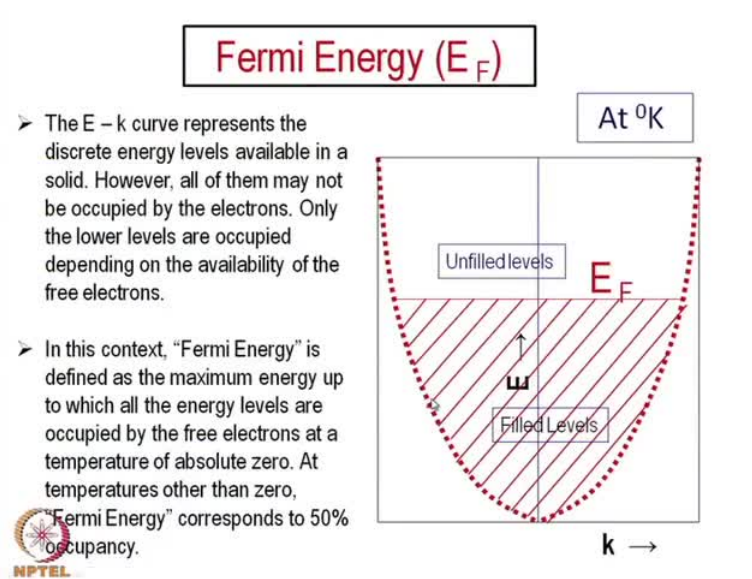


**Advanced Ceramics for Strategic Applications**  
**Prof. H. S. Maiti**  
**Department of Mechanical Engineering**  
**Indian Institute of Technology, Kharagpur**

**Lecture - 12**  
**Electrical Conduction in Ceramics (Contd.)**

This is in continuation of our discussion on electrical conduction in ceramic materials. We have earlier discussed about the two basic concepts of electrical conduction and parameters, which are important in describing the electrical phenomena in different materials. We have also started discussion about the various theories, would forward for the explanation of conduction behavior particularly in metals to start with. We have already considered the, so called ideal gas model for the electrical behavior of metals and then took up the field electronic theory of the metals.

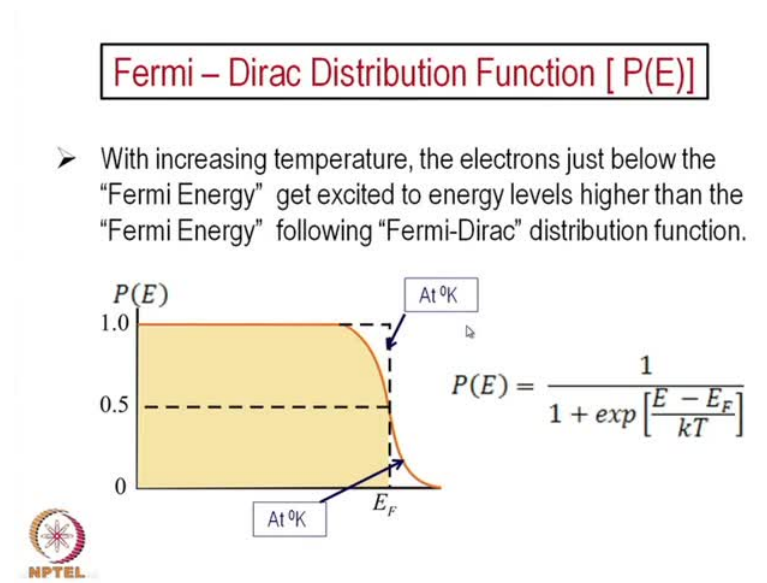
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In that context we saw the energy diagram with respect to k factor and it was a parabolic function and we are also derive defined the fermi energy, that is the highest energy up to which the energy states are filled up depending on the available free electrons in electrical solid, and although it has been, we have drawn at two-dimensional curve, but actually it is a three-dimensional figure, and in also we mentioned that this energy are actually discrete energy levels, they are not a continuous energy levels as per the poly (( )) principles.

So, there all which is expected in any free electron. So, they are actually quasi continuous carves and that is the reason some dots have been (( )), they are along the line. Next we talk about what is the temperature effect? When you... This is what we get at absolute 0 the e verses k curve is propositional to k square.

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If we want to look at the temperature effect of this distribution of the kind of occupancy, we had seen either there is a 100 percent occupancy or there is a 0 percent occupancy. So, depending on the available electrons, these are fully occupied 100 percent occupancy and then about that there is a 0 present occupancy, there is absolutely no electron available, although energy states are there. If the energy if the electrons can somehow acquire higher energy from external sources, it can go to the higher level.

However, there are two ways by which the energy electrons can basically acquire some additional energy. One is the external electric field; so, that is possible, so under that conditions some of the electrons will acquire higher energy and go to the higher energy level about, so called fermi energy. There is other way of acquiring energy that is post by temperature. So, if the electrons acquire additional energy from the thermal energy supplied to it. Then, we have to consider how this distribution changes and that is given by, so called fermi-dirac distribution function P E P, as a function of E.

