Introduction to Solid State Physics
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Lecture – 62
Band theory of metals, insulators and semiconductors

So, recall last week we had discussed the Bloch's theorem and how the periodic potential leads to energy bands and energy gaps at Brillouin zone boundaries.

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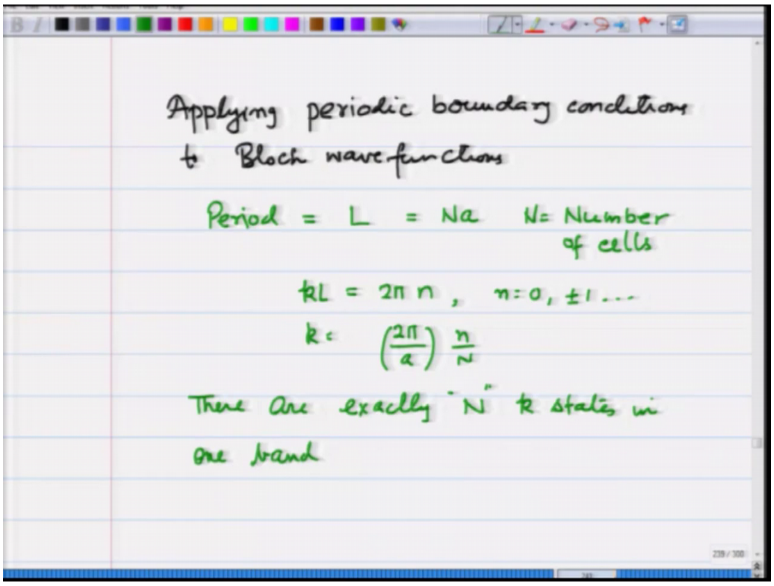

And finally what we discussed was applying periodic boundary conditions to Bloch wave functions and we got that when the Periodic boundary condition is applied over a length L. Periodic boundary condition is applied over a length L which is N times a N is the number of cells. In that case you get k L equals 2 pi n where n equals 0 plus minus 1 and so on and k equals 2 pi over a n over N. And there are exactly N k stats in one band.

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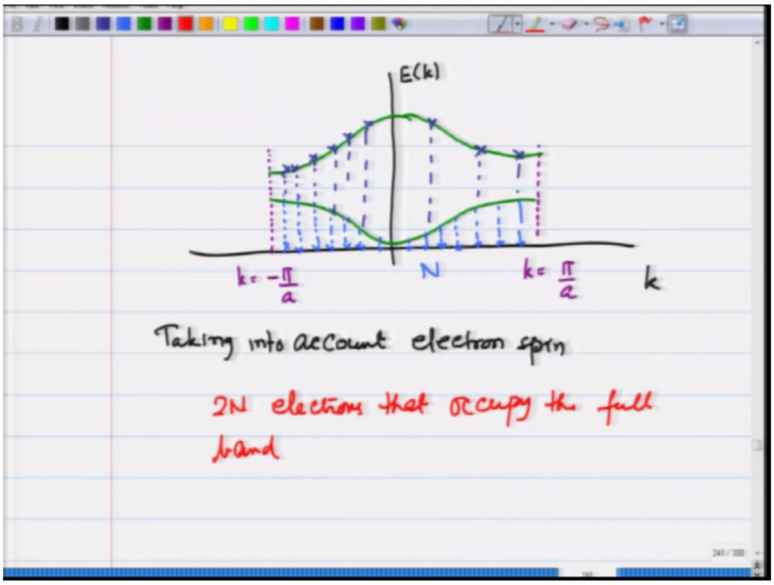

This is where we are stopped last week and what it meant was that if I have a, an energy band k E k I will just make two of them up to the Brillouin zone. k extends from minus pi by a to a and here is the first band here is the second band. Then the total number of states in this, total number of k values k is quasi continuous because n is interior. So, all these number of k values that are their independent stats are going to be any number in this band as well as in the upper band exactly same k values will exist here also.

So, I am just indicating these are the quasi continuous k values and I have E versus k. I have shown some points and taking into account electron spin which can take 2 values, we have 2 N electrons that occupy a full band. So, when the band is full, it will accommodate 2 N electrons. All the stats in the Brillouin zone are occupied including the number electrons spin when the band is full and this has implications.

