Course Summary
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Lecture No. # 40
Physics of Nano Scale Materials
Course Summary

Hello, welcome to this the fortieth lecture in our physics of materials course. We have looked at variety of different topics through this course and. So, with this class we come to the conclusion of this course and in this class we will spend a fair bit of time looking at one of the topics that I would like to discuss with you which is the physics of nano scale materials.

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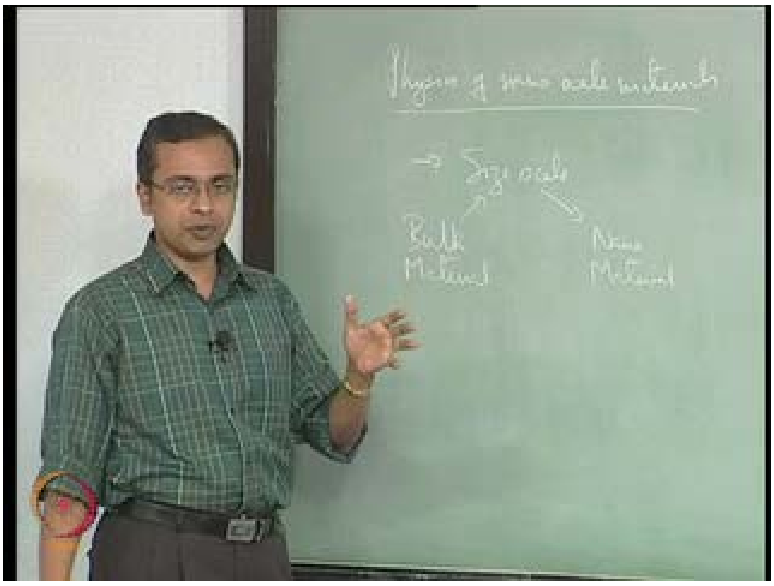

So, in this class we will look at several aspects associated with the physics of nano scale materials and some of the reasons why this is of interest and also get a feel for how what we have learnt will someway enable as to understand, what it what this physics of nano scale materials means and perhaps how we can go head and you know appreciate the literature that is available in this in this area. So, through this class we will do that and then we will summarise this course and look at the various things that we have done through this course right. So, of course, as you know these there is a lot of emphasis on nano materials in general, the basic idea being that you can get variety of properties in materials that we are already familiar with, but often when you take the same material and you keep reducing its particles size then you eventually reach a stage where there is for most properties there is there is a dependence on particles size for the property or at least several properties you will see at dependence on particles size on the of the property and that may have a certain trend, but often it is seen that when you get down to the nano meters scale size scale this trend can be either dramatically ex-saturated or could even be dramatically different. So, so you see some of these effects.

Sometimes, you see properties were actually there is no real great size dependence up to some point and then after that point suddenly as you drop the size parts some point there is a dramatic change in the property of the material. So, what this is useful for is the is the general idea that you can now get the same material essentially chemically the same material giving you a variety of difference properties, something that you can tune you can you can say affront that you would like certain chemical composition, but certain particular value of a property and then you can deliberately choose to prepare that combination and within a within reason you should be able to do this depending on the general applicability of that composition or that system for the kind of property that you are trying to put it to use for.

So, so this is the reason why there isso much of interest in nano materials. Why there is so much of research in nano materials and so much of funding in the area of nano materials. So, this is what it is. We will look at these nano materials from the perspective of the kinds of properties that we looked at which is optical properties, electronic properties and such and from that perspective what is it that is of interest to us. In this context as I said there is there is a sense of size scale. So, so there is some particular size that you have to cross before this kind of change in property occurs as a result of the size scale. Now, that size we are talking of is not a fixed size. It is not that you know there is a universal size of 50 nano meters or 25 nano meters that if you go below 25 nano meters everything will change that is not how it is. For every property that you are looking at there may be a particular size scale or is even a range of sizes across which this property change might become more and more apparent.

So, that maybe true for every, that may vary for every different that you are investigating. Not just that even within a single property even within a particular property that you are chosen maybe a mechanical property, maybe a chemical property or an electronic property even within that property based on the material you are choosing the size scale where this the effects of the nano scale begin to show up may vary from material to material. So, it may vary the size scale that causes this changes to occur as a result of the being in being such a small sized particle, being a material made out of small sized particles that may change depending on property if the scale were that effects shows up and also within the same property the size scale may vary from material to material based on the property that you are looking at. So, this it is an important concept that we should keep in mind.

So, there is no universal size scale at which everything happens, but we have to really look at the property and the composition and get a sense of what is that size scale which is now of interest and when you get to that size scale you sees properties of interest. So, this is the important concept that you should look at. So, it is important to keep in mind size scale in other words when it that it is a nano material of interest. You may have nano material, but it may still not be interesting because it may not be doing anything different from a bulk material. So, you have bulk material and a nano material and it is this size scale that gets you there and exactly what that size scale is varies from material to material, varies from property to property.

So, this is what you are looking at. Now, we will look at it from the context of what we have discussed in our course. So, in that relationship we will first start with something that we have that we are familiar with and we will see what features of it starts becoming of relevance from the perspective of nano materials.

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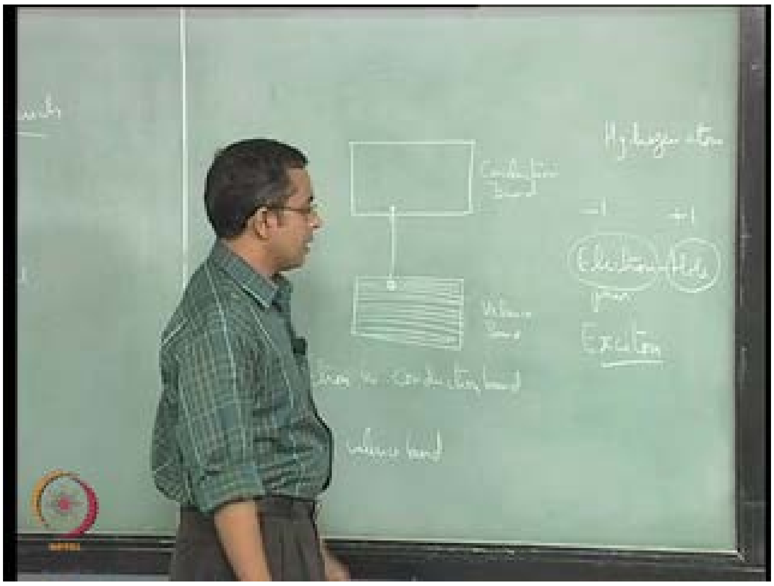

So, let us look here we have drawn band diagrams before and we will for this purpose will simply strict to a flat band diagram. So, we have some we have some valance band and then we have conduction band. So, so for in our discussion we have really looked at how this bands come about and sort of what are the what happens I mean what is the phenomena related to this transfer of an electron from the valance band to the conduction band. So, will assume it is a semiconducting material. So, so this band gap is less than two electron volts will say and it is a semiconducting material which means this valance band is full, the conduction band is empty.

So, we have looked at you know direct band gab semiconductors, indirect band gab semiconductors. So, that talks about this process of the electron transfer from the valance band to the conduction band. What we will now discussed today is what happens after this transfer. So, we have talked about the transfer, the factors affecting the transfer and what it is the significance of it in terms of you know optical properties. How it tells you what is it in terms of what wavelengths will be observed all those things we have discussed, but we will now see what happens after we do this transfer. So, what have we done after we have done this transfer? We got an we have we now have an electrons setting here in the conduction band and we have a hole setting here in the valance band.

So, there is an electron here, we have when we do one transfer we have electron in conduction band and we have a hole in the valance band. So, this also we have we are quite familiar with this happens. What is special about this situation, what is special about the situation is that we are now have you know pair of oppositely charged entities, you have an electron which is negatively charged and you have hole that is positively charged and they are separated by some energy gab in the material.