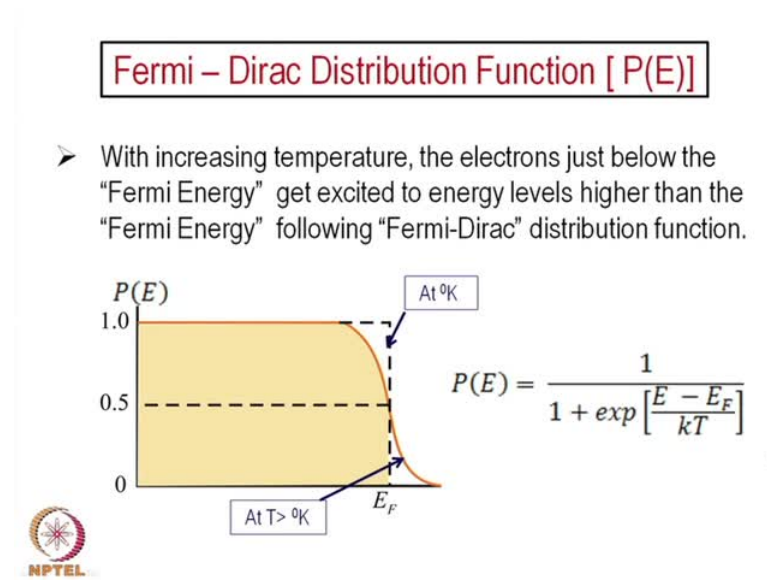
So, it increasing temperature the electrons just below the fermi energy get excited to the energy levels higher than the fermi energy, following fermi-dirac distribution function.

This has been the energy diagram brought as. So, this is the energy, which was there in the vertical axis, here in the horizontal axis and here it is the probability. Is the probability function of occupancy of a particular energy stack that means this energy take what is the occupancy factor. That is 0 percent occupancy, 5 percent occupancy or 100 percent occupancy.

So, this one means it is fully occupied. So, these energy levels up to this is fully occupied and the distribution function is, can we express in this manner  $P = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$ , once again  $k$  is the boltzmann constant and  $T$  absolute temperature,  $E$  the actual energy of consideration and then  $E_F$  is this energy that is the fermi energy, which we have seen earlier as this energy. So, this is fermi energy, we are plotting this called in this manner. So, this was the vertical axis  $E$  here and they are it is the horizontal axis. There is no  $k$  term is not there it is  $k$  is a boltzmann constant here, that one as remember.

So, this probability function, if you plot it looks like this. So, this is at  $T$  equal to 0 at 0 degree Kelvin, that means this is a rectangular curve rectangular plot. Which means up to  $E_F$  up to  $E_F$  the fermi energy the probability value factor is 1, which means fully occupied or full occupancy factor is 1 of 100 percent occupancy is 1. So, that happens at 0 degree kelvin or absolute 0. So, the curve is like this as per the dotted line here, suits a rectangular or a complete discontinuity at  $E_D$  from 100 percent occupancy to 0 percent occupancy, here and then it continuous. Where as if... I think there is some mistake here, it is not at 0 degree Kelvin, it is  $T$  greater than 0 degree Kelvin. Let me see whether I can make this change here itself.

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At T greater than 0 degree Kelvin, this is at 0 degree Kelvin. Whereas at T greater than 0 this becomes the kind of situation, it changes more or less in this passion, we look in to that later more details. Basically, what it means very close to the E F very close to the E F, the electrons which we are having the energy is very close just below E F, will acquires some additional energy from thermal energy there will absorbs thermal energy, because of the hot temperature and they will cross over cross over the fermi energy and go to the higher level.

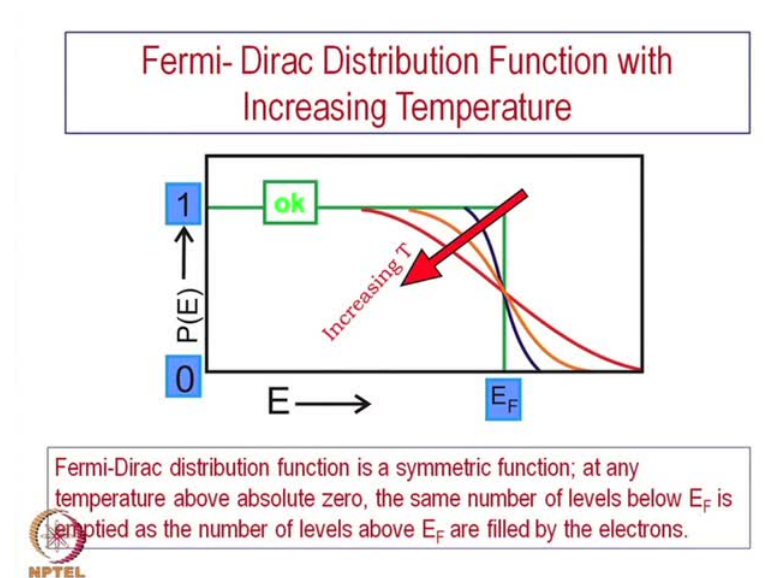
So, some of the energy, some of the electrons will be empty in this place will empty this place and go to the additional space here, for this is higher energy then E F. So, there will be again a distribution from 0 it will increase to 1 occupancy, but higher is the energy level, lower is the occupancy factor and closer to the energy level, that means the closer to E F higher the occupancy factor. So, it will increase from here, from it is 0 occupancy factor beyond this point there will be no occupancy the energy states will be completely empty, but up to this there will be some finite occupancy and then that quantity will increase slowly and becomes 1 at a temp at a energy little lower than the fermi energy.

So, basically it means that some of the electrons have been very energy is very close to the E F, we acquired additional energy and go above E F. So, that original definition is not going to hell in more. So, in this condition at temperature is greater than absolute 0, it

is not be highest energy level occupied the occupancy there, it is more than that, but at  $E_F$  the occupancy is 50 percent.

So, this line crosses this vertical line at 0.5. So, for  $E_F$  the at fermi energy the occupancy factor will be 50 percent and less 50 percent will be empty. Whereas, more electrons will go above, some amount of the electrons are some fraction of the electrons will go above  $E_F$  and occupy higher energy levels. That precisely it says the fermi-dirac statistics or fermi-dirac distribution function that is a very very important concept, where it looks at the temperature effect of the occupancy of the energy levels of the electrons at different temperatures.