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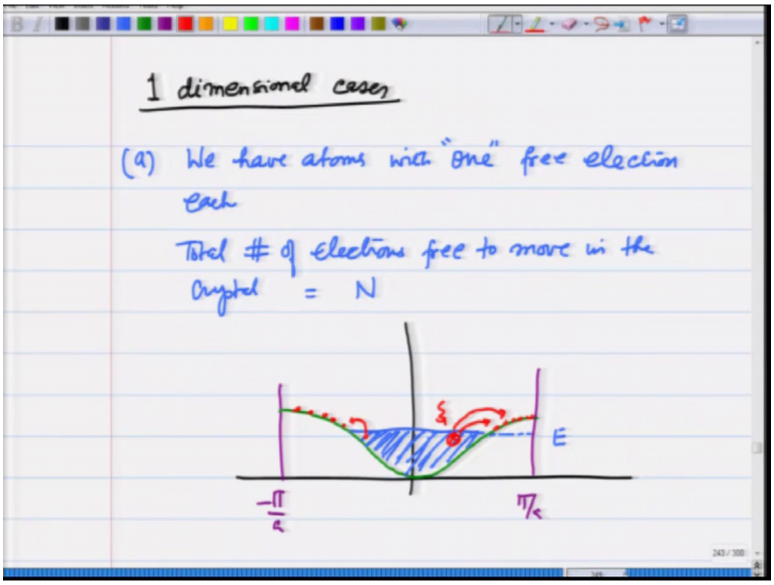

Now, let us take it case by case and I want to remind you again that I am dealing with 1 dimensional cases. When we go to 2 or 3 dimensions there will be little more certainly involved. But general conclusions that we arrive at right now are going to be valid with little changes and I will give you examples of that. So, let us take them case by case suppose a, we have atoms with "one" free electron each. In that case total number of electrons that are free to move in the crystal, free to move in the crystal is going to be N and therefore if I look at the band it is going to be only half filled.

So, it has all the states upto certain energy E that are filled, so all these are filled and these are upper stats are all empty. In that case if I give even small energy to an electron here let us say this red one, if I give even small energy by any means it can gain energy and go to the next level, it can gain energy and go to the next level. You can gain energy from here and go to the next level. So, I can excite these electrons. If I do that by applying an electric field and let us see what happens.

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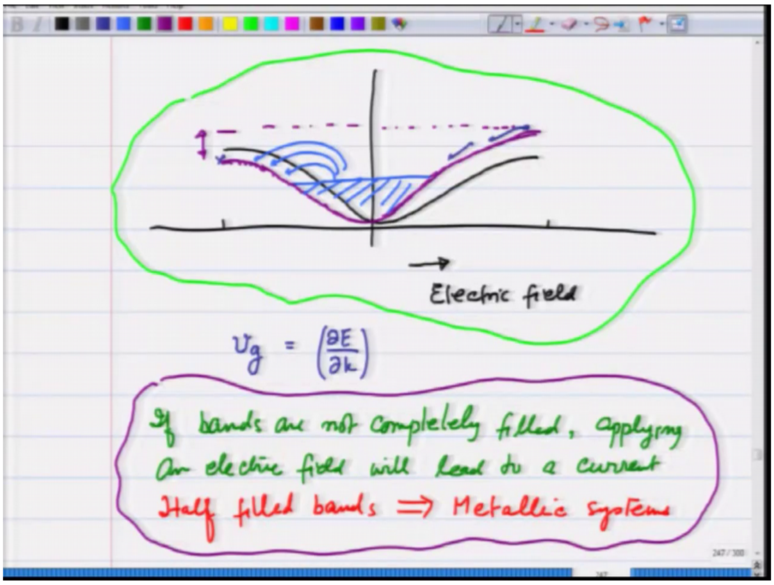

So, I have this band and suppose I apply the electric field in this direction, in that case in the first very first qualitative approximation what I can say is that the potential energy for electrons in this direction on the left hand side, on the in the direction opposite to the electric field would be lower and because they will tend to move that way and on the right side it will be higher.

So, I can think of this band as if it has tilted a bit where this there is a finite difference in the energy on the right hand side, in the left hand side. So, what could happen is electrons out here in the filled bands would gain energy and come to the other side. So, they will start occupying these empty states and they start as occupying these empty states they are moving because, they are going to a different k state right and velocity I will talk about it later, we have you can guess the velocity of electron will be given by the group velocity which is d E by d k. It will start gaining velocity. once they reach on the left hand side, they start moving from here. So, when they start moving that means they will be a correct.

