Semiconductor Optoelectronics
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Lecture - 12
Strained–Layer Epitaxy and Quantum Well Structures

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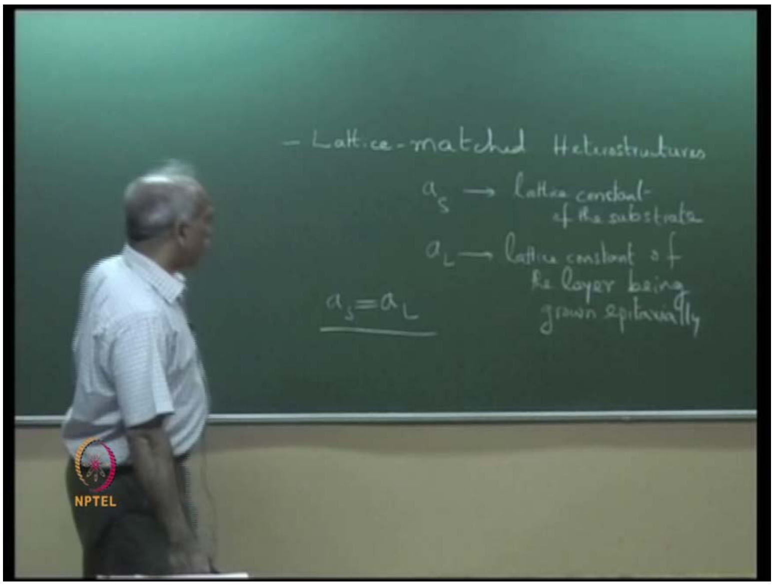

So we start with this lecture on strained-layer epitaxy. In the last class I discussed about lattice matched hetero structures, growth of lattice-matched hetero structures. So this is what we discussed in the last class and I had mentioned that if there is a lattice mismatch, if the lattice constant of the substrate a S, if a S is the lattice constant of the substrate of the substrate and a L is the lattice constant lattice constant of the layer that is being grown of the layer the epi-layer actually the layer being grown epitaxially. Then we wanted that a L a S must be equal to a L. So this is lattice matching, but what would happen if a S is not equal to a L?

In the last class in our discussion I showed that if a S is not equal to a L, there are some atoms which do not participate in the bonding and then there are dangling bonds which are defects in the medium. And the defects always increase the possibility of non-gradiative recombination’s which is detrimental to the performance of optoelectronic devices.

Is it true that we cannot grow this at all if a S is not equal to a L? If a S is not equal to a L, even then we can grow defect free structures provided, there are certain conditions, provided the thickness of the layer is below a critical thickness. If the thickness of the layer that is being grown is less than a critical thickness, then it is possible to grow defect free structures and this is called strained-layer epitaxy. It is called strained-layer epitaxy, because in that case there will be built-in strain in the medium.

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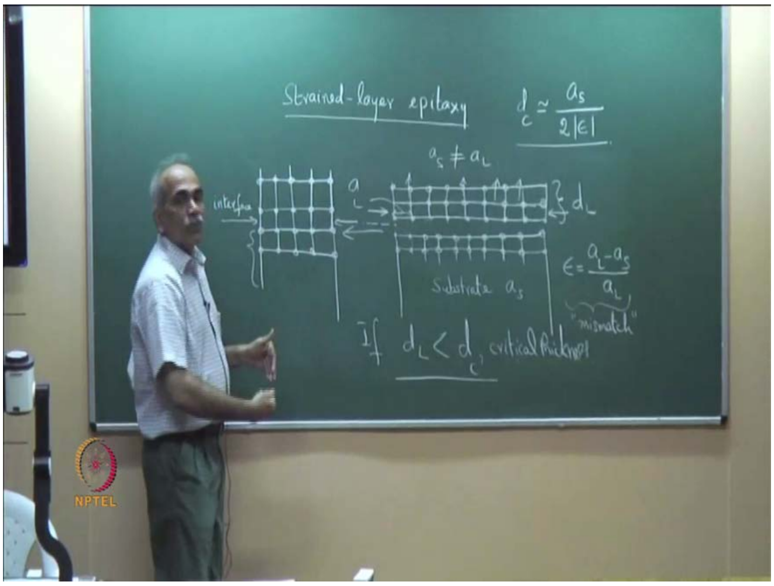

