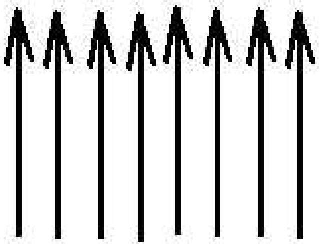
The magnetization in ferromagnetic material is linear and gets saturated when a large magnetic field is applied at low temperature.

The examples of paramagnetic materials are Mg, gaseous and liquid oxygen , ferromagnetic material (Fe), and anti-ferromagnetic materials at high temperature and ferromagnetic material (Fe_3O_4) at high temperature.





Ferromagnetic materials

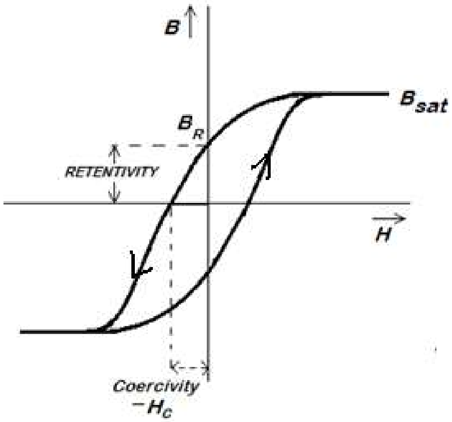


Atoms or molecules of ferromagnetic materials have permanent magnetic moment. In ferromagnetic materials all the dipoles are aligned parallel as shown in the figure if a small value of magnetic field is applied, a large value of magnetization is produced. As the ferromagnetic material have permanent magnetic dipole moment and the susceptibility is positive. The magnetization in ferromagnetic material is non linear and gets saturated when a large magnetic field is applied.

A ferromagnetic materials exhibits two different properties. It behaves as a ferromagnetic material below a certain temperature known as ferromagnetic ***curie temperature***. Above the temperature it behaves as a paramagnetic material. In the ferromagnetic region, it exhibits well known curve known as hysteresis curve as shown in the figure.

The susceptibility of a ferromagnetic material above the ferromagnetic curie temperature is given by $\chi = \dfrac{C}{T-\theta_f}$

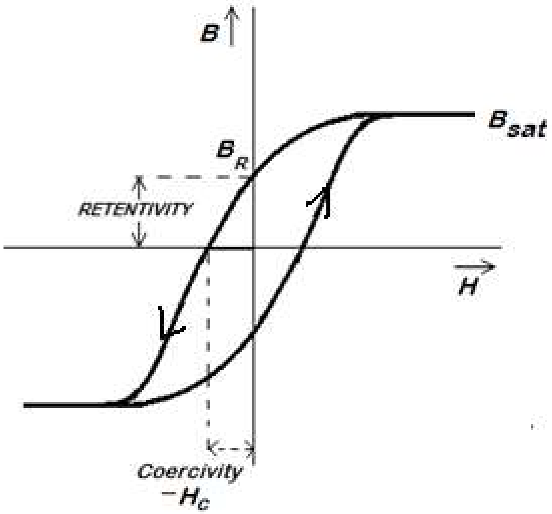
Where C is the Curie constant and θ_f is the ferromagnetic Curie temperature.The transition and rare earth metals such as Fe ,Co, Ni ,Gd are the examples of ferromagnetic materials.



Hysteresis in ferromagnetic materials (B-H curve)

Below the ferromagnetic Curie temperature (T < θ_f) Ferromagnetic material exhibits a well known curve called hysteresis curve. The variation of B(magnetic induction) with H(applied field) can be represented by a closed curve called hysteresis loop or curve. This refers lagging of magnetization behind the magnetising field.

If a magnetic field is increased gradually, the flux density increases and it becomes maximum. The maximum value of flux density is called saturated magnetization.If the field is reversed, the ferromagnetic materials is found to have magnetization in the absence opf external field. This is called as retentivity or remanent magnetization (B_R) and this property is called as spontaneous magnetization. If the field is further reduced the flux density reduces to zero. The field requird in the opposite direction to bring magnetization to zero is called as coercive field or coercivity ($-H_c$). If the field is increased in oposite direction it attains saturation magnetization. If an alternating field is applied a closed loop as shown in the figure is obtained.



According to Weiss, a virgin specimen of ferromagnetic material consist of number of regions or domains($\approx 10^{-6}$ m or above) which are spontaneously magnetized. When magnetic field is not applied the direction of spontaneous magnetization varies from domain to domain. The resultant magnetization may hence be zero or nearly zero.

These domains are separated from other by a wall known as domain wall or Bloch wall The domain concept is used to explain the hysteresis property. When an external field is applied two possible ways of alignment domain growth are possible one by domain wall motion and other by rotation of domain wall and domain growth is also reversible. Hysteresis curve is explained by domain concept.

Antiferromagnetic matériels : These are the ferromagnetic materials in which equal no of opposite spins with same magnitude such that the orientation of neighbouring spins is in antiparallel manner are present.
Susceptibility is small and positive and it is inversely proportional to the temperature.

$$\chi = C/(T+\theta)$$

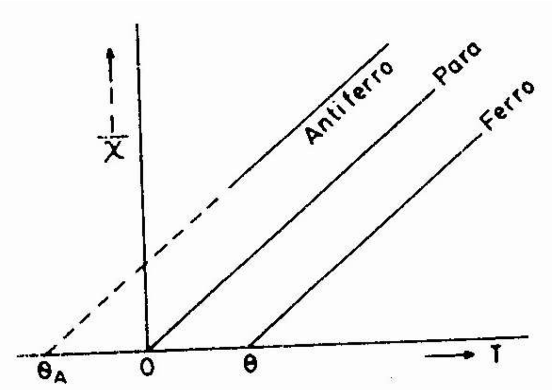
the temperature at which anti ferromagnetic material converts into paramagnetic material is known as Neel's temperature.

Examples: FeO, Cr_2O_3.

Ferrimagnetic materials: These are the ferromagnetic materials in which equal no of opposite spins with different magnitudes such that the orientation of neighbouring spins is in antiparallel manner are present.
Susceptibility positive and large, it is inversely proportional to temperature

$\chi = C/(T \pm \theta)$ $T > T_N$ (Neel's

temperature) Examples : $ZnFe_2O_4$, $CuFe_2O_4$



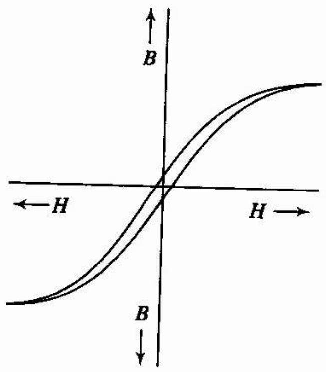
Soft and Hard magnetic materials

Soft magnetic materials

The magnetic materials that are easy to magnetize and demagnetize are called as soft magnetic materials.

Properties:

1. Low remanent magnetization
2. Low coercivity
3. Low hysteresis energy loss
4. Low eddy current loss
5. High permeability
6. High susceptibility



HYSTERESIS CURVE FOR SOFT MAGNETIC MATERIAL

Examples of soft magnetic materials are

i) Permalloys (alloys of Fe and Ni)
ii) Si – Fe alloy
iii) Amorphous ferrous alloys (alloys of Fe, Si, and B)
iv) Pure Iron (BCC structure)

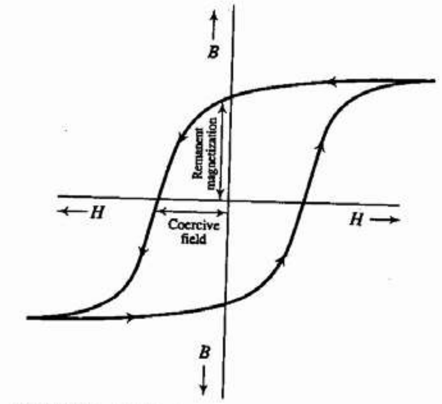
Applications of soft magnetic materials: Mainly used in electro- magnetic machinery and transformer cores. They are also used in switching circuits, microwave isolators and matrix storage of computers.

Hard magnetic materials

The magnetic materials that are difficult to magnetize and demagnetize are called as hard magnetic materials.

Properties:

1. High remanent magnetization
2. High coercivity
3. High saturation flux density
4. Low initial permeability
5. High hysteresis energy loss
6. High permeability



HYSTERESIS CURVE FOR HARD MAGNETIC MATERIAL

7. The eddy current loss is low for ceramic type and large for metallic type.

Examples of hard magnetic materials are, i) Iron- nickel- aluminum alloys with certain amount of cobalt called Alnico alloy. ii) Copper nickel iron alloys. iii) Platinum cobalt alloy.

Applications of hard magnetic materials: For production of permanent magnets, used in magnetic detectors, microphones, flux meters, voltage regulators, damping devices and magnetic separators.

Hard magnetic materials	**Soft magnetic materials**
Difficult to magnetize and demagnetize	Easy to magnetize and demagnetize
large hysteresis loop area	small hysteresis loop area
Have large hysteresis loss	Have very low hysteresis loss
The domain wall movement is difficult and it is irreversible in nature	Domain wall movement is relatively easier. Even for small change in the magnetizing field ,magnetization changes by large amount
The coercivity and retentivity are large	The coercivity and retentivity are small
Magnetostatic energy is large	Magnetostatic energy is small.
Small values of permeability and susceptibility	Large values of permeability and susceptibility
Used to make permanent magnets Examples- *Iron-nickel-aluminium alloys (alnicol)* *Copper nickel iron (cunife)*	Used to make electromagnet Examples- *Fe-Si , Ferrous nickel alloys ,Ferrites,Garnets*

Sample Questions:

Dielectric Materials:

1. Explain the phenomenon of electric polarization in dielectric materials?.
2. Describe in brief
   (a)electronic polarization
   (b) ionic polarization
   (c) Orientation polarization
   (d) Space charge polarisation with diagrams. Also find the total polarizability.
3. Differentiate between polar and nonpolar dielectrics.
4. Drive an expression for internal field in solids and liquids. Or Derive an experession for for internal field by Lorentz method?
5. Derive Clausius-Mossoti equation.
6. What are ferroelectric materials? Describe in detail the Ferroelectric hysteresis.
7. Applications of Dielectric materials.
8. Derive the relation between dielectric polarization and dielectric constant?
9. What is its dielectric constant? Explain its importance in dielectric materials?
10. Which of the following properties are typical for dielectrics?
11. Write a note on
    (a) Ferroelectricity (b) Dielectric constant (c) internal field in solids
12. Discuss the frequency dependence of various polarization processes in dielectric materials.
13. What is dielectric loss? And also explain *Dielectric Breakdown*.
14. Describe the frequency dependence of dielectric constant.
15. Explain the applications of dielectric materials as insulators.

Magnetic Materials:

1. Define magnetization and show that B= $\mu_0(H+M)$
2. Explain the classification of magnetic materials in detail?
3. Give important features of ferromagnetic materials. Explain the hysteresis curve on the basis of domains.
4. What is hysteresis loss? Explain.
5. Distinguish between soft and hard magnets.
6. What is ferromagnetic Curie temperature? Discuss the behaviour of a ferromagnetic material below the Curie temperature.
7. What are ferrites? Explain the magnetic properties of ferrites and mention their industrial applications.
8. Write the importance of hard magnetic materials in engineering applications?
9. What are the applications of soft and hard magnetic materials?

Important formulae:

1. Dipole moment, $\mu = ql$.

2. Flux density, $D = \varepsilon_0 \varepsilon_r E$.

3. $D = \varepsilon_0 E + P$.

4. Dielectric susceptibility, $\chi = (\varepsilon_r - 1)$.

5. Polarization, $P = \varepsilon_0 (\varepsilon_r - 1) E$, $P = N\alpha E$.

6. Induced dipole moment, $\mu = \alpha E$; $\mu_e = \alpha_e E$.

7. Electronic polarizability, $\alpha_e = \dfrac{\varepsilon_0(\varepsilon_r - 1)}{N}$.

8. Orientational polarizability, $\alpha_o = \dfrac{\mu^2}{3kT}$.

9. Internal field, $E = E + \left(\dfrac{\gamma}{\varepsilon_0}\right) P$

10. Lorentz field, $E_{\text{Lorentz}} = E + \dfrac{P}{3\varepsilon_0}$

11. Clausius - Mossotti relation

$$\frac{(\varepsilon_r - 1)}{(\varepsilon_r + 2)} = \frac{N\alpha_e}{3\varepsilon_0}$$

12. The energy loss in a dielectric material is due to the phase lag of voltage behind the current under a.c. conditions. It is also called tangent loss given by, $\tan\delta = \dfrac{\varepsilon_r''}{\varepsilon_r'}$.

13. Curie-Weiss law, $\varepsilon_r = \dfrac{C}{T - \theta}$ for $T > T_c$.

2. $B = \mu_o \mu_r H$, $\mu_o = 4\pi \times 10^{-7}$ H/m.

3. $\chi = \dfrac{M}{H}$.

4. $B = \mu_o (H + M)$.

5. Curie Weiss law, $\chi = \dfrac{C}{T - \theta}$ for $T > \theta$.

Problems

An air-filled parallel plate capacitor has a capacitance of 1.5 pF. If the separation between the plates is doubled and wax is inserted between them, the capacitance increases to 3 pF. Compute the dielectric constant of wax.

Data :

Capacitance when air is dielectric, $C_1 = 1.5 \text{ pF} = 1.5 \times 10^{-12}$ F.

Capacitance when wax is dielectric, $C_2 = 3 \text{ pF} = 3 \times 10^{-12}$ F.

To find :

For wax, $\varepsilon_r = ?$

Solution :

Let the capacitance be C_1 while air is the dielectric,

$$\therefore \quad C_1 = \frac{\varepsilon_0 \varepsilon_r s}{d}.$$

But for air, $\varepsilon_r = 1$.

$$\therefore \quad 1.5 = \frac{\varepsilon_0 \times 1 \times s}{d} \qquad \text{......(1)}$$

When d is doubled and wax is inserted,

let the capacitance be C_2.

$$\therefore \quad C_2 = \frac{\varepsilon_0 \varepsilon_r s}{2d}.$$

$$\text{or,} \quad 3 = \frac{\varepsilon_0 \varepsilon_r s}{2d}. \qquad \text{......(2)}$$

Dividing Eq(2) by Eq(1), we have,

$$\frac{3}{1.5} = \frac{\varepsilon_0 \varepsilon_r s}{2d} \times \frac{d}{\varepsilon_0 s}.$$

$$\therefore \quad \varepsilon_r = 4.$$

∴ **Dielectric constant of wax is 4.**

2. **A parallel plate capacitor has an area of 7.45×10^{-4} m^2 and its plates are separated by a distance of 2.45×10^{-3} m across which a potential of 10 V is applied. If a material with dielectric constant 6 is introduced between the plates, determine the capacitance, the charge stored in each plate, the dielectric displacement *D* and the polarization.**

Data :

Area of the plates, $s = 7.45 \times 10^{-4}$ m^2.

Distance of separation of the plates, $d = 2.45 \times 10^{-3}$ m.

Applied potential, $V = 10$ V.

Dielectric constant of the material, $\varepsilon_r = 6$.

To find :

Capacitance of the capacitor, $C = ?$,

Displacement, $D = ?$

Charge stored, $Q = ?$

Polarization, $P = ?$

Solution :

We have for capacitance of a capacitor,

$$C = \frac{\varepsilon_0 \varepsilon_r s}{d} = \frac{8.85 \times 10^{-12} \times 6 \times 7.45 \times 10^{-4}}{2.45 \times 10^{-3}},$$

$$= 16.147 \times 10^{-12} \text{ F} = 16.147 \text{ pF}.$$

Charge stored on the plates,

$$Q = CV = 16.147 \times 10^{-12} \times 10,$$

$$= 16.147 \times 10^{-11} \text{ C}.$$

Polarization is given by,

$$P = \varepsilon_0 (\varepsilon_r - 1) E.$$

But,

$$E = \frac{V}{d}.$$

$\therefore$

$$P = \varepsilon_0 (\varepsilon_r - 1) \frac{V}{d},$$

$$= \frac{8.85 \times 10^{-12} (6-1) 10}{2.45 \times 10^{-3}}$$

$$= 1.806 \times 10^{-7} \text{ Cm}^{-2}.$$

Displacement D is given by,

$$D = \varepsilon_0 \varepsilon_r E = \varepsilon_0 \varepsilon_r \frac{V}{d} = \frac{8.85 \times 10^{-12} \times 6 \times 10}{2.45 \times 10^{-3}},$$

$$= 2.167 \times 10^{-7} \text{Cm}^{-2}.$$

$\therefore$ **The capacitance, the charge stored, the polarization and the displacement are 16.147 pF, 16.147×10^{-11} C, 1.806×10^{-7} Cm^{-2}, and 2.167×10^{-7} Cm^{-2} respectively.**

3. **The dielectric constant of Sulphur is 3.4. Assuming a cubic lattice for its structure, calculate the electronic polarizability for Sulphur.**
Given: Sulphur density= 2.07 gm/cc, and atomic weight =32.07

Given data:

Dielectric constant, $\varepsilon_r = 3.4$.

Density, $D = 2.07$ gm/cc $= 2.07 \times 10^3$ kg/m^3.

Atomic weight = 32.07.

Crystal structure of sulphur is cubic.

find :

Electronic polarizability for sulphur, $\alpha_e = ?$

Solution :

Since the crystal structure of sulphur is cubic we can apply Clausius - Mossotti eqruation,

$$\frac{(\varepsilon_r - 1)}{(\varepsilon_r + 2)} = \frac{N\alpha_e}{3\varepsilon_0}.$$

$$\therefore \qquad \alpha_e = \frac{3\varepsilon_0}{N}\left[\frac{\varepsilon_r - 1}{\varepsilon_r + 2}\right]. \qquad \text{......(1)}$$

Now, N the number off atoms/unit volume can be written as,

$$N = \frac{N_A \times 10^3 \times D}{\text{atomic weight}}.$$

$$\therefore \qquad N = \frac{6.025 \times 10^{26} \times 2.07 \times 10^3}{32.07}.$$

$$\therefore \qquad N = 3.89 \times 10^{28} / \text{m}^3.$$

By substituting the values for various parameters, Eq(1) becomes,

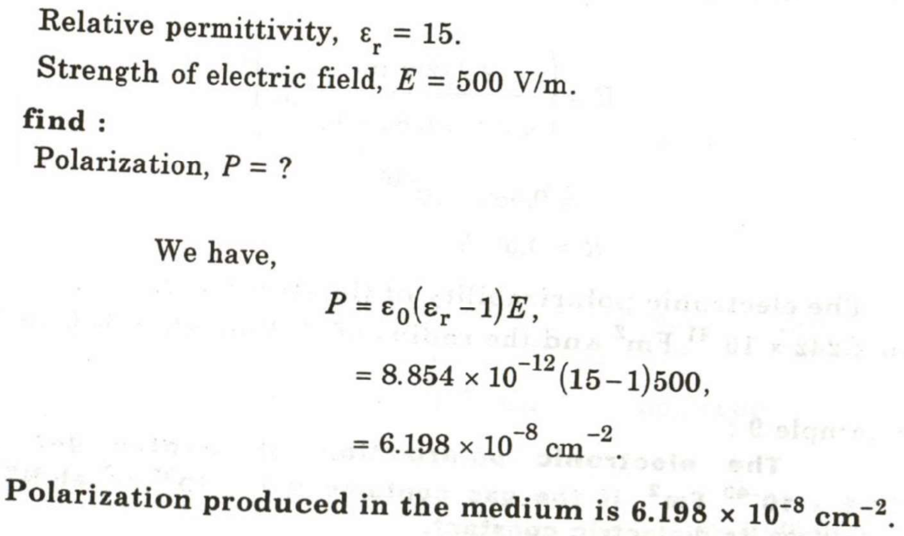
$$\alpha_e = \frac{3 \times 8.854 \times 10^{-12}}{3.89 \times 10^{28}}\left[\frac{3.4 - 1}{3.4 + 2}\right]$$

$$\therefore \qquad \alpha_e = 3.035 \times 10^{-40} \text{ Fm}^2.$$

$\therefore$ **Electronic polarizability of sulphur is 3.035×10^{-40} Fm^2.**

4. **Find the polarization produced in a dielectric medium of relative permittivity 15 in presence of an electric field of 500 V/m.**

Given data:



Relative permittivity, $\varepsilon_r = 15.$

Strength of electric field, $E = 500$ V/m.

find :

Polarization, $P = ?$

We have,

$$
\begin{aligned}
P &= \varepsilon_0(\varepsilon_r - 1)E, \\
&= 8.854 \times 10^{-12}(15-1)500, \\
&= 6.198 \times 10^{-8} \text{ cm}^{-2}.
\end{aligned}
$$

Polarization produced in the medium is 6.198×10^{-8} cm^{-2}.

1. In a magnetic material, the field strength is 10^6 Am^{-1}. The magnetic susceptibility of the material is $0.5\text{X}10^{-5}$. Calculate the intensity of magnetization and the flux density of the material.

$$\chi = \frac{M}{H}$$

$$M = \chi H = 0.5 \times 10^{-5} \times 10^6 = 5$$

$$
\begin{aligned}
B &= \frac{\phi}{A} = \mu_0(M+H) \\
&= 4\pi \times 10^{-7}(5 + 10^6) \\
&= 1.257 Wbm^{-2}
\end{aligned}
$$

2. If a magnetic field of 1800Am^{-1} produces a magnetic field 3×10^{-5} Wb in an iron bar of cross sectional area 0.2cm^2, Calculate permeability.

$$B = \frac{\phi}{A} = 1.5 Wbm^{-2}$$

$$B = \mu_0 \mu_r H$$

$$\mu_r = \frac{B}{H\mu_0} = \frac{1.5}{4\pi \times 10^{-7} \times 1800} = 663.14$$

3. Calculate the saturation magnetization for Ni ferrite. The lattice parameter of a cubic unit cell of Ni ferrite is 0.835nm and the magnetic moment per unit cell is $18.4\mu_B$.

($\mu_{B=}9.27 \times 10^{-24}$)

$$M = \frac{Magneticmoment}{volume} = \frac{18.4 \times 9.27 \times 10^{-24}}{(0.8353 \times 10^{-9})^3} = 2.929 \times 10^5$$

Lecture 1: Electronic materials

Contents

1 Introduction

When we think of electronic materials the physical property that is important is *resistance*. Based on resistance materials can be classified into 3 major types

- Conductors
- Semiconductors
- Insulators

The unit of resistance is Ohm (Ω) and is related to the applied voltage and current by Ohm's law

$$V = IR \tag{1}$$

where V is the applied voltage (units Volts), I is the current (units Amperes) and R is the resistance. Resistance depends on the sample dimensions. Reducing the thickness of a film or decreasing the diameter of a wire would lead to an increase in resistance. We can define a material independent property

Table 1: Resistivity values of some typical metals

Metal	ρ ($\times 10^{-9}$ Ωm)
Copper	15.7
Gold	22.8
Platinum	98
Silver	14.6

Table 2: Resistivity values of some typical semiconductors

Semiconductor	ρ (Ωm)
Germanium	10^{-3} - 10
Silicon	0.1 - 10^{3}
Zinc oxide	10^{-2} - 10^{-4}
Gallium Arsenide	10^{-6} - 10^{-2}

called **resistivity** (ρ) which removes this dependence on sample dimensions. Resistance is related to resistivity by

$$R = \frac{\rho l}{A} \tag{2}$$

where l is the length of the sample and A is the cross sectional area. The unit of resistivity is Ωm. **Conductivity** is defined as the inverse of resistivity. The symbol for conductivity is σ and unit is $\Omega^{-1}m^{-1}$. We can compare typical values for resistivity for conductors, semiconductors, and insulators. When we deal with conductors they will mostly be metals. Some typical values of metal conductivity are shown in table 1.

Metals are characterized by low resistivity. The values quoted in table 1 are in the range of nano Ωm. Compared to metals, semiconductors have higher resistivity values, as seen in table 2. Semiconductor resistivities usually have a range since they depend on the impurity level and also on the crystalline state (single or poly crystalline). Overall, semiconductor resistivities are 5-6 orders of magnitude higher than metals. Insulators have the highest resistivities, these are tabulated in 3.

Thus, we have a range of values for resistivity for different materials and this is related to their electronic properties. To understand this range we need to understand how band gap evolves in materials. We will look at a basic picture of how band gap forms, with a focus mainly on metals and then semiconductors. We will also introduce some concepts on density of states, Fermi energy, and Fermi-Dirac statistics to understand the difference in conductivity.