So, if bands are not completely filled applying and electric field will lead to a current, if it leads to a current that means these are metallic systems. Half filled bands imply systems. Once that I have explained this just a word of caution. The word of caution is I have very qualitatively when I made this picture up here, let me encircle this the green color thing when I made this picture here I tilted the band it is a very very qualitative picture, because remember this band has been plotted in k space which is not the same as the regular x space.

So, when I said it is tilted, it has to be taken with a little very qualitatively, what is actually happening is the electron is gaining energy and it is going to an higher energy state. It can move to a higher energy state so that there is a disbalance between the electrons which are filled on one side and on the other side there is a velocity display balance and that leads to the current. So, bottom line is that when you have these half filled bands, electrons can gain energy from the applied electric field and lead to a current, so Half filled bands are going to be metallic.

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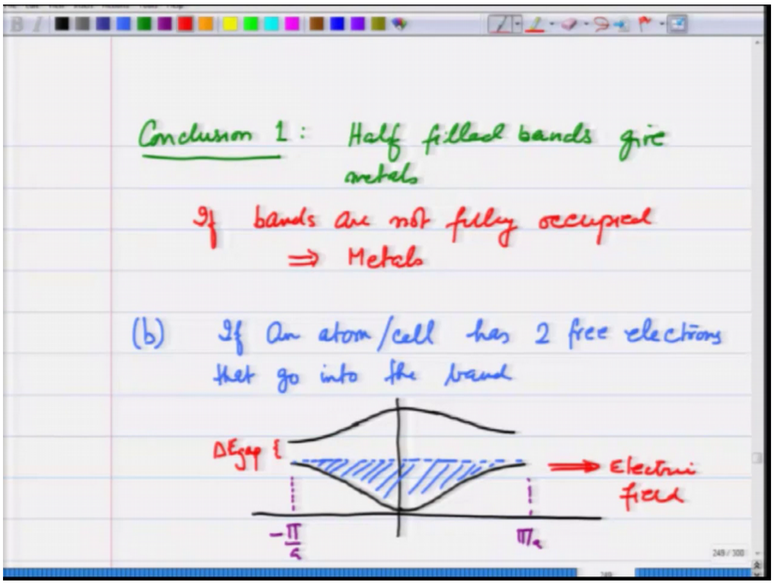

So, Conclusion number 1: Half filled bands give metals along same line I can say that if bands are not fully occupied this implies metals. Now let us see what happens if an atom per cell suppose there is only 1 atom per cell has two free electrons that can go into the band. In that case let me make this picture again the band diagram I have minus pi by a to pi by a and this whole band is filled with electrons it is occupied all the stats and the next band has a gap. So, if I apply a weak electric field, so let us apply an Electric field, it would require for electron to gain minimum this energy equal to the gap. Let us call it delta E gap so that it can go to the next band. If it does not acquire that much energy it cannot move to the next band. On the other hand if it remains in the same band it has nowhere else to go. A little like when you take atomic states unless you apply some minimum energy the electron does not go to the higher level. So, it does not accept that energy. Similarly here if I apply a weak field, the electron would not accept any energy from it. It will not move and the electron does not move that means there can be no current.

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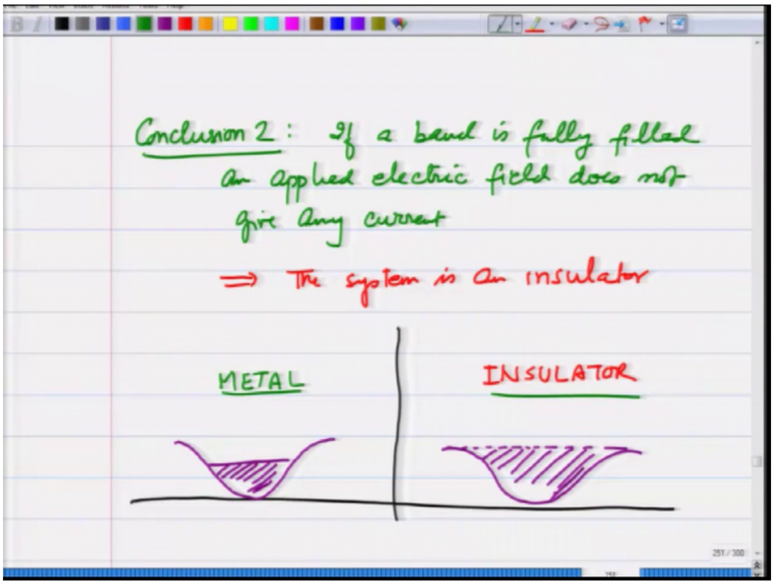

So, conclusion 2: If a band is fully filled then an applied electric field does not give any current and this implies the system is an insulator. So, these are the two pictures that are emerging from the band theory that if I have a fully filled band there will be an insulator, the system would be insulating and if I have a partially filled band then the system will be metallic.