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This is also almost the same curve, but at different temperatures, same portability function  $E$  as a function of  $E$  and one can see at  $E_F$  there are three different temperatures; temperature is increasing in this direction. So, this is at 0 k or absolute 0 green one, I just take step jump a step this connectivity, step change here from suddenly from 100 percent it goes to 0 percent at  $E_F$  and that happens at 0 absolute 0, at as you increase the temperature the curve changes and from steeper to it becomes a more flatter curve if more flatter curve. But all through curves go through this point  $T$  equal to 0.5. So, 50 percent occupancy, that do not change that is independent of the temperature.

So, only at 0 degree kelvin it is 100 percent occupancy otherwise any temperature about 0 degree kelvin it is always 50 percent occupancy. So, that value do not change

irrespective of the temperature and that is very important aspect or important aspect of this distribution function, the fermi dirac distribution function. So, it also means that this area under the curve this area actually is proportional to volume total number of the electrons, which we acquire higher energy and go to the higher energy level acquire additional energy and go to the higher energy level.

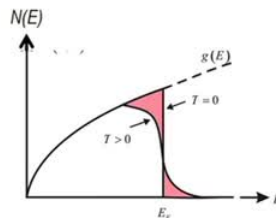
So, this area under the curve, this area bound by curve actually and this area bound by this lower portion because it should be equal. So, this volume this area and this area must be equal. Similarly, for other curves also, the exactly equal number of at the same number of electrons, which leaves their energy level and goes to the higher energy level, so the total number is con. So, with increasing temperature more and more electrons acquire higher energy level, higher energy from the thermal energy, thermal systems and it goes to the higher level above  $E_F$ .

The fermi dirac distribution function is a symmetric function at any temperature above absolute 0, the same number of levels below  $E_F$  is empty as the number of levels above  $E_F$  are filled by the electrons. So, that is what I explained that the area under enclosed by this curves the same on this side as well as on this side, irrespective of the temperature. Whatever, maybe the temperature this area and this area must be same. So, which means basically the same number of electrons will be on the both sides. So, whatever sides will be empty it will be filled up here. So, that is very important aspect of fermi dirac statistics or fermi dirac distribution function, which can be applied for the fermi energy.

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## Density of States

- The “density of states” is the number of electronic energy states per unit energy ( $dN/dE$ ), which is often written as  $g(E)$ .
- The number of electrons per unit energy,  $N(E)$  also depends upon the probability that a given state is occupied,  $F(E)$ .



In addition to normal energy or energy distribution, one can also have another parameter that is known as the density of states. Now, the density of states is the number of electronic energy states per unit energy that is the derivatives  $dN/dE$ , which is often written as  $g(E)$ , sometimes  $N(E)$  also. The number of electrons per unit energy, what is the total number of electrons at any particular level what is the energy energy states. So,  $N(E)$  also depends upon the probability that given state is occupied, that is  $F(E)$  the fermi dirac statistics.

So, it is basically  $g(E)$  is multiplied by  $F(E)$  becomes  $N(E)$ . So, this is  $N(E)$  the... once again this is the energy scale and this is any if you plot this then this also becomes a parabolic function and here it will be the  $E_F$  here will be  $E_F$ . So, what you have plotted earlier is basically a probability and here it is the number of actually actual number of electrons, which will be available at particular energy level. So, this has a some amount of similarity the earlier curve for example; at  $t$  is equal to 0 this up to  $E_F$  everything will be again filled up and this will be the distribution function, that means at lower temperature. The lower energy less number of electrons will be there, as higher energy more number of electrons will be there, more number of energy states will be available. So, that is also we can get from  $E_k$  curve.

So, at this temperature this energy level, this will be the number of energy states available, whereas, and this pre this will be the particular line will be the energy levels available. So, higher is the energy level more and more number of energy states are


available and at  $E_F$  it will be the maximum. Once again one can apply the fermi dirac distribution function here and at the temperature greater than 0, this will be the situation.

Some of the electrons closer to the electron just below the  $E_F$  or fermi energy will be excited above the fermi level and again the number of states below and above will be equal. So, this is the variation of what we call the energy density of states at any particular energy level how many states are available, how many energy states are available. So, at 0 it is only 0 whereas, as we increase the energy more and more number of energy states are available, following a parabolic curve.

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**Alternative Definition of Fermi Energy ( $E_F$ )**

➤ As per Fermi Dirac Distribution Function, "Fermi Energy" is the energy at which the occupancy factor is always 50% irrespective of the temperature.



These are mentioned earlier as per fermi dirac distribution function fermi energy is the energy at which the occupancy factor is always 0 irrespective of the temperature. So, this is the definition, which is useful for higher energy higher temperatures, at 0 temperature or absolute temperature, it is the highest energy level up to which the states are occupied. Whereas, if it is a non 0, the temperature is non 0 then this will be a better definition or actual definition that means  $E_F$ , at the under that situation  $E_F$  for the fermi energy is not the highest energy level up to these electrons are available are electrons are occupied energy states are occupied. So, it is only fifty percent occupancy and that is a constant irrespective of whatever the temperature is used.