So let me illustrate this strained-layer epitaxy. So epitaxy is growing on top epitaxies. So if you start with a substrate as before let me show a one dimensional structure which means, I have atoms sitting in a one dimensional lattice. So this is the top monolayer that I am showing this is the substrate, which is characterized by a S.

If I want to grow a layer on top of this which has a larger let us say I want to grow a monolayer of this, which has a slightly larger. So this layer has a L the lattice constant here in one dimension the separation between two atoms is a L lattice constant. This is now not matching. In the last class I had said that there this will result in dangling bonds and defects.

However if the thickness of the layer is very small, what is this very small we will quantify. If the thickness of the layer is very small, it is possible to form lattice matching, what would happen is the atoms in this layer which is a very small thickness, adjust themselves reduce their lattice constant, that is there would be a built-in strain in this direction, a compressive strain a compressive strain from the sides which will result in a compressive strain here will lead to an elongated strain or tensile stress strain in this direction, a compressive strain from the sides and a tensile strain in this direction.

So these atoms will feel a tensile strain in the vertical direction, compressive strain from here. To match these atoms exactly to match this, so what would happen is this would result in a structure I will show a smaller portion here. I am taking a square lattice just to illustrate the point. So this is square, this was also square before they formed bond but when they formed what happens is let me draw it and then it will become clear.

This was the interface, please see this was the substrate, this is the interface, this gap interface here. So the interface has is here so it had square lattice here but what has happened in this direction is when it tried to adjust itself in this direction by experiencing a compressive strain, then it gets extended in this direction, it has become rectangle in this direction because the atoms have been pushed to accommodate the size here. So at the interface we have a S equal to a L before this, so this was a L.

So a S not equal to a L a S not equal to a L but it has adjusted itself. So that a S has become equal to a L in this direction at the interface but there is a built-in strain now and hence they are called strained-layer epitaxy. It is a strained layer epitaxy, because there is built-in strain on the layer that you have grown. Hence the name strained-layer epitaxy but there is a restriction when can the atom adjust itself when can the layer adjust itself, provided the thickness of the layer that you are growing here the thickness if I call this as this thickness was d, this is d L then if this thickness d L, if d L is less than a critical thickness d C. So d C is the critical thickness critical thickness.

This critical thickness d C is given by an empirical relation approximately equal to a S divided by twice mod epsilon, where epsilon is called the mismatch parameter. So epsilon is equal to a L minus a S divided by a L a L minus a S divided by a L is called the mismatch parameter or mismatch. It is a measure of mismatch when epsilon equal to 0; that means, a L equal to a S it is perfectly lattice matched structure but when epsilon is not 0 it means a L is not equal to a S therefore, epsilon is the mismatch parameter.

If the thickness of the layer epitaxial layer which is being grown, if it is less than a critical thickness then it is possible for the atoms in the layer lattice here to get adjusted although there will be a built-in strain. In the resulting structure there will be a built-in strain but the layers can get adjusted. You can think of an example of a sheet of rubber rubber rubber sheet. If it is very thin you can stretch it, rubber you can stretch if it is thin. If I give a thick block of rubber you just cannot stretch. It is just like a solid you just cannot stretch it but if the rubber sheet is thin then it is possible to stretch it, it is exactly that what is happening that if the thickness of this layer is very small, then it will adjust itself. So that it matches this lattice with the additional feature that there are compressive strains built-in strains and this is called strained-layer epitaxy.

There are no defects, no dangling bonds it has adjusted itself but in the process of adjustment there is built-in strain in the structure hence, the name strained-layer epitaxy. Let us put some numbers into this and see what kind of thicknesses are acceptable which will make it more clear and then we will also quantify this parameter which is the mismatch parameter.