So, let me make this partially filled band here and fully filled band here this is an Insulator and the left hand side I have a Metal. So, you can also say that if I have in a crystal 1 atom per unit cell and each item gives only 1 electron I will have a metal. If one that each atom gives two electrons, I will have an insulator and there is something in between and that is known as a Semiconductor.

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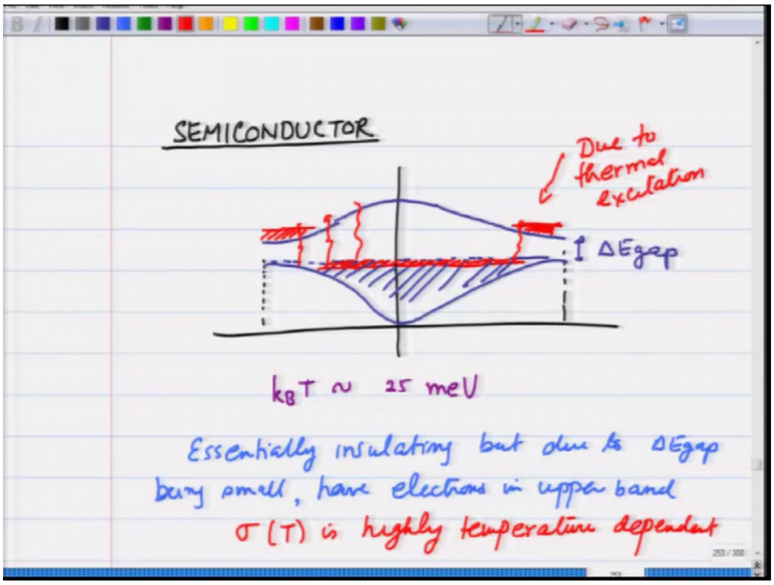

There will be a whole lot of lectures in Semiconductors but right now let us just introduce the idea and the idea is that again I have band which is fully filled. However the next band has this gap delta E gap which is very small, if it is small there could be these electrons going up due to thermal energy they will. Obviously, reside at the bottom of the band and they will go from here so some part here will become empty and this is due to thermal excitation, remember thermal excitation kBT at room temperature is of the order of 25 meV.

So, this band gap has to be very small so that these electrons are excited to the upper band and in that case I have these electrons which can move in an empty band and there will be some conduction, that conduction would be temperature dependent. So, these are semiconductors which are essentially insulating but due to delta E gap being small have electrons in upper band and therefore that leads to conduction. You can easily see that the conductivity of these systems, conductivity is going to be highly temperature dependent. So, this is the band theory explanation of the materials metals, insulators and semiconductors.

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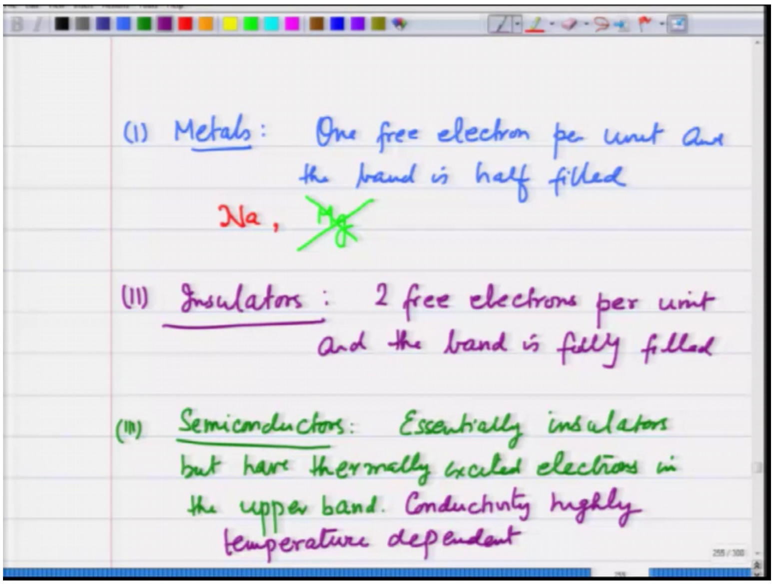

So, let us conclude again. One, Metals. One free electron per unit and the band is half filled. Examples for this will be sodium and all the alkali earth in that, then in that case magnesium will not be a metal because it has 2 electrons free electrons Mg is remember 3 s 2 it will not be a metal. However, it is. So, I will talk about that in a minute and number 2 this is general observation. Insulators, 2 free electrons per unit and a band fully filled and third category semiconductors essentially these are insulators. But have thermally excited electrons in the upper band. Conductivity highly temperature dependent, because basically these electrons are thermally excited and therefore conductivity depends on the number of electrons and it becomes highly temperature dependent.