And location wise they may they are; obviously, not at the same location otherwise they would just recombined so, but anyway you have you have got this a transfer in energy now what happens is because this is negatively charged and this is positively charged there is a columbic attraction between the two of them. So, there is a columbic attraction between the 2 of them. So, therefore, they tend to actually maintain some connectivity with respect to each other. So, you when you. So, talk of a band you normally talk of it you know as though once the electron as gone there it is free to run across the extend of the material.

So, the and. So, and that is how you talk of conductivity and so on. What I am telling you is that in that process every time you do this this electron and hole entities which we have sort of tended to talk of them as independent entities, what I am trying to point out this they tend to have some force of attraction between them because they are oppositely charged and as a result there is an attempt on their part to sort of stay connected, to sort of maintain stay within certain distance of each other and so when they move they sort of move with keep maintaining this distance or staying within the limits of this distance. So, the force of attraction between them makes them more stable than on completely independent electron and completely independent hole. So, and it is that and it is it is a result of that they tend to stay connected and within a certain range of influence between each other.

So, so that is how it happens. This electron hole pair. So, the electron hole pair is given a name it is called an exciton. So, if you read articles and physics you read articles on a, in a which are about the physics of materials various articles you read popular articles for even books in books you will see this term exciton. It refers to this electron hole pair which forms whenever you have this electron getting a transmitted through this as a which when it is observes an energy and its goes up to the conduction band. So, now, we see some new thing that we have not really discussed. We see that this pair actually is a sort of moving in tandem, it has some connection to each other they have connection to each other and so they, they have. So, now, you can sort of expect therefore, that they may have certain properties associated with them, they may have certain limitations on what they can do what they cannot do and that may itself impact the properties of the material that you see.

So, first thing we realize now is that it is combination called an exciton. The other aspect of this which is of interest is the fact that what do we have here we have one negatively charge species an electron. So, minus 1 and one positively charged species plus 1. Where do we a see a combination like this? So, that is a question we should ask ourselves. Where we do a combination like this in or rather where have we seen a combination like this which is which were very familiar with? We have seen this in a hydrogen atom. In a hydrogen atom you have nucleus which has a plus 1 charge and an electron around it which has a minus 1 charge. So, in terms of charge and in terms of the number of entities involved these two situations are exactly the same. The main difference of course, is that in a hydrogen atom we are talking of a proton, we are talking of a proton an electron combination.

Here we are talking of a hole and an electron combination. So, this is in that sense they are different they are not the same, but there is suddenly reason to see that there can be similarity between the two of them, there is can be similar similarity. So, it is sort of like a hydrogen like system that you are talking of here and therefore, in sort of the manner in which bore has treated the hydrogen atom in that same, in the same context we can think of sort of a characteristics distance that may exist between the electron in the hole and this is therefore, refer to as the exciton bore radius.

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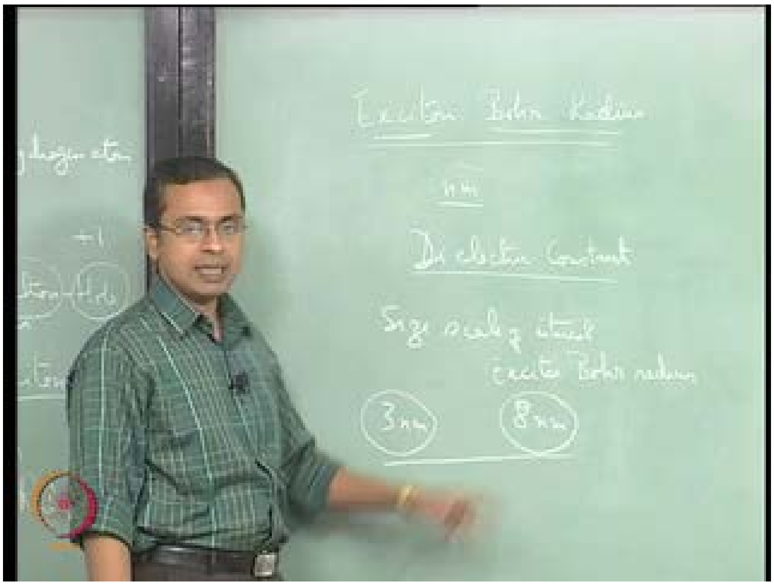

So, we have here. So, we now see that an entity called the exciton can show up and it can have something called an exciton bore radius associated with it, which then represents the kinds of distance that the electron hole pair can have between them while still maintaining this kind of a contact with each other or this connection each other. So, to speak. So, this is the exciton bore radius and as it turns out unlike that for a hydrogen atom where you are talking of you know an atom is within an angstrom, this exciton bore radius can be of the order of nano meters of several nano meters, it could be 3 nano meters, 10 nano meters and so on.

So, that is a large distance nano meter is 10 angstroms. So, 10 nano meters is 100 angstroms and so that means, it is of the order of 50 atomic distances. So, anywhere from 10 to 50 atomic distances is the kinds of values we are looking for in a, in a bore radius sorry in an exciton bore radius. So, it can be relatively large number, it is not in that sense you can see that it is not exactly it is not exactly equal to a hydrogen atom. So, so this is an exciton bore radius right and what is a and this is affected these exciton bore radius as I mentioned you know when you talk of materials it really each material has its own properties, the phenomenon is the same. Your seeing this, this formation of an exciton is essentially the same regardless of what you are looking at, what semiconducting material you looking at, but the actual radius is going to vary from material to material simply because each material may will have a different dielectric constant.

So, each material has its own dielectric constant. Now, when the dielectric constant is different it impacts the extend a manner in which the extent to which the electron hole pair are able to interact with each other or and therefore, have a influence on each other. Because they are oppositely charge they would like to have an they are they have a tendency to have a influence an each other which is what causes this exciton, but what is the extend of this interaction and how far they can get away from each other and still maintain that interaction depends on the dielectric constant of the material. So, therefore, as a result you find that the phenomenon of an exciton will show up in the semiconducting materials, but the corresponding exciton bore radius can vary significantly from material to material. So, this is one concept that we have. Now, what happens?

So, when I said you know the size scale is important we have to understand what is the size scale at which we start seeing this nano material based effects occurring for the that particular system. I said the size scale is impacted by the material we choose and also by the property that we choose. In our case with respect to the band gab type of properties, the electronic properties. For many of the electronic properties the size scale of interest is directly impacted by this exciton bore radius. So, for a nano material which is being used for electronic purposes where you are reaching, where you are trying to take advantage of some phenomenon that is occurring at the nano scale and its impact on the material property as long as you are talking of an electronic property. So, to speak electronic or optoelectronic property the size scale of interest is not some arbitrary fixed nano meter.

It is rather the specific exciton bore radius of the particular material, given a material, given it dielectric constant and such you can actually come up with an exciton bore radius. So, once you know that exciton bore radius whatever it is you know it may be 3 nano meters for some material, it may be 8 nano meters for some other material and so on. So, we may have different values for the exciton bore radius and based on the material you have chosen this would then be the scale of interest, size scale of interest for you to start seeing nano scale effects and here for another material this would be the size scale of interest.

So, clearly you know this factor of three differences here. So, when you make a sample out of this material when you reach a certain size scale and starts seeing the effects of the nano scale on the properties of the material, you will have to go to one third the size before you starts seeing the effects the same sort of effects on this material. So, so it reiterates my comment in the beginning both the property that you are choosing as well as the material you are choosing impact the size scale that you are looking at, which is where the effects of the nano material begin to take impact. So, this is 1 issue and incidentally when.