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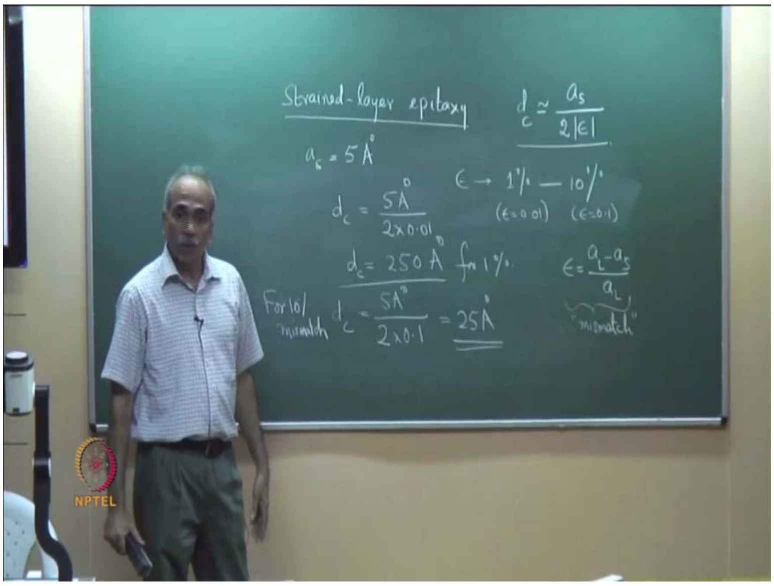

Let us say the substrate the substrate lattice constant a S is equal to 5 angstrom as you know typically most of the semiconductors have a S substrate lattice constant anywhere from 5 point 5 to 6 angstroms.

So let me take a S equal to 5 angstrom. If epsilon generally, people talk in terms of percentage, if eplison is 1 percent to 10 percent. This is the kind of mismatch which is 1 10 percent means, epsilon equal to 0.1 expressed in percentage is 10 percent, this ratio is 0.1, that is 10 percent mismatch, 1 percent means epsilon equal to 0.1.

So let us see what is d C? The critical thickness equal to if I put 1 percent then a S is 5 angstrom divided by twice into epsilon is this much that is 2 into 0.01, 1 percent how much is this? 250 angstrom. The critical thickness is 250 angstrom. So if a lattice mismatch of 1 percent can be tolerated provided the thickness of the layer is less than 250 angstrom. If you are growing only a thin layer with thickness less than 250 angstrom then that lattice mismatch can be tolerated.

If you put 10 percent mismatch 10 percent so d C will be equal to so this is for 1 percent for 1 percent because most of the times the mismatch is talked in terms of percentage but it remember that it means epsilon is this much. So d C will be equal to for 10 percent mismatch. What do you expect the thickness of the layer to be? Much smaller because mismatch is more therefore, only it has to adjust more itself therefore, a thinner layer would get adjusted. So d C is equal to 5 angstrom divided by 2 into 0.1 which is 25 angstrom. So if that layer that is being grown is less than 25 angstrom then that material can stretch itself and get adjusted with a built-in strain. The numbers are very small 250 angstrom, 10 angstrom, 25 angstrom are this practical? Do they have any practical significance? Yes.