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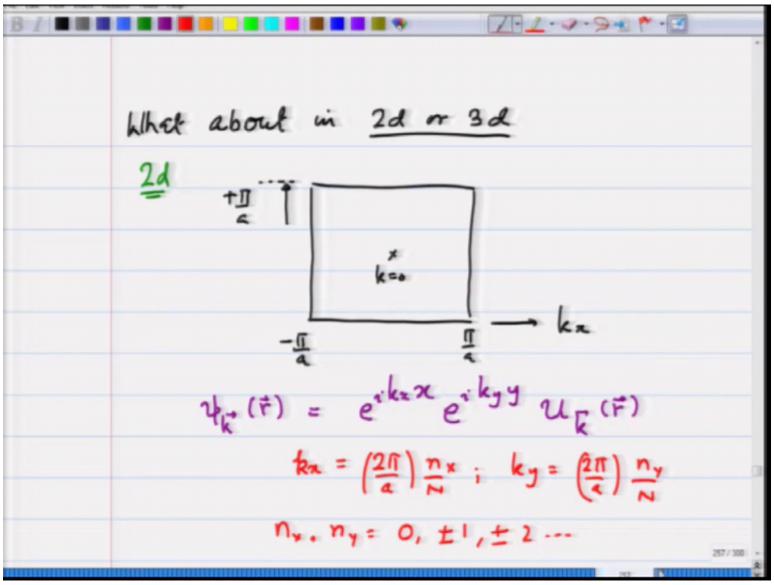

Now, the question what about in 2 d or 3 d? Is the picture the same? Essentially the same, but with a subtle difference. Let us consider a 2 d case and that is sufficient to explain what happens in a dimension higher than 1 d. So, in 2 d, suppose I have this square lattice, so that this is the Brillouin zone. Brillouin zone 1 would extend this is 0. Let us say this is k equals 0. So, Brillouin zone will extend from minus pi by a to pi by a in the x direction and minus pi by a to plus pi by a in the y direction. This is the Brillouin zone, first Brillouin zone and the Bloch wave function psi k where k is now 2 dimensional is going to be e raise to i k x x e raise to i k y y times this function u k bar which is periodic.

Now, the periodic boundary conditions are going to be applied over the x and y directions and they are going to lead to k x equals 2 pi over a n over N and k y equals 2 pi over a n over N. I may as well write this as n x and n y, we are both n x and n y go as 0, plus minus 1, plus minus 2 and so on. So, the picture is really what we are doing is going into the 2 dimensions. So, I just include one more dimension and the boundary conditions and everything or all those things remain essentially the same.

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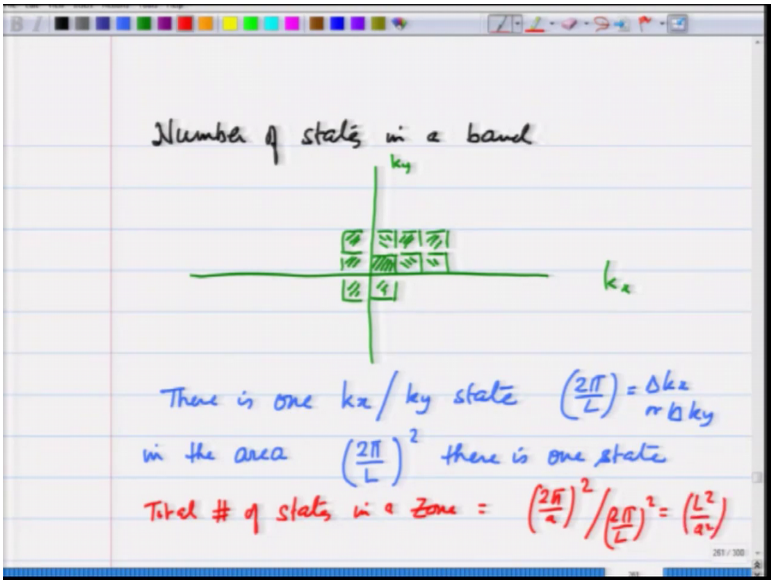

Now, the number of states in a bands are going to be counted by counting states in both x and y exactly like we did for free electrons. So now, if I go to make this picture of k x and k y there is one state in each 2 pi by L and so on. So, there is one k x or k y state in each 2 pi by L equals delta k x or delta k y and therefore in the area 2 pi by L square there is one state. The total number of states in a zone is going to be equal to 2 pi by a whole square the area of the zone divided by 2 pi over L square which is L square over a square.