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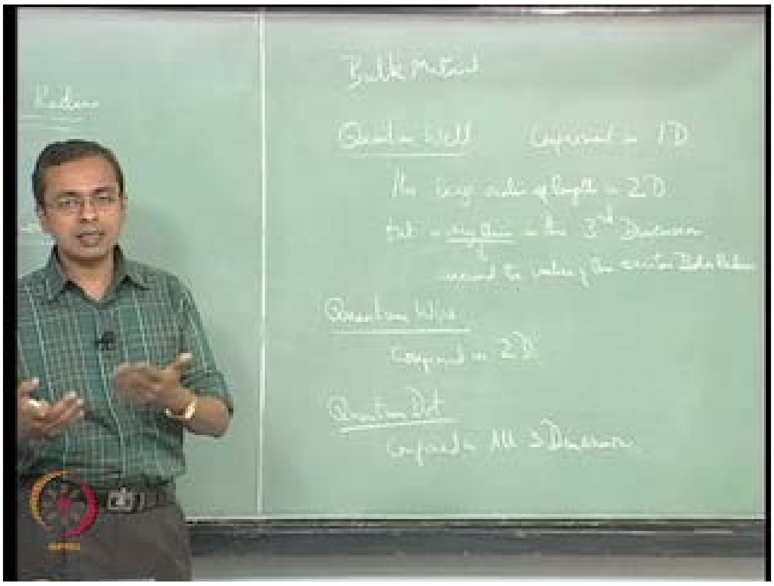

So, what it means is now a nano material has to be made in the dimensions for those respective materials before you start seeing the impact. What is done in terms of nano materials for this size scale? From an electronic perspective there are 3 terms that are often used, 1 is called a quantum well. In this what is being done is you these are all things that we will compare with a bulk material. A bulk material has a large crystal size and. So, on now you take a large bulk material and you start making it thinner, thinner and thinner till you finally, get an extremely thin sample of that same material.

So, it is now a 2 dimensional material what are a bulk material is large 3 dimensional material from which you remove material tell you get a two dimensional material. In principle in fact, with they do not normally do it that way rather they grow it up that way. So, you start with nothing and you growth atoms of whatever it is that you are growing till you get a very thin layer of whatever it is that you want or you can you may even sandwiched between two different materials. So, when you do that you have what you have got is a material which has has large dimensions in 2 dimensions, but it is thin in 1 dimension.

So, you have a very large piece of material, but it is very thin in 1 dimension and so the 3 dimension is extremely thin and when we say extremely thin, this very thin is a very descriptive sense this means you should get it to the around the exciton bore radius . So, you have to get it get the value of this dimension to be very close to the lengths scale in that direction to be of the order of the exciton bore radius, then you start seeing the impact of that material. If you, if it much thicker than this you will it will still look like a bulk material you will not know the difference, you have to get it to the size scale before you start seeing that difference. So, this is when you do it in when you do this only in 1 dimension and you are actually the electron is now actually free to move the we in this case we are actually we discussed that we are we have now discussing about this excitons, in this case this excitons as sort of free to move in 2 dimensions, but in the third dimension they have very limited mobility. So, they when you talk of a quantum well the exciton is now confined in 1 of the dimensions.

So, the exciton this is with respect to the exciton that we are talking of. So, with respect to the exciton, the exciton which has also this same kind of size scale is now confined in 1 of those dimensions where you have made it extremely thin and the other 2 dimensions its free it’s relatively unconfined. So, this is a quantum well then we have a quantum wire where you make a extremely thin wire of this material that you are interested in. So, it is confined in 2 dimensions and in 1 dimension it is free to go as far as it may there is no confinement in that sense and finally, we have something that we call quantum dot where essentially you are trying to make an extremely tiny particle of the material such that in all 3 dimensions it is confined to near about the exciton bore radius or even less.

So, in 3 dimensions confined in all 3 dimensions. So, on top we have the bulk material from that we can convert to a material which is confined. So, there is no confinement at all in all the 3 dimensions you get a material which can be confined where confinement of the exciton occurs in only in 1 dimension that is a quantum well, in typically a very thin film of the material you can confine it in 2 dimensions that is the quantum wire. So, that is actually a very thin wire and then finally, you can confine it an all 3 dimensions in which case you are essentially having out tiny particle of the material and that is called a quantum dot. There are of course, lot of very interesting scientific challenges in doing this because when you make such tiny particles they are usually very highly reactive.

So, they will not stay as tiny particles for too long if you make such tiny particles they are simply reactive with each other and they will (( )). So, when you make such tiny particles 1 of the scientific challenges is to freeze them such that they do not get in touch with each other and grow. So, normally for example, what is done one of the ways this is accomplished is to actually grow them inside a polymer metrics. So, many of the polymers will typically have pores inside them which are in the nano scale. So, you and. So, this would save as a host metrics. So, you take a host metrics consisting of this polymer. So, will have to analyze the polymer to understand what is what kind of porosity it has in it or what kind of internal voiced or present within it and pick a host material which has a voids in the size the size scale that you are interested in, which is the exciton bore radius of the particular material that you have planning to test. Then you grow this material inside this polymer.

So, and that can be done by various ways you can actually make a salt solution of this material, get it to penetrate into the polymer and then expose it to some gas. So, that it reacts and then forms the semiconducting material that you wish to have in that particular region. So, therefore, there are some interesting ways in which you can do this. So, there are lot of challenges here to get this materials made in the form that you wish to use. So, that you wish to test it in. So, in the process you will you can create all this thing,s you can create quantum wells, quantum wires and quantum dot. In each of these things in each of these cases you are doing you are confining the exciton in some one dimension either 1 dimension or 2 dimensions or in 3 dimensions you confining.

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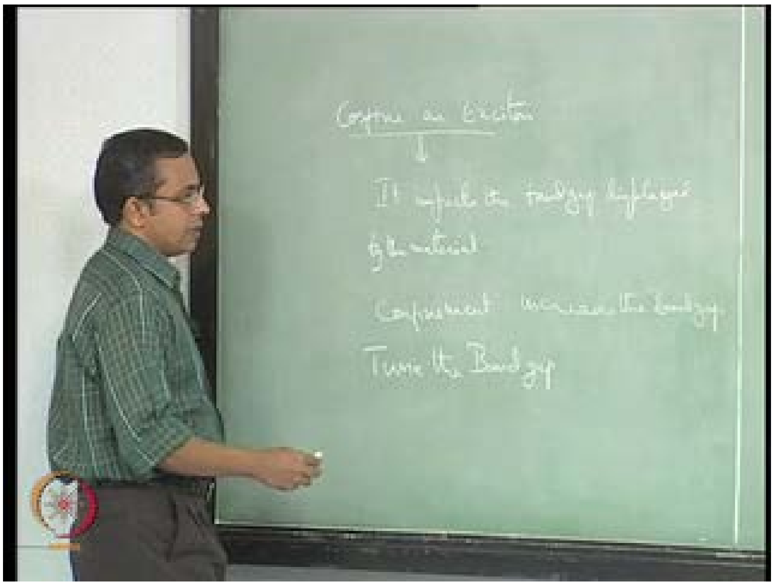

So, what is the impact of confining an exciton. When you confine an exciton within dimensions that is of the order of the bore exciton bore radius then what happens is it impacts the band gab. So, it impacts the band gab displayed by the material all right. So, what you now have is a situation where the bulk material has certain band gab and by simply making it a nano material you can change the band gab. So, because that changes the way in which the exciton is it is it is impacting the exciton combination and as a result it is causing changes to the band gab because they exciton has a certain interaction between the electron and the hole and this is a impacting it by making it in the same size scale the with the particle size being in the same size scale.

So, it impacts the band gab displayed by the material and in general confinement increases the band gab. So, it increases the band gab. Now, this is this is of the lot of interest because what this means is you can actually say for a some particular purpose, some particular purpose you wish to have semiconductors of different band gabs arranged next to each other. So, that you can make specific semiconducting devices let us say that that is the that is of interest. Often what happens is when you do this you can have with heat and so on, you can have some material diffusing to each other and as a result over a period of time dissimilar material contact is usually a bad idea to have in most engineering senses.

So, in many places in engineering we find that when we have dissimilar material contact there are lot of problems associated with them in terms of selling, in terms of any diffusion that might occur between them, any corrosion that might occur with between as a result of that contact and so on. There is several problems associated with dissimilar material contact, but there are many places in the in the electronic devices field where you end of having to use a dissimilar material contact because the band gabs that you are looking for and other such details maybe different for different materials and therefore, you may need that combination to make it to work.