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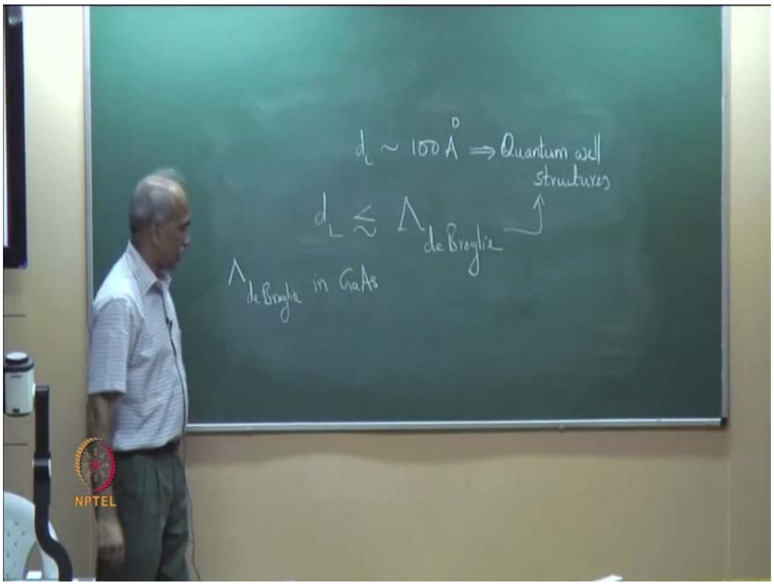

If you are talking of layers with the d L of the order of 100 angstrom what are we talking of? We are thinking of quantum well structures. If the thickness is of the order of 100 angstrom then we are talking of quantum well structures. Why are we talking of quantum well structures? What are quantum well structures? Quantum well structures are structures where the dimension of the layer when the dimension of the layer is less than or of the order of the de Broglie wavelength of electrons in the medium. So structures in which the dimension that is d L is less than or of the order of de Broglie wavelength are called quantum well structures. What is the de Broglie wavelength? De Broglie wavelength did I calculate earlier? The De Broglie wavelength lambda De Broglie. Let me calculate De Broglie for a semiconductor let us say in for example, in gallium arsenide I want to calculate lambda de Broglie of electrons in the semiconductor gallium arsenide.

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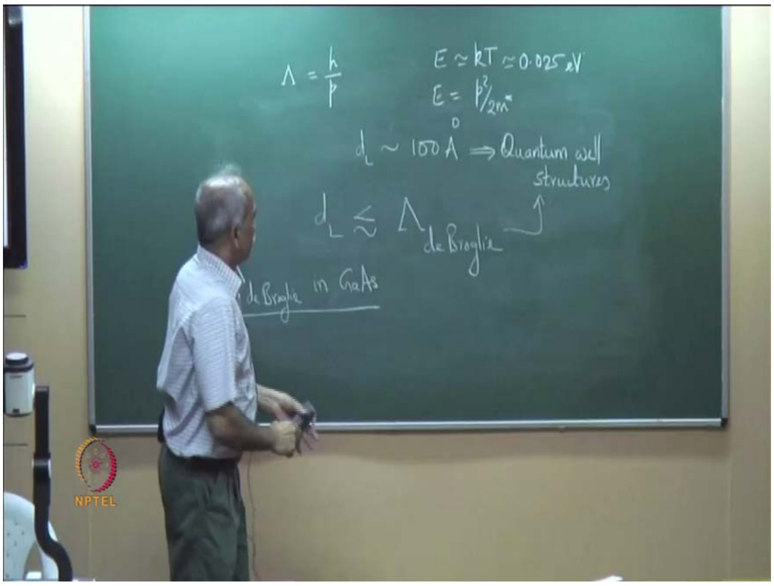

How to calculate lambda De Broglie? So we know that lambda is equal to h by p, where p is the momentum h is the planks constant. The thermal energy of electrons, electron has thermal energy E is of the order of k T corresponding to these electrons thermal electrons I want to find out what is the corresponding de Broglie wavelength. So this is E is equal to p square by 2 m star in the medium.