Table 3: Resistivity values of typical insulators

Insulator	ρ (Ωm)
Wood (damp)	10^3 - 10^4
Deionized water	10^5
Glass	10^{10} - 10^{14}
Fused quartz	10^{17}

2 Molecular orbital formation

Energy levels in an atom are sharp and well defined. To understand what happens when these atoms come together to form solids, we can start with the simplest atom, hydrogen (H). Hydrogen has 1 electron located in the K shell with electronic configuration $1s^1$. When 2 H atoms come together there are 2 $1s$ atomic orbitals (AOs) and these form 2 molecular orbitals (MOs). For simplicity, let us denote the atomic orbital of H atom by ψ_{1s}. In quantum mechanics ψ refers to the wave function of the electron in the $1s$ orbital. The wave function can be solved using Schrödinger's equation in spherical coordinates and the wavefunction solution for the $1s$ orbital is

$$\psi(r) = \frac{1}{\sqrt{\pi}}(\frac{1}{a_0})^{3/2}\exp(-\frac{r}{a_0}) \tag{3}$$

Here, a_0 refers to the Bohr radius and has a value of 0.53 Å. This is an exponential function with the maximum when $r = 0$, corresponding to the nucleus and exponentially decreasing away from the nucleus.
Consider two H atoms A and B, with AOs ψ_{1s}^A and ψ_{1s}^B. There are two ways in which the 2 AOs can come together to form two MOs. The two AOs can be added, this the bonding orbital, σ or they can be subtracted, giving the anti-bonding orbital, σ^*. This can be represented by

$$\begin{aligned} \sigma &= \psi_{1s}^A + \psi_{1s}^B \\ \sigma^* &= \psi_{1s}^A - \psi_{1s}^B \end{aligned} \tag{4}$$

The bonding orbital represents the symmetric MO while the anti-bonding orbital represents the anti-symmetric MO. They are shown pictorially in figure 1. The bonding orbital shows a local minimum in the wavefunction in the region between the 2 H atoms but the function does not go to zero. Thus there is a finite probability of finding the electron between the 2 atoms. The anti-bonding orbital wavefuntion goes to zero between the 2 atoms and hence the probability of finding the electron between the 2 atoms is zero. This is called a **node**. Thus, the bonding orbital has zero nodes and the

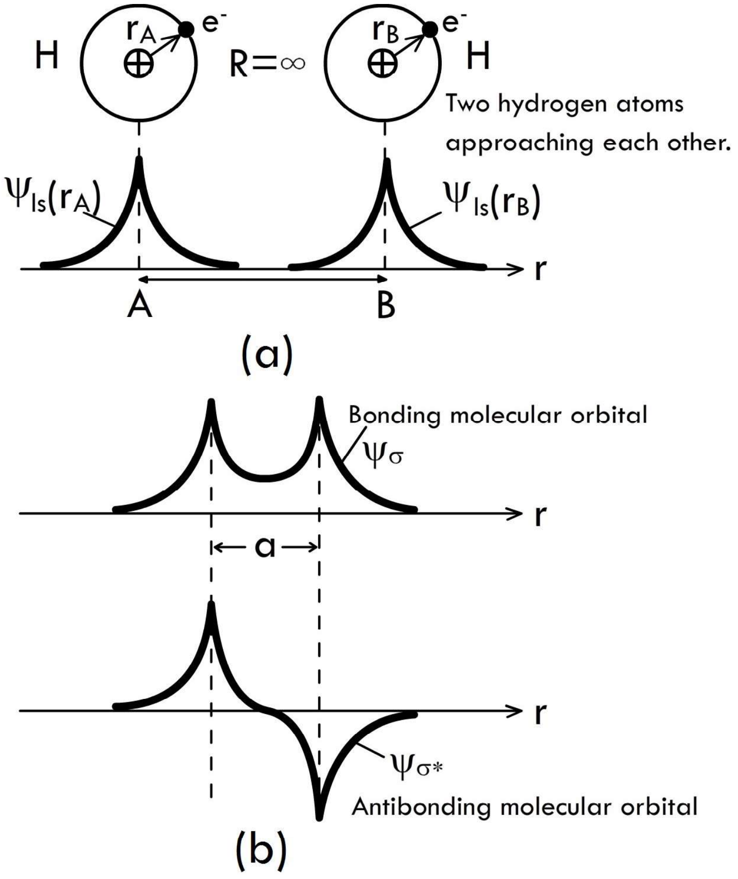


Figure 1: Formation of (a) bonding and (b) anti-bonding orbitals when 2 H atoms come together. Adapted from *Principles of Electronic Materials - S.O. Kasap.*

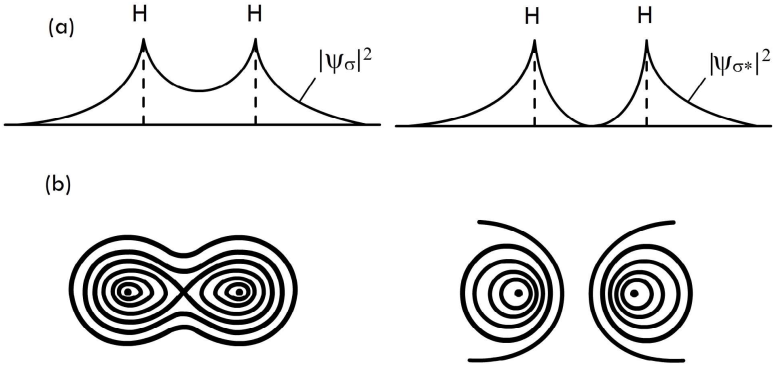


Figure 2: Electron probability distribution in (a) bonding (σ) and (b) anti-bonding (σ^*) orbitals. Lines of constant probability are shown. For the anti-bonding orbital there is zero probability of finding the electron betwen the two atoms i.e. node. Adapted from *Principles of Electronic Materials - S.O. Kasap.*

anti-bonding orbital has 1 node. The electron probability distribution is shown in figure 2.

In terms of energy the bonding orbital has a lower energy than the individual orbitals which have a lower energy than anti-bonding orbital. This is because in σ the electron can be influenced by both the nuclei which leads to a lower energy. If two H atoms come together then both electron will go to the bonding σ orbital (with opposite spin) since this will lower the overall energy of the system. This can be represented by a energy vs. bond length plot. This is shown in figure 3. At large interatomic distances the H atoms have individual atomic energy levels. When they start to come together (R starts to reduce) the 2 atoms start to 'see' the influence of each other. The atomic orbitals start to mix and form the MOs σ and σ^*. There is an equilibrium distance of separation when the energy of the system is at a minimum. Both electron occupy this minimum in the bonding orbital. Figure 3 also shown the schematic representation of the formation of the MOs and the energy minimization using horizontal lines to represent the orbitals. From this diagram it is clear why He_2 will not form. Each He atom has 2 electrons so that there are a total of 4 electrons. Out of these 2 electrons will go to σ and two to σ^* since each MO can only take a maximum of 2 electrons (opposite spin). The overall energy of the He_2 molecule will then be higher than the energy of 2 individual He atoms and hence He_2 will

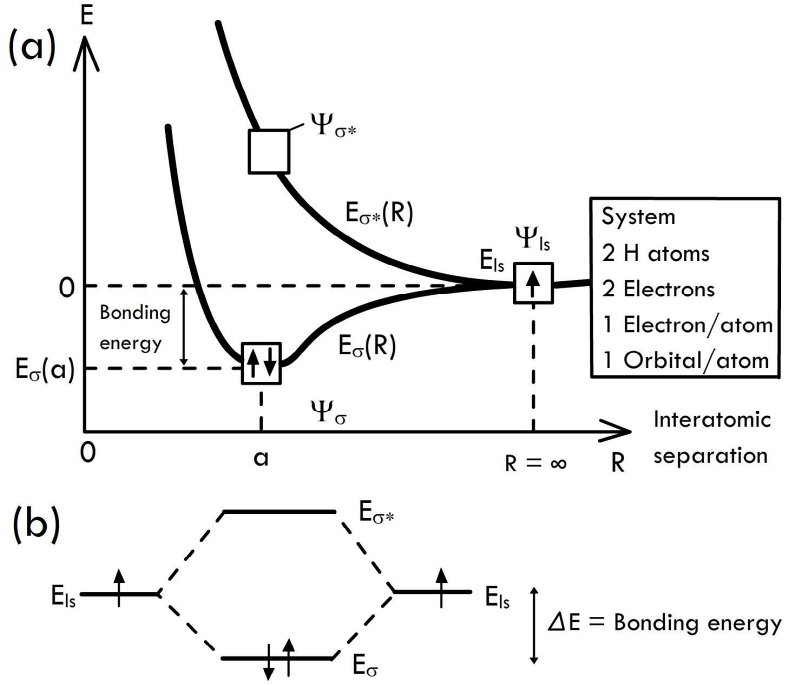


Figure 3: (a) Energy vs. bond length plot for 2 H atoms. (b) The schematic representation of the formation of the H_2 molecule. Both electrons go to the bonding orbital while the anti-bonding orbital is empty. Adapted from *Principles of Electronic Materials - S.O. Kasap.*

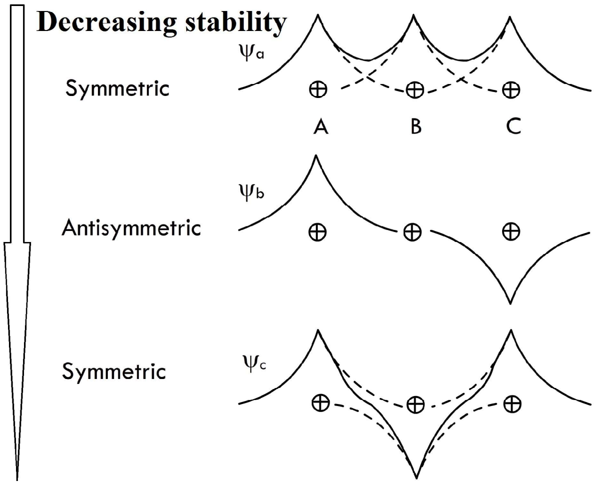


Figure 4: MOs formed when 3 H atoms come together. The number of nodes increases while the stability decreases. The configuration with the lowest number of nodes is most stable. Adapted from *Principles of Electronic Materials - S.O. Kasap.*

not form.

3 Molecular orbitals in extended systems

Consider the case when we have 3 H atoms. Each atom has a ψ_{1s} atomic orbital and these 3 AOs will come together to form 3 MOs. Let the 3 H atoms be A, B, and C with atomic orbitals ψ_{1s}^A, ψ_{1s}^B, and ψ_{1s}^C. The 3 AOs can be put together to form 3 MOs while maintaining symmetry of the resultant wave function in the following way.

$$\begin{aligned} \sigma_a &= \psi_{1s}^A + \psi_{1s}^B + \psi_{1s}^C \\ \sigma_b &= \psi_{1s}^A - \psi_{1s}^C \\ \sigma_c &= \psi_{1s}^A - \psi_{1s}^B + \psi_{1s}^C \end{aligned} \tag{5}$$

σ_a, σ_b, and σ_c are the 3 MOs that are formed. This formation is shown in figure 4. σ_a is the symmetric solution with no nodes. σ_b is the antisymmetric solution with a node in the location of the middle atom (this is the reason for no contribution from B in equation 5). σ_c is again a symmetric solution but with 2 nodes, between the 2 sets of atoms. In terms of energy σ_a is the lowest followed by σ_b and then σ_c. The energy vs. bond length diagram for

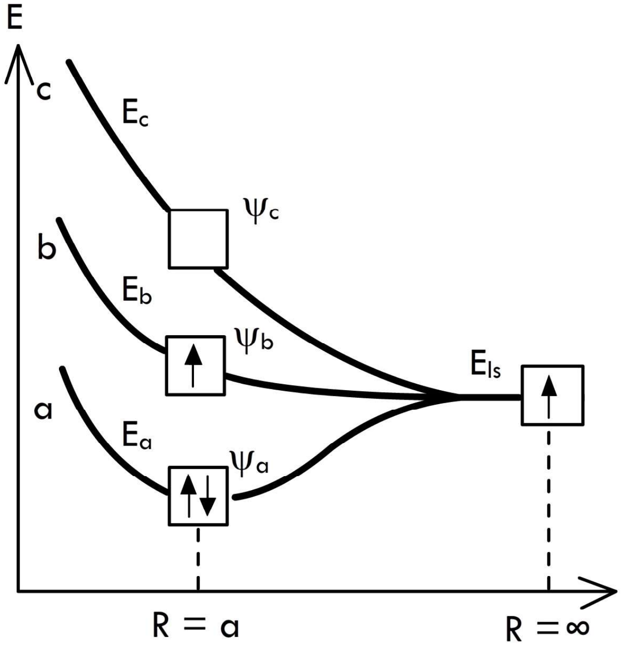


Figure 5: Energy vs. bond length diagram for 3H atoms forming 3 MOs. The 3 electrons occupy the configuration with 0 noes (2 electrons) and 1 node (1 electron). Adapted from *Principles of Electronic Materials - S.O. Kasap.*

3 H atoms is shown in figure 5. Out of the 3 electrons that are available 2 go to the lowest energy MO i.e. σ_a with 0 nodes and the remaining one goes to σ_b with 1 node. More the number of nodes greater is the energy of the MO. Instead of 3 H atoms, if we have 4 atoms then there are 4 AOs which form 4 MOs with 0, 1, 2, and 3 nodes (arranged in order of increasing energy). Each of these MOs can take 2 electrons (opposite spin) so that there are a total of 8 **energy states** (including spin). The argument can be generalized saying that if there are **N** atoms, there are **N** atomic orbitals, and hence **N** molecular orbitals, and **2N** energy states. As long as the energy of the configuration is lower than the individual atoms the solid will be stable.

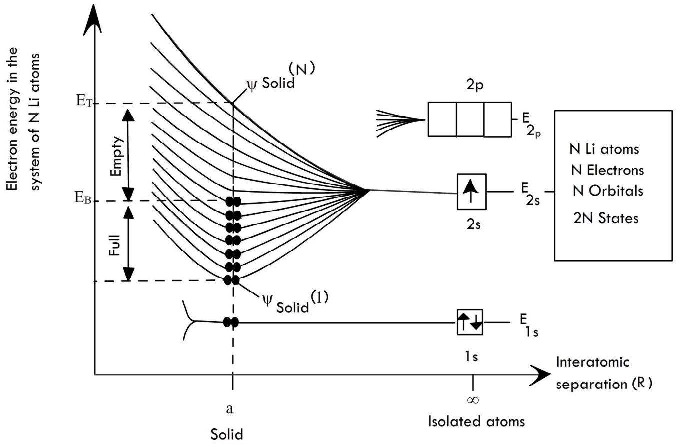


Figure 6: Energy vs. bond length diagram for N Li atoms. There are a total of 2N energy states (including spin) out of which N are occupied, half full. This makes Li a metal. Adapted from *Principles of Electronic Materials - S.O. Kasap.*

4 Energy bands in metals

We can try to extend this model beyond H. Consider the case of Li, which has 3 electrons. The electronic configuration is $1s^2 2s^1$. The $1s$ electrons form the inner shell and are usually not involved in bonding. Hence, for bonding we have the $2s$ shell with 1 electron and this can be considered similar to the H atom. So, if we have **N** Li atoms, there will be **N** MOs, and **2N** energy states (including spin). This is shown schematically in figure 6.

The spacing between the individual MOs depends on the equilibrium interatomic spacing and the value of N. Larger the value of N, closer the individual levels. For really large N (e.g. if we have 7 g of Li then N will be 6.023×10^{23} or Avogadro's number) the individual MOs are so close that we can consider them to be continuous. Thus an **energy band** will be obtained. This band is called the **valence band** since it is obtained from the outermost shell. The band formation for Li is shown in figure 7. In the case of Li the band formed from the outer $2s$ levels is half full since there are a total of $2N$ energy states and only N electrons.

The *separation between the filled states and the empty states* is called the **Fermi energy** and is denoted by E_F. Another way of defining the Fermi energy is that *this is the highest filled state in a metal at 0 K.* The energy required to remove an electron from the Fermi level to vacuum level (where

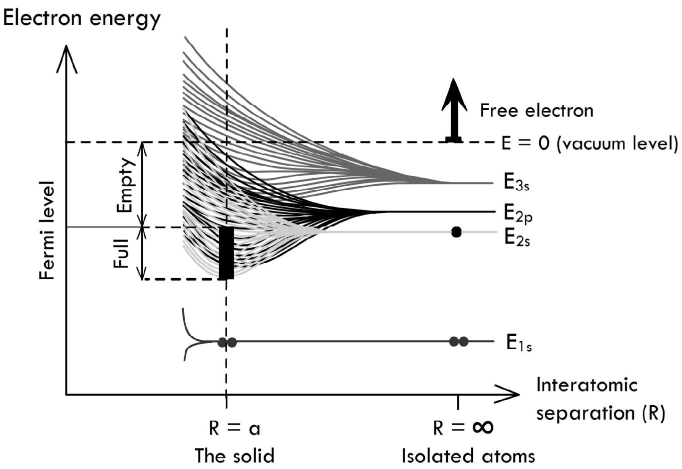


Figure 7: Energy vs. bond length diagram for large values of N showing a continuous band formation. The overlap between the $2s$, $2p$, and $3s$ levels are also shown. Adapted from *Principles of Electronic Materials - S.O. Kasap.*

the electron is free of the influence of the metal) is called the **work function**. The Fermi level and work function for Li are shown in figure 8. Energy levels can be referenced either with respect to the vacuum level (takes as zero) or with respect to the bottom of the valence band. Thus, metals like Li have a partially filled valence band.

We can extend this model to Be, which has 2 electrons in the outer $2s$ shell. According to the model we developed for Li where we have a band with $2N$ energy states and N electrons we have now have $2N$ states and $2N$ electrons so that the band should be completely full. So how is Be a metal? The reason is because Be has empty $2p$ shells which are close in energy to the $2s$ shell and they overlap. Because of this overlap there are empty states available for conduction. There are overlap states in Li as well, but we do not need these to explain conduction since the starting band is half full anyway. We can call the band formed by the empty $2p$ shell as the **conduction band**. In metals, the valence and conduction band overlap to give a continuous band of filled and empty states. This is shown schematically in figure 9. In the presence of an electric field electrons can move by occupying these empty energy states and this makes metals good conductors of electricity.

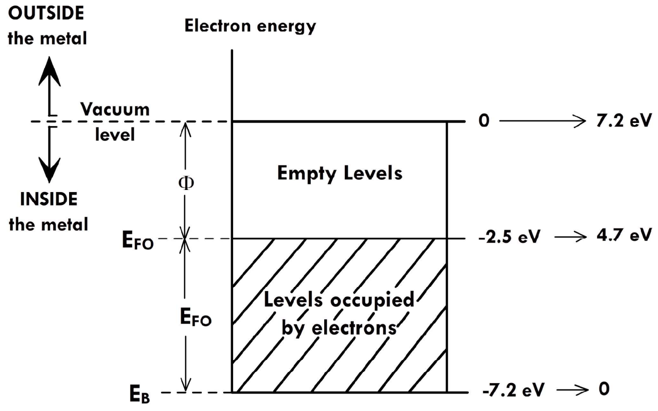


Figure 8: Fermi energy and work function in Li. By convention the vacuum level is taken as zero and energy levels within the metal are shown as negative. If the lowest energy level in the valence band is used as reference all these energy levels become positive. Adapted from *Principles of Electronic Materials - S.O. Kasap.*

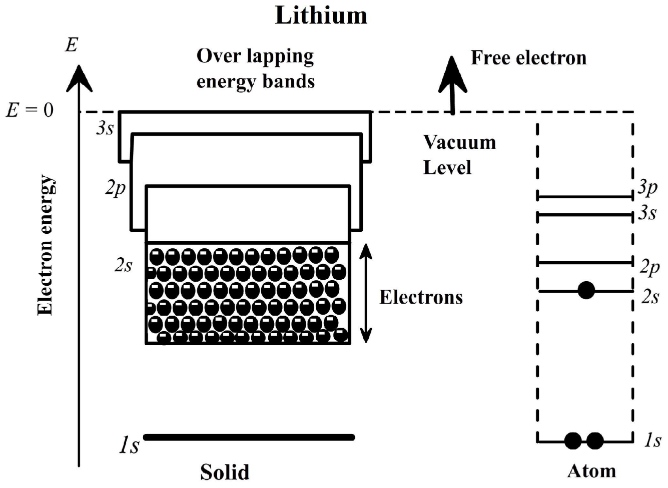


Figure 9: Energy band in a metal formed through overlap of individual bands. This diagram is similar to figure 7, at the equilibrium distance. Adapted from *Principles of Electronic Materials - S.O. Kasap.*

Condensed Matter Physics

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Department of Physics
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Lecture - 18
Optical Properties of Metals; Ionic Polarization in Alkali Halides; Piezoelectricity

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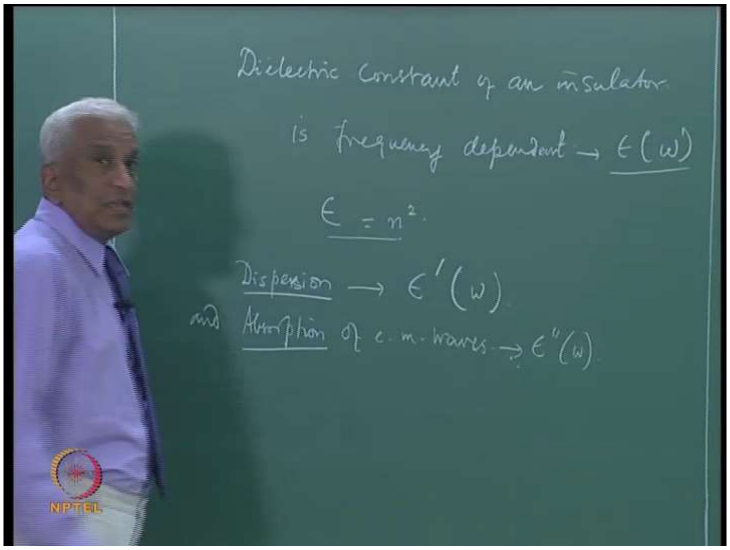

Dielectric constant of an insulator
is frequency dependent → $\underline{\epsilon(\omega)}$
$\underline{\epsilon} = n^2$.
$\underline{\text{Dispersion}} \rightarrow \epsilon'(\omega)$.
and $\underline{\text{Absorption}}$ of e.m. waves → $\epsilon''(\omega)$

We have discussed the mechanism by which the dielectric constant of an insulator becomes frequency dependent. So, we represent this by the function - the dielectric function epsilon omega. We also noted that this epsilon since this is equal to this square as a refractive index, so this frequency dependence also leads to a frequency dependence of the refractive index. In particular, this leads to the phenomenon of dispersion and absorption of electromagnetic waves when propagating through a medium, which is characterized by this dielectric function epsilon omega. So, this is related to the real part of the dielectric constant, while absorption is related to the imaginary part which in turn leads to an absorption. So, we discuss the theory of this in a dielectric media.

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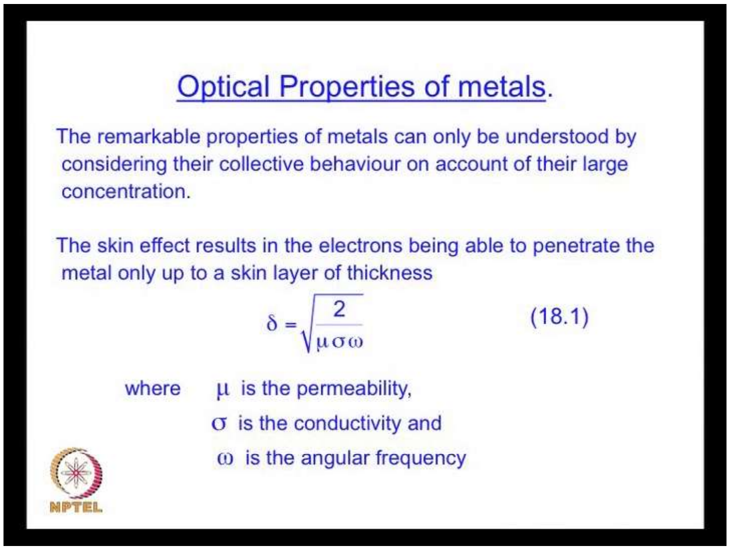

Optical Properties of metals.

The remarkable properties of metals can only be understood by considering their collective behaviour on account of their large concentration.

The skin effect results in the electrons being able to penetrate the metal only up to a skin layer of thickness

$$\delta = \sqrt{\frac{2}{\mu\sigma\omega}} \qquad (18.1)$$

where μ is the permeability,
σ is the conductivity and
ω is the angular frequency

Just by way of digression, we will just read up back to the case of a metal which we have been discussing in some detail earlier and the incidentally want to see how this behavior this dispersive and absorptive nature is reflected in the properties of metals, metals as you know are highly conducting media. So, the question is, whether there will be any change, any difference in the optical behavior of metals in the response to light, because these are all know it is a matter of common experience that metals are highly reflective in contrast to insulate existences which are not so. We would like to see whether this treatment of dispersion and absorption can lead to a detailed understanding of the optical behavior of metals. Now one thing we know is that the metals have a very large concentration of conduction electrons.