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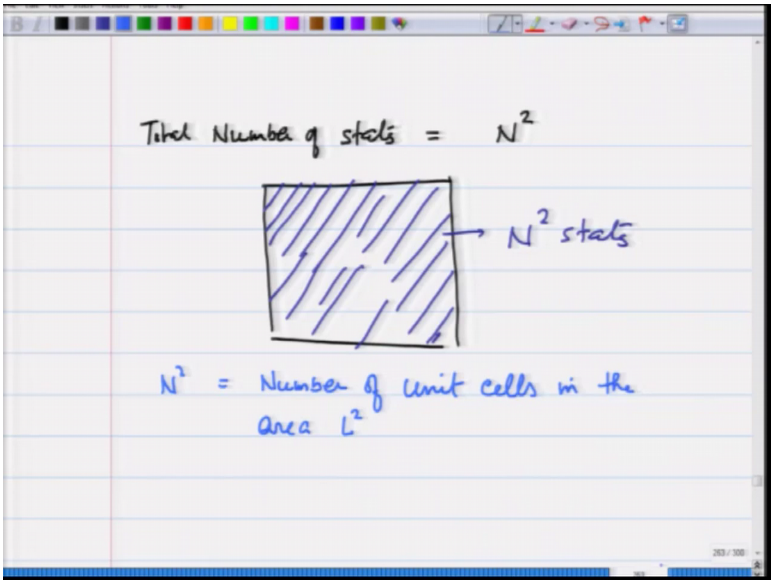

So, the total number of stats is equal to N square and that is perfectly fine, because now in this entire below zone. I will have this whole thing filled with N square states and this

N square is the number of unit cells in the area and L square because in the real space I have this crystal of size L over which I am applying the boundary condition and I am taking each cell size to be of a.

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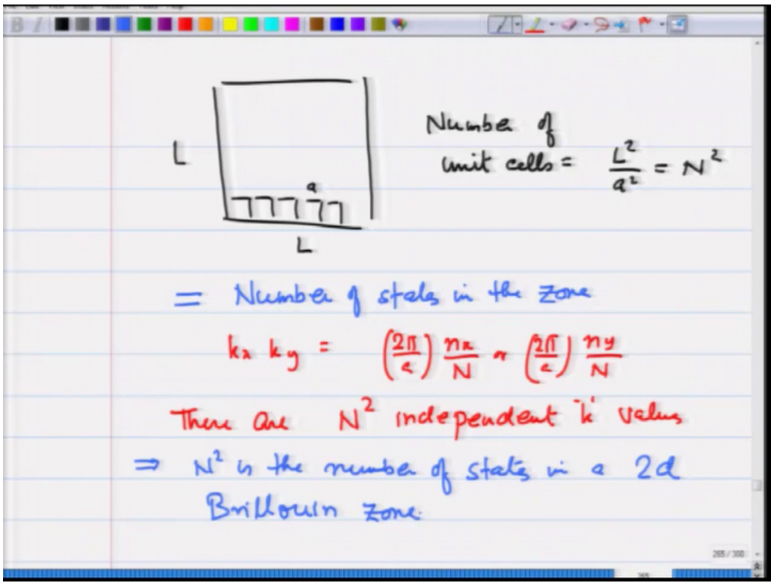

So, number of unit cells is equal to L square over a square which is N square and that is precisely equal to the Number of states in the zone. Now when I apply the periodic boundary conditions and take this k x k y to be equal to 2 pi over a n x over N or 2 pi over a n y over N what it is giving me is there are N square independent k values. So, this will be the number of stats and in the Brillouin zone or in the band, so this implies N square is the number of stats in a 2 dimensional Brillouin zone.