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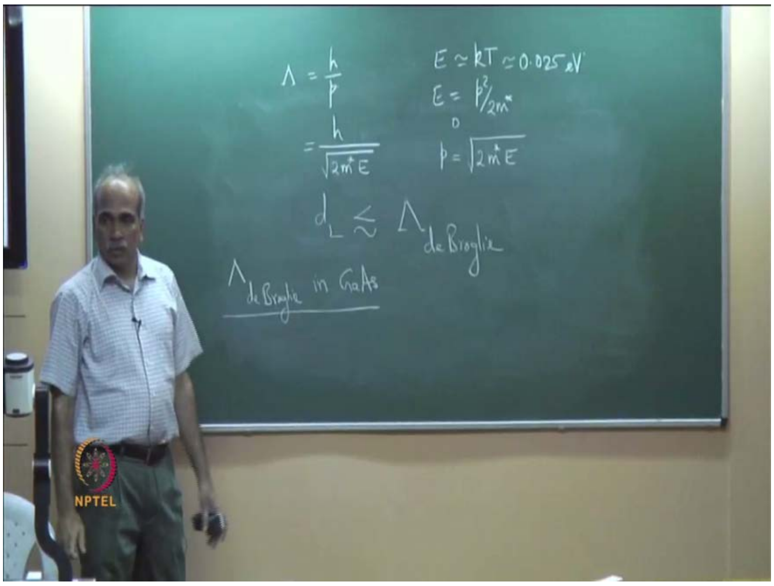

Or p is equal to square root of twice m star E and lambda is equal to h by p. So this is equal to h by square root of 1 m star E. I am calculating the average de Broglie wavelength of electrons in a semiconductor.

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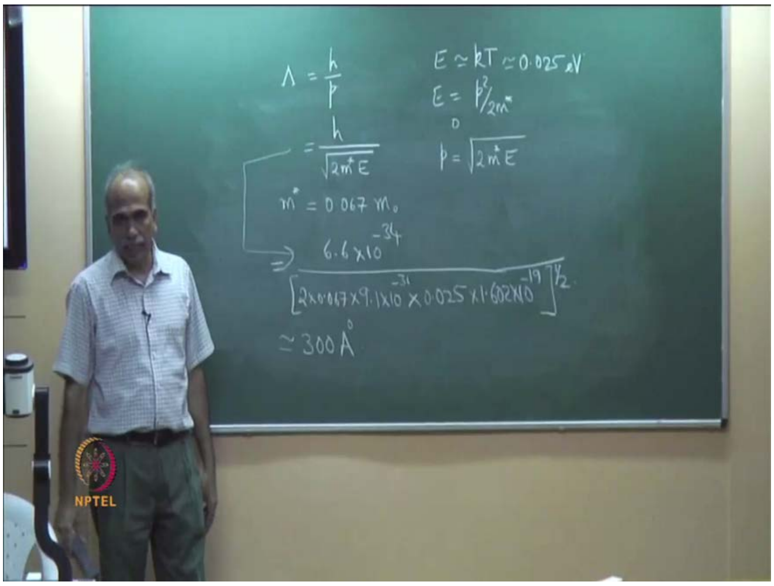

And if I take gallium arsenide for example, then we know m star for the conduction band electrons is equal to 0.067 into m 0. So if I substitute in this expression here h is equal to 6.6 into 10 to the power of minus 34 divided by square root of so to the power half 2 into m star 067 into m 0, it is 9.1 into 10 to the power of minus 31 k g, m star is this much into m 0 into E k T is equal to 0.025 e v, but rest are all in S I unit. So you have to convert this into joules 1.602 into 10 to the power of minus 19 whole to the power half, simplify this and you will see that this comes out to be approximately I think 297 angstrom or approximately 300 angstrom.

I think 297 please check use the calculator and check approximately 300 angstrom. This is the de Broglie wavelength of electrons of electrons in a semiconductor in gallium arsenide. We have calculated for gallium arsenide therefore, if the dimension if the thickness of the layer is less than 300 angstrom or of the order of 300 angstrom, we have a quantum well structure, a structure in which quantum size effects become important. So, quantum size effects refer to the effects which lead to discrete energies for electrons discrete energies for electrons.