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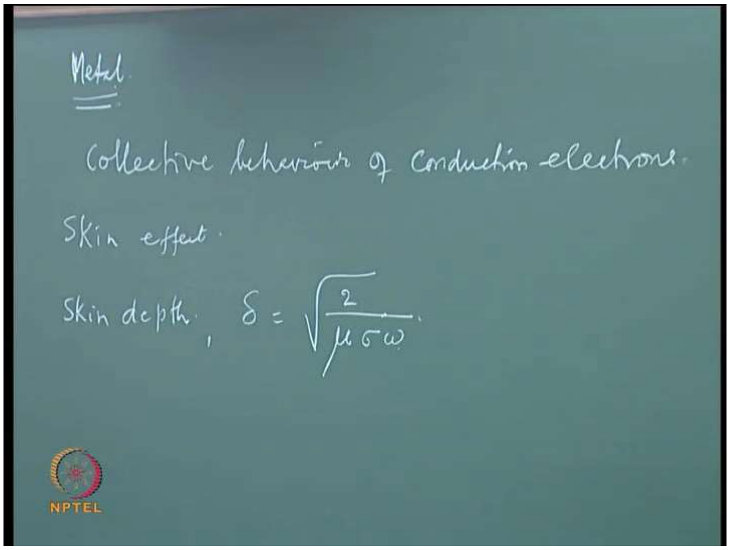

Metal

Collective behaviour of conduction electrons.

Skin effect.

Skin depth, $\delta = \sqrt{\dfrac{2}{\mu \sigma \omega}}$.

And therefore, the main properties of metals are usually understood in terms of the collective behavior of conduction electrons. In particular, one remembers there is a phenomenon called skin effect, which is characteristic of metals and this result in the electrons being able to penetrate the metal only up to a short distance named our skin layer or skin depth. And this depth is usually given by the root of 2 by mu sigma omega; mu is the permeability, sigma is the conductivity and omega is the angular frequency.

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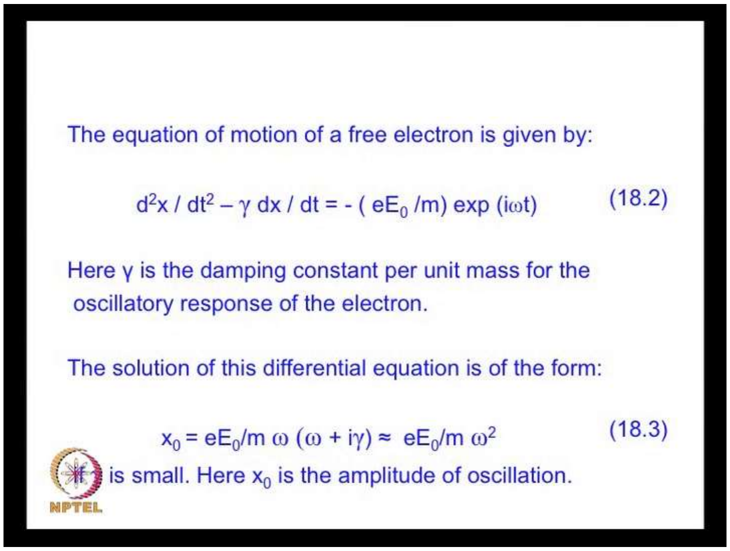

The equation of motion of a free electron is given by:

$$d^2x / dt^2 - \gamma\, dx / dt = -(eE_0 /m) \exp (i\omega t) \qquad (18.2)$$

Here γ is the damping constant per unit mass for the oscillatory response of the electron.

The solution of this differential equation is of the form:

$$x_0 = eE_0/m\, \omega\, (\omega + i\gamma) \approx eE_0/m\, \omega^2 \qquad (18.3)$$

is small. Here x_0 is the amplitude of oscillation.

So, this is one thing you will keep in mind before discussing this, and going back to our discussion of the response of a free electron unlike the response of a bound electron in an insulator.

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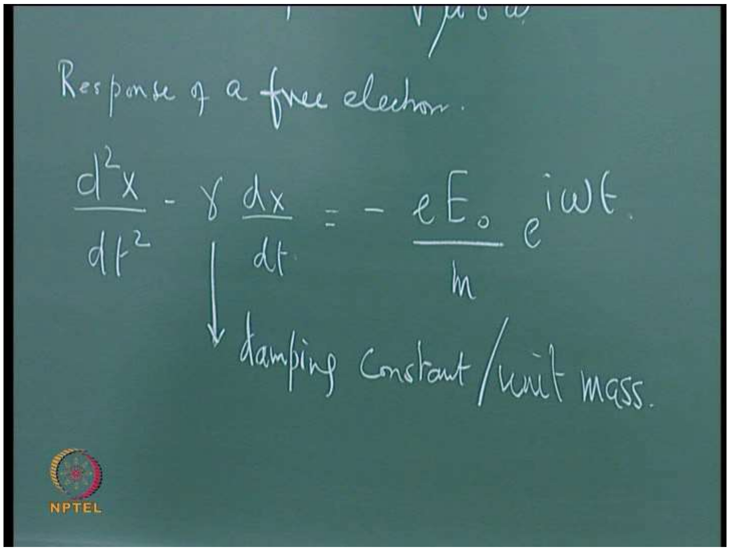

Response of a free electron.

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

$\gamma \downarrow$ damping constant/unit mass.

The response of a free electron, in what way is it different from that of the bound electron insulator. We will see by writing the equation of motion as before as d square x by dt square minus gamma dx by dt, this is the dissipative or resistive term. So, there was in addition in the case of a bound electron, there was a natural frequency of oscillation which is in the form a restoring force here in the equation of motion. Now in the case of a frequency electron, there is no restoring force, there is no natural frequency, it free to move under the influence of an applied electric field. So, this term we seen in the equation of motion and we have. So, this is the equation of motion in case of a free electron in a metal this gamma is the damping constant per unit mass and be seek a solution to this differential equation in the usual way by saying that.

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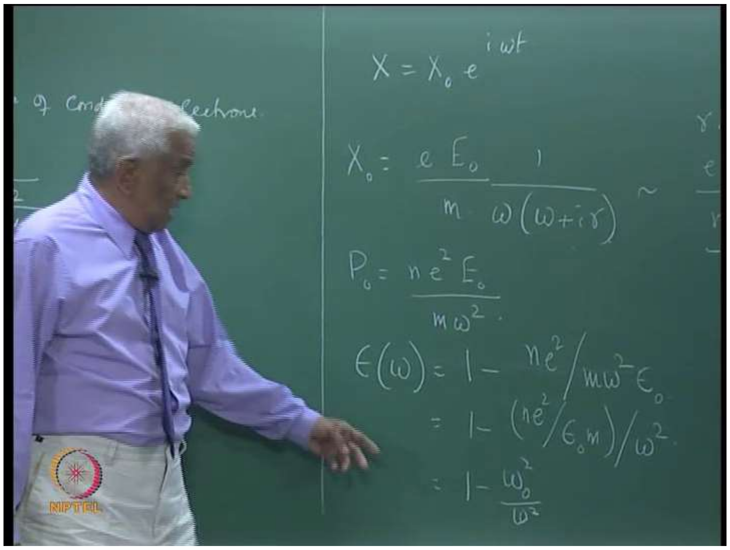

The response is also of the firm of x naught e to the power I omega p the probably a phase shift and as plugging this back we get x naught equal to and this for a small then gamma is very small compared to one we can just write this as e naught by m omega square.

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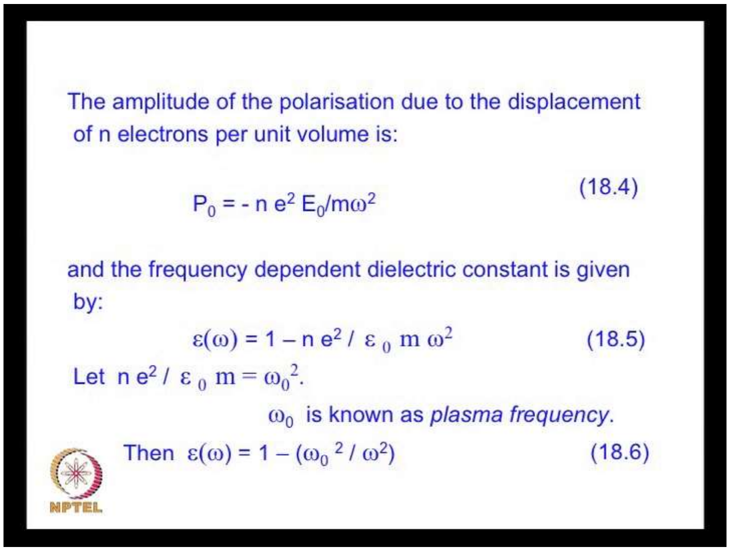

The amplitude of the polarisation due to the displacement of n electrons per unit volume is:

$$P_0 = - n e^2 E_0/m\omega^2 \qquad (18.4)$$

and the frequency dependent dielectric constant is given by:

$$\varepsilon(\omega) = 1 - n e^2 / \varepsilon_0 m \omega^2 \qquad (18.5)$$

Let $n e^2 / \varepsilon_0 m = \omega_0^2$.

ω_0 is known as *plasma frequency*.

Then $\varepsilon(\omega) = 1 - (\omega_0^2 / \omega^2)$ (18.6)

This will lead to a polarization usual way once we have the displacement we can write the polarization and that take this farm and… So, this leads to the frequency dependent dielectric constant if the case of a metal following the same procedure we get now this dump n e square by m x let me rewrite this. So, that this can be written let n e square by m epsilon naught d call this is a term which has the concentration of the electrons the electronic charge mass and the permutative of this space. So, this is the constant which is characteristic in the metal.

Now, that is take as omega naught is known as last month frequency once you have that substitution is simply arrive at a simple relation like this and. So, what is this say. So, it the dielectric function of as metal as simply form one minus omega naught square by omega square. So, this can be again related to the real and to the imaginary part of the dielectric constant this has the form which is shown in the figure. At very low frequencies, the epsilon one is a there negative and then it rises to 0 then omega approaches the frequency and then you goes up to the value one at high frequencies. So, that the behavior which is shown in the figure.

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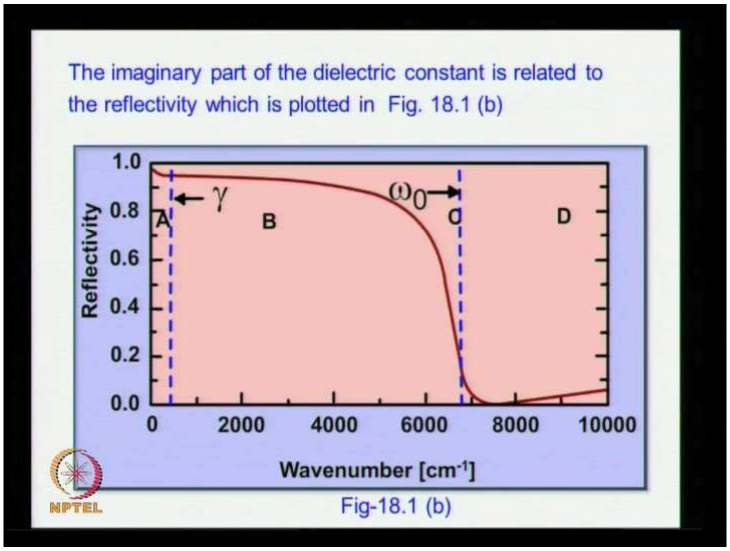

The imaginary part of the dielectric constant is related to the reflectivity which is plotted in Fig. 18.1 (b)

Fig-18.1 (b)

Next figures show the imaginary part of the dielectric constant which is related to the reflectivity. So, in this figure the reflectivity is blocked as a function of a frequency. So, this shows that the reflectivity is one at low frequencies which means that at low frequency the metal reflects all the incidental electromagnetic radiation except when the frequency approaches the plasma frequency.

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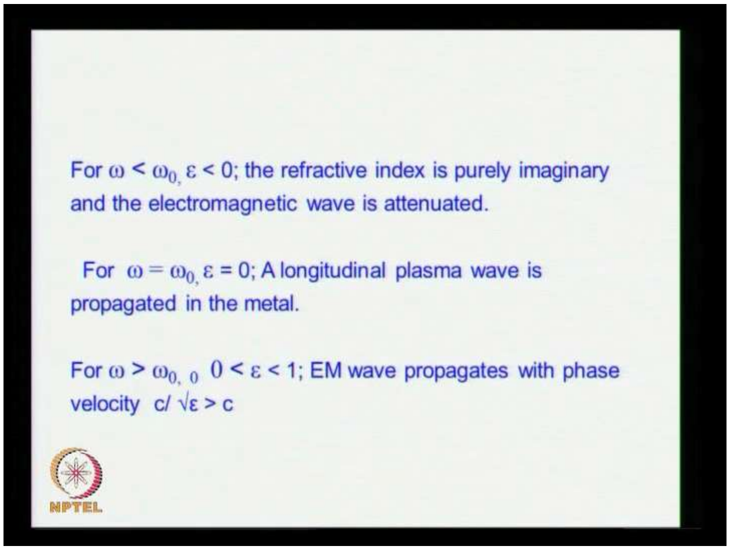

For $\omega < \omega_{0,}$ $\varepsilon < 0$; the refractive index is purely imaginary and the electromagnetic wave is attenuated.

For $\omega = \omega_{0,}$ $\varepsilon = 0$; A longitudinal plasma wave is propagated in the metal.

For $\omega > \omega_{0,\ 0}$ $0 < \varepsilon < 1$; EM wave propagates with phase velocity $c/\sqrt{\varepsilon} > c$

Then this behavior is did explain for omega very small compared to omega naught there is a negative dielectric constant and a correspondingly the refractive index which is the square of the dielectric constant is purely imaginary and I imaginary effective index means that the electromagnetic wave is attenuated. So, it does not propagate inside the medium inside the metal and it is perfectly reflected which is the reason why a metallic surface highly reflective shines. When the frequency approaches the plasma frequency, the dielectric constant approaches zero and you have a longitudinal plasma wave which is propagated in the metal. And for higher frequencies, higher than the plasma frequency, the dielectric function change the varies from 0 to 1. And this is the usual behavior in which they are electromagnetic real propagates to the phase velocity which is given c by root epsilon.

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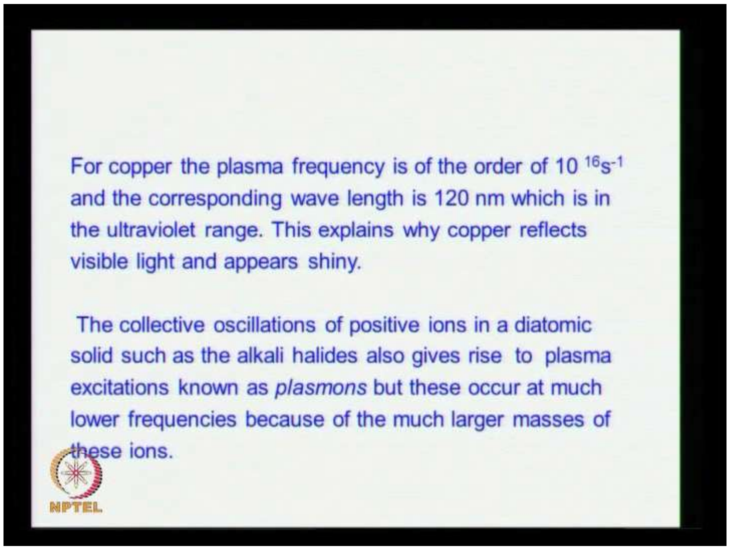

For copper the plasma frequency is of the order of $10^{16} s^{-1}$ and the corresponding wave length is 120 nm which is in the ultraviolet range. This explains why copper reflects visible light and appears shiny.

The collective oscillations of positive ions in a diatomic solid such as the alkali halides also gives rise to plasma excitations known as *plasmons* but these occur at much lower frequencies because of the much larger masses of these ions.

So that is the overall behavior and in the case copper corresponding wave length is about 120 nanometers. This is in the ultra violet rate that is way copper reflects visible light and appears shine. The collective oscillations also take place in the case of the past two iomans a diatomic solid that at the which also give rise to plasma executions which are known plasmas, but these plasmas occur at much lower frequency because the ion masses much larger it is shifted with the infrared range.

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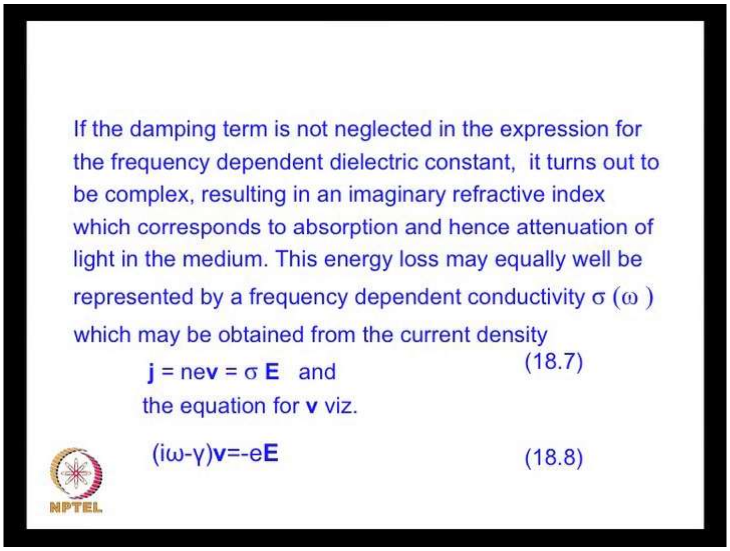

If the damping term is not neglected in the expression for the frequency dependent dielectric constant, it turns out to be complex, resulting in an imaginary refractive index which corresponds to absorption and hence attenuation of light in the medium. This energy loss may equally well be represented by a frequency dependent conductivity $\sigma(\omega)$ which may be obtained from the current density

$$\mathbf{j} = ne\mathbf{v} = \sigma \mathbf{E} \quad \text{and} \qquad (18.7)$$

the equation for $\mathbf{v}$ viz.

$$(i\omega - \gamma)\mathbf{v} = -e\mathbf{E} \qquad (18.8)$$

Now, we have in this treatment taken gamma as very small compared to one and neglected the damping term. Now if the damping term is not neglected in the frequency dependent direct constant then epsilon omega turns out to the complex, and this results again in an imaginary ineffective index this corresponds to absorption and hence attenuation like the media, because this light is attenuated. There is an energy loss and this energy loss may equally well be described in terms of a frequency dependent conductivity. So, this is known as the a c is the electrical connectivity then the when the incident radiation incident wave has a time dependence.

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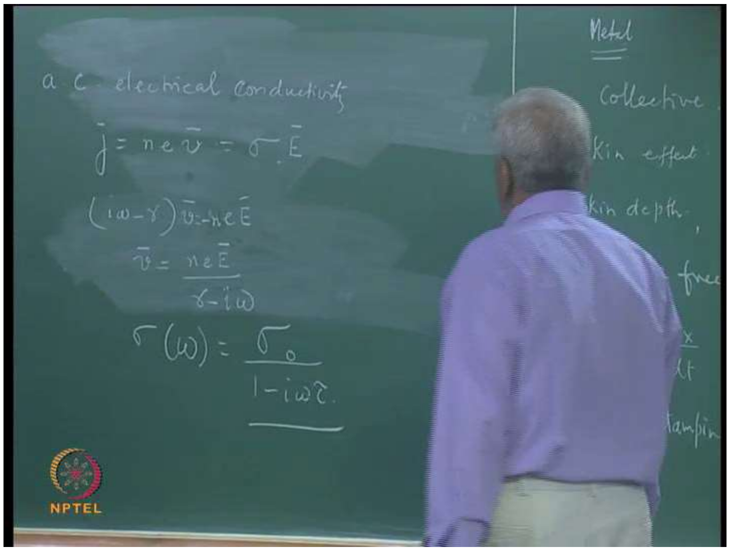

a c electrical conductivity

$$\bar{j} = ne\bar{v} = \sigma \bar{E}$$

$$(i\omega - \gamma)\bar{v} = -ne\bar{E}$$

$$\bar{v} = \frac{ne\bar{E}}{\gamma - i\omega}$$

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau}$$

So, you have an a c response and therefore, this known as the a c electrical conductivity in contrast to the d c connected which we have already discussed. If a metal now this can be discussed again the same formalism that which we discussed the conductivity in terms of the current density which is n e v and this is equal to the sigma e by owns law. And the for we the velocity is a I omega minus gamma and v equals e on to take it account to sign of the charge is the. So, this means that v is and the e gamma minus i omega me. So, this can be a rewritten because we know that gamma is by 1 by tau we remember tau is the relaxation time for connecting trans. So, this can be written in terms of using this and this we can write the sigma the frequency dependent conductivity as sigma naught by one minus I omega now. So, that is the expression for the frequency dependent a c conductivity of a metal.

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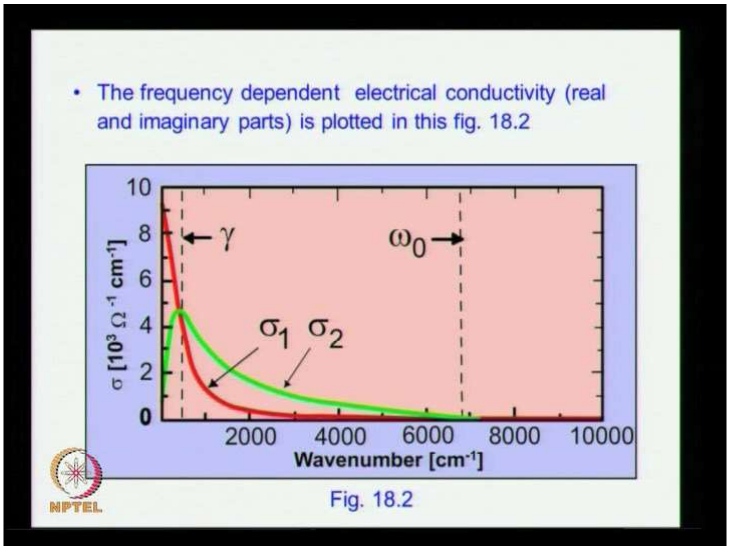

- The frequency dependent electrical conductivity (real and imaginary parts) is plotted in this fig. 18.2

Fig. 18.2

And this again displayed in the next figure where the real and imaginary parts of the electrical conductivity of a metal you shown again as a function of frequency are very not well and you can see the hole behavior is the different from that the d c conductivity.

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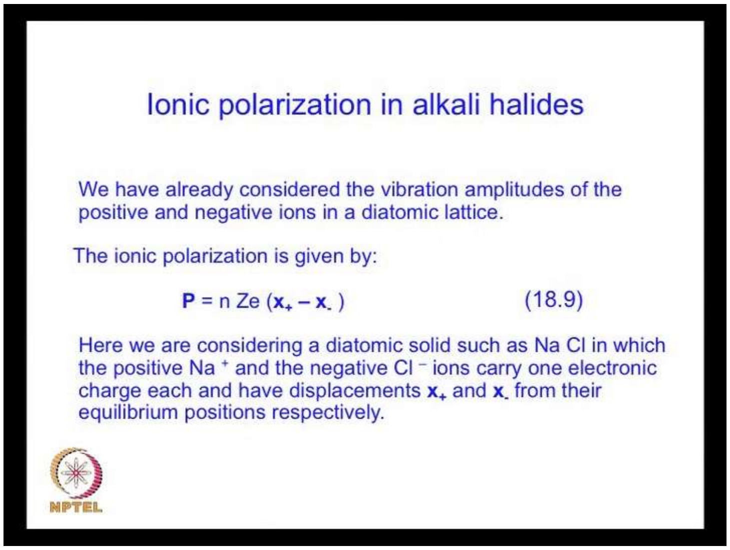

Ionic polarization in alkali halides

We have already considered the vibration amplitudes of the positive and negative ions in a diatomic lattice.

The ionic polarization is given by:

$$\mathbf{P} = n Ze (\mathbf{x}_+ - \mathbf{x}_-) \qquad (18.9)$$

Here we are considering a diatomic solid such as Na Cl in which the positive Na $^+$ and the negative Cl $^-$ ions carry one electronic charge each and have displacements $\mathbf{x}_+$ and $\mathbf{x}_-$ from their equilibrium positions respectively.

Now, we turned to a discussion of the ionic polarization we discuss. So, for the electronic polarization and be now turned to a discussion of the ionic polarization.

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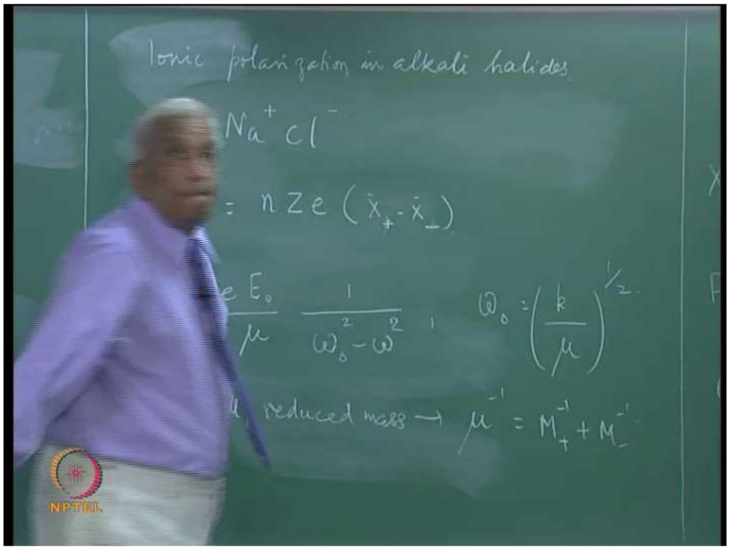

So, in simple alkali halides an example sodium chloride we have sodium plus chlorine ions sitting alternately in a diatomic. Now the ionic polarization is again given by and z e into x one minus x two where that is the relative net displacement of the ion from the equilibrium position are we can write plus and again following the same procedure.