So, now, you have a situation where by doing this confinement for the same material you can change the band gab. What is more important is you can actually the tune the band gab meaning if you do this carefully enough you can get a collection of particles of roughly the same size all of which are different from, all of which are near that exciton bore radius dimension and since you get a collection of particles of essentially the same size they will all have more or less the same band gab, but it will be different from the bulk band gab. So, you can have set of particles which are now different from the bulk band gab, but they have a distinct band gab associated with them. So, you can actually get variety of band gabs with the exact the same chemical composition you can get a variety of different band gabs.

So, you now have the possibility where you can put together something where you have pieces of that component each of which has different band gab, but has the same chemical composition. So, you can now eliminate dissimilar material contact, but still have the property variation that you desire. So, that you can actually get the component to work the way you wish to, you wish for it to work. So, confinement increases the band gab and we by using this nano scale all the impact of this nano scale structure you can actually tune the band gab and get materials with the band gab that you desire and therefore, you can use it with some of several advantages associated with the fact that the chemical composition is the same. And so, that is the big advantage.

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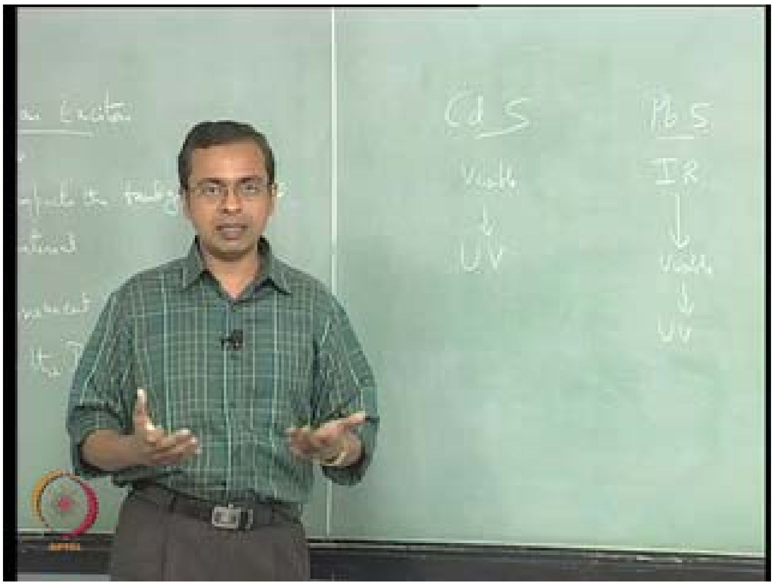

So, for example, you know some of the materials that people work on or materials such as cadmium sulfate and lead sulfate. So, this has a band gab which is sort of in the somewhere in the visible region of the spectrum and when you raise the band gab of course, it means that you can now it will now respond to the radiation of only higher wavelength. So, you can go from visible to u v. So, the same material you can get with the wide range of band gabs going from the visible spectrum to the ultraviolet spectrum. This is a material which actually has band gab more closer to the infrared region infrared which is represented by I r and with this material the infrared region you can actually change its band gabs going all the way through visible to u v.

So, you can change the band gabs in a dramatic way and so, the beauty of this is if you are looking for color of the material when you are talking of material which are actually going through this range of band gabs which goes through the visible range what it means is you can actually make a series of samples, where all the samples have exactly the same composition, but they span the entire spectrum of colors that you are looking at. So, you can sort of get paint of variety of different colors if use this as you are pigment for example, I mean we and I mean we do not want use lead, but I am just giving you the as an example. You basically in terms of color you can get all the colors with the composition being exactly the same and that is a very interesting and interesting and in a sense a very visible way in which you are seeing the quantum confinement effects on some of these materials.

So, therefore, and that is just the that is something just for our visual perception of course, in term of actual usage you may find much more interesting band gabs and variations of those band gabs, which you can cause by this quantum confinement effect on the based on the exciton bore radius of those radii of those materials. And therefore, lot of there is lot of technological interest in the nano scale materials and what they represents in terms of the physics and in terms of what they can represents in terms of the devices that you can create using those nano scale materials.

So, we have seen here that you know you we understand now why is it that the nano scale material has a certain property that we can manipulate and that is not as I said with the fact this exciton’s form and those exaction’s have some characteristics radii associated with them, in a sense behave likes hydrogen atoms and then this is impacted by the materials properties such as the dielectric constant and then once you know this information for a particular system you can manipulate it. There are lot of scientific ah on technical challenges in being able to do this manipulation this is easy to say here to go from I r to u v, but to get any particular wavelength consistently is a challenge, but you can do it, people have done it and demonstrated it and that is how this these materials are used.

So, that is a brief over view of the physics of nano scale materials from the within the per view of what we have discussed through this course. Of course, there is a lot of as I mentioned this lot of research into this kinds of materials and there is a lot of literature available which looks at this in great detail. they look at cut off wavelengths were something is observed and how that wavelength changes, there is lot of studies on how this materials age with time and what are the factors that impact how stable those nano particles are and where you can use them. Even for solar cell application you can perhaps finds something which has a which is a cheaper material, but has the right kind of a band gab. So, that it observes most of the radiation that is falling on that material because you the solar energy has spectrum associated with it only as certain fraction of it is the visible spectrum that we see. There is a lot of energy available in the spectrum which we do not directly see through our eyes and if you and therefore, if you want to capture solar energy in its entirety and the. So, that you can make use of solar power you need a materials which have the right kind of a band gabs to observes all of that energy and to do show very efficiently.

So, so that you capture as much percentage of what is falling within that unit area that would help you have smaller solar cells which are cheaper because it is of a materials that you have chosen which is cheaper, but it is small because it is able to efficient to capture of all the energy that is falling incident an it and you are able to tap it. So, very. So, what we have just discussed is a very important input towards work that people carry out towards finding out alternate material for collecting capturing solar energy and using it as an alternate source of power. So, with this we will conclude our discussion on these, its brief discussion on the physics of nano scale materials. This is relatively an advanced topic because a lot of research is being done on this it is still an on going research topic and in that sense it is not the, in the same sense of a conventional undergraduate topic were basic theory and understanding is very sound and everything is a currently known.

There is lot of work going on and this in this area it is a relatively its typically more of post graduate topic. So, you may you may see post graduate courses which do well more on to this kinds of nano scale materials and the physics of nano scale materials. This gives you an overview of the major features associated with such types of topics and the discussions associated with them. So, with this we will conclude this topic what we will now do briefly is a we will review what we have done through this course with through a series of slides and conclude this course with a few specific comments related to where this course stands with respect to everything else that we have you are studying.

So, will now look at a few slides. So, as we come to the conclusion of this course we will now briefly review what it is that we have done through this course more or less on a class by class basis and that will give a very good feel for what it is that we have covered through this course and perhaps how it is connects to anything else that you are presently learning. So, we will do that and that will give a summary of the course that we have and the material that we have looked at at this point.

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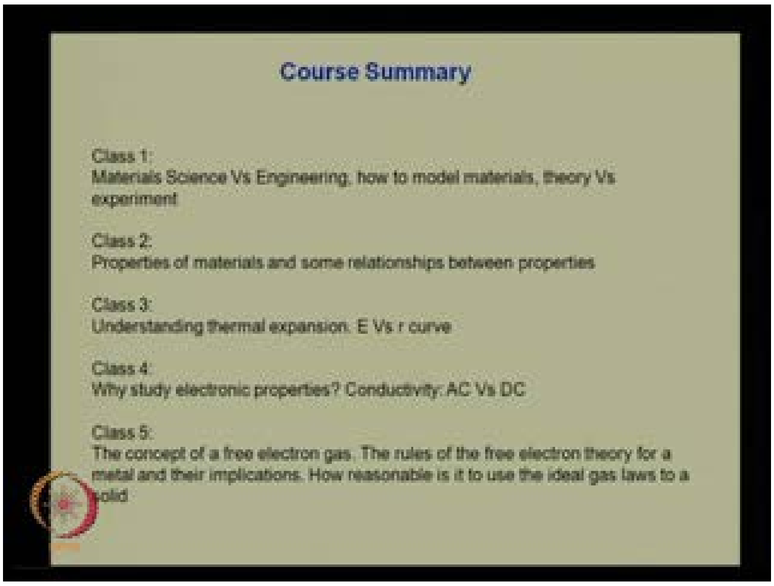

Course Summary

Class 1:
Materials Science Vs Engineering, how to model materials, theory Vs experiment

Class 2:
Properties of materials and some relationships between properties

Class 3:
Understanding thermal expansion. E Vs r curve

Class 4:
Why study electronic properties? Conductivity: AC Vs DC

Class 5:
The concept of a free electron gas. The rules of the free electron theory for a metal and their implications. How reasonable is it to use the ideal gas laws to a solid

So, to begin with we looked at a we started off by looking at material science verses material engineering and in particular we looked at how we need what kind of a approaches we would need to do model materials. And also we considered the difference between a theory verses experiment in the sense that I particularly highlighted the fact that at the end of it all it is the experiment that is supreme, in the sense that if you write if you are able to come up with a theory that is that cannot be proven by experimental in any in any in any sense with by experiment or if there is strong experimental evidence that that is contradicting a theory then in principle the theory is not going to be accepted.