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### Consequences of the Free Electron Theory (I)

➤ At  $T = 0$  K 
$$E_F(0) = \frac{\hbar^2}{2m_e} (3N\pi^2)^{2/3}$$

Where,  $N$  is the electron density, i.e. the number of electrons per unit volume of the metal

➤ calculations show that  $E_F(0) \sim 5 - 10$  eV

➤ However, thermal energy at room temperature:

$$kT \sim 0.025 \text{ eV} \Rightarrow kT \ll E_F(0)$$



Now, consequences of this free electron theory, these are some of the considerations of free electron theory, we have a  $E$   $K$  curve and there is a energy called fermi energy up to these electrons are occupied and temperature about 0 degree kelvin, some electrons will occupy attain or get excited to a higher level. So, these are the major observations of this theory are outcome of this this theory. So, at 0 degree consequences of what happen at 0 degree kelvin  $E_F$  at 0 is  $\frac{\hbar^2}{2m_e} (3N\pi^2)^{2/3}$ .

So,  $N$  is the electron density, the energy states that is number of electrons per unit volume of the metal, not at density of states it is the number of electrons per unit volume of the metal and calculations show that  $E_F$  at  $E_F(0)$ , that means at temperature 0, it is about 5 to 10 e V electron volt. However, thermal energy at room temperature is much much less, it is about  $kT$  0.025 eV. So,  $kT$  is much much less than the  $E_F$  or the fermi energy at 0 degree kelvin.

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### Consequences of the Free Electron Theory (II)

- Only electrons occupying levels close to the Fermi Energy will participate in the conduction phenomenon since only these electrons can be excited into the higher energy states by the electric field.
- From Quantum Mechanical consideration, energy supplied by the electric field is sufficient to excite electrons from lower to higher energy levels close to the Fermi energy.



Only electrons occupying level close to Fermi level from energy will participate in the conduction phenomenon. Since, only the electrons can be excited into the higher energy states by the electric field. So, that also another important aspect, that only the electrons occupying levels very close to the Fermi level, not because other energy other electrons will need much much larger energy to be excited half of the Fermi level only very only the electronic level are the electrons occupying having energy very close to the Fermi level will get excited, both by thermal as well as by external electric field. From quantum mechanical consideration, energy supplied by the electric field is sufficient to excite electrons from lower to higher energy level close to the Fermi level.

So, all though we have also seen in the Fermi Dirac statistics or Fermi Dirac distribution function, that as a function of temperature or as temperature is increased or more thermal energy is delivered to the system, electrons very close to the Fermi level gets excited. Similar is the case with the applied field, applied field to this system in addition to the temperature. Once again the same thing will happen no electrons having this level of energy will get excited here, only the electrons having very close to the Fermi level energy close to the Fermi level, you will crossover and go to the higher level.

So, that another important aspect is not only the thermal energy, but the interesting are the electrical energy also have similar effect. So, that is what is mentioned here from quantum mechanical consideration energy supplied by the electric field is sufficient to

excite electrons from lower to higher energy levels close to the fermi level or fermi energy. So, that also another aspect of this theory.

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### Temperature Dependence of Resistivity of Metals(I)


If an electron possesses the kinetic energy equivalent to  $E_F$ , one can write:

$$E_F = \frac{1}{2} m_e v_F^2 \quad v_F = \sqrt{\frac{2E_F}{m_e}}$$

Where,  $v_F$  is Fermi velocity, in terms of which

$$\sigma = \frac{e^2 n l_f}{m v_F}$$

Where  $l_f$  is the mean free path



With this one can find out what will be the temperature dependence, if an electron possesses kinetic energy equivalent to  $E_F$ . One can write  $E_F$  is equal to impact it introduces a velocity in terms of the kinetic energy, the fermi energy and that velocity is termed as  $v_F$  fermi velocity. So, half  $m v$  square once again the kinetic energy if the kinetic energy  $E_F$  than and the velocity of the electron is  $v_F$  fermi velocity, than half  $m_e v_F$  square,  $v_F$  is equal to  $\sqrt{2 E_F / m_e}$ . So, the energy of the electron having, the electron having energy of  $E_F$  will have a velocity of this provided  $m_e$  is the mass of that electron.

So,  $v_F$  is the fermi velocity in terms of which,  $\sigma$  the conductivity because the  $(v_F)$  velocity term in the conductivity. So, it becomes  $e^2 n l_f / m v_F$ , where  $l_f$  is the mean free path again again. Some kind of collision as been assumed what exactly its means did not be understood, but this term is some kind of a mean free path because in the way you have define the conductivity term it contains some velocity term, it also contains the distance covered by the charge spices. So,  $\sigma$  is the expression of that, this is the velocity term and this is the distance term. So,  $e^2 n l_f / m$  and the mass.

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### Temperature Dependence of Resistivity of Metals(II)

- It may be shown that because of the wave – particle duality of the electrons the collision is not between the electron and the stationary ion but due to the interaction of the electron wave and the lattice vibration or the phonons.,
- In case of phonon scattering the mean free path is inversely proportional to temperature (K) and thus

$$\sigma \propto \frac{1}{T} \quad \text{As per experimental observation}$$



So, to continue that it may be shown that because of this, the wave-particle duality of the electron the collision is not between the electron and the stationary ion, but due to the interaction of the electron wave and the lattice vibration of the phonons. Since, by this time we are not considering only the particle nature of the electron, we are also considering the wave nature, and that is how the wave vector came and the brown de broglie wavelength also came. So, it is basically a wave and that wave is interacting with the lattice vibration, because the lattice is also vibrating and it has a different modes of vibration and those are called phonons.

So, the collision here is not with the static ion core, but it is the vibrational mode of the ion core and that is possible because you had a wave nature of the electron. So, the electron is also a wave and lattice vibration is also generating some form of waveforms. So, this two will interact and that is what we are talking about the collision. So, this collision and the earlier collision which we consider in the ideal gas theory is a little different. So, their characteristics is also will be different in case of phonon scattering, the mean free path is inversely proportional to the temperature and thus sigma because the term which we are used earlier, is the mean free path is proportional to the mean free path and this mean free path is inversely proportional to temperature.