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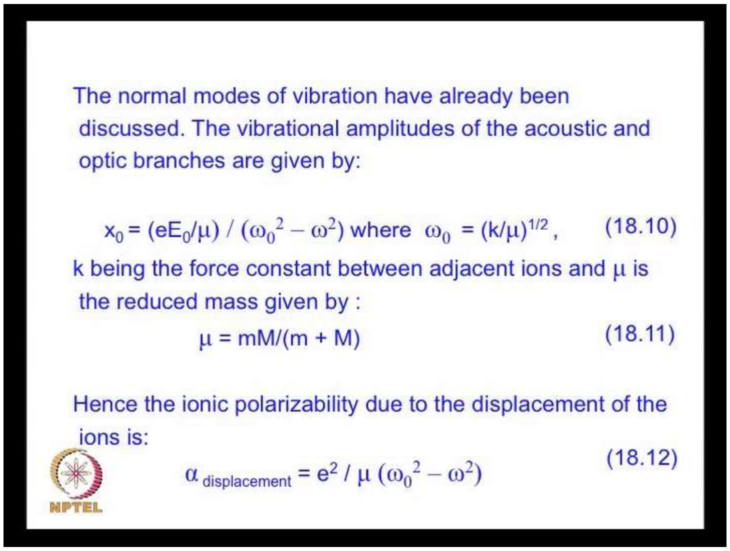

The normal modes of vibration have already been discussed. The vibrational amplitudes of the acoustic and optic branches are given by:

$$x_0 = (eE_0/\mu) / (\omega_0^2 - \omega^2) \text{ where } \omega_0 = (k/\mu)^{1/2}, \quad (18.10)$$

k being the force constant between adjacent ions and μ is the reduced mass given by :

$$\mu = mM/(m + M) \quad (18.11)$$

Hence the ionic polarizability due to the displacement of the ions is:

$$\alpha_{\text{displacement}} = e^2 / \mu\,(\omega_0^2 - \omega^2) \quad (18.12)$$

We arrived a situation where x naught to the equation motion and solid salt it and law where this omega naught this k by mu and mu is reduce mass of the two ions given by from this once we know the displacement.

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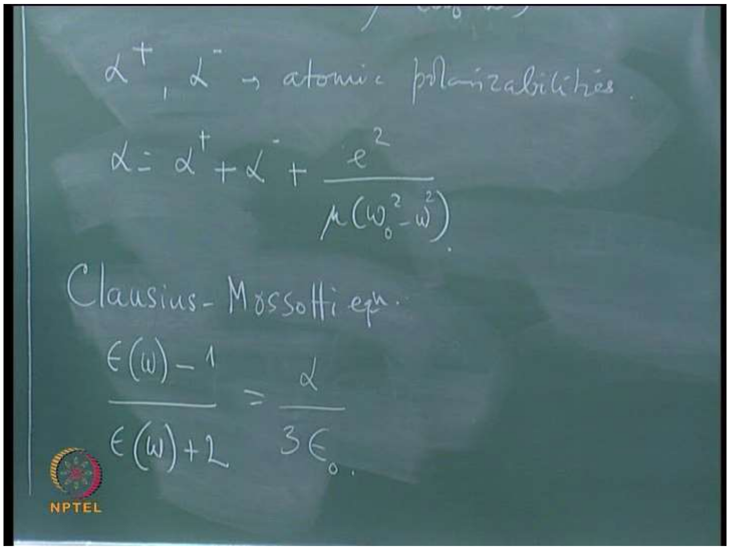

$\alpha^+, \alpha^- \rightarrow$ atomic polarizabilities.

$$\alpha = \alpha^+ + \alpha^- + \frac{e^2}{\mu(\omega_0^2 - \omega^2)}.$$

Clausius-Mossotti eqn.

$$\frac{\epsilon(\omega) - 1}{\epsilon(\omega) + 2} = \frac{\alpha}{3\epsilon_0}.$$

We can write the ionic polarizability in the ionic polarizability due to the relative lead to displacements of the two ions of the form following the same procedure which we followed up to now.

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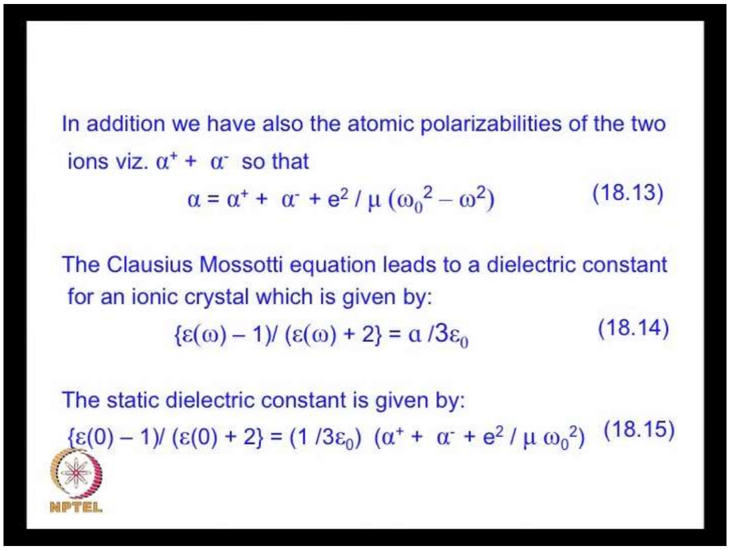

In addition we have also the atomic polarizabilities of the two ions viz. $\alpha^+ + \alpha^-$ so that

$$\alpha = \alpha^+ + \alpha^- + e^2 / \mu\,(\omega_0^2 - \omega^2) \quad (18.13)$$

The Clausius Mossotti equation leads to a dielectric constant for an ionic crystal which is given by:

$$\{\varepsilon(\omega) - 1)/ (\varepsilon(\omega) + 2\} = \alpha / 3\varepsilon_0 \quad (18.14)$$

The static dielectric constant is given by:

$$\{\varepsilon(0) - 1)/ (\varepsilon(0) + 2\} = (1 / 3\varepsilon_0)\ (\alpha^+ + \alpha^- + e^2 / \mu\,\omega_0^2) \quad (18.15)$$

Of course, we have neglected here the individual atomic polarizabilities, which are alpha plus and alpha minus therefore, alpha total polarizability this plus this plus this term and this lead to the clausius mossotti equation we discussed already for the dielectric function an where alpha is given by this and therefore, going to the different limits define.

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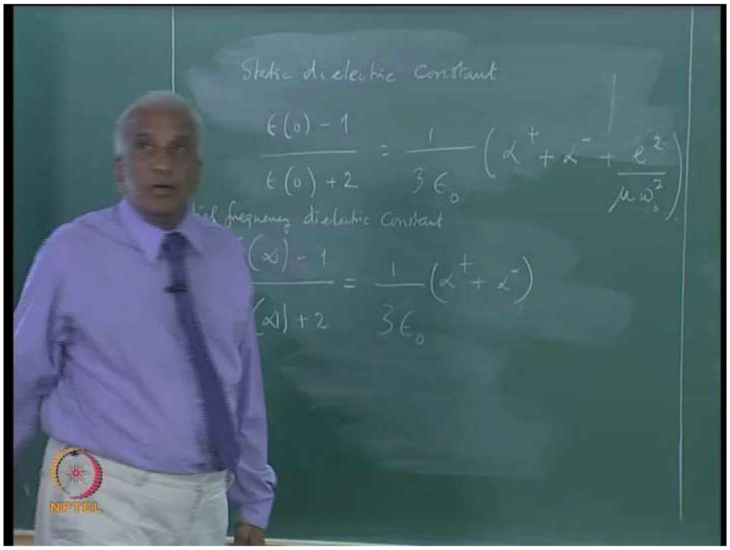

Static dielectric constant

$$\frac{\epsilon(0)-1}{\epsilon(0)+2} = \frac{1}{3\epsilon_0}\left(\alpha^+ + \alpha^- + \frac{e^2}{\mu\omega_0^2}\right)$$

...l frequency dielectric Constant

$$\frac{(\infty)-1}{(\infty)+2} = \frac{1}{3\epsilon_0}\left(\alpha^+ + \alpha^-\right)$$

For example, the static dielectric constant static omega equal to zero there that will be and we have in this omega becomes zero.

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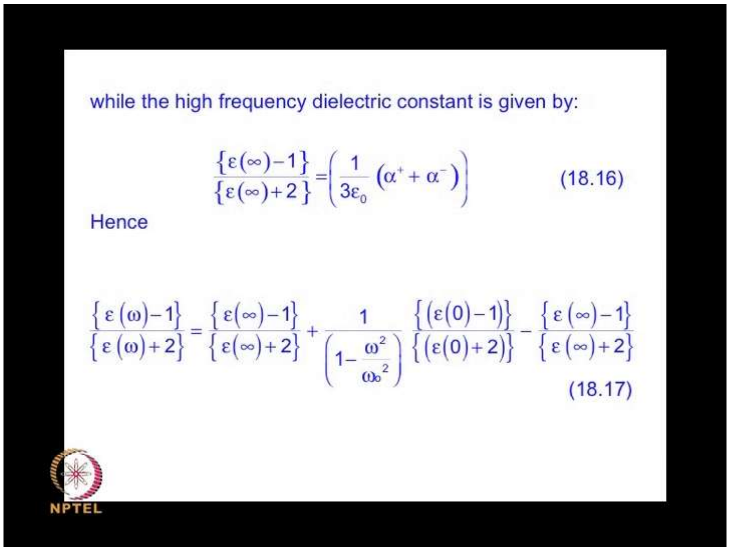

while the high frequency dielectric constant is given by:

$$\frac{\{\varepsilon(\infty)-1\}}{\{\varepsilon(\infty)+2\}} = \left(\frac{1}{3\varepsilon_0}\left(\alpha^+ + \alpha^-\right)\right) \qquad (18.16)$$

Hence

$$\frac{\{\varepsilon(\omega)-1\}}{\{\varepsilon(\omega)+2\}} = \frac{\{\varepsilon(\infty)-1\}}{\{\varepsilon(\infty)+2\}} + \frac{1}{\left(1-\frac{\omega^2}{\omega_0^2}\right)}\left[\frac{\{(\varepsilon(0)-1)\}}{\{(\varepsilon(0)+2)\}} - \frac{\{\varepsilon(\infty)-1\}}{\{\varepsilon(\infty)+2\}}\right] \qquad (18.17)$$

So, I have whereas, the high frequency dielectric function which we write as epsilon infinity is is one is got in the same way by setting omega equal to infinity there. So, the frequency dependent term goes off. So, using these two limit we can write the epsilon omega the dielectric constant at any frequencies of omega.

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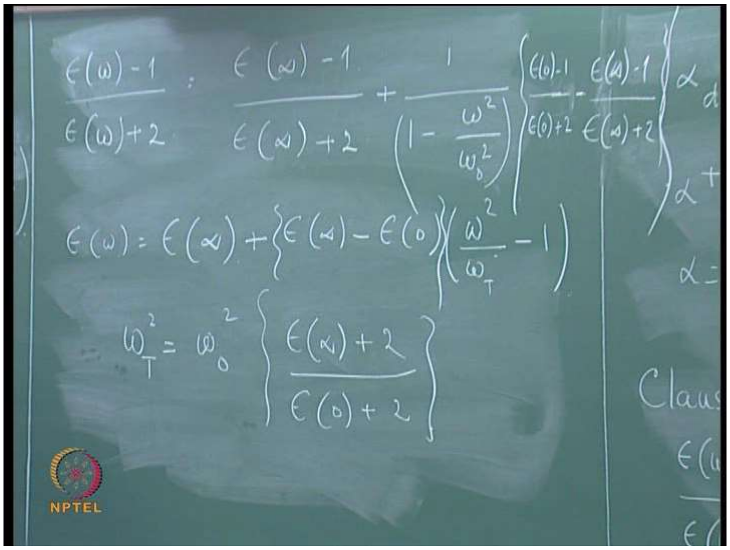

$$\frac{\epsilon(\omega)-1}{\epsilon(\omega)+2} = \frac{\epsilon(\infty)-1}{\epsilon(\infty)+2} + \frac{1}{\left(1-\frac{\omega^2}{\omega_0^2}\right)}\left\{\frac{\epsilon(0)-1}{\epsilon(0)+2} - \frac{\epsilon(\infty)-1}{\epsilon(\infty)+2}\right\}$$

$$\epsilon(\omega) = \epsilon(\infty) + \{\epsilon(\infty) - \epsilon(0)\}\left(\frac{\omega^2}{\omega_T^2} - 1\right)$$

$$\omega_T^2 = \omega_0^2\left\{\frac{\epsilon(\infty)+2}{\epsilon(0)+2}\right\}$$

This take the form that will be plus minus. So, solving for epsilon omega we get? Where omega t square, this is something which we one can figure out rather straight forward algebra.

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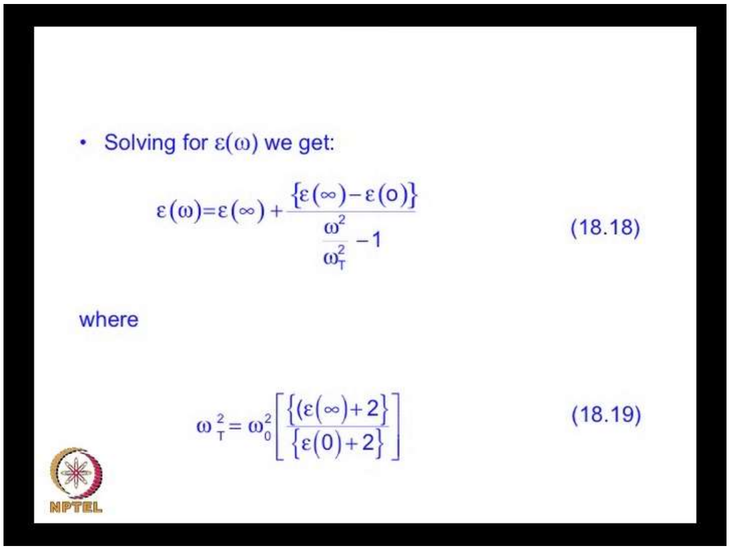

- Solving for $\varepsilon(\omega)$ we get:

$$\varepsilon(\omega)=\varepsilon(\infty)+\frac{\{\varepsilon(\infty)-\varepsilon(o)\}}{\frac{\omega^2}{\omega_T^2}-1} \qquad (18.18)$$

where

$$\omega_T^2=\omega_0^2\left[\frac{\{(\varepsilon(\infty)+2\}}{\{\varepsilon(0)+2\}}\right] \qquad (18.19)$$

So, what is the meaning of all this we have now returned the frequency-dependent dielectric constant at any frequency in terms the high-frequency dielectric constant and then the static dielectric constant and have a frequency the defined in this way. So, this helps us to visualize what is going on in terms of what I have known in the longitudinal and transverse of pick more.

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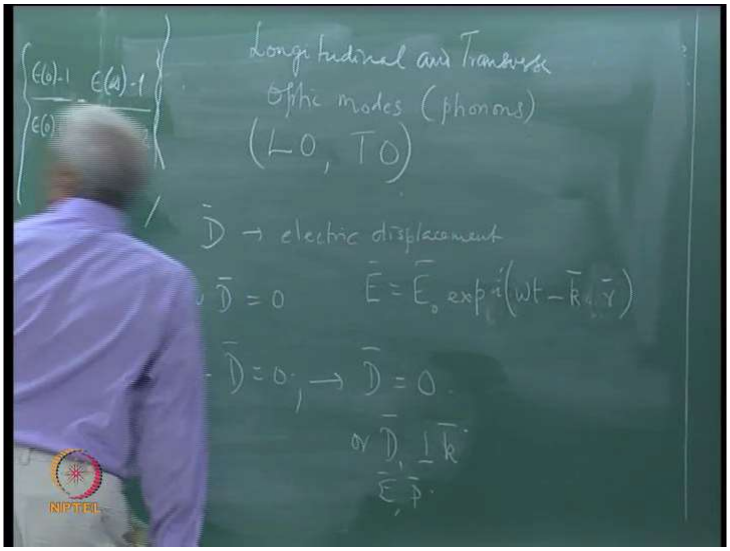

So, we now go on discuss the longitudinal and transfers optic modes and optic on usually they go by the contraction at the abbreviation l o and t o for us. So, in an optic mode of an ionic crystal, there is an non varnishing polarization p and associated with this is the electric displacement d and when there are no free charger. We have the general relation divergent to be vanishes now the apply an alternating field the e equal to e naught exponential I minus k or k dot r in general. So, using this, you can see d gives rise to k dot d equal to zero, because the divergence is going to taking the divergence means it would be replacing this by I k div d equal to zero goes to the equation k dot d equal to zero. And what the consequences of this this means that I either d itself is zero or d need is perpendicular to k if d is perpendicular to k take care e also is and p also that is the significance of this condition div d equal to zero.

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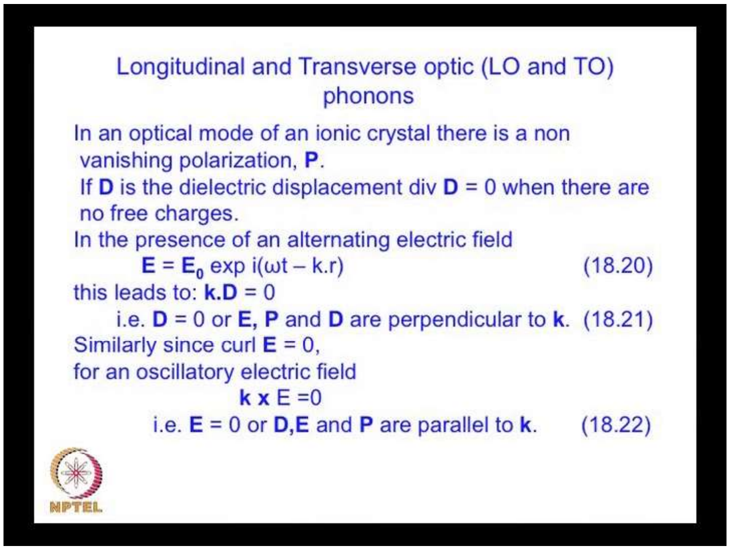

Longitudinal and Transverse optic (LO and TO) phonons

In an optical mode of an ionic crystal there is a non vanishing polarization, **P**.

If **D** is the dielectric displacement div **D** = 0 when there are no free charges.

In the presence of an alternating electric field

$$\mathbf{E} = \mathbf{E_0} \exp i(\omega t - k.r) \qquad (18.20)$$

this leads to: **k.D** = 0

i.e. **D** = 0 or **E, P** and **D** are perpendicular to **k**. (18.21)

Similarly since curl **E** = 0,

for an oscillatory electric field

$$\mathbf{k} \times E = 0$$

i.e. **E** = 0 or **D,E** and **P** are parallel to **k**. (18.22)

Now, in addition we also have for the electric case the additional relation donation going equal to zero.

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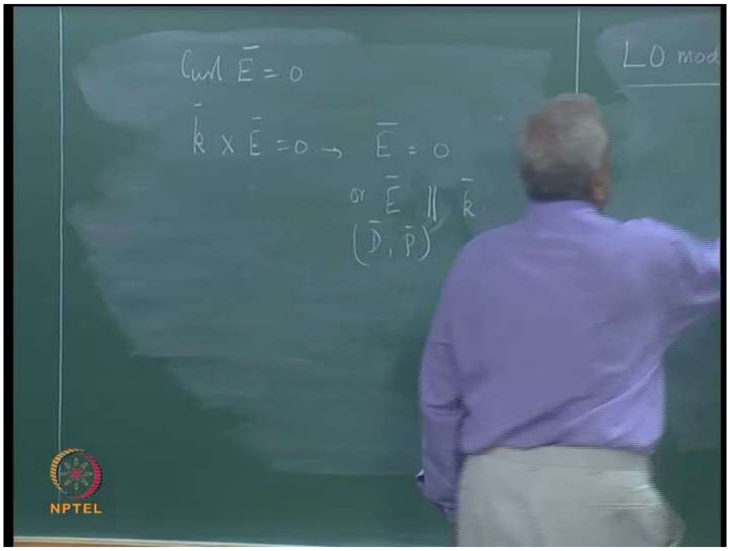

Now, curly cord is you know foreign hostility electric field again give rise to the relation k cross e equal to zero this means either e itself is zero or e is perpendicular to keep no parallel if is all. So, is the and p. So, that these are the two possibilities.

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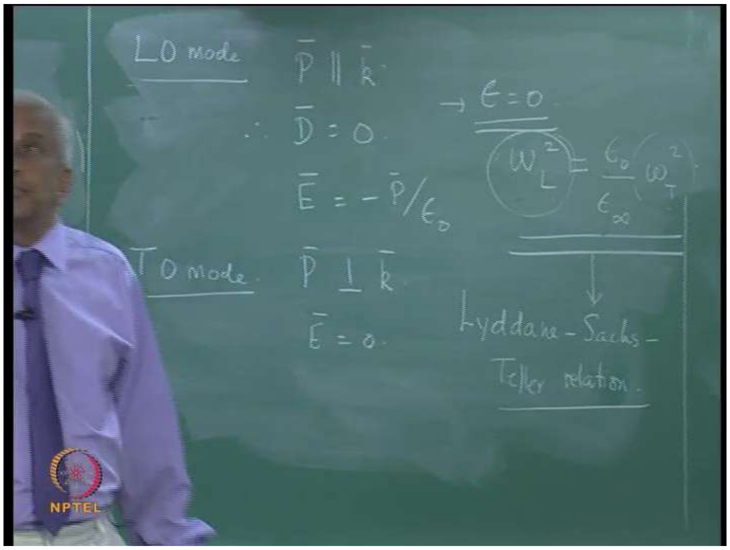

LO mode

$\bar{P} \parallel \bar{k}$

$\therefore \bar{D} = 0$

$\bar{E} = -\bar{P}/\epsilon_0$

$\to \epsilon = 0$

$\omega_L^2 = \frac{\epsilon_0}{\epsilon_\infty} \omega_T^2$

TO mode

$\bar{P} \perp \bar{k}$

$\bar{E} = 0$

Lyddane - Sachs - Teller relation.

Now, we can discuss an l o mode a longitudinal in an optic mode in an l o mode what happens it is defined by the polarization being parallel to keep. So, if p is parallel to k naturally this condition is ruled out there for only we have the d equal to zero and therefore, e is minus p value where as for the t o mode p is perpendicular to k which means that p s parallel to k therefore, e zero. So, this is the main difference between l o mode and the t o mode.

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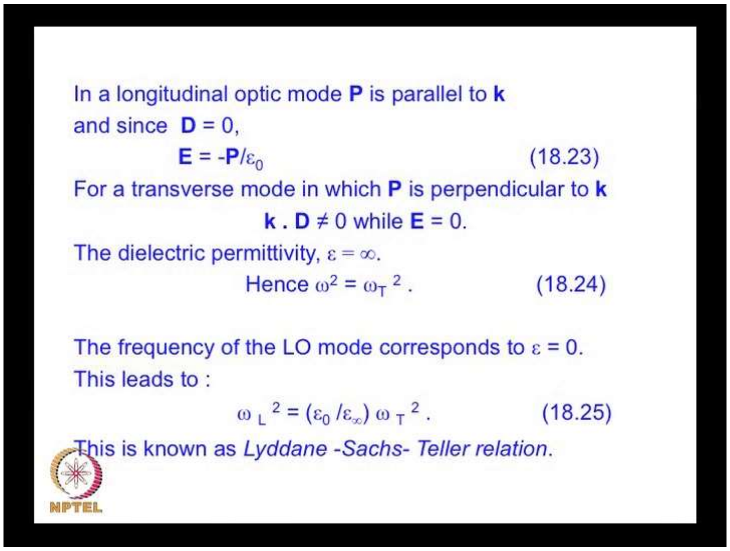

In a longitudinal optic mode **P** is parallel to **k**
and since **D** = 0,

$$\mathbf{E} = -\mathbf{P}/\varepsilon_0 \qquad (18.23)$$

For a transverse mode in which **P** is perpendicular to **k**

$$\mathbf{k} \cdot \mathbf{D} \neq 0 \text{ while } \mathbf{E} = 0.$$

The dielectric permittivity, $\varepsilon = \infty$.

$$\text{Hence } \omega^2 = \omega_T^{\ 2}. \qquad (18.24)$$

The frequency of the LO mode corresponds to $\varepsilon = 0$.
This leads to :

$$\omega_L^{\ 2} = (\varepsilon_0/\varepsilon_\infty)\, \omega_T^{\ 2}. \qquad (18.25)$$

This is known as *Lyddane -Sachs- Teller relation*.