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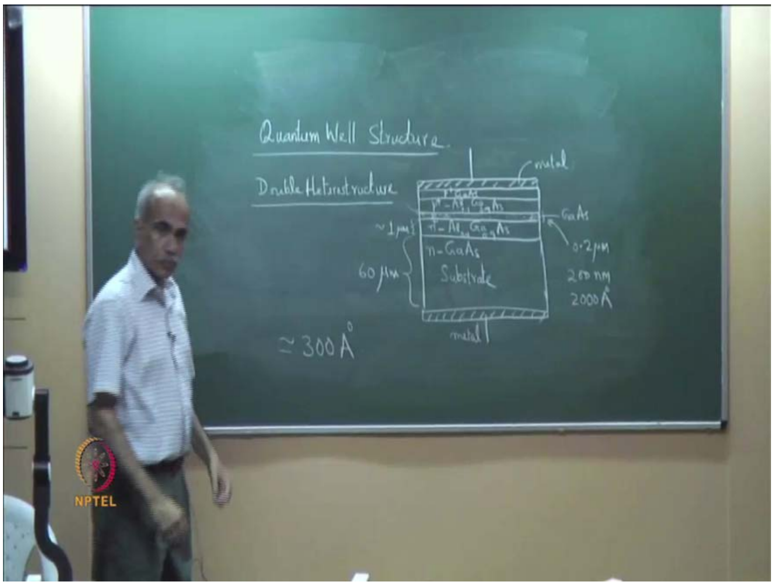

Let me go a little bit further therefore, what is a quantum well structure? And how does a quantum well structure form? We have talked about double hetero structures, where you heard a substrate a substrate on top of this, you grow a layer. Let me put typical materials say gallium arsenide on which n gallium arsenide, n plus I am taking a typical structure which is used in laser diode for example, n plus gallium arsenide or aluminum gallium arsenide Al 0.1 today's example Al 0.1 gallium 0.9 and arsenic.

So n plus aluminum gallium arsenide on top of this we grow a thin layer, let me put some typical numbers if you take a substrate, then generally this is anywhere from 60 to 100 micron. So let us say 60 micron is not to scale and on top of this you grow a layer here generally, 1 to 2 micron. So let us say 1 micron or 2 micron, 3 micron just a kind of numbers 1 micron. This layer and on top of this we grow a thin layer, let us say gallium arsenide intrinsic or lightly doped p or lightly doped n gallium arsenide this layer thickness is generally I am drawing the layer thicknesses of a double hetero structure double hetero structure gallium arsenide thickness of 0.2 micrometer, some numbers will make it a it will give you a good idea. So this layer here intermediate is 0.2 micrometer on top of this we grow another layer which is p, p plus or p aluminum gallium arsenide Al 0.1, gallium 0.9, arsenic 0.9. This is again let us say about 1 micron, almost 1 micron on top of this generally one grows a p plus layer of gallium arsenide, p plus gallium arsenide. Why does why do one need all this layers this is a technological reasons and also physics involved and on top of this you have the metal for contacts.

At the bottom electrode metal electrode, so this is also metal and top electrode here top contact and then we have a p plus layer. You will discuss this, this forms an ohmic-contact, there are short key contacts and ohmic-contacts. So this forms an ohmic-contact if this the p plus and a metal or an n plus n metal and this is a double hetero structure and there are two hetero junctions as we have already discussed, you can see here. So this is p gallium arsenide, then there is a p n junction here, there is a p p junction here. So there is 1 hetero junction here and 1 hetero junction here, hetero junction is junction between two dissimilar semiconductors. So we have two hetero junctions here hence this there are this is say double hetero structure. I have given typical numbers for the thickness of the layer so 0.2 micron is the thickness of this intermediate layer which is the active layer as we will see later, 0.2 micron is 200 nanometer or 2000 angstroms this is a double hetero structure.

If we reduce this dimension of the active layer, if we go on reducing bring down to 200 angstrom or 100 angstrom what results is a quantum well structure. It is a double hetero structure that the thickness of the active layer is very thin or very small, the thickness is very small. It is of the order of 100 angstrom. So a where is a quantum well structure? What is a quantum well structure? You can define it in different ways, quantum well structure is a double hetero structure it is a semiconductor double hetero structure where the thickness of the active layer is of the order of 100 angstrom, where the thickness is less than the de Broglie wavelength of electrons in the medium. So quantum well structure is basically a double hetero structure but the thickness has been reduced. If you see the now why quantum well structure varies the well will be the next question if you want to ask where is the well? In this let us see where is the well?