So, have the temperature is lower is the mean free path greater is the possibility of the calcium, if the phonon modes of the lattice vibrations. So, ultimately it is the lattice

vibrations which are much more important than just the static ion core. So, the temperature dependence now, becomes  $\sigma$  is proportional to  $1/T$ , as per our experimental observations which we have seen earlier.

So, this therefore, this so far as this particular aspect is concern the temperature dependence, give free electron theory is certainly satisfactory and one can explain the temperature dependence that the conductivity will decrease as function of temperature or in other words the resistivity will increase as a function of temperature. So, far this is useful, but it has also its limitations, we will also see what are these limitations.

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**Thermal Scattering**

Temperature increases atomic vibration leading to increased collision and therefore enhanced resistivity. However, the dependence is different at different ranges of temperature.

- **At Low T**, both  $l_f$  and  $\tau$  are proportional to  $1/T^3$
- **At high T**, they are proportional to  $1/T$

**Impurity Scattering (Mattheissen Rule)**

- The resistivity of a metal increases with addition of impurity (alloying element) content at all temperatures.



Now, some more fundamental logical observations, the temperature increases atomic vibrations leading to increased collision and therefore, enhanced resistivity that we have just seen. However, the dependence is different at different ranges of temperature, you have earlier seen just the earlier slide that  $\sigma$  is proportional to  $1/T$  inversely proportional to  $1/T$ , but this linear proportionality is not always true, that is what it is been shown here that both  $l_f$  and  $\tau$ ,  $\tau$  is the relaxation time. I think it introduced earlier, but not discussed that much.

$\tau$  is the relaxation time that the time elapsed between the two collision or two consecutive collisions. So,  $l_f$  is the actually the distance and  $\tau$  is the time. So, both  $l_f$  the mean free path and  $\tau$  are proportional to  $1/T^3$ , when the temperature is very low. So, where as it is slightly elevated temperature there are proportional to  $1/T$ . So,

that is what we have already discussed that there is a  $1/T$  dependence on  $\sigma$ . However, at very low temperatures again the slope changes, this the variation of  $\sigma$  enhances more or same, but the actual quantitatively the slope is different. So, it becomes more flatter.

Now, in addition to temperature there is always have solution experimental curves, in which we have seen that addition of impurity alloying elements also increases the resistance or decreases the conductivity. The resistivity of a metal increases with addition of impurities are the alloying elements, content at high temperatures, irrespective of temperature. This is an almost an independent phenomena irrespective of temperature and this is also very important particularly when we are dealing with very high conductivity materials like silver copper or gold and so on.

So, where conductivity is place a very very important role many many technological applications, whether it is a hi power application like over a cables or underground cables or even microelectronic circuits, where conductors often used as a as a charge transport path, the conductivity of very great importance. So, the alloying elements whether we should have a alloy or a pure metal that is determine the effect of the, what is the effect of the alloying elements and it has been seen that the resistivity of metal increases with additional impurity alloying element content at all temperatures.

And well these are the basically explanation is very to a largest and simple that we have more barriers the motion of the charge species that is the electrons. So, the electrons not only collide with the are interacts with the phonon modes of the vibrate lattice vibrations, but also with there is a impurity it also acts, it is the motion of the electrons and that is how they actually return the momentum. So, the conductivity gets decreased.

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### Combined Effect of Temperature and Impurity

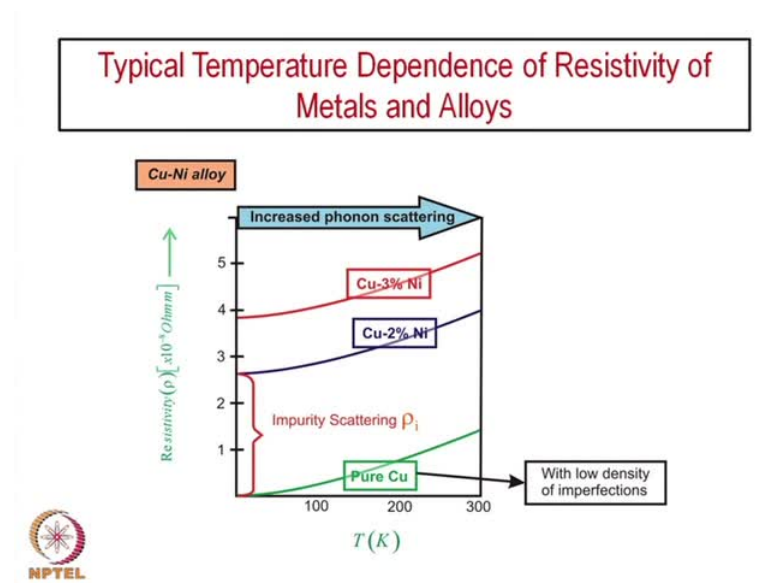
As resistivity of a metal increases both with temperature and impurity content the overall resistivity may be expressed as :

$$\rho = \rho (T) + \rho (I)$$



And this combined effect this is particular, this system this effect actually called Mattheissen rule, where this catering is by impurities, so this one is by the scattering by the lattice vibration are thermal scattering and this is called the impurity scattering and that is empathetically actually its more or less than empathetically described by the Mattheissen rule. So, the combined effect is in terms of resistivity now, resistivity is row T, which is a function of temperature are also resistivity is function of impurity concentration. So, both of them more or less independent of each other, the temperature as its one effect whereas, row has its own effect and finally, these are there is a combined effect both of them.