Therefore you have the frequency a the L O mode corresponds to epsilon equal to zero in; that means, omega l square plugging back into the expression for the along L O mode omega l square is epsilon naught by epsilon in finite a into omega q square. So, this very interesting relation between a frequency of a L O mode and the frequency of a t o mode goes by a special name lezyne sects tailor this can be experimentally verify because no one can measure the static dielectric constant the high frequency the frequency angular frequency that the L O and T O modes. Therefore, one can check this relations now this in general gives back omega is usually greater than omega t. So, the frequency-dependent dielectric constant its variation for an ionic crystal is shown ionic the next figure.

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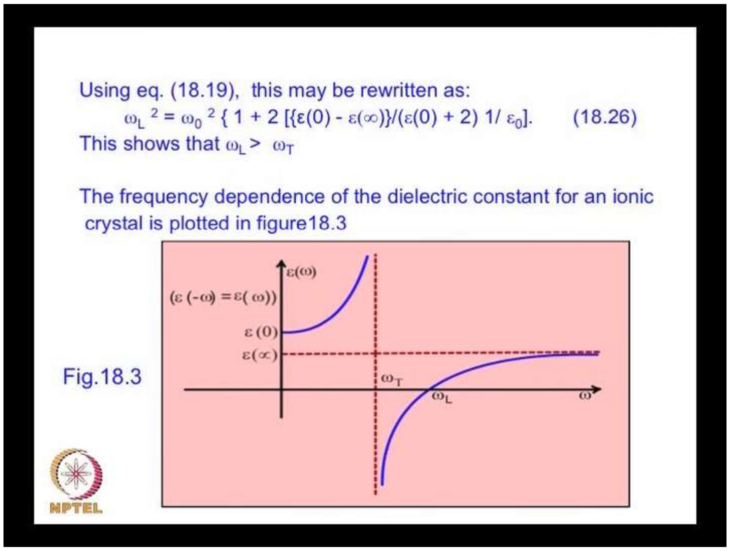

Using eq. (18.19), this may be rewritten as:

$$\omega_L{}^2 = \omega_0{}^2 \{ 1 + 2 [\{\varepsilon(0) - \varepsilon(\infty)\}/(\varepsilon(0) + 2) 1/ \varepsilon_0]. \qquad (18.26)$$

This shows that $\omega_L > \omega_T$

The frequency dependence of the dielectric constant for an ionic crystal is plotted in figure18.3

Fig.18.3

And one can see that indeed frequency range between omega l and omega t there is a again and negative dielectric constant and on the ionic crystal is highly reflective.

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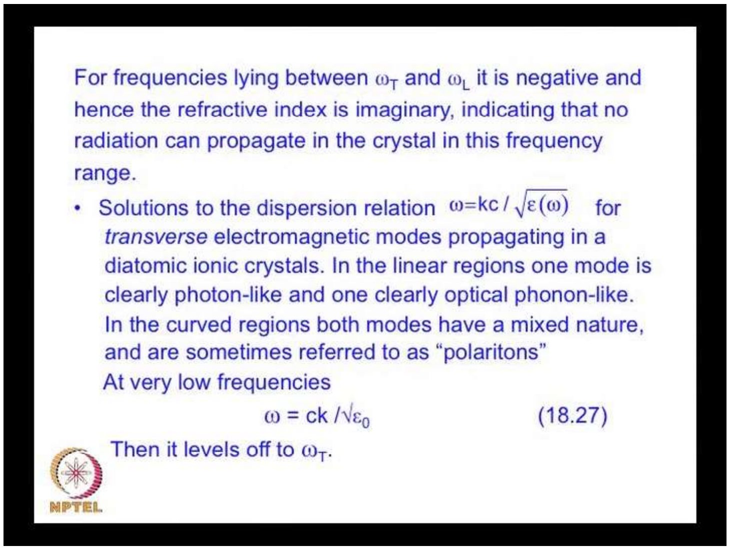

For frequencies lying between ω_T and ω_L it is negative and hence the refractive index is imaginary, indicating that no radiation can propagate in the crystal in this frequency range.

- Solutions to the dispersion relation $\omega = kc/\sqrt{\varepsilon(\omega)}$ for *transverse* electromagnetic modes propagating in a diatomic ionic crystals. In the linear regions one mode is clearly photon-like and one clearly optical phonon-like. In the curved regions both modes have a mixed nature, and are sometimes referred to as "polaritons"

  At very low frequencies

  $$\omega = ck/\sqrt{\varepsilon_0} \qquad (18.27)$$

  Then it levels off to ω_T.

So, no radiation can propagate in the crystal this frequency region laying between the transverse and longitudinal optical modes. Now we can also solve for the dispersion relationship for the transfers electromagnetic wave and modes and this gives you dispersion relationship and solved gives you a behavior like this. So, the dispersion relationship has to branches one laying below omega t and another laying above omega l. So, you have in the region there are linear regions one mode is clearly found like and one is clearly optical.

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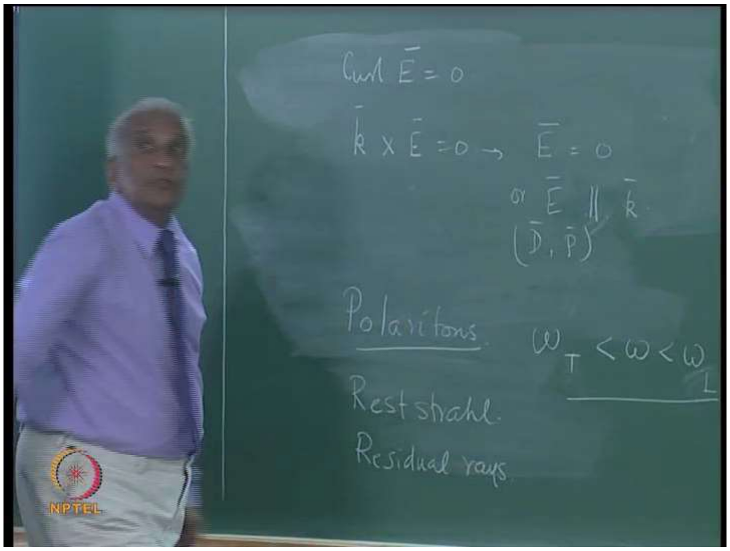

So, this excitation is known as polarity dance at at very low frequency is we see omega goes as linear and it is levels of the omega t and at highly frequencies about the other branch.

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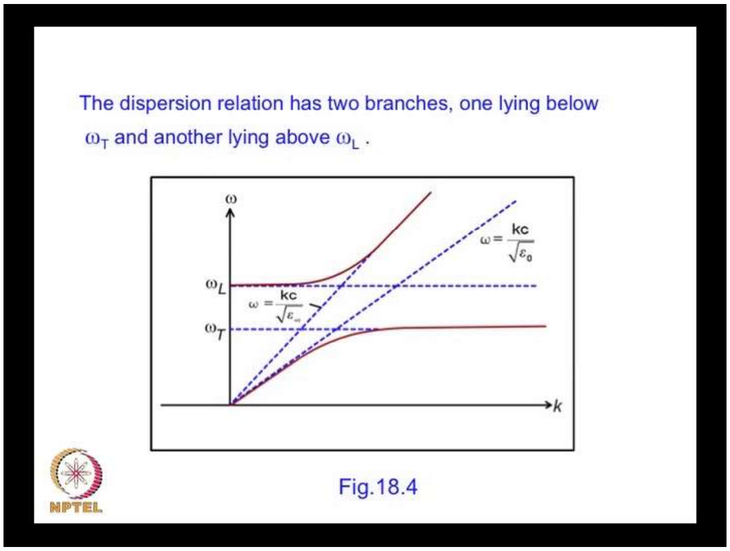

The dispersion relation has two branches, one lying below ω_T and another lying above ω_L .

Fig.18.4

You have again in linear region at very low frequency is it levels off to omega t and again you have at high frequencies you have a linear region again it levels of up a syntactically to the longitudinal optical.

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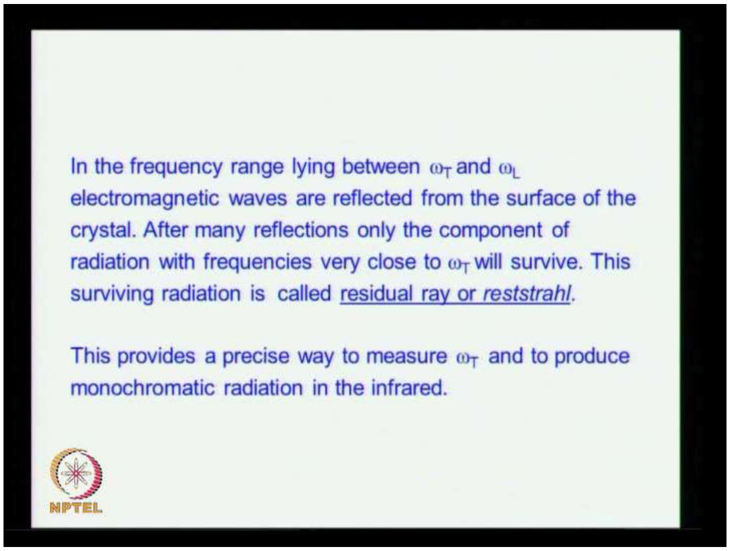

In the frequency range lying between ω_T and ω_L electromagnetic waves are reflected from the surface of the crystal. After many reflections only the component of radiation with frequencies very close to ω_T will survive. This surviving radiation is called residual ray or *reststrahl*.

This provides a precise way to measure ω_T and to produce monochromatic radiation in the infrared.

So, in the region between omega on in this frequency range you have highly reflected behavior and the e m waves are reflected from the surface at the custom. So, you can after many reflections only the component of radiation frequencies very close to omega t will survive. So, you can have a surviving radiation which is known as a rest trial or in English is a German-term which means residual unease. So, you can have a very precise to measure the transfers of the pick mode frequency and also produced monochromatic radiation gross e to omega t which lies in the intranet. So, these are some vacations of this behavior.

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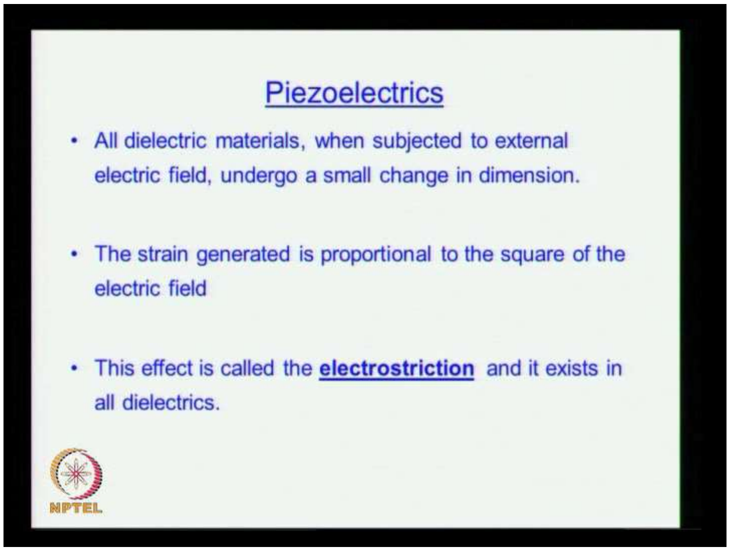

Piezoelectrics

- All dielectric materials, when subjected to external electric field, undergo a small change in dimension.
- The strain generated is proportional to the square of the electric field
- This effect is called the **electrostriction** and it exists in all dielectrics.

We know all closed is that their discussions brief discussion of very remarkable you kind a substances known as b. So, electric's.

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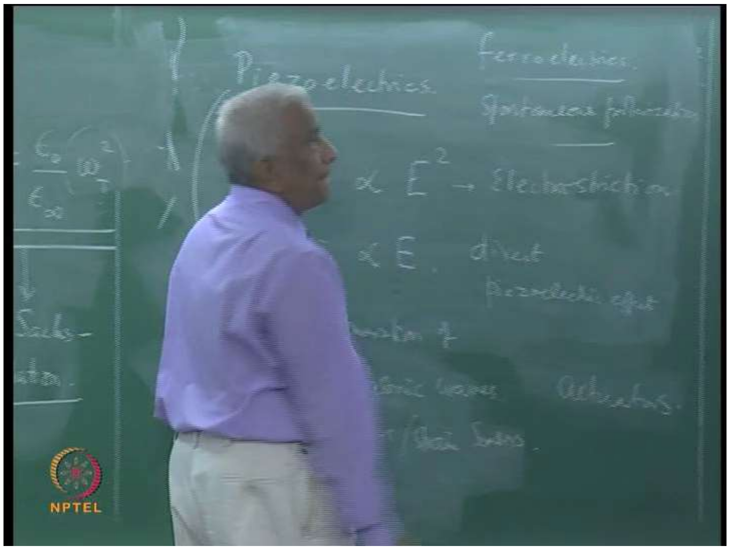

In general all the dielectric material when you subject it to an external electric field have sufficiently large magnitude undergoing a small chain in a dimension. So, there is a strain generated which is proportional this cure of the electric feed at high enough fields.

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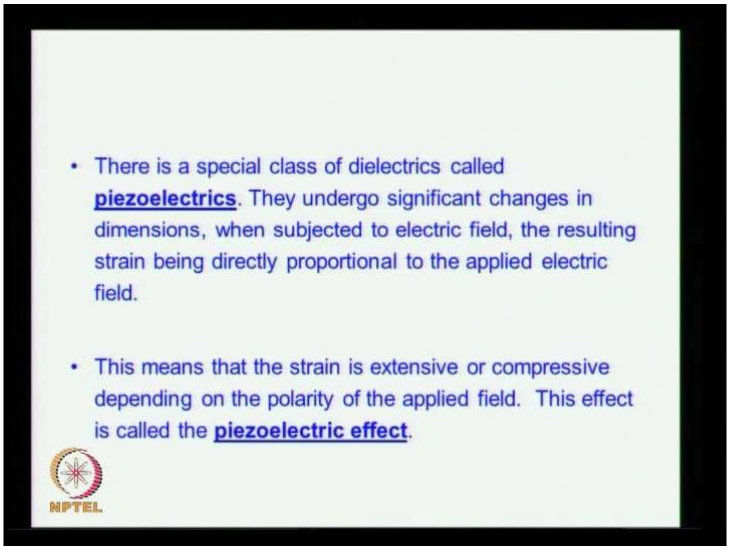

- There is a special class of dielectrics called **piezoelectrics**. They undergo significant changes in dimensions, when subjected to electric field, the resulting strain being directly proportional to the applied electric field.
- This means that the strain is extensive or compressive depending on the polarity of the applied field. This effect is called the **piezoelectric effect**.

So, this effect is known as an electron structure and this is observed in all the dielectric materials at high enough electric fields, but piezo electrics is different. This is a one special class electric where there is a significant change in dimension in and subjected to an electric field backed in a piezoelectric strain is proportionately to the field. So, they strain depending on whether what is the polarity the field you can have a compressive if you are extensive string.

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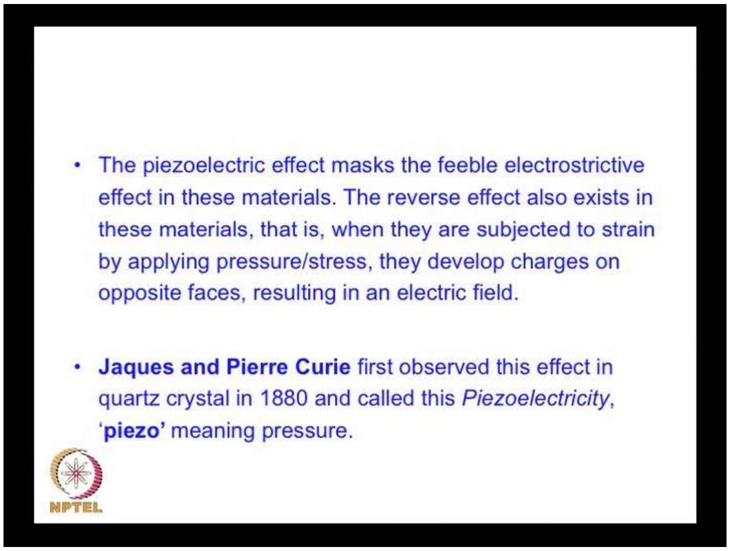

- The piezoelectric effect masks the feeble electrostrictive effect in these materials. The reverse effect also exists in these materials, that is, when they are subjected to strain by applying pressure/stress, they develop charges on opposite faces, resulting in an electric field.
- **Jaques and Pierre Curie** first observed this effect in quartz crystal in 1880 and called this *Piezoelectricity*, '**piezo**' meaning pressure.

So, this is piezoelectric, now usually the electric effect mass the electrostrictive effect. Now you can have not only a direct electric effect best, but also in direct reverse effect in in which you have a field resulting and their an a electric field resulting from and applied strain jacks on the acuity first observed this effect in eighteen eighty and all means, but if that. So, that is the reason for the terminology.

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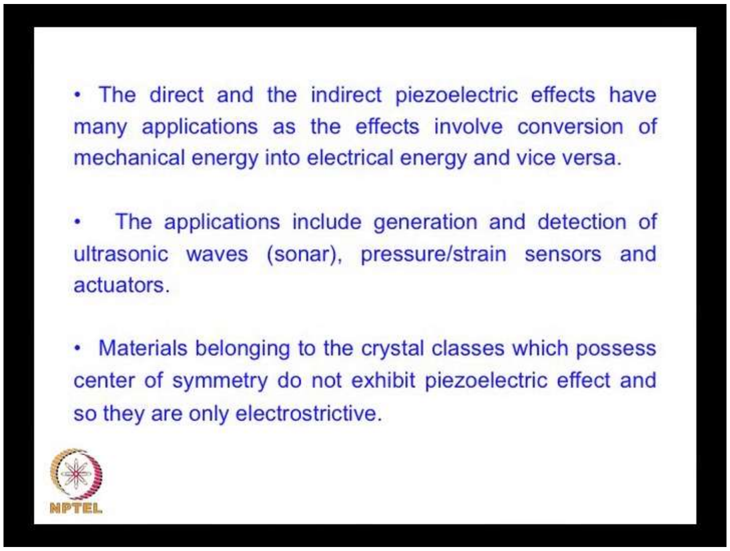

- The direct and the indirect piezoelectric effects have many applications as the effects involve conversion of mechanical energy into electrical energy and vice versa.
- The applications include generation and detection of ultrasonic waves (sonar), pressure/strain sensors and actuators.
- Materials belonging to the crystal classes which possess center of symmetry do not exhibit piezoelectric effect and so they are only electrostrictive.

Now, this is interests comes because of the applications apply it well generation all ultra sonic it is because it is trained needs used in sauna and then you can also have pressure are strain since we I based on director reverse piezoelectric effect you can also have actuators these electric actually. So, usually materials belonging to crystal which classes these processes and center of symmetry do not exit it piezoelectric effect because the linearity. So, it is only the non centro symmetric crystals which produce the piezoelectric effect.

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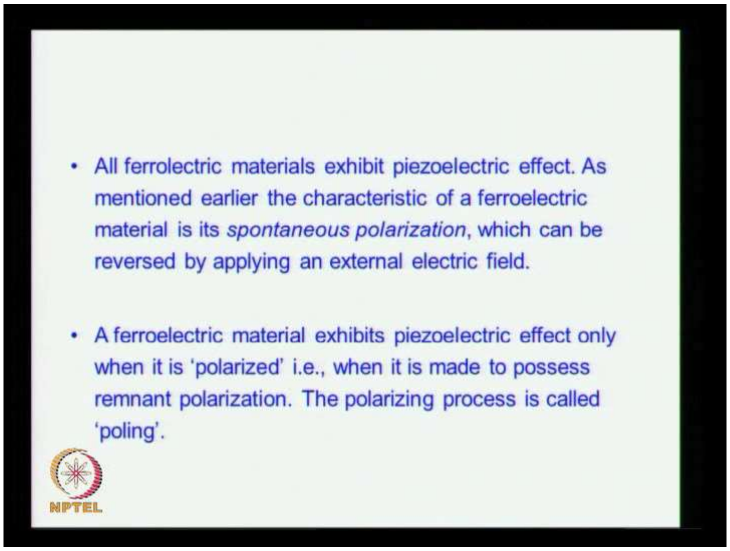

- All ferrolectric materials exhibit piezoelectric effect. As mentioned earlier the characteristic of a ferroelectric material is its *spontaneous polarization*, which can be reversed by applying an external electric field.
- A ferroelectric material exhibits piezoelectric effect only when it is 'polarized' i.e., when it is made to possess remnant polarization. The polarizing process is called 'poling'.

Now, that shown in next couple of figure direct and the indirect is addicting effect I and that usually we have already discussed faro electrics all faro electrics display piezoelectric. Now in the case of a faro electric material the important characteristic is that there exists a spontaneous polarization which can be the reverse by applying the external electric field. So, a faro electric material exhibits a piezo effect only when it is polarized in this way that is when it is made to process ramnant and polarization the polarizing processes is call only the error that.

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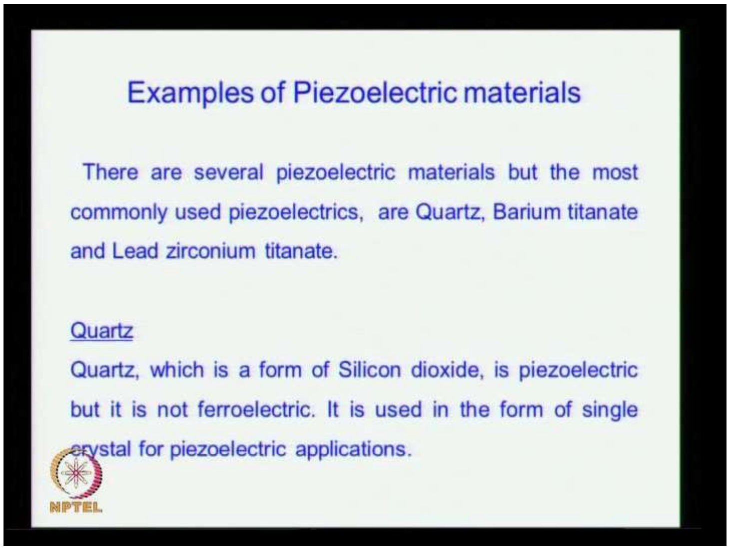

Examples of Piezoelectric materials

There are several piezoelectric materials but the most commonly used piezoelectrics, are Quartz, Barium titanate and Lead zirconium titanate.

Quartz

Quartz, which is a form of Silicon dioxide, is piezoelectric but it is not ferroelectric. It is used in the form of single crystal for piezoelectric applications.

What are the material typical examples one as the material which is very well known a piezoelectric material is quarts.

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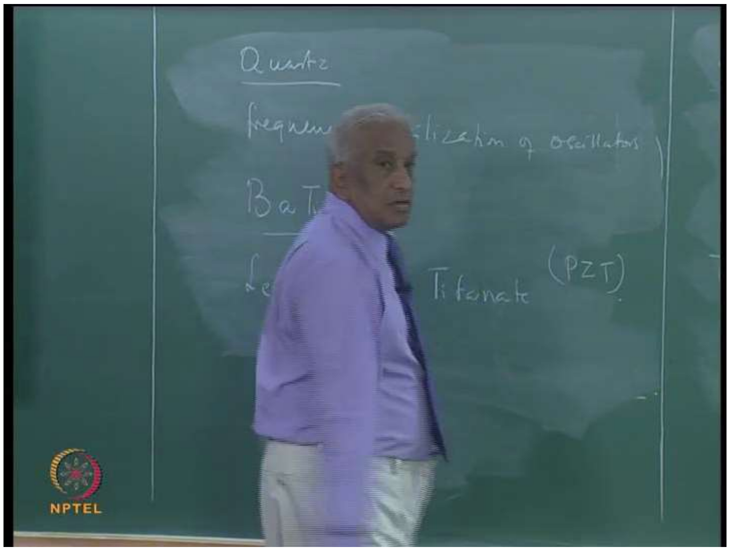

Quat the silicon dioxide usually piezoelectric, but not faro can used in the form of a single crystal and when have quat crystal.

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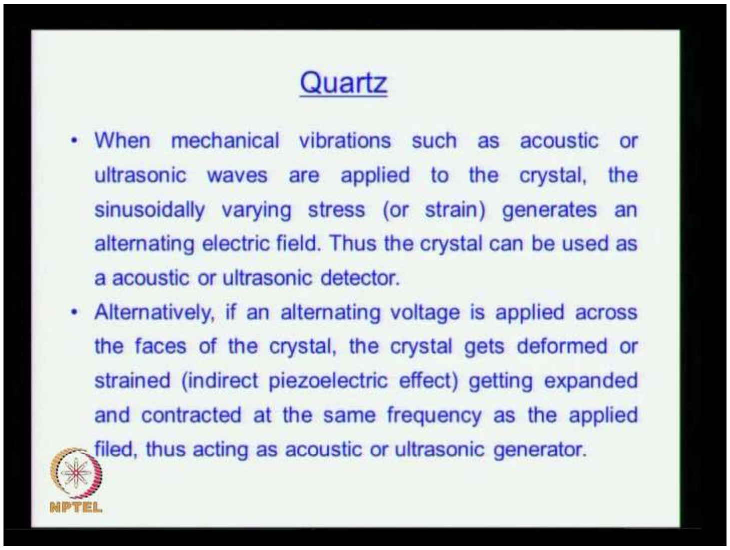

Quartz

- When mechanical vibrations such as acoustic or ultrasonic waves are applied to the crystal, the sinusoidally varying stress (or strain) generates an alternating electric field. Thus the crystal can be used as a acoustic or ultrasonic detector.
- Alternatively, if an alternating voltage is applied across the faces of the crystal, the crystal gets deformed or strained (indirect piezoelectric effect) getting expanded and contracted at the same frequency as the applied filed, thus acting as acoustic or ultrasonic generator.