So, in that sense in hierarchy experiments in higher than the theory; however, theory may suggest that you have to try out new experiments or perhaps have a better control on how you run your experiments. So, that possibility is always there. We then went and looked at properties of materials and some relationships between those properties to see what are the kinds of things that we should attempt to module. So, that we can see if our models are actually correct because as I said the model will be some kind of a theory which then has to match the experimental data given by those properties.

Then we looked at the thermal expansion process and in particular the e verses r curve and we did this because in a single instance we could in a single class we could actually see how we could build a model for a material from fun first principles and see and they experimentally observed property which we could, which we can then and see how it matches that experimentally observed property and so we spend, we did we focused on this for an entire class. After that we got on to electronic properties which required as to look at a lot of back ground material, but we started off by trying to understand why we why there is a focus an electronic properties and in particular if you are looking at conductivity the fact that you know there is AC conductivity and there is DC conductivity and what are the similarities between them what are the differences between them and under what conditions one of the property is one way of measuring it is more relevant than the other way of measuring it and so on.

So, we did that in some detail then we moved on to the concept of a free electron gas which we used for our initial theory of a trying to understand conductivity. We looked at the rules that are used for this free electron theory for a metal and they are implications. We also try to reason whether or not it is reasonable to use the ideal gas loss to a solid. We looked at what are reasons why it may be acceptable and also what are the reasons why it may be questionable to use such a such a approximation.

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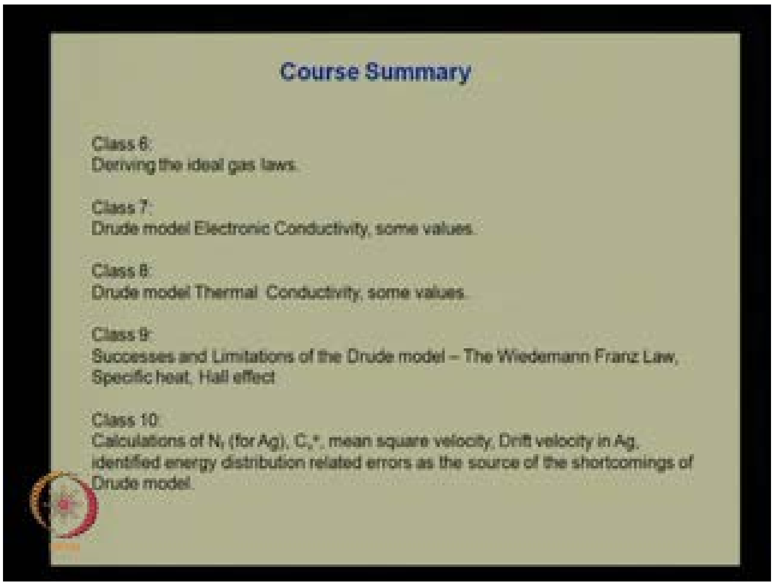

Course Summary

Class 6:
Deriving the ideal gas laws.

Class 7:
Drude model Electronic Conductivity, some values.

Class 8:
Drude model Thermal Conductivity, some values.

Class 9:
Successes and Limitations of the Drude model – The Wiedemann Franz Law, Specific heat, Hall effect

Class 10:
Calculations of N_f (for Ag), C_v*, mean square velocity, Drift velocity in Ag, identified energy distribution related errors as the source of the shortcomings of Drude model.

In this context since we were going to use specific relationship that are obtained in the ideal gas loss as part of our derivation of the free electron theory for the metallic systems. We actually went ahead and derive those particular relationships of the free of the ideal gas theory. So, that we could use them with confidence in our modules for the electrons in the metals The first module that we looked at in detail was the Drude model for the electronic conductivity and particularly how that Drude model was helping to explain electronic conductivity. What it gave as a trend for electronic conductivity, for the values for the electronic conductivity for various materials that was the focus of our class here and in we compared of the what model predicted with several experimental values and we found that it actually did a very good job in explaining electronic conductivity.

We then looked at the same Drude model which is a free electron gas model a classic free electron gas model were the electrons are treated as classical particles and similar to an ideal gas set of atoms and then tried to see if how good it was in trying to explain thermal conductivity and again we looked at values from the literature to see if the thermal conductivity predicted by the Drude model was reasonable and once again it turned out that those values were pretty good. So, both of these were considered successess of the Drude model and in particular the Wiedemann Franz law which relates the electronic conductivity and the thermal conductivity was a very accurately, I mean quite accurately predicted by that Drude model and so, that was considered as a remarkable success for that Drude model.

However, we also pointed out that the Drude model had some limitations in the sense that it was not able to explain everything that we saw in a experiment. In particular specific instances of the hall effect you were not clearly explained using the Drude model and most importantly from the with respect to the prediction of the electronic contribution to specific heat, the Drude model over estimated this prediction in a very significant way. So, in this context we try to explore the Drude model and aspect associated with it in greater detail and we went ahead and did some calculation for the number of free electrons per unit volume, the specific heat at constant volume, electronic contribution to specific heat at constant volume and related mean square velocity it drift velocity and silver and we realize that at as at a fundamental level when we looked at this models, we were using an energy distribution amongst the electrons as a very fundamental aspects of the model.

So, somewhere hidden in the model even though we did not state it upfront was the assumption that electrons were distributed across energy levels in a particular manner and whatever we were predicting for the material was based on how this distribution existed. What was this distribution and therefore, how did the distribution change as a function of say temperature of the system. So, this was something we identified as a very fundamental aspect of the model which was not immediately apparent when we did the model. And so, we thought that we looked at the possibility that there may be errors related to this model which were the source of the short coming of the Drude model.

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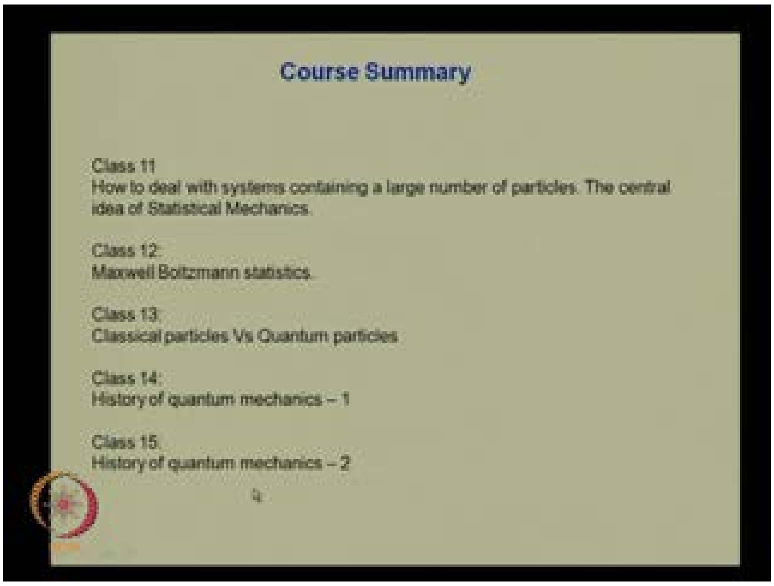

Course Summary

Class 11
How to deal with systems containing a large number of particles. The central idea of Statistical Mechanics.