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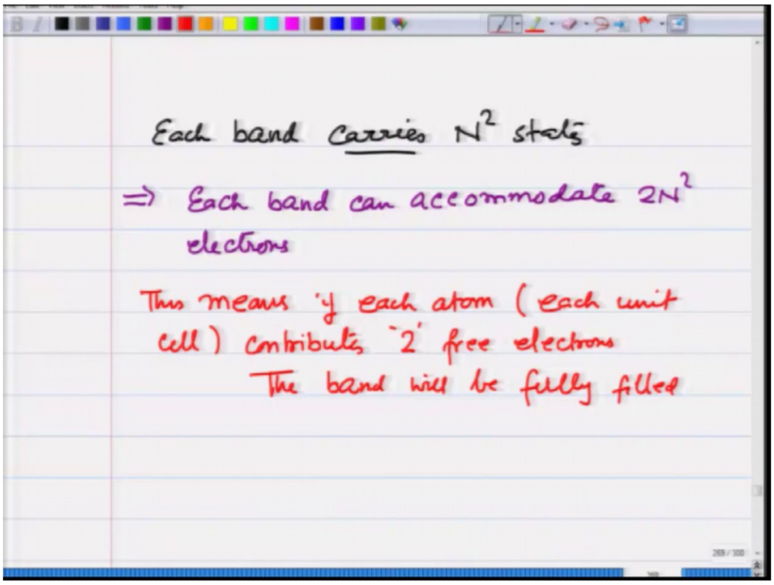

And therefore each band which occupies all these k x and k y stats carries N square states and this implies each band can accommodate 2 N square electrons. So, now whatever we discussed in terms of a 1 d model, if I have N square unit cells in the sample and each unit cell take carries 1 atom and each atom gives 2 electrons then the band will be fully occupied.

So, this means that if each atom means each unit cell which carries one atom contributes 2 free electrons, the band will be fully filled. Normally yes, but in general there could be subtleties and that is what I want to discuss now and that is precisely what makes magnesium a metal so let us understand that.

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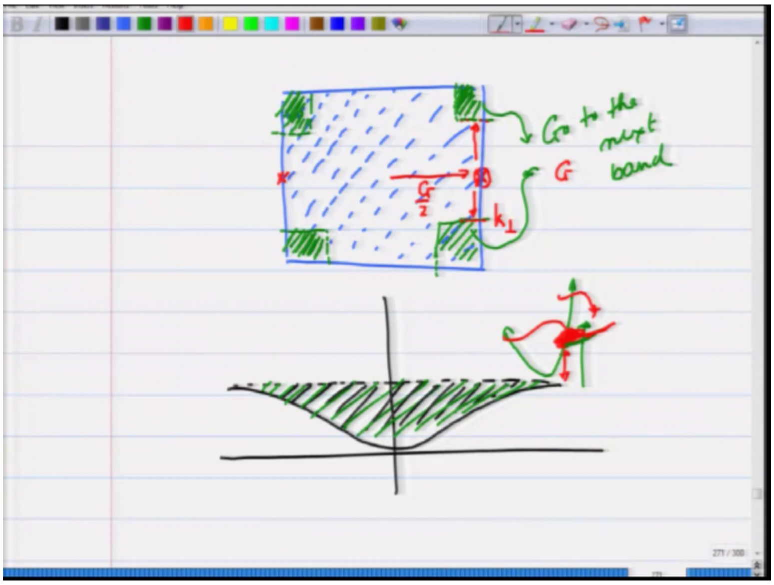

So, let us make this Brillouin zone which is fully filled because, there are 2 N square electrons this is fully filled. So, in the band picture let me make it like this, in the band picture if I have this band I would expect that this is fully filled and 1 d this is precisely what happened.

But let us look at it slightly carefully. There is a gap at the zone boundary right here and the next band has this band gap out here. Now in 2 d, if I start going let us say from this point that I have made up or down along k perpendicular to this G by 2, electrons at these levels, other levels are going to have higher kinetic energy. If they have higher kinetic energy it may so happen that at a certain point let us say this point onwards all right.

So, let me show this point by green, let us say this point onwards and the same thing would happen on the other side this point onwards because of the symmetry. So, all these points have kinetic energy such that the total energy of the electrons with these cases becomes higher than the energy at the top of the band plus the gap. So, if I keep increasing the kinetic energy of the electrons in the first band, the total energy may become higher than the lowest of the next band.

In that case what would happen? All these green electrons or electrons in this green area would go to the next band. It is a settle point because the gaps arise at G by 2. So, the arise G by 2. If I go away from that point in 2 d I can do that. The kinetic energy of the electrons goes up.