This is use very often in frequency stabilization of as electives appeaser piezoelectric quad crystal gives you frequency stabilization.

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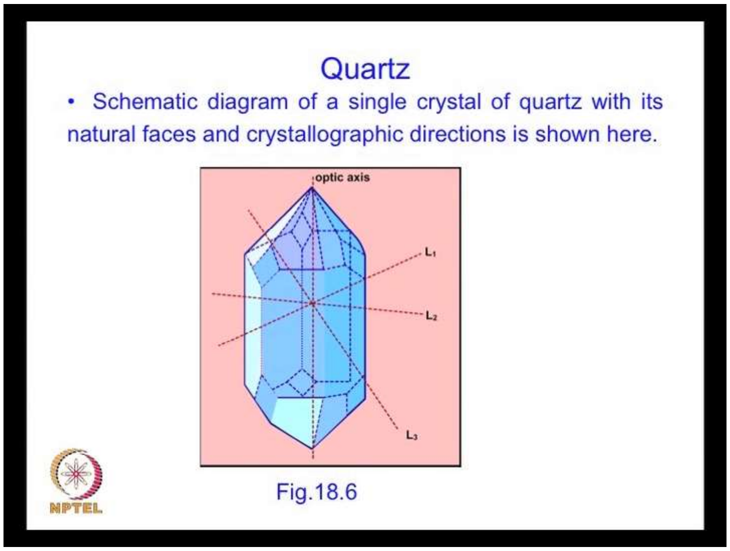

Quartz

- Schematic diagram of a single crystal of quartz with its natural faces and crystallographic directions is shown here.

Fig.18.6

This figure shows a single crystal of quad's in the different cuts type which are implied for production of x piezoelectric slices with the different frequencies are shown in the figure.

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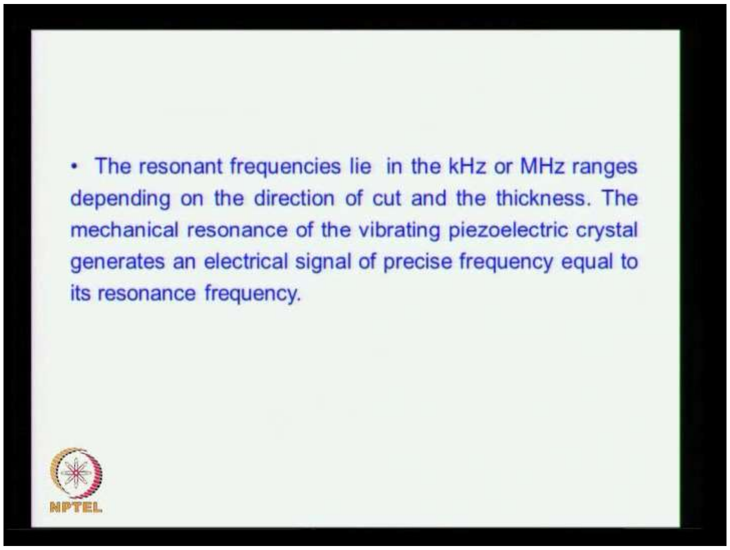

- The resonant frequencies lie in the kHz or MHz ranges depending on the direction of cut and the thickness. The mechanical resonance of the vibrating piezoelectric crystal generates an electrical signal of precise frequency equal to its resonance frequency.

Now, they evident frequencies can lay in the kilohertz are mega hertz in depending on the direction of correct and the thickness of the custom.

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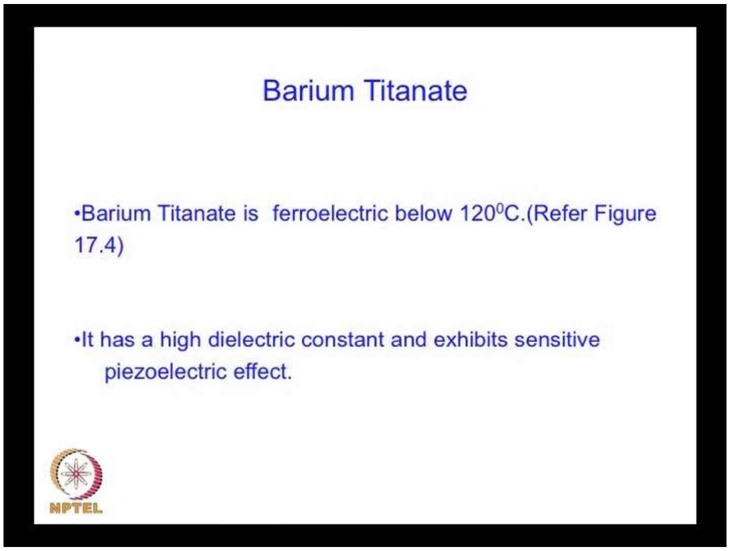

Barium Titanate

- Barium Titanate is ferroelectric below 120^{0}C.(Refer Figure 17.4)
- It has a high dielectric constant and exhibits sensitive piezoelectric effect.

So, that is the oscillator the next material is barium title it we already discussed this material it becomes a fero electric head phone under on twenty d b celsius and as I a high dielectric constant exhibits a very sensitive piezoelectric.

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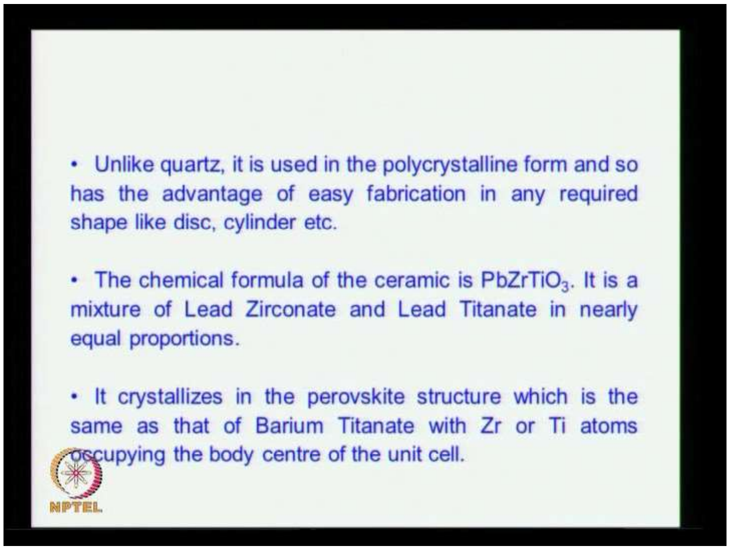

- Unlike quartz, it is used in the polycrystalline form and so has the advantage of easy fabrication in any required shape like disc, cylinder etc.
- The chemical formula of the ceramic is $PbZrTiO_3$. It is a mixture of Lead Zirconate and Lead Titanate in nearly equal proportions.
- It crystallizes in the perovskite structure which is the same as that of Barium Titanate with Zr or Ti atoms occupying the body centre of the unit cell.

Another one is lead zirconate well it is lead zirconate titanate is it is that on. So, this is the widely used a piezoelectric it looks at me, but plans to use application now it is also used in the polycrystalline farm.

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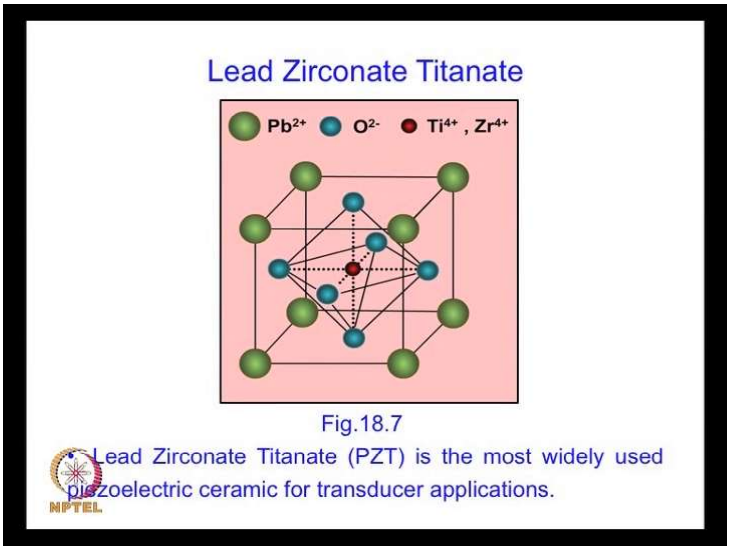

Lead Zirconate Titanate

Fig.18.7

- Lead Zirconate Titanate (PZT) is the most widely used piezoelectric ceramic for transducer applications.

So, it as an advantage of easy fabrication that is the crystal structure of let us open it paid and this there the most widely used piezoelectric material.

Condensed Matter Physics
Prof. G. Rangarajan
Department of Physics
Indian Institute of Technology, Madras

Lecture - 17
Dispersion and Absorption of Electromagnetic Waves In Dielectric Media: Ferro-and Antiferroelectrics

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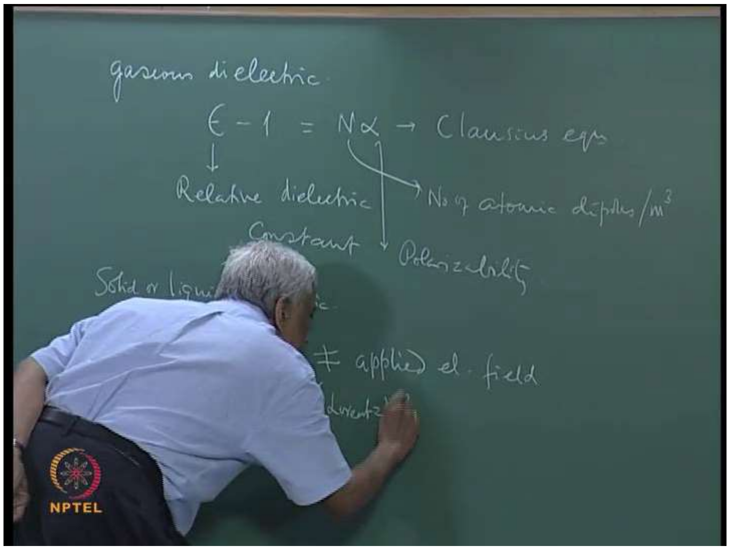

In the last lecture, we discussed the basic mechanism of polarization of a dielectric medium, and we saw that in the case of gaseous dielectric gases so we have the relation epsilon minus one equal to n alpha this is known as a Clausius equation. Here epsilon is the relative dielectric constant, n is the number of dipoles atomic or molecular dipoles per meter cube, and alpha is the polarisability. We also saw that when we come to a condensed phase like a solid or liquid, we saw that this equation is not valid anymore, because of the presence a local field which is not equal to the applied electric field because of the presence of an internal field which is also known as the Lorentz field.

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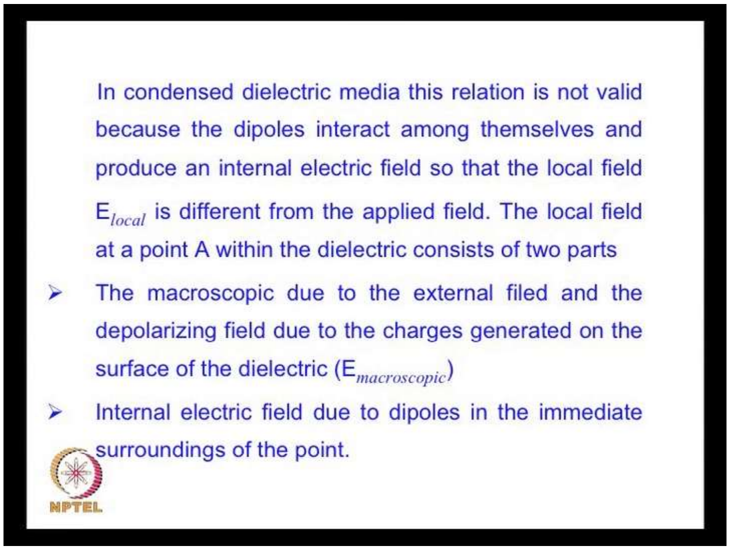

In condensed dielectric media this relation is not valid because the dipoles interact among themselves and produce an internal electric field so that the local field E_{local} is different from the applied field. The local field at a point A within the dielectric consists of two parts

- The macroscopic due to the external filed and the depolarizing field due to the charges generated on the surface of the dielectric ($E_{macroscopic}$)
- Internal electric field due to dipoles in the immediate surroundings of the point.

So, it is this E local which has to be used here in this equation, and this leads to a modification of the Clausius equation in the form and this is known as the Clausius-Mossotti equation and this is what is valid for solids and liquid dielectrics.

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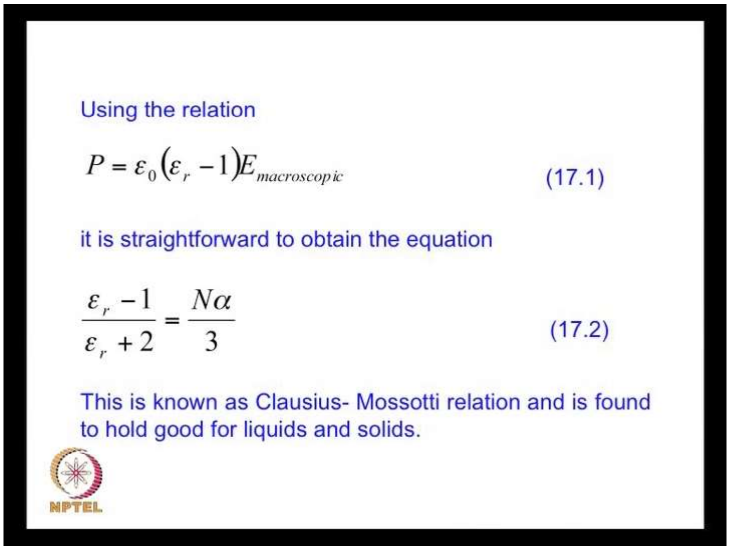

Using the relation

$$P = \varepsilon_0 (\varepsilon_r - 1) E_{macroscopic} \qquad (17.1)$$

it is straightforward to obtain the equation

$$\frac{\varepsilon_r - 1}{\varepsilon_r + 2} = \frac{N\alpha}{3} \qquad (17.2)$$

This is known as Clausius- Mossotti relation and is found to hold good for liquids and solids.

So, this is the Clausius Mossotti equation which has to used for solid and liquid dielectric, and therefore of relevance class.

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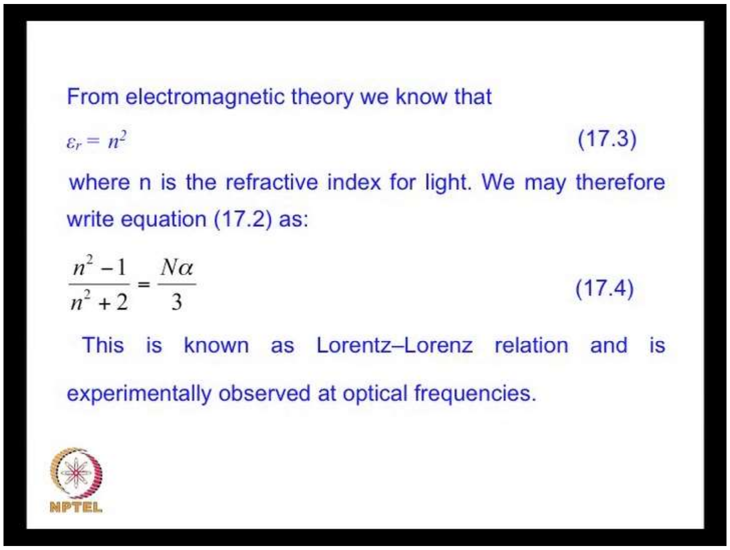

From electromagnetic theory we know that

$$\varepsilon_r = n^2 \qquad (17.3)$$

where n is the refractive index for light. We may therefore write equation (17.2) as:

$$\frac{n^2-1}{n^2+2} = \frac{N\alpha}{3} \qquad (17.4)$$

This is known as Lorentz–Lorenz relation and is experimentally observed at optical frequencies.

Since we also know that the dielectric constant is proportional to n square from em theory we can also write this as in this form this is known as the Lorentz relation.

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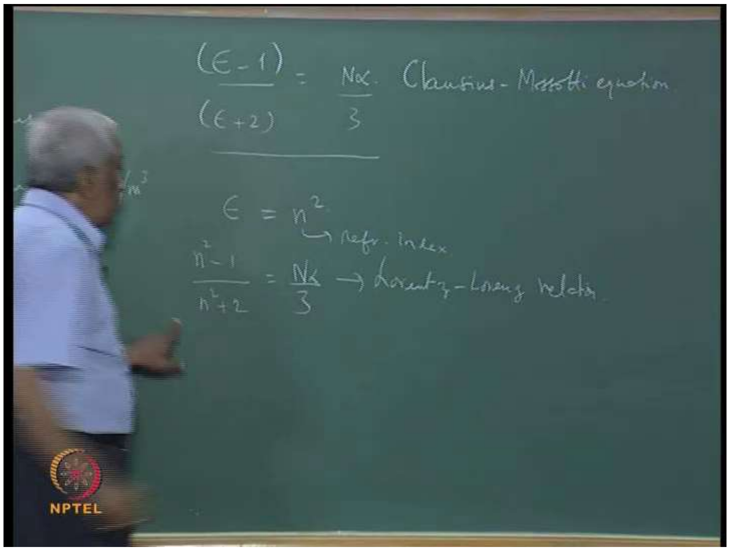

So, if you measure the refractive index n, this is the reflective index, you can use this equation at optical frequencies.

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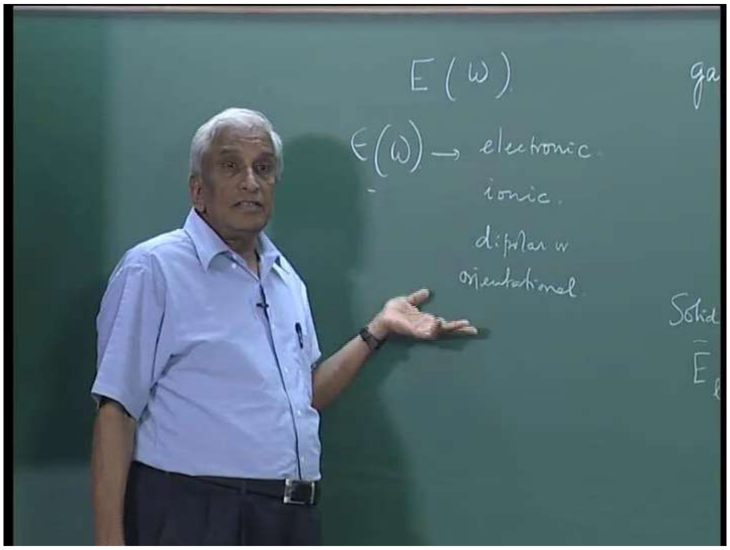

So, this is the overall situation and we also saw how when we go from the static to the dynamic situation where the applied field is a function of omega the frequency, so it is an alternative field for example, ((Refer Time: 04:36)) field. Then you have the frequency dependent dielectric constant, which is basically because of the polarization of various entities in the medium. The mechanism of polarizations can be different electronic, ionic and dipolar or orientation. Last time we discuss these with specific reference to examples such as sodium chloride and water and so on. Sodium chloride is the ionic material and the ionic contribution will not be able to keep phase, will not be able to follow the past frequency variations of the applied dielectric field. And therefore, it will not contribute to the polarization at high frequencies.

Whereas, the electronic polarization will go all the way will be able to follow the polarizations follows the field variations right up to the ultraviolet across the visible spectrum. And for example, if you have a polar molecule like water in which there is a permanent electric dipole moment then there is an orientation of these dipoles in the applied electric field and this also has a certain time constant. And therefore, depending on the relaxation of these dipoles, this will also contribute only up to a certain frequency such as microwaves.

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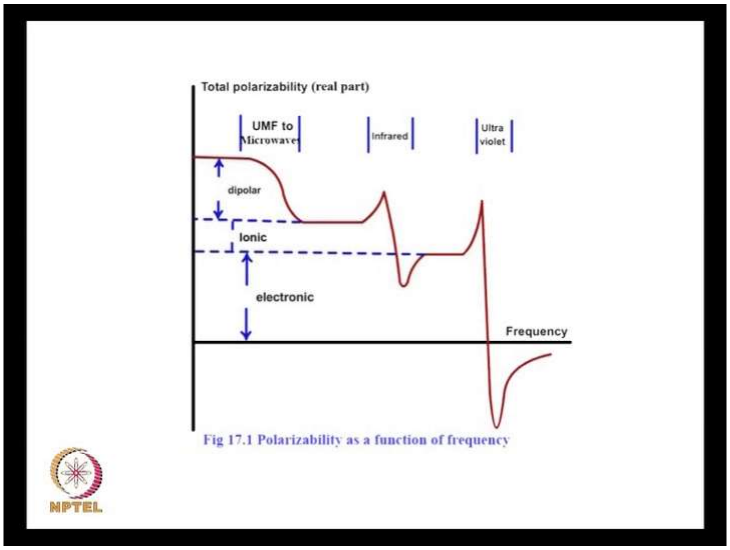

Fig 17.1 Polarizability as a function of frequency

So, this is what we saw last time, and all these three together are illustrated in the next figure, where we have plotted the polarisability as a function of frequency. Now what we see is that at low frequencies, you have the dipolar mechanism, so you have something like this.

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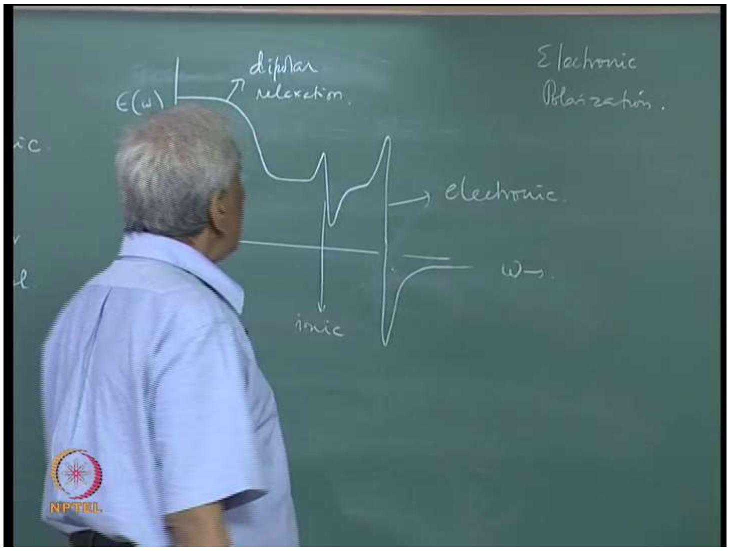

So, the epsilon omega function of omega starts from this zero static value and goes down and then there is the region here and then region here. So, that is the overall shape of the polarisability as a function of frequency. So, this is the dipolar region, dipolar relaxation this is the ionic and this is the electronic, so that is the overall behavior of the polarized ability and we will consider these in some detail next.

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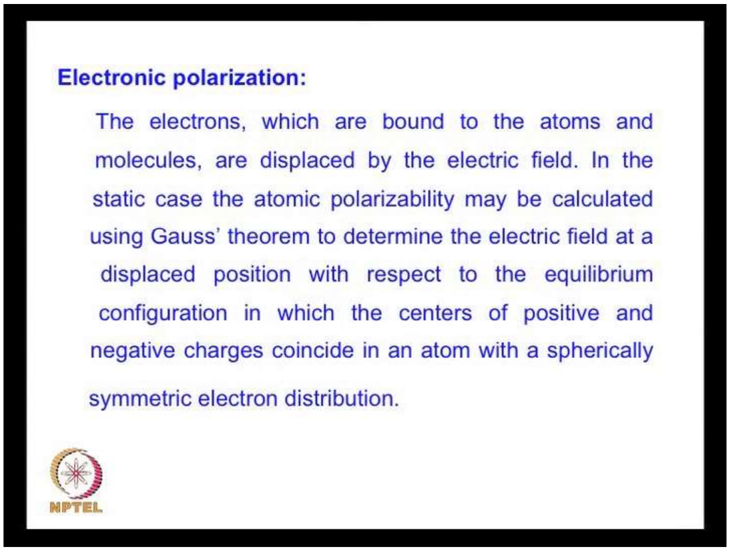

Electronic polarization:

The electrons, which are bound to the atoms and molecules, are displaced by the electric field. In the static case the atomic polarizability may be calculated using Gauss' theorem to determine the electric field at a displaced position with respect to the equilibrium configuration in which the centers of positive and negative charges coincide in an atom with a spherically symmetric electron distribution.