Class 12:
Maxwell Boltzmann statistics.

Class 13:
Classical particles Vs Quantum particles

Class 14:
History of quantum mechanics – 1

Class 15:
History of quantum mechanics – 2

So, this is something that we wanted to explore in greater detail. In this context, we recognized that that system that we were dealing with were actually a electrons in a solid which were a large number of particles essentially 10 power 28 electrons per unit volume and to deal with such a system we cannot just like that find out even if you want to find out the mean square velocity, we cannot actually physically calculate the velocities of each of those particles and then find out the mean square velocity. So, if there has to be a different system to way of approaching such a large collection of particles and that is the statistical idea of statistical mechanics and in this context we discussed the central idea and central approach, central idea of the approach of the statistical mechanics and how it says that you know if you look at large collection of particles then the most probable distribution of those particles is then the equilibrium distribution of those particles and

so, if you understand what is the most probable description distribution of those particles you get a good sense of what is the average property that the material is going to demonstrate as a result of assuming that that is the distribution of those particles.

Having understood this idea of statistical mechanics we went on to the math we went on and derived the Maxwell Boltzmann statistics. The Maxwell Boltzmann statistics applies to a series of a set of particles a large collection of particles which are called classical particles and so, that is what this derivation was all about and in therefore, this is exactly the statistical distribution that the Drude model assumes in by saying that the electrons are behaving like atoms of a of an ideal gas. And therefore, errors in say estimating the velocity or the energies of those electrons traces itself back to the fact that we have assuming that this is the distribution of energy of those electrons. So, the distribution itself is the statistical distribution is correct, it is just that or assumption that it applies to electrons is not correct.

So, the it is not that the math associated with the distribution is wrong, the math is fine it is just that our assumption that this distribution applies to as collection of electrons is not correct. In this context we examined in detail what we mean by a classical particle and what and what are quantum particles. Classical particles particularly I mean these are terms that we here often and it therefore, it was necessary to explore this in detail to understand exactly what is different between the 2 of them. So, that we can incorporate those differences into the statistical the ideas of this statistics of those particles. So, so that is a reason why we looked at this in greater detail. And having understood that you know the particles that we are dealing with or not classical particles electrons, they are quantum particles.

We recognize that we have to now use approaches which are relevant to quantum mechanics to understand what the how the solid is going to behave. In this context we looked at the history of quantum mechanics and particularly we did it because there is usually a lot of difficulty amongst too lot of people to understand quantum mechanics or to use it and this is hardly surprising if you understand the if you look at the history of quantum mechanics and the difficulty that the most spectacular scientist involved in this process had in also accepting quantum mechanics. People like Einstein lived there life time with lot of doubt that quantum mechanics was correct. They actually, see he seriously doubted that it was right he was of the firm opinion that there was the much more fundamental science that would sooner or later we discovered which would not requires the sort of what look like arbitrary steps in arbitrary assumptions of the quantum mechanical of quantum mechanics and so, there is a lot of difficulty, inherent difficulty in quantum mechanics simply because of what it is represents. Simply, because many of the things stated about quantum mechanics or not very intuitive for many of us.

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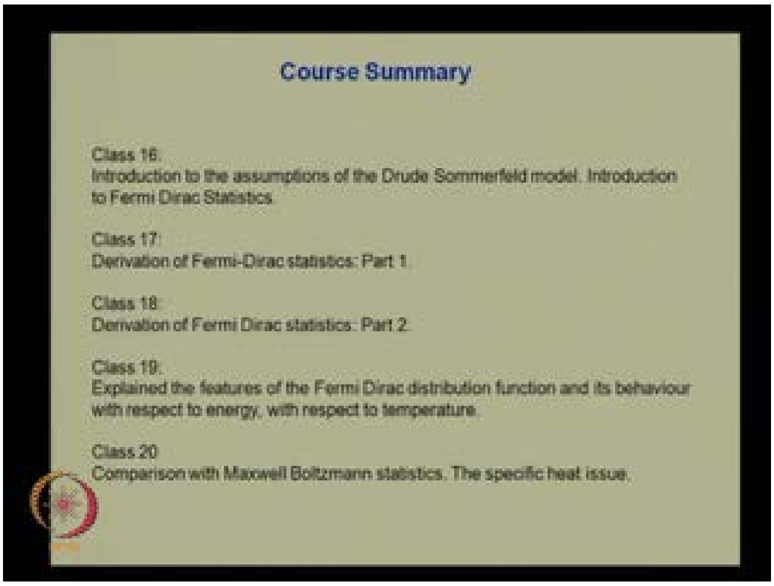

Course Summary

Class 16:
Introduction to the assumptions of the Drude Sommerfeld model. Introduction to Fermi Dirac Statistics.

Class 17:
Derivation of Fermi-Dirac statistics: Part 1.

Class 18:
Derivation of Fermi Dirac statistics: Part 2.

Class 19:
Explained the features of the Fermi Dirac distribution function and its behaviour with respect to energy, with respect to temperature.

Class 20
Comparison with Maxwell Boltzmann statistics. The specific heat issue.

So, there that is why there is a lot of difficulty and so, the at least we recognize that we need not be so surprised that we have such a difficulty in dealing with this subject. Then having looked at quantum mechanics, we looked at the assumptions of the Drude Summerfield model which is the model that takes the quantum mechanical behavior and imposes it on the. So, on the original Drude model and therefore, tries to correct for some of the errors associated with the Drude model and in particular it does so, by changing these statistical distribution that is being assumed for the electrons whereas, previously the fermi the Maxwell Boltzmann distribution was being assumed for the electrons the Drude Summerfield models specifically introduce the Fermi dirac statistics and looked at how the Fermi dirac statistics can be imposed the fact this would be the more appropriate set of statistics the statistical distribution to use for the collection of electrons that are there in a solid.

In this context we derive the Fermi dirac statistics. So, that we get a good feel of what those how the statistical distribution is, how the fundamental nature of the particle impacts the manner in which we count the possibilities that can exist and therefore, how we incorporate the fact that it is a quantum mechanical particle rather than a classical particle into the statistical distribution.

So, that was the important reason why we looked at this statistical distribution and we derived it in full detail. So, that we can take the result with confidence and understand what each of those terms means. Then we looked at the features of the Fermi Dirac distribution function and it is a behavior with respect to energy and with respect to temperature. This is very important because the properties of the electrons in terms of the electronic contribution to specific heat which was the big problem with the original Drude model are all associated with these two aspects.

The distribution of electrons across energy and how they behave with respect to temperature. So, this is the very important aspect of that correction to that models and so, this is why we looked at it in detail here. So, we compare then with the with our results up until that point with what had that we obtained for the using the Maxwell Boltzmann statistics and in particular we looked at the specific heat issue and how the Maxwell Boltzmann statistics or the Drude model dealt with a specific heat issue and as suppose to how the Fermi Dirac distribution and therefore, the Drude Summerfield model which is an improved model dealt with a same specific heat issue.

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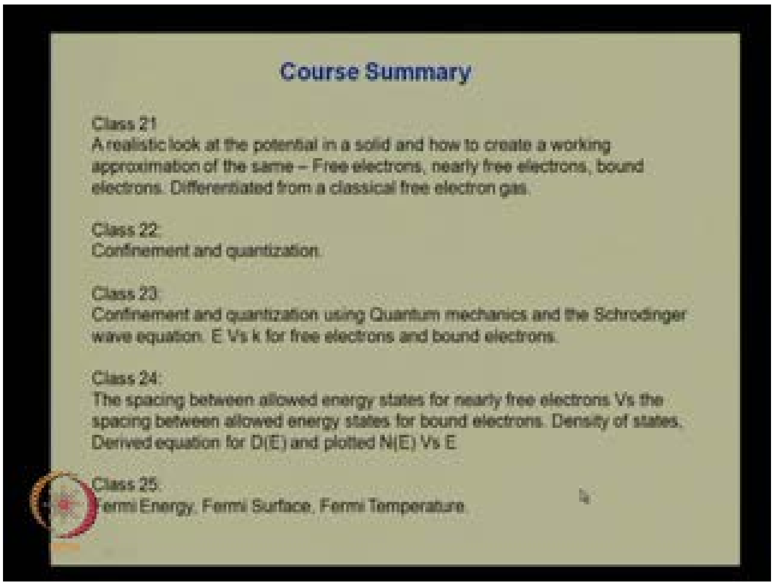

Course Summary

Class 21
A realistic look at the potential in a solid and how to create a working approximation of the same – Free electrons, nearly free electrons, bound electrons. Differentiated from a classical free electron gas.