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And this is the curve which, this is the plot which we have already presented and but just for completeness for sake of completeness once again, we are giving this because this describes many different other point we have discussed so far. For example; this is the resistivity carbo pure copper, where is basically there is no impurity of at it is primarily the temperature effect. So, it is the temperature effect which changes the curve and you can see here you have two different slops this is linear, where is closer to the absolute 0 as we approach absolute 0 there is a slight change in slope which we have just mention, this is 1 by T cube. So, this is at high temperature this is 1 by T and closer to absolute 0 is 1 by T cube.

So, on this same curve both of them have been reflected and so, for as the impurity effect is concern, it is in dependant of temperature at all temperature there is a impurity effect so, there is a vertical shift as soon as you would some other impurity there is a vertical shift at all temperatures and its almost parallel to each other. So, the impurity effect is almost independent of the temperature and the temperature is also independent of impurity and it is proportional to the impurity content. So, higher is the impurity content more and more solid atoms are put in the more resistance change.

So, higher is compared to pure copper to copper nickel allow either 2 percent or 3 percent nickel has increased resistivity are increase resistance. So, this is what their said the increased the phonon scattering, as we increase the temperature there is a increase




phonon scattering and the vertical direction as increase the impurity content there is a more impurity scattering. So, ultimately both of them actually actually impurity scattering, here it is mention in impurity scattering and one can see this gap this distance of separation is more or less constant true of the temperature. So, once again it is independent of temperature.

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**Obstacles / Barriers (Scattering Centers)**

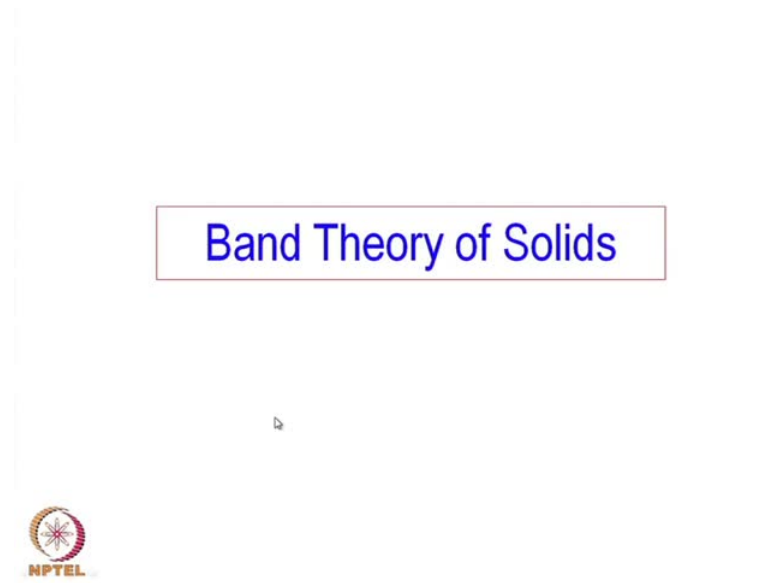
Following are the barriers with which the charge carriers may collide and thus act as the scattering centers so as to reduce the drift velocity:

- Other charge carriers of the same or different type
- Vibrating atom core (Phonons)
- Crystalline defects (Point, line or surface defects )
- Impurity atoms



While to complete this discussion, so ultimately we find as the obstacles are different kind of obstacles, scattering centers give rise to resistance of the metals temperature has an effect, but the obstacles are like this other charge carriers of the same or different type if it is cartance and alignes and they can also collide others electrons can collide of course, they can collide primarily with the phonon mode. By getting atom core the phonons the crystalline defects; the point defects, line defects and surface defects. These are also add to the in these of resistance of the metals. So, it is not only the crystal structure as such, but the crystal defect crystal defect are sometime this locations, all of them do contribute some additional resistance to the system and if you want a very very low resistance material one must have devoid of all this interactions and impurity atoms we have already discussed in details.

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So, that discussed two different models ideal gas model and free electron theory model. While ideal gas model do not is not satisfactory to explain the particularly great temperature, dependence of the electrical conductivity of the metals. Free electron theory do rise to that, but in addition it also has some other importance which will be simulator, but one thing the free electron theory does not is not satisfy is not satisfied to explains that is the.. why only metals have so have conductivity and semiconductors have different kind of conductivity, different kind of temperature variation of resistance and conductance and why some other materials are insulators.

What is the commonality between them, is there any commonality, can we have universal theory and you have universal theory, which explains the property is electrical property is of all the materials together because, you have seen the conductivity has conductivity levels are resistance level widely different from material to material at some of them extremely good insulators, some are extremely good conductors.

Is there any co relation between them is there any common factors, which actually control this parameters. So, at both this theory is free electron theory as well as ideal gas theory is not just sufficient to explain these properties and explain this behavior of the solids of the hole. So, we should then look for some other model or some other theory, which can possibly explain many of this properties or many of this behaviors. So, in that

context band theory becomes very and band theory is very very important, as well as today's knowledge is concerned.

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## Electrons in Solids

- Free Electron Theory can explain many of the properties of metals but it can not fully explain why some solids are insulators or semiconductors?
  - For metals we assumed that electrons are free
  - We know, however, that there are no free electrons in insulators
- More exhaustive quantum mechanical approach is necessary. A realistic potential for the electrons is required to be considered.



So, once again we are talking about the electrons free electrons, because those are the major charge carriers here. So, to the free electron theory can explain in many of the properties metals, but cannot fully explain why some solids are insulators are semiconductors. Well for conductors it is ok, but the behavior of the semiconductors and insulators are quite different and one major in addition to the level of conductivity the absolute value of a resistance conductance, they are temperature depends completely opposite in that of metals.