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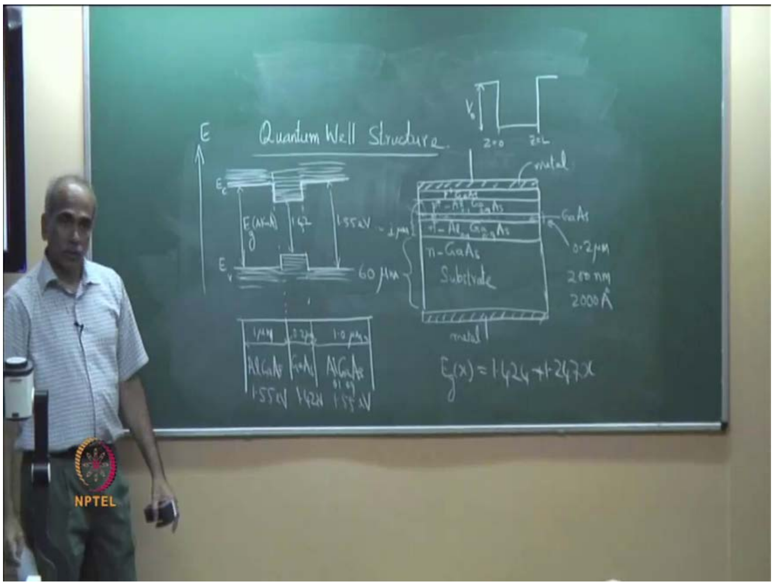

So the well here refers to the potential well, if you zoom this what I am doing is I will rotate this through 90 degree and zoom only this region, zoom this region only aluminum gallium arsenide has a larger band gap compared to gallium arsenide. You remember that E g of x was equal to 1.424 plus 1.247, I had truncated to 4 to 5 and 25 x which means for x greater than 0, it is greater than that of gallium arsenide this is that of the gallium arsenide therefore, these layers have higher band gap.

So two things I am doing, I am rotating this at 90 degree. So I am showing the layers here, this is that gallium arsenide layers which was 0.2 micron and this is 1 micron. So I have rotated this through 90 degree. So 0.2 micron and 1 micron I want to plot the band diagram of these this is gallium arsenide and this is aluminum gallium arsenide 0.1, 0.9 arsenide. What is the band gap? Corresponding to x equal to 0.1 so we calculated this it was 1.55. So this is 1.55 e v, this is 1.42 e v, 1.55 e v. I plot the band diagram here corresponding to each of this medium, the energy band diagram. So I have this is E g so this is E c E v and this is E g of aluminum gallium arsenide, that is 1.55 and this is 1.42.

So this is gallium arsenide, so this is 1.42 and this is again 1.55. What is this axis? Energy, there is a difference in band gap energy and what we have here is if you see this conduction band here, what we have is a finite potential well. The famous problem in quantum mechanics particle in a potential box this is V 0. So let us say x equal to 0 or z equal to 0 particle in a potential box, if it is a infinite potential then this goes continuously otherwise these a finite potential well. So what you have here is a potential well and this well is quantum well, this is the potential energy variation, potential energy well so that is that quantum well.

When will this become a quantum well? This will become a quantum well when the structure is thin enough. So that quantum size effects come into play right now there are large number of allowed states here because it is a bulk semiconductor, here also you have very large number of allowed states, here also you have very large number of allowed states, allowed states for electrons, electrons can occupy any of the states similarly, you have large number of allowed states for holes and large number of allowed states. This is a double hetero structure, this is not a quantum well, right now this is a double hetero structure but if you reduce the dimension, then the number of allowed states decrease and you reach a stage when you call that it is a quantum well and when the dimension of the well becomes less than the de Broglie wavelength, then we have finite number of solutions the allowed electron energy values are finite.

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