Class 22:
Confinement and quantization.

Class 23:
Confinement and quantization using Quantum mechanics and the Schrodinger wave equation. E Vs k for free electrons and bound electrons.

Class 24:
The spacing between allowed energy states for nearly free electrons Vs the spacing between allowed energy states for bound electrons. Density of states. Derived equation for D(E) and plotted N(E) Vs E

Class 25:
Fermi Energy, Fermi Surface, Fermi Temperature

In this context we, we then decided that you know even though we had understood now at least in a pictorial sense what was the difference between the Drude model and the Drude Summerfield model and why the Drude Summerfield model was better. Why Fermi dirac statistics was doing a better job than the Maxwell Boltzmann statistics, we decided we needed to have a better feel for what was going on the material. So, we needed more quantification of what was going on the material is more specifically as we discussed when we looked at the Fermi Dirac statistics the statistical distribution was giving as the probability of occupancy. It never told as how many electrons were occupying those state or how many electrons could even consider occupying those states.

So, it was necessary for us to understand how many states were available at each energy level, which required as understanding more about how those energies are quantized and how we can calculate those numbers. So, in this context we would we looked at we built a realistic model to look at a potential in a solid and how to work creating working approximation of the same. So, we looked at how if you move an electron from infinity towards an ionic core, how with a potential would change. If you had a series of ionic cores what kind of potential atmosphere it would experience as it moves through the solid and then we came up with an approximation for it. So, that we could do calculation with respect to it.

So, that the potential wells looked a little bit more square. In this context we recognize what are free electrons, what are nearly free electrons and what are bound electrons and we differentiated these from a classical free electron gas. Having done that we looked at the fact that electrons in a solid or confined and we looked at the idea that when we do confinement you get quantization and we explore this in great detail because this is a very central part of how the behavior of solids is seen and experienced when you look at it in this context. And then we looked at quantization using and the confinement and quantization using quantum mechanics and the Schrodinger equation and therefore, we were able to see come up with an energy verses k relationship for free electrons, nearly free electrons and for bound electrons. And we also found that the that there was a spacing between allowed energy states for the nearly free electrons and we compared it with the spacing between allowed energy state for bound electrons.

We calculated density of states and derived the equation of density of density of allowed states as a function of energy and the density of occupied states verses energy and this is what really enables us to understand the to quantify the electronic contribution to specific heat. In this context we also looked at important concepts such as Fermi energy, Fermi surface and fermi temperature and we looked at their significance in terms of the properties of those materials. Then

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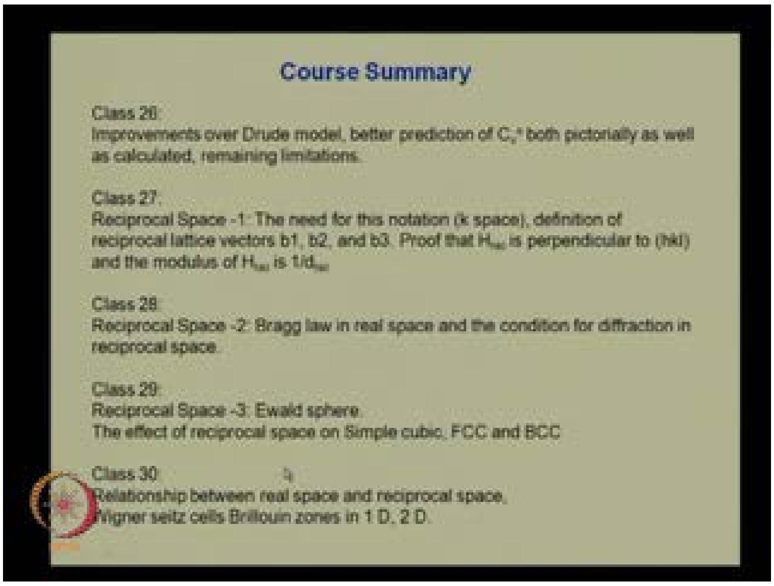

Course Summary

Class 26:
Improvements over Drude model, better prediction of C_v^e both pictorially as well as calculated, remaining limitations.

Class 27:
Reciprocal Space -1: The need for this notation (k space), definition of reciprocal lattice vectors b1, b2, and b3. Proof that H_{hkl} is perpendicular to (hkl) and the modulus of H_{hkl} is $1/d_{hkl}$

Class 28:
Reciprocal Space -2: Bragg law in real space and the condition for diffraction in reciprocal space.

Class 29:
Reciprocal Space -3: Ewald sphere.
The effect of reciprocal space on Simple cubic, FCC and BCC

Class 30:
Relationship between real space and reciprocal space.
Wigner seitz cells Brillouin zones in 1 D, 2 D.

we looked at improvements over the Drude model and as I said now that we had all the tools in place we were able to look at the electronic contribution to specific heat at constant volume, as a calculated process comparing the Drude model with Drude Summerfield model and we identified the remaining limitations such as the and an isotropy of solid which had not yet been understood. We then looked at reciprocal space in considerable detail.

We looked at its construction. We looked at how diffraction occurs in reciprocal space, what is the condition for diffraction and what it is represents how it can be represented pictorially and what it does in terms of how it relates to real space in the sense that what happens to lattices which are simple cubic FCC and BCC in real space, what happens to them when you looked at them in reciprocal space. And in that sense we looked at the relationship between real space and reciprocal space. We define what are Wigner Seitz cells and what are brillouin zones in 1 dimension, in 2 dimensions.

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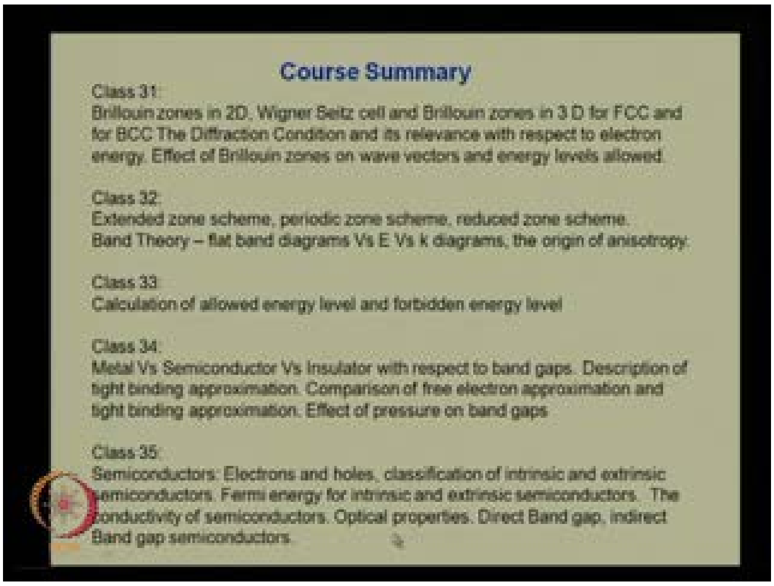

Course Summary

Class 31:
Brillouin zones in 2D, Wigner Seitz cell and Brillouin zones in 3 D for FCC and for BCC The Diffraction Condition and its relevance with respect to electron energy. Effect of Brillouin zones on wave vectors and energy levels allowed.

Class 32:
Extended zone scheme, periodic zone scheme, reduced zone scheme.
Band Theory – flat band diagrams Vs E Vs k diagrams, the origin of anisotropy.