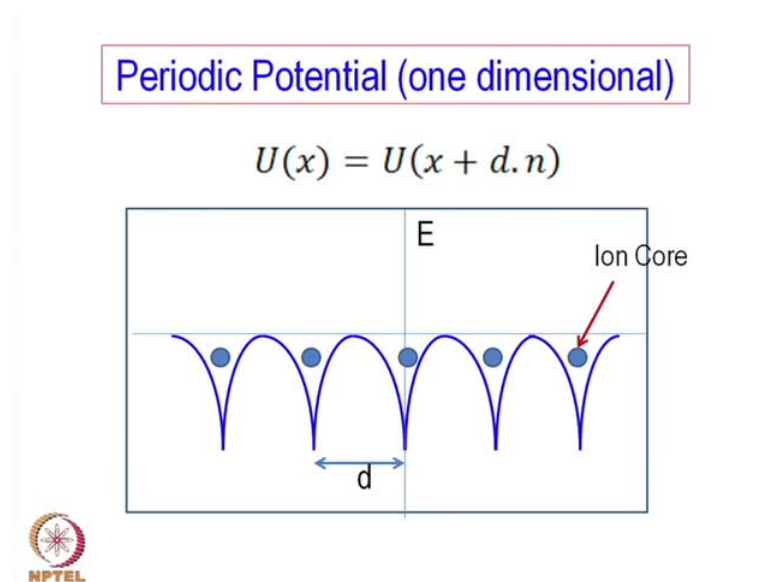
So, free electron theory from that point to cannot explain the temperature dependence of the a resistivity of insulator are conductors, so a semiconductors. For metals we have seen that the electrons are free. However, there is a question mark, we still we not know how free are there in different solids in metals certainly there quite free, but in many other solids possible they are not that free, there in some kind of localization then kind of attractiveness with the ion cores. So, as such the bonding, the chemical bonding is different in metals, insulators as well as semiconductors.

So, the electrons which, I seen that there are completely free may not be sure. So, the more exhausted quantum mechanical approach is necessary, a realistic potential what the electrons require to be consider. So, if we remember that, in the free electron theory, we

have seen or we have considered that the potential is constant. So, the electron is moving in a potential constant potential which, is we are low potential negative potential compact to the end end of the solids. So, at the end of the solid there is a very high potential these elections are not able to crossover.

So, the electrons are confined within the value of this solids, that is understandable, but is it true that the electron is actually moving the constant potential across the volume of the material and length of the material, possibility not and that is the basics this is of the band model. The mode exhaustive quantum mechanical approach is necessary realistic potential for electrons is required to be considered. So, what is that realistic potential.

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We have seen earlier we have considered in the free electron theory that the potential is constant. Infact in this band model, it has been assume that the potential is really not constant and which now, everybody believes that is more realistic. So, it had some ion cores these are the position of the ion cores lattice sites, where the atoms are the side and these are the potential these are the electrical potential variation of the electrical potential of the electrons with respect to its position. So, earlier we have seen we have seen that it is a constant potential although.

Now, I saying it is not a constant potential is a variable potential and particularly just near the ion cores these are the positions of the ion cores, so near the position of ion core the potential is very low. Whereas the form the ion cores potential is high. Which means the residence time of the electrons is not uniform throughout of the length and breadth of the solid? So, more time it spends near than ion core then i from the ion core. So, that is a more realistic situation and of course, that makes the mathematics little complex, much complex than what we have seen earlier. So however, it possibility gives us a more realistic representation of the situation.


So, this is what the call a periodic potential, one dimensional once again it can be considered a one dimensional or two dimensional and three dimension solutions are much much more difficult. However, people have tried one dimensional problems and try to solve the solve them a and found what is the ultimate effect. So, this is a in one dimensional, this is the what we call the periodicity this is an exposition of periodicity  $U$  is a function potential as a function of  $x$ ,  $x$  is this horizontal distance and so, this function is equal to the  $U \times$  plus  $d$  into  $n$ .

So, at any point any point at distance  $d$  multiplied by integer integer is a number of lattice sites. So, at different it is a multiplied, it is a kind a multiplied and  $d$  is the distance between in the two consecutive lattice sites two neighboring lattice sites. So, that is so, then what ever is the value of  $U$ , here it will be exactly the same here. So, it is periodically vary coming back to the same value. So, that is the description how the periodicity of the potential can be describe mathematically. So,  $d$  is the distance between the two consecutive. This is symmetric way symmetric distribution, but a variable distribution.

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### Bloch's Theorem

- Each electron in a crystalline solid belongs to each and every atom of the solid forming an Electron Cloud.
- The probability of finding an electron at any of the atomic sites of the solid is same

$$P(x) = P(x + d).$$
$$P(x) = |\Psi(x)|^2$$


So, this is the distribution which has been which has been consider and then of course, it is a much more complex problem may not be able to discuss each and everything and may not need that also except that we need that what is the ultimate continuation and what is the outcome of this mathematical analysis, to do the mathematical analysis there are some theorems, certain constitution, certain assumptions and so on. So, just try to introduce the names of the particular idea, the each electron in a crystalline solid belongs to each and every atom of the solid forming and electron cloud.

Once again we have the electron cloud no doubt, but electron cloud means that is the definition of the electron cloud, basic that means the electrons are actually not specific to any particular lattice sites although, there is some kind of probability function because we have a periodicity and the near the lattice sites there is the potential is less so the probability is more, but it belongs it is not static at any particular point. So, it is moving around, but with some with some kind of a time saving basis, more time it is near the positive charges than it is higher from the positive charges.