So, what I have shown here is 1 d picture which I am again you know writing, making marks with green. If I go perpendicular to this, the energy goes up. So, in the perpendicular direction the energy goes up and as the energy goes up it may go higher than the lowest of this orange band and therefore all these upper electrons will start coming to the bottom of this band. As a result neither the lower band nor the upper band would be fully filled.

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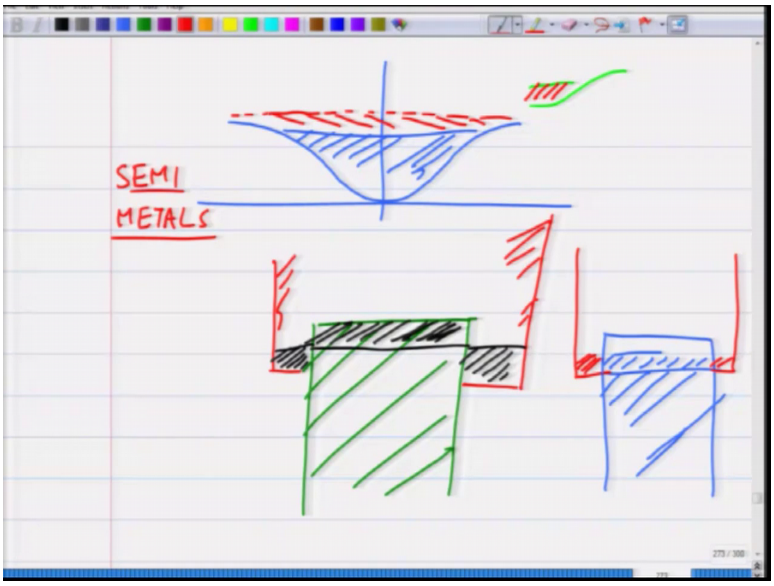

What would happen is that, in this case some of these electrons once shown by red will go to the higher band here and this is because as you go perpendicular to this plane the energy of the electrons goes higher. If I make another picture this is the first band. These are the energies up to the top and the second band has an overlap with it. This is the second band in some other direction.

So, if it has an overlap what will happen is half of these electrons here would move out and come here. The result being that I am going to have this band which is partially empty and the outer band which is partially filled and these systems will conduct these are known as Semi Metals. These are not metals in the conventional sense in that the bands are not well separated they have overlap and therefore some electrons from one band the lower band start moving into the upper band and both are therefore partially filled bands and they start conducting.

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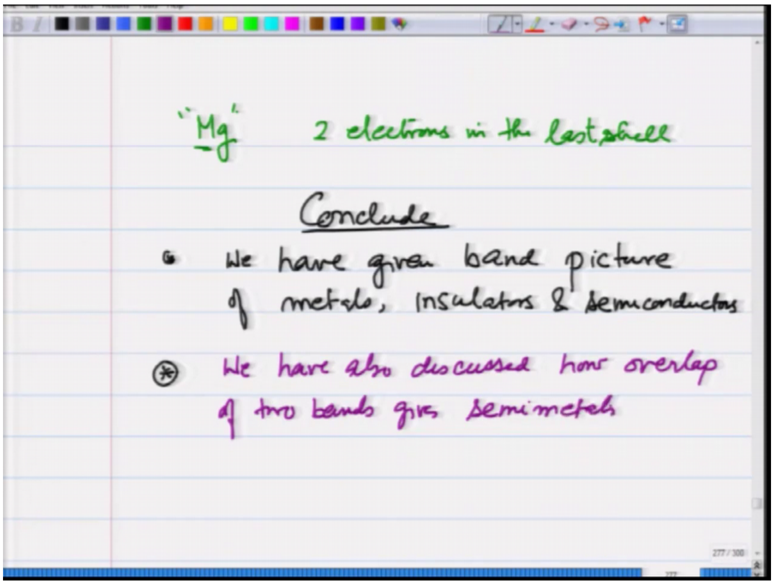

The example best example for this is the Magnesium which has 2 electrons in the last shell and those could be free and move. In 1 dimensional cases, they will fill. The entire band and the material would be a non conducting or insulating but in 2 d and 3 d it conducts because of the overlap of the bands. So, same argument applies to 3 d so I have illustrated with the example of 2 d that bands may overlap if you go to dimensions higher than one d and materials may become conducting.

So, to conclude, we have even band picture of metals, insulators and semiconductors and we have also discussed how overlap of 2 bands gives materials called semi metals.

Thank you.