Class 33:
Calculation of allowed energy level and forbidden energy level

Class 34:
Metal Vs Semiconductor Vs Insulator with respect to band gaps. Description of tight binding approximation. Comparison of free electron approximation and tight binding approximation. Effect of pressure on band gaps

Class 35:
Semiconductors: Electrons and holes, classification of intrinsic and extrinsic semiconductors. Fermi energy for intrinsic and extrinsic semiconductors. The conductivity of semiconductors. Optical properties. Direct Band gap, indirect Band gap semiconductors.

And we also defined what they are in 3 dimensions for in FCC and BCC and more importantly we also looked at the diffraction condition which we had independently looked as separate entity, but we now looked at it with its relevant with respect to the electron energy. In particular we looked at the effect of Brillouin zones on wave vectors and the energy levels allowed and therefore, how the energy gabs are likely to appear in the materials. In this context we drew diagrams which we called the extended zone scheme, the periodic zone scheme and the reduces zone scheme.

And we saw how the flat band diagrams which is the which is what the band theory is all about, how it compares with the e verses k diagrams and how in this context of understanding that depending on the direction in the lattice the bands can appear at different locations in energy. We can understand the origin of an isotropy. The Fermi surface is the same, but were the Brillouin zone is different in different directions and that is why we get an isotropy. We looked at a detail calculation of how we can see based on or understanding of the material and how by using the Schrodinger wave equation and solving for a what the electron for do when the potential is 0 and the potential is v naught using that as a framework, how we can calculate what are the energy L levels that are allowed and what are the energy levels that are forbidden. This context we looked at metals verses semiconductor verses insulator and we compared the free electron approximation to the tight banding approximation. We built up this tight banding approximation and compared these 2 free electron approximation and tight banding approximation. We also got of sense of how pressure my change band gabs by changing the inter atomic spacing with respect to the tight banding approximation.

Then, we delt in detail with semiconductors. We looked at the classification of intrinsic and extrinsic semiconductors. What happens to electrons and holes. What are electrons and holes what happens to them in this context. We looked at a Fermi energy for these semiconductors and how it changes form an intrinsic semiconductor to an extrinsic semiconductor and we also looked at how the conductivity of semiconductors is impacted by whether or not it is intrinsic or extrinsic. In this context we also looked at optical properties and we looked at direct band gab and indirect band gab semiconductors and they are use for opto electronic materials. In the last few classes

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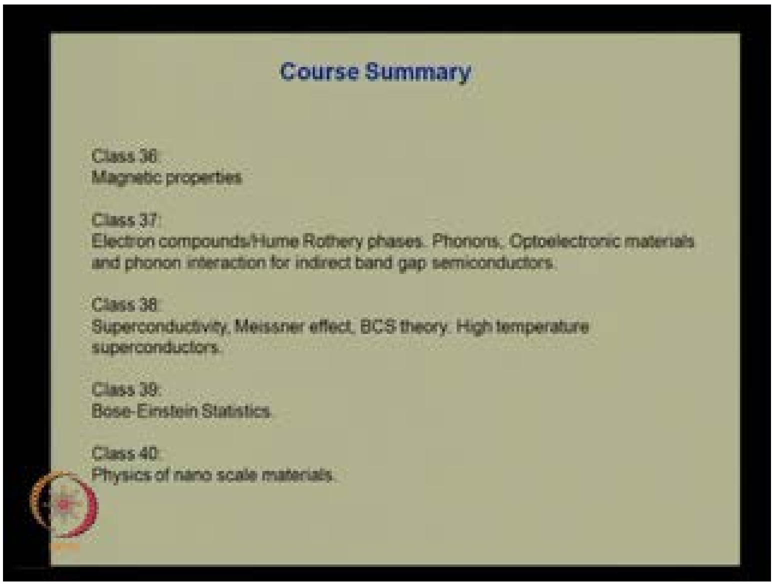

Course Summary

Class 36:
Magnetic properties

Class 37:
Electron compounds/Hume Rothery phases. Phonons, Optoelectronic materials and phonon interaction for indirect band gap semiconductors.

Class 38:
Superconductivity, Meissner effect, BCS theory. High temperature superconductors.

Class 39:
Bose-Einstein Statistics.

Class 40:
Physics of nano scale materials.

we looked at magnetic properties in detail. We will try to understand what the properties are what are features of this magnetic properties and also how the density of occupied states that we have that we have understood through this course helps us understand magnetic properties. Then we went on to look at electron components hume rothery phases and again understand how our picture of the density of occupied states helps us understand why 1 phase is more stable than the other phase in relation to electron energies and then we looked at phonons and how what they are, what they represent, how they interact in the case of optoelectronic materials and what phonon interaction does for indirect band gab semiconductors.

We then went on to superconductivity in detail we looked at the Meissioner effect. We consider the BCS theory discussed it and we also looked at high temperature superconductors and we notice that in both in terms of the photons that we have discussed, the phonon that we have discussed and the cooper pairs that we have discussed in the BSC theory that an integral part of all this was the fact that they were all bosons and so, in that context we looked at the Bose Einstein statistics.

And finally, we finished of by looking at the physics of nano scale materials by trying to understand what is so special of the nano scale that it impacts the physics of it and how perhaps we could take advantage of it. So, this is a then this summary of the course. So, we would now we now come to the conclusion of our course we have gone through all these topics and we have also looked at summary of it in the last few moments.

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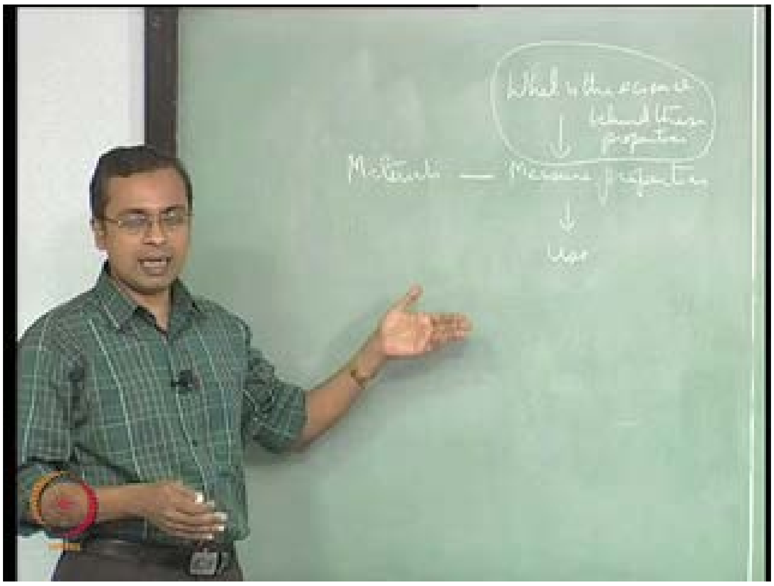

So, what we have actually done is through this course we started off this course at a stage where we basically said we have materials, we can measure their properties and therefore, we can use them. So, this is the framework within which most of work, most of what is done in material science operates. What we have now done is we have write to understand what is the source of, what is the science behind this properties. This is then the important contribution of this course. In this course we have looked in great detail at this science behind this properties. So, that we now have a better sense of why is it that we are measuring the property, why is it that the value of the property is what it is when we measure it and by understanding this we have a better capability of manipulating the materials to get the properties the way we desire them to be and therefore, this is important contribution to the general field of our ability to function effectively as material scientist. So, that is why that is the important contribution of this course.

Of course, a no course is ever going to be entirely complete. So, this is what we have discussed here will be able to will set the framework for you the base for you to look at a lot of other courses advanced courses in material science in electronic materials, in devices and so on. Where you can take all the basic concepts that we have learnt here and understand the material that they are they are going to expose you to in those courses and then make and in the process help you become a more effective material scientist. So, with this we will conclude the course. I hope it has taken you from being able to nearly use the materials to understanding how you can what is the science behind them. So, that you can manipulate them and get them to serve you are purpose even better. Thank you. .