So, let us consider electronic polarization. So, we have a medium in which there are bound electrons, the electrons are not free in a dielectric like unlike in a metal. So, they are bound electron. So, when the electric field is acts upon them the electrons are only slightly displaced by the electric field. So, first let us see how this polarisability may be calculated in the static case.

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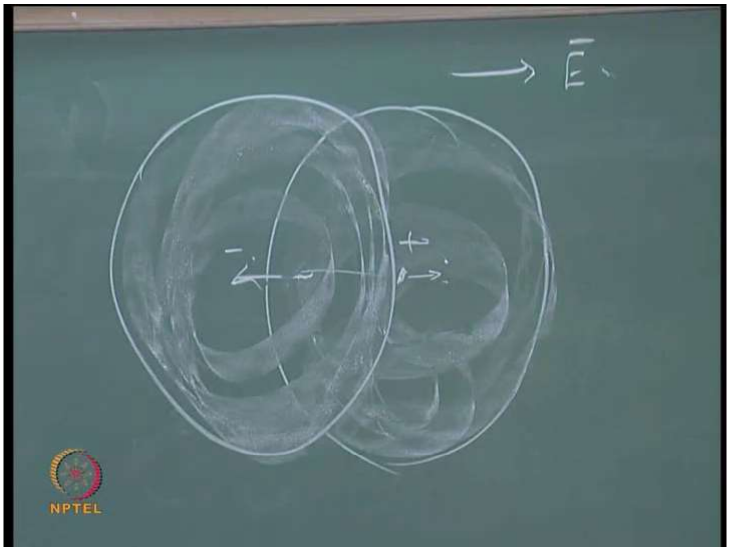

So, this can be done because we have already seen how in the presence of an applied electric field in the case of spherical atom the electronic cloud with the nucleus, the nucleus in the presence of an applied electric field how is the nucleus gets displaced slightly while the electronic cloud is replaced much more. And so there is the rigid shift of this electronic cloud. So, the centers of positive and negative chargers are displaced relative to each other say by an amount x. So, now, we can use Gauss theorem to calculate the polarisability.

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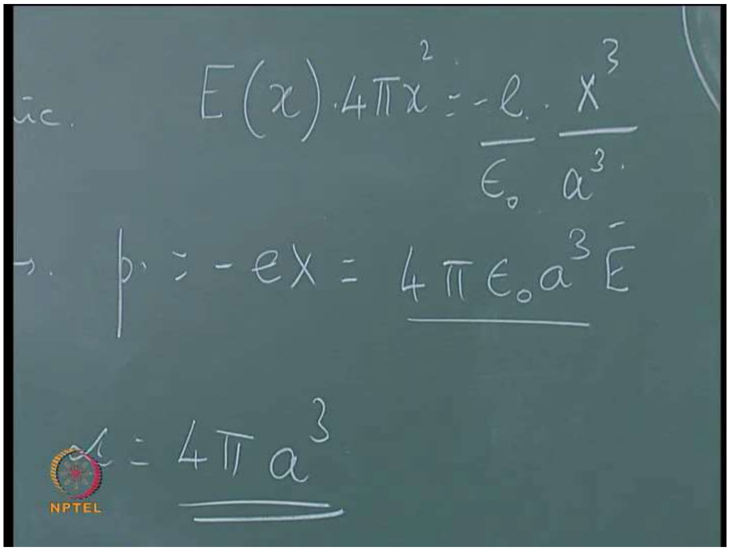

$$E(x) \cdot 4\pi x^2 = \frac{-e}{\epsilon_0} \cdot \frac{x^3}{a^3}$$

$$p = -ex = \underline{4\pi\epsilon_0 a^3 \bar{E}}$$

$$\alpha = \underline{\underline{4\pi a^3}}$$

Because Gauss theorem say that is the flux due to an electric field and that is equal to the charge which is minus e is the electronic charge times x cube by a cube. Because in both cases will be four-third pi x cube and four third pi a cube I am writing four third pi cancels of and this is all we are left with. So there we have e x equal to 4 pi epsilon naught a cube E, and this is what we call the dipole moment induce dipole moment. And therefore, we can see from the definitions of the polarisability that the polarisability alpha is four pi a cube, so it is proportional to the atomic volume, this is of course, in the static situation.

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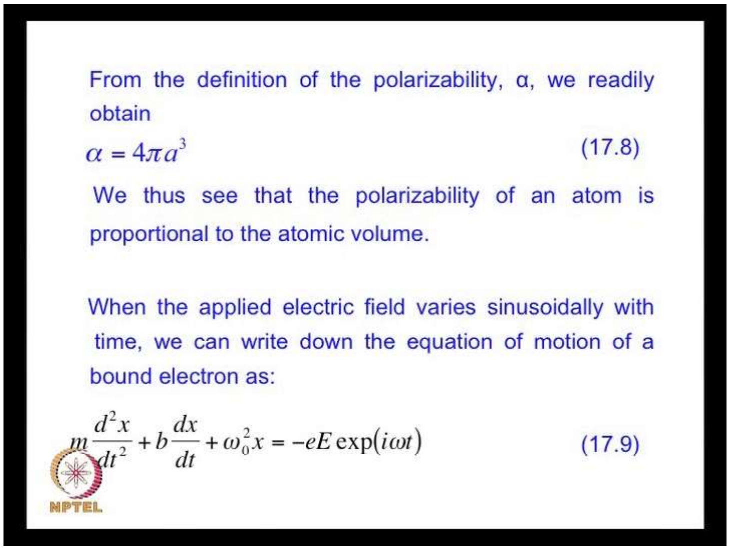

From the definition of the polarizability, α, we readily obtain

$$\alpha = 4\pi a^3 \qquad (17.8)$$

We thus see that the polarizability of an atom is proportional to the atomic volume.

When the applied electric field varies sinusoidally with time, we can write down the equation of motion of a bound electron as:

$$m\frac{d^2x}{dt^2} + b\frac{dx}{dt} + \omega_0^2 x = -eE\exp(i\omega t) \qquad (17.9)$$

But when there is a time dependent or an oscillating electric field the response of the electron a given electron can be written using the equation of motion which is m d square x y d t square that the Mossotti acceleration by Newton's law plus b times d x by dt. This is because the electronic motion always experiences a resistance for its motion. And this resist the force by unit moss is the taken to be proportions to this speed or velocity then the bound electron has it is bound with a kind of elastically or to the atom with a kind of force which can be represented in the simple approximation.

The simplest model by harmonic oscillators of natural frequency x omega naught, so that I can write omega naught square x equal to minus v e e to the power of i omega t, so that is the equation of motion which is to be solved and be assume, since I am writing only the time-dependent here. So, i has so assume that the displacement also has a form e to the power i omega d, so that there might be a full shift, but we will just consider this omega naught square here is just the k by m where k is the time force constant.

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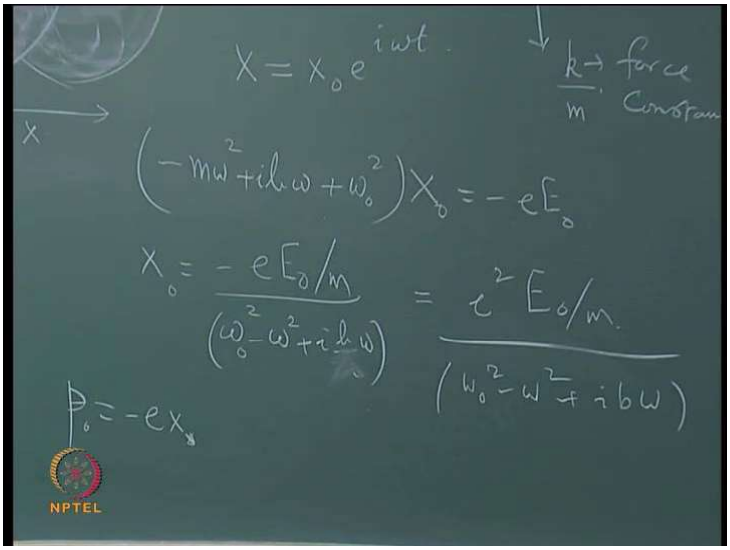

So, using the, we can immediately write m omega square plus be omega i plus omega naught square times x naught equal to minus e naught. So, that x can be written it is not in written as well we will write a b by m as b you will just define this by the damping per unit moss, so that the simpler left with this. So, immediately we can calculate the dipole moment because the dipole moment in this case is minus e x naught at the amplitude of the oscillating dipole moment and therefore, this will be and since we have the dipole moment the protocol polarization is just n times p.

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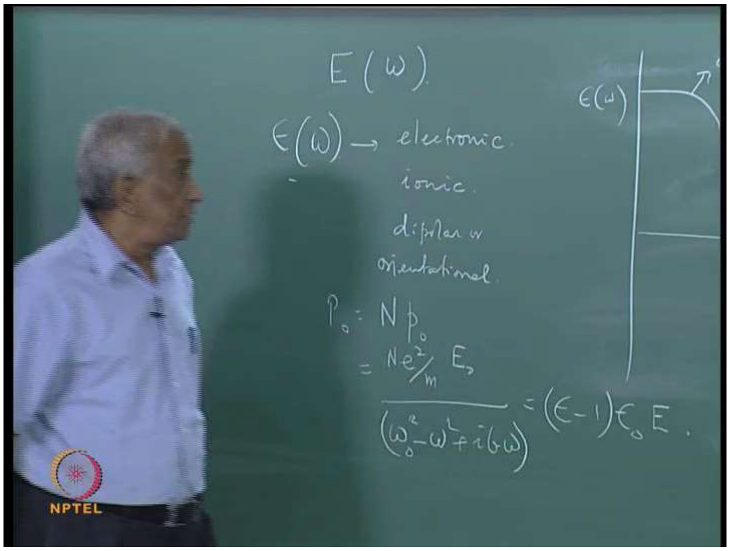

So, this is the naught and therefore, this will simply be n is square by m e naught by omega holes square minus omega square plus i b omega and therefore, since the relation between this is what gives you the epsilon. So this can be written as epsilon minus one, so that we get the directory constant and because of this factor, i here this becomes a complex quantity and therefore, the epsilon is in general complex.

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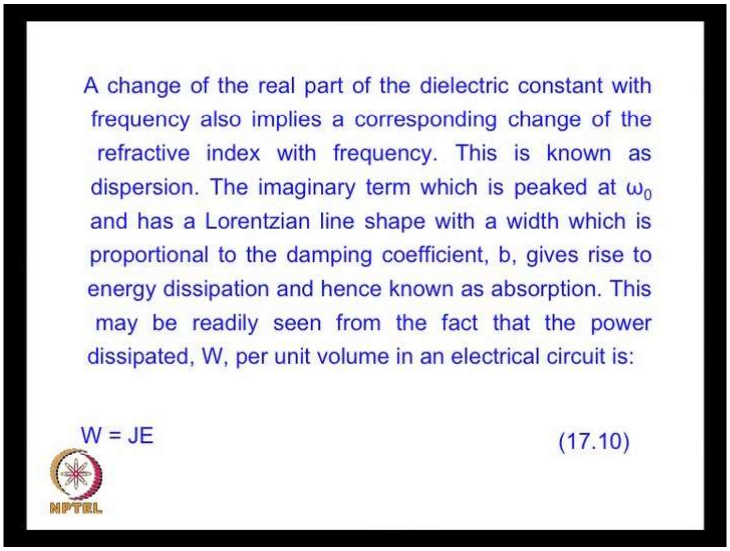

A change of the real part of the dielectric constant with frequency also implies a corresponding change of the refractive index with frequency. This is known as dispersion. The imaginary term which is peaked at ω_0 and has a Lorentzian line shape with a width which is proportional to the damping coefficient, b, gives rise to energy dissipation and hence known as absorption. This may be readily seen from the fact that the power dissipated, W, per unit volume in an electrical circuit is:

$$W = JE \qquad (17.10)$$

So, let us write it as epsilon prime plus i epsilon double i. So, we have the complex dielectric constant. So, the real and imaginary parts are there. So, it can be separated into real and imaginary part and we have these are plotted here.

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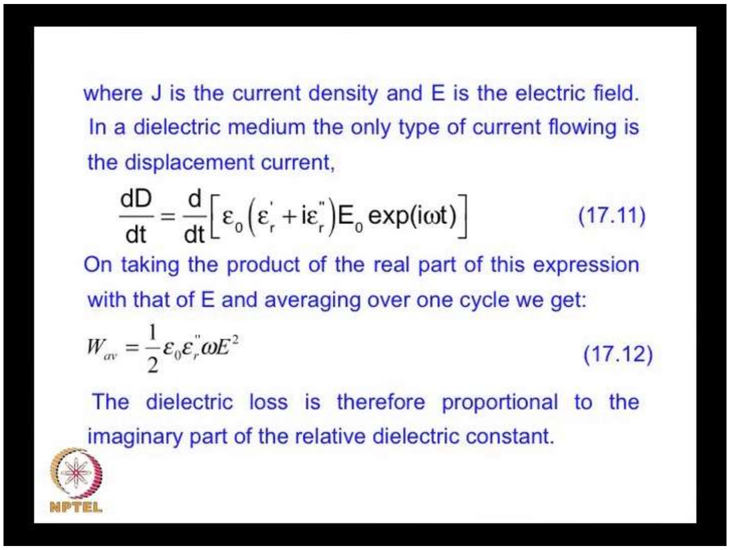

where J is the current density and E is the electric field. In a dielectric medium the only type of current flowing is the displacement current,

$$\frac{dD}{dt} = \frac{d}{dt}\left[\varepsilon_0\left(\varepsilon_r' + i\varepsilon_r''\right)E_0\exp(i\omega t)\right] \qquad (17.11)$$

On taking the product of the real part of this expression with that of E and averaging over one cycle we get:

$$W_{av} = \frac{1}{2}\varepsilon_0\varepsilon_r''\omega E^2 \qquad (17.12)$$

The dielectric loss is therefore proportional to the imaginary part of the relative dielectric constant.

They are given the real and imaginary parts are given in the equation here and therefore, you can see that they are plotted here the real and imaginary parts of the direct constant as a function of frequency.

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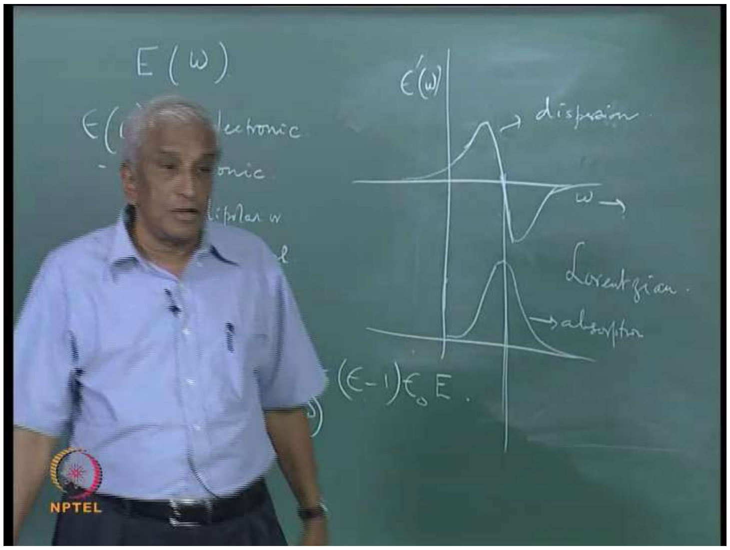

So, the real and imaginary parts look like this. So, I take epsilon prime omega as a function of frequency in the neighborhood a resonances then I have something like. So, that is the kind of response. So, this is real part of the dielectric constant while imaginary part below. So, these two so the imaginary part is the maximum. So, this is what is known as a Lorentzian, because these the dispersion part and this is the absorption. So, dispersion and absorption the real part in the dielectric constant is a associated with dispersion while the imaginary part of the dielectric constant is relative to the absorption. Now we saw that there are several other mechanism will not consider the ionic in detail. Now we will instead go to the other case where there are permanent dipoles in the system.

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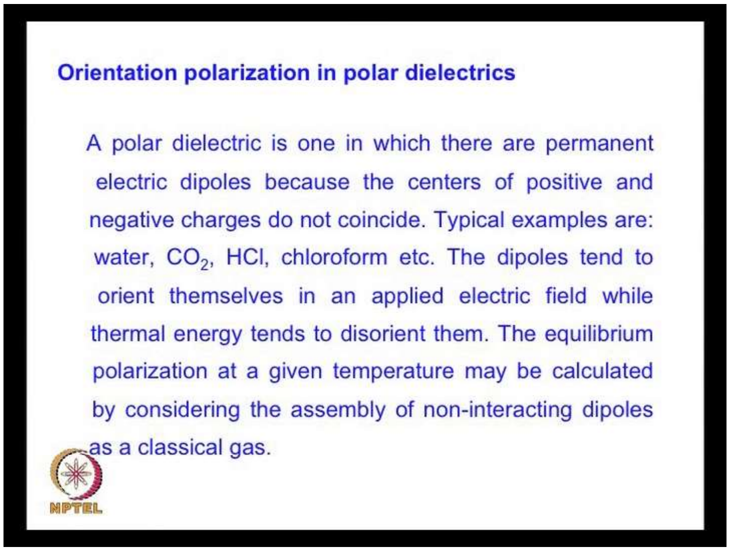

Orientation polarization in polar dielectrics

A polar dielectric is one in which there are permanent electric dipoles because the centers of positive and negative charges do not coincide. Typical examples are: water, CO_2, HCl, chloroform etc. The dipoles tend to orient themselves in an applied electric field while thermal energy tends to disorient them. The equilibrium polarization at a given temperature may be calculated by considering the assembly of non-interacting dipoles as a classical gas.

So, the medium in the dielectric medium is what is called the polar dielectric for example, water water has a large dipole moment.

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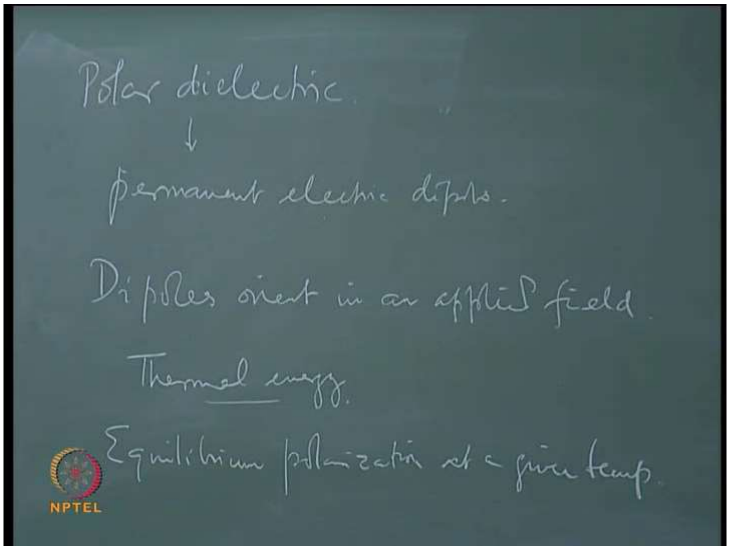

Polar dielectric

↓

permanent electric dipoles.

Dipoles orient in an applied field.

Thermal energy.

Equilibrium polarization at a given temp.

So, if you have a polar electric this means that there are permanent electric dipole moment as the distinct from induce electric dipoles which persist only as long as there is an applied electric field, for example, some typical is abstractions are water carbon dioxide. So, a hydrogen chloride chloroform etcetera they are all highly polar dielectric. So, what happens is that these dipole tend to orient themselves orient in an applied field. So, it is this orientation which gives you the polarization. In this cases because if do orient more as a orient more and more like get aligned alone the electric field there is the the polarization increases. Now this orientation tendency is opposed by the thermal energy this is some as thermal energy which tends to restoral the disorder, which tends to thermal energy is always lens leads to disorder the dipoles.

So, there is a ordering influence due to the applied field and which completes with these this ordering influence the equilibrium polarization at any given temperature at a given temperature that is what determine the dielectric constant. So, this can be easily calculated and this is the temperature dependent process unlike the induce dipole mechanism or the electronic ionic mechanism. So, this is the temperature dependent because the thermal energies more. So, there is a temperature dependence for the orientational polarized ability. So, this is now the orientational contribution to the polarized ability can be separated from the electronic for ionic contribution because you measure the dielectric constant as a function of temperature a different temperature and then the temperature dependent part comes from the orientation of mechanism. So, let us consider this mechanism, we have let us write down what is the polarization.

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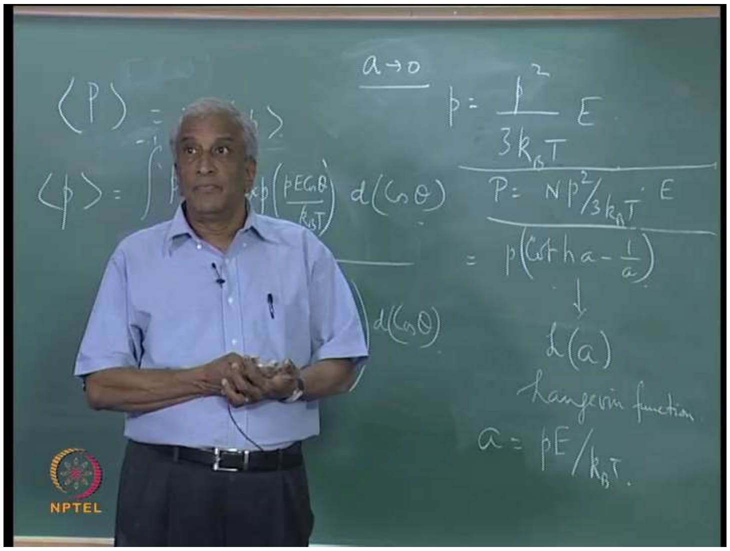

The polarization is P - it is a thermal average statistical average which is n times the individual average of the individual dipole moment. Where this average p is integral p cos theta, this is the projection of the dipole moment of the permanent dipole in the direction of the applied field times. There is the usual Maxwell Boltzmann factor statistical factor times b f cos theta zero to pi zero to one minus one point to minus one exponential p e cos theta by k b t and d of cos theta.

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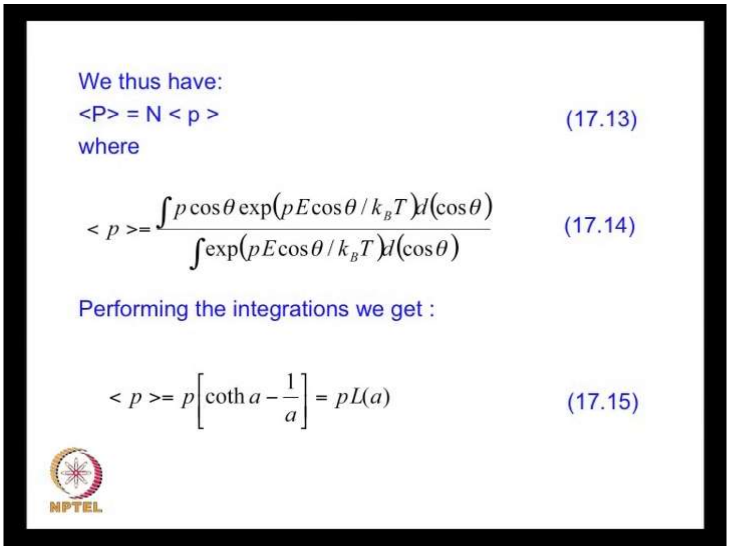

We thus have:

<P> = N < p > (17.13)

where

$$< p >= \frac{\int p\cos\theta \exp(pE\cos\theta / k_B T) d(\cos\theta)}{\int \exp(pE\cos\theta / k_B T) d(\cos\theta)} \quad (17.14)$$

Performing the integrations we get :

$$< p >= p\left[\coth a - \frac{1}{a}\right] = pL(a) \quad (17.15)$$

Now this can be evaluated you get this as this is the functional dependent this function is usually known as the langevin function l of a.

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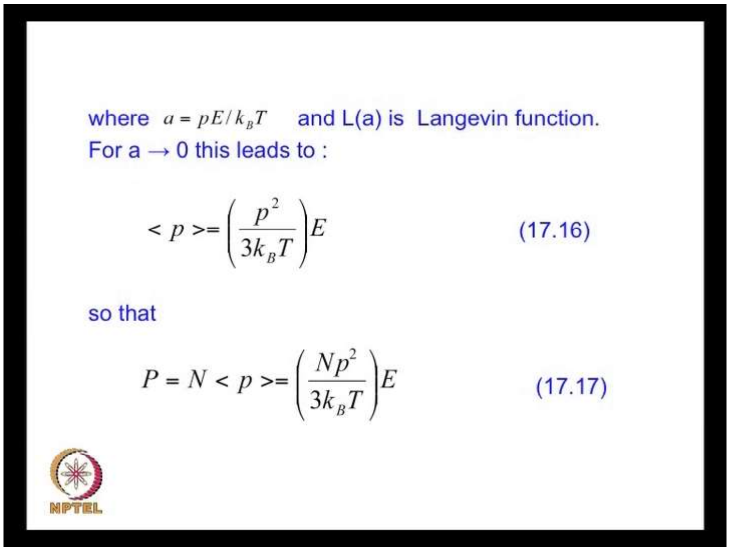

where $a = pE/k_B T$ and L(a) is Langevin function.

For a → 0 this leads to :

$$< p >= \left(\frac{p^2}{3k_B T}\right)E \quad (17.16)$$

so that

$$P = N < p >= \left(\frac{Np^2}{3k_B T}\right)E \quad (17.17)$$

Now, a is p E by k B T for a tend into zero that is p E by k B T tends to zero that is in small applied fields at very high temperatures P goes to p square by 3 k B T times E. So, the orientation of all receptivity is just is square by 3 k B T. And therefore, the total polarization is p equals. So, that is why orientational polarization as of and it has an inverse temperature of one temperature dependence for the absolute temperature T. So, you have a dielectric susceptibility which varies inversely with the temperature and like the electronic ionic contribution.

So, if you measure the dielectric constant as a function of temperature and plot it as of versus 1 by T, you will get a straight line for the orientational contribution which may therefore, be separate. Now this alignment, which we talk about these the equilibrium alignment of the dipoles is not of course, an instantaneous process and is govern by a relaxation time. So, there is a time dependent polarization which is due to the alignment of these dipoles this time dependence can be written.

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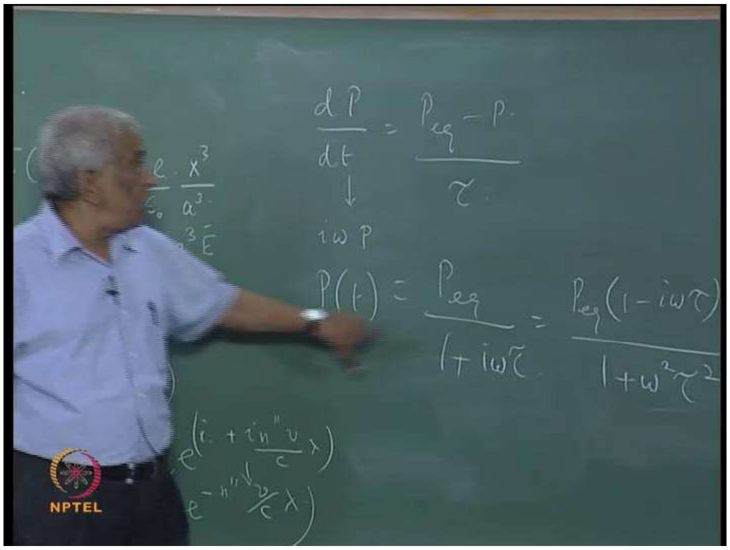

In terms of the time dependence of the polarization can be written as p equilibrium minus p by tau where tau is a characteristic relaxation time for the dipoles to get align and p equilibrium the equilibrium polarization. So, if you have this we can write this as i omega p therefore, this give you the rate equation which is p equal to p equilibrium by one minus i tau. And so one plus and this is p equilibrium one minus i omega tau by one plus omega square holes square. So, again you can see that the equilibrium polarization is complex and therefore, the relative dielectric constant due to this mechanism is also a complex quantity again the real part of which is the dispersive part and the imaginary part is the absorption. So, this is the contribution which we showed in the figures.

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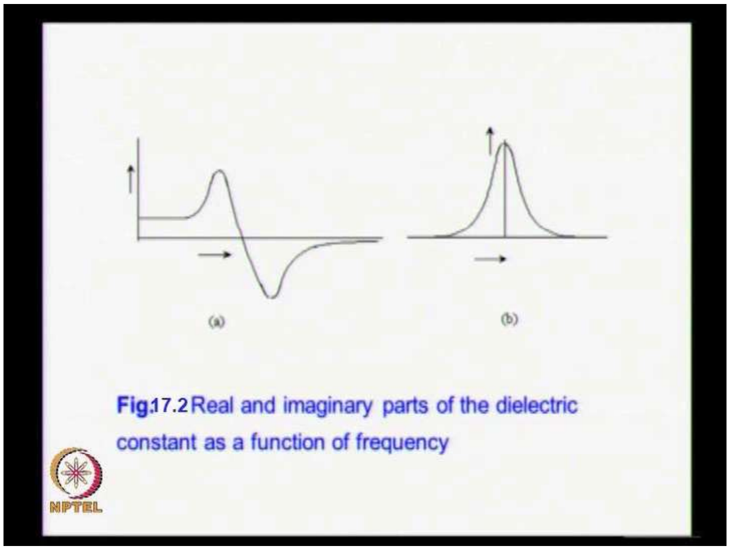

Fig17.2 Real and imaginary parts of the dielectric constant as a function of frequency

We now come to a very important related concept namely that of ferroelectric phase transition. We talk at the beginning of this lecture course about thermodynamic phase transition such as the gas to liquid transition and then the liquid to solid phase transitions.

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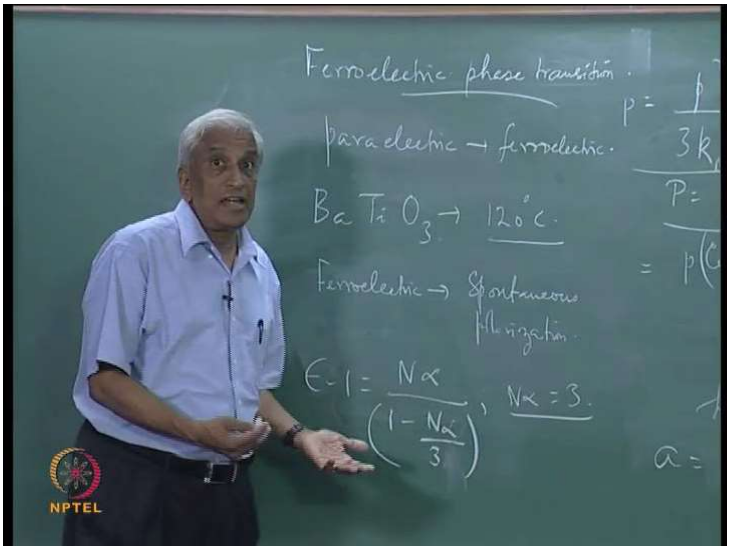

We are going to talk about another kind of phase transition, which takes place in the dielectric material which is known as the ferroelectric phase transition. So, an important this is an important class of phase transitions which go which take the material from a para electric to a ferroelectric this at low-temperature. For example, variant barium titanate is a very well-known ferroelectric material which has a ferroelectric phase transition temperature in the neighborhood of 120 degrees Celsius. So, belong hundred and twenty degrees Celsius it is ferroelectric about this it is a paraelectric. What do you mean by a ferroelectric material a ferroelectric material is characterized by existence of what is known as a spontaneous polarization there is a spontaneous polarization normally till now we have been talking about situation where an applied electric field.

Hence to create a polarization induce a polarization or orient the dipoles to produce a polarization net polarization. So, here these an entirely different situation where even in the absence of an applied electric field there is a polarization a polarization is present even when there is no applied electric field. So, it is call spontaneous polarization ferroelectrics are materials which are characterized with the existence of a spontaneous polarization whereas, a para electric is one in the there is no spontaneous polarization and you need an applied electric field in or at create a polarization now this ferroelectric behavior may be qualitatively understood from the Clausius Mossotti relationship.

Now if you take this we have something like so this let you recall this this is the cloud of Clausius Mossotti relation and look at if you look at the denominator this denominator will become zero than n alpha equal to three then there's become zero and therefore, the a dielectric constant singular it blows up. So, this means there would be a non- zero polarization even than the field is zero this is known as the polarization catastrophe where they are dielectric constant the polarization blows up and goes to infinity because of this behavior. So, when this condition is made.

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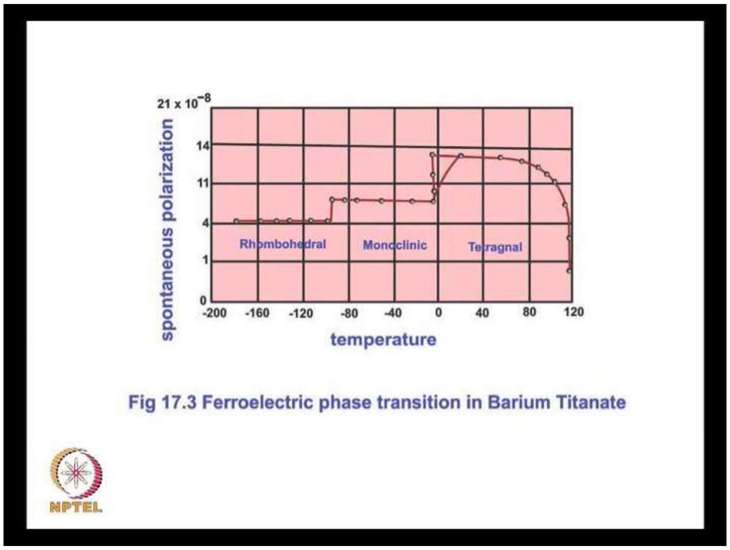

Fig 17.3 Ferroelectric phase transition in Barium Titanate

So, this behavior is illustrated in the next picture where the ferroelectric phase transition is shown in barium titanate at 120 degree Celsius. So, there is a polarization catastrophe.

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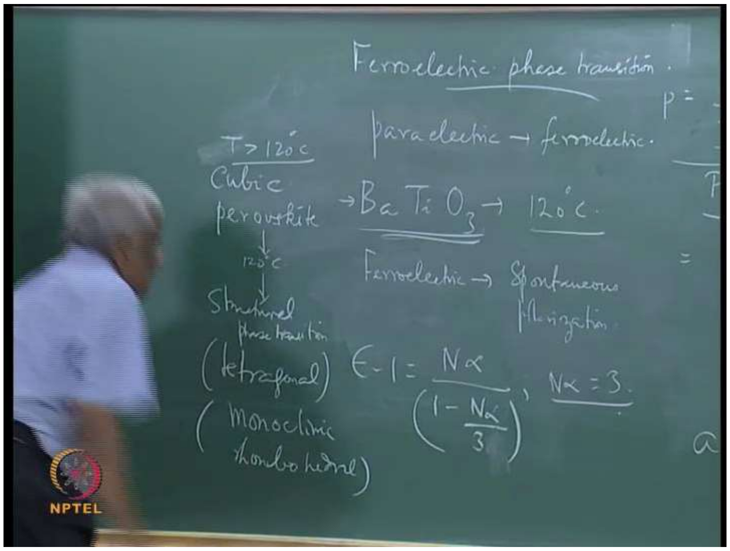

Ferroelectric phase transition.

$T > 120°C$
Cubic
perovskite
↓ 120°C
↓
Structural
phase transition
(tetragonal)
(Monoclinic
rhombohedral)

paraelectric → ferroelectric.

→ $BaTiO_3$ → 120°C.

Ferroelectric → Spontaneous polarization.

$\epsilon - 1 = \frac{N\alpha}{\left(1 - \frac{N\alpha}{3}\right)}$, $N\alpha = 3$.

So, above the transition temperature of a 120 degrees Celsius barium titanate exist in the cubic phase. This structure is a cubic structure which is known as the perovskite structure above where a conceive cool it below 120 degrees Celsius. There is a structural phase transition the structure the crystal structure changes along with the ferroelectric phase transition this becomes a tetragonal structure below 120 Celsius. So, and then subsequently becomes some monoclinic rhombohedral.

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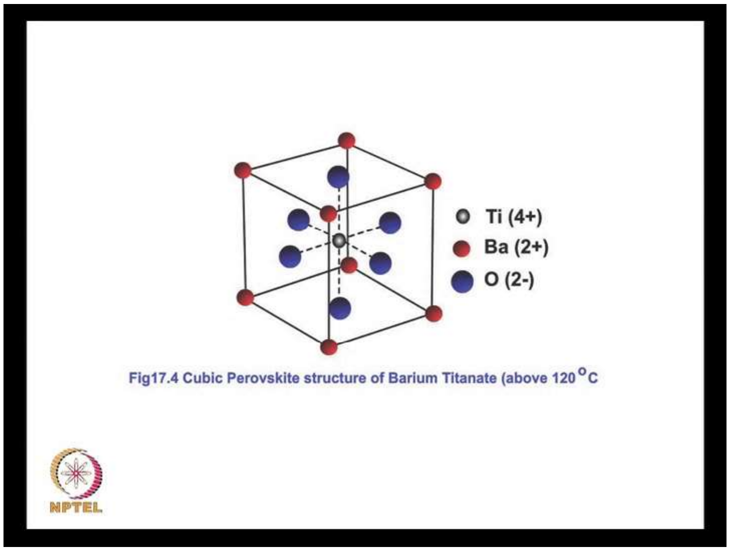

Fig17.4 Cubic Perovskite structure of Barium Titanate (above 120 °C

So, this is shown in a this picture the cubic ferrite structure a barium titanate is shown in the figure. This is the structure of the barium titanate the titanium ions or at the centre of this cubic cell and surrounded by an oxygen atoms and then the barium atom occupy the corners of this cube.

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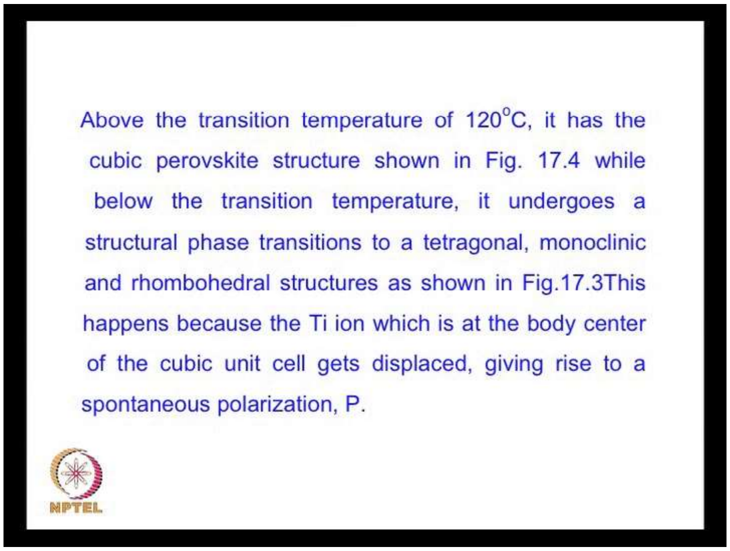

Above the transition temperature of 120°C, it has the cubic perovskite structure shown in Fig. 17.4 while below the transition temperature, it undergoes a structural phase transitions to a tetragonal, monoclinic and rhombohedral structures as shown in Fig.17.3This happens because the Ti ion which is at the body center of the cubic unit cell gets displaced, giving rise to a spontaneous polarization, P.

So, this is the structure at high temperatures, but once you cold the low 120 Celsius. This goes interior tetragonal structure because the titanium ion which is at the body centre of the cubic unit cell get displace and because of these displacement there is a spontaneous polarization this is the mechanism of the buildup of the spontaneous polarization in the ferroelectric.

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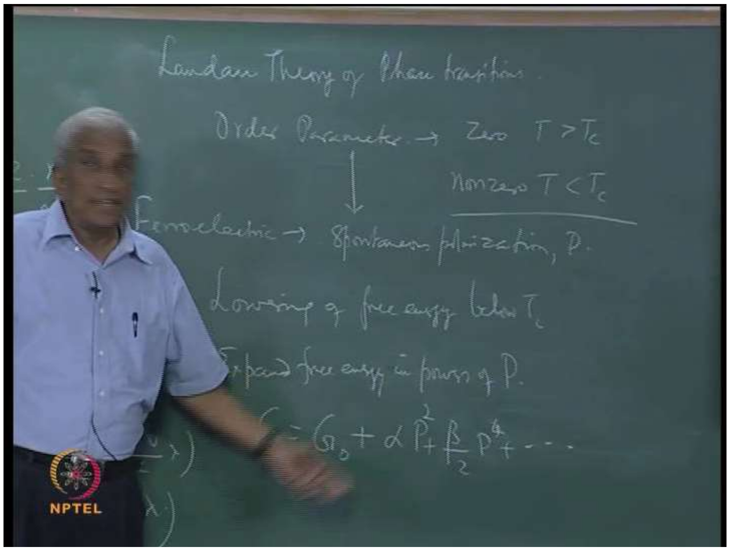

Landau Theory of Phase transitions.

Order Parameter → Zero $T > T_c$

Nonzero $T < T_c$

Ferroelectric → Spontaneous polarization, P.

Lowering of free energy below T_c

Expand free energy in powers of P.

$$G = G_0 + \alpha P^2 + \frac{\beta}{2} P^4 + \dots$$

Now, the general features of a ferroelectric phase transition understood in terms of landau theory of phase transition the general approach of landau theory is to define an order parameter. So, this is the crucial feature of the landau theory of phase transition defined an order parameter the order parameter can be any physical quantity which is zero or about the transition temperature and non-zero below. So, that the general definition of the order parameter in this presence case of a ferroelectric material the order parameter is the spontaneous polarization; obviously, the there is a no spontaneous polarization above t c the transition temperature and heat the spontaneous polarization existent therefore, is nonzero below t c. So, that is the order paramagnetic in this case the next step in the landau theory which is a thermodynamic theory.

This thermodynamic theory always says why should there be a phase transition, the phase transition takes place and the change there is a change in phase in this case the structural phase. And therefore, the ferroelectric phase because of a lowering of the free energy below T c. So, the free energy becomes lower in the order phase and therefore, this lowering as the free energy favors the existence of the order phase over the disorder phase. So, that is the basic explanation thermodynamic information given by the landau theory. So, how do you find this. So, you expand the free energy in powers of the order parameter in this case these spontaneous polarization.

So, we write this is the gift free energy g which is written as G naught plus alpha P plus beta by 2 p square plus etcetera P square meter the power four etcetera terms in p p cube etcetera do not exist because this as such as favorite state and central symmetry. And therefore, order powers will be vanished under the operation of the centre inversion therefore, only even powers p square p to the power four etcetera are there; all for beta are constants which have to be determine by the minimization of the ferroelectric.

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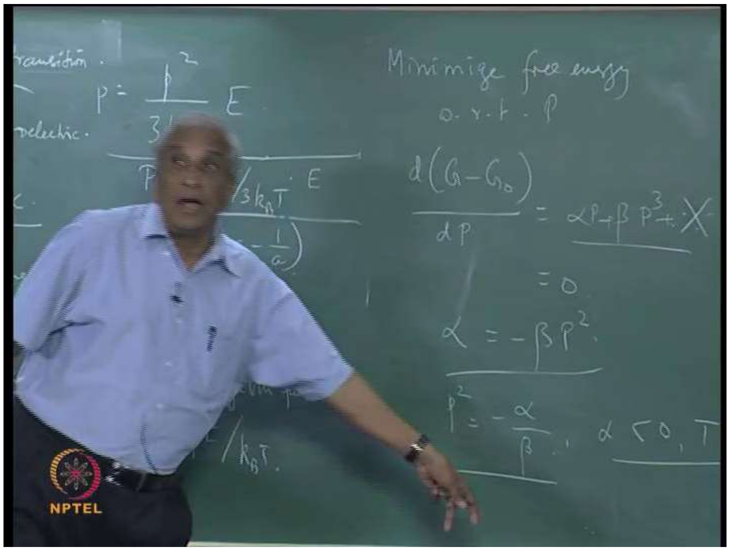

So, the entire exercise is to minimize this free energy with respect to variations in the order parameter changes in p. So, if i do that this is the free energy deference and this is minimize by taking the differential coefficient with respect to p and that will be alpha plus alpha p plus beta b cube neglecting the higher order terms was etcetera which are neglect. So, this is the derivative all the free energy difference with respect to p and we set this equal to zero for a minimum this give me alpha equal to minus beta p square or the square is minus alpha by beta. So, the minimum is characterized by a spontaneous polarization, which is minus alpha by beta. So, this is the order parameters. So, we expected to be zero above t c and nonzero below t c. So, in order that this should happen and p will be real. So, p square should be a positive definite quantity therefore, we take alpha to be less than zero for t less than t c alpha is negative, so that minus alpha by beta is positive when beta is also positive.

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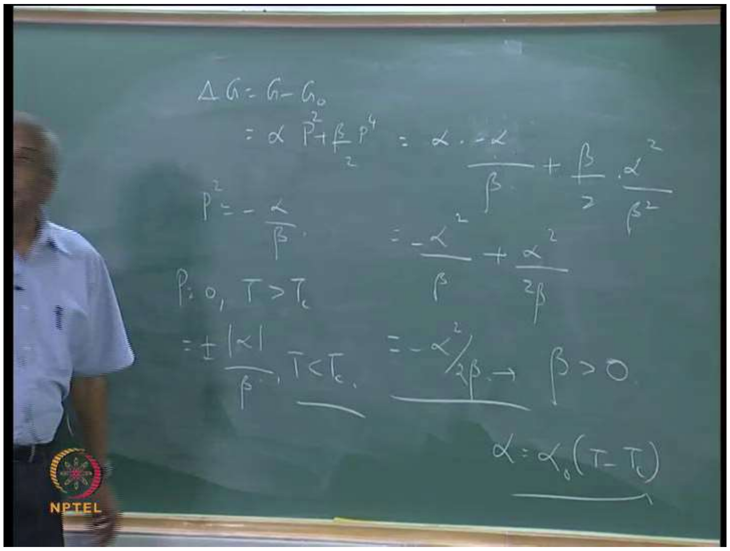

And the corresponding free energy difference when we substitute this delta G equal to G minus G naught equal to alpha P plus beta by 2 alpha P square plus beta by 2 P to the power 4. And substituting p square equal to minus alpha by beta for the minimization condition, we get this to be alpha time minus alpha or mod alpha by beta plus beta by two into alpha square by beta square. So, this gives me alpha square by beta minus plus this. So, this will be I can write this as alpha by 2 into minus alpha. So, this becomes minus alpha square plus alpha square by two beta which gives me minus alpha square by… So, one can see that there is a reduction in the free energy below T c. So, the free energy is lower we expect provided beta is positive and alpha now can be taken to be a function of T.

So, alpha can be written as alpha naught times T minus T c, so linear function of the temperature. So, we take these to be a alpha changes sign at t c and become positive making the para electric very energetically more stable at higher temperatures. So, the simplest analytical form is this and therefore, we have equal to zero for t equal to t c and p equal to zero for t greater than t c and equal to plus minus mode alpha by beta for t less than this to the power half taking square root for p square. So, the landau theory thus predicts a spontaneous polarization which goes as alpha to the power half or p goes as T minus T c or T c minus T, so half so the temperature dependence predicted by the landau theory for the spontaneous polarization.

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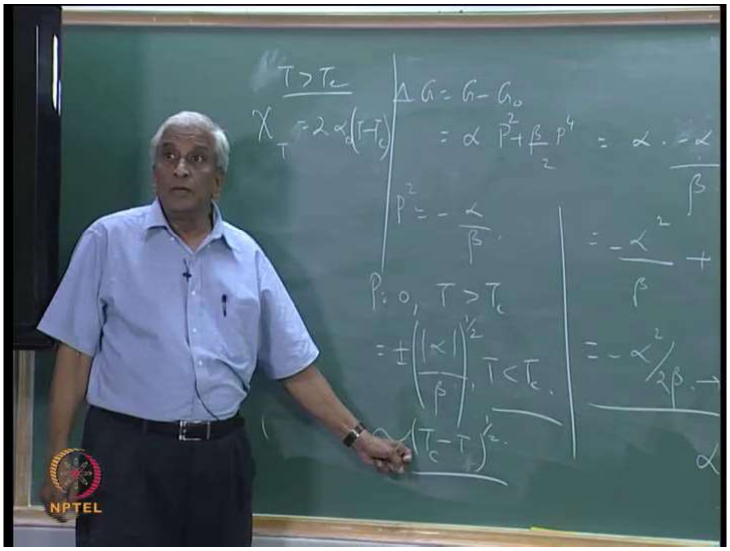

And above T c the para dielectric susceptibility goes as T greater than T c, the susceptibility goes as two alpha naught into T c, T minus T c as we conjunct readily. So, this is the temperature dependence for the susceptibility above the phase transition and this is the temperature dependence predicted for this spontaneous temperature dependence as the spontaneous polarization below T c. So, these are features which have been verify. Ferroelectric compounds in general fall into three main classes. One is the perovskite such as the barium, titanate, which you have discussed. Then there is another family, which is called the roselle salt type compound. And then a third class for which the prototype is the potassium dihydrogen phosphate type known as hydrogen bound it ferroelectrics. Dielectric in which adjacent dipoles are lined up not parallel to each other as in this case, but anti parallel to each other also exhibit a shop discontinuity in the relative dielectric constant at the transition temperature, these are known as anti ferroelectrics. In the next lecture, we will consider piezoelectric another important class of dielectric material.