So, but the electron cloud still exist and the concept of the electron cloud still exist. The probability of finding an electron at any of the atomic sites of the solid is same, that means irrespective of the irrespective of the particular site the probability at this site and the site is same, that is what it also assumes. So, that is a perfectly periodical lattice. So,

one can say the more or less in the same manner as the potential distribution either you seen, the potential is the  $U \times U \times \text{plus } d \text{ n}$ . Here it is not the potential, but it is probability.


So, probability of finding the electron at  $x$  is exactly equal the probability of finding the same electron at  $x$  plus  $d$ . So, it is moving at very fast speed and the probability of finding on that electron at particular space or particular site this side, of course, now everywhere, but at on a periodic manner. And this probability is actually nothing, but the size  $x$  square, which means the size the studying this functionality, studying this equation studying this function so, size  $x$  square is actually the probability. So, that actually size squared that actually the potential distribution of the how one can express the potential of the electron in the periodical lattice.

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Schrodinger Equation

$$H(k)|\Psi\rangle = E(k)|\Psi\rangle$$

$$\Rightarrow H(k) = \frac{(\hbar k)^2}{2m}$$

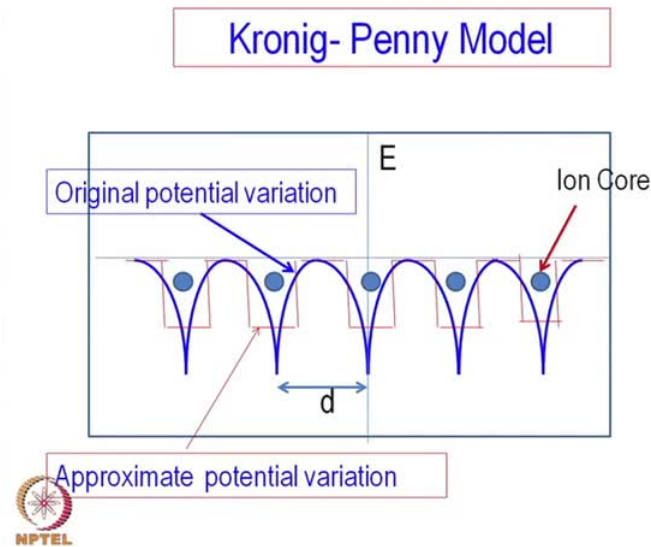


Free Electron Kinetic  
Energy Hamiltonian

$k$  = Momentum vector  
 $E$  = Kinetic Energy  
 $m$  = Effective mass

While once again I will not go to details of that, just one or two points, this is what we write and studying this equation, this is hamiltonian of  $k$  of  $\psi$  and then it gives rise to this value of  $k$   $H$ , the hamiltonian  $\hbar$  again. Once again we are bringing coming back to the similar equation, similar term that  $k$  term, the vector term as well as the flanks constant and  $2m$  is the  $2m$  is the mass and  $m$  is the mass effective is called the effective mass. So, the  $E$  again is the kinetic energy, which we have discussed earlier in terms of the field electronics theory,  $k$  is the momentum vector and then this is what we called the field electronic kinetic energy Hamiltonian.

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So, ultimately becomes this value and to solve some some of these equations, we have to take some kind of assumptions. Although this may be a more realistic potential variation, but for solving the equations, the complex equations one is to take the thinks little simplify, a kind of square well kind of well instead of a varying wave continuously varying wave like that potential like that. So, the approximate potential variation has been use by under the Kronig Penny model and the basic philosophically and just till let you know that this variation, instead of this variation one as used a more simpler variation, although it may not be exactly realistic this may be a more realistic, but it provides as more and the same outcome.



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## Bragg Diffraction

$$n\lambda = 2d \sin \theta \quad \text{For } \theta = 90^\circ \quad n\lambda = 2d$$

$$k = \frac{n\pi}{d \sin \theta}$$

$$\lambda_{critical} = \in \left[ 2d, d, \frac{2d}{3} \dots \right]$$
$$k_{critical} = \in \left[ \pm \frac{\pi}{d}, \pm \frac{2\pi}{d}, \pm \frac{3\pi}{d} \dots \right]$$



So, using that concept the assumption and also at this point one has to consider this called Bragg diffraction, because electrons are actually waves here. So, these waves are passing through the lattice. So, as know that where ever there is a periodic lattice and through which there is a electric magnetic wave passing through the some scattering and that is scattering sometimes at some under certain conditions it becomes a constructive interference and that is given by so called Bragg diffraction, that is the  $n \lambda = 2 d \sin \theta$ .

So, that also applies because electrons are is being consider here as a wave, a kind of electromagnetic wave. So, if that this, so these electrons scattered or diffracted through a periodical lattice and the Bragg diffraction actually be quiets periodical lattice, without a periodical lattice Bragg diffractions cannot be expected. So, since we have a periodical lattice here, we are talking about the periodic lattice the potential is vary. So, we also have the possibility of Bragg diffraction of the electron itself. So, in this case the Bragg diffraction means at certain planes graphic planes they are electrons gets detracted, not detracted a constrictive interference takes place and it is actually reflected back.

So, electron cannot pass through electron as if it is absorbed in mirror plane and the electron comes back. So, that is a duct allowed this concept also important or dislike to this kind of a situation. Therefore, you have some kind of a Bragg diffraction taking places within the lattice, periodical lattice and that is also including the motion of

electrons. So, the motion electrons becomes at certain levels, the electrons becomes it becomes the energy barrier becomes so high, the electron cannot go through. So, it comes back and reflect, so there will be some kind of for bin labels for bin energy gaps, which, will be discussing a maybe in the next class. Time for this class over now.

Thank you, thank you for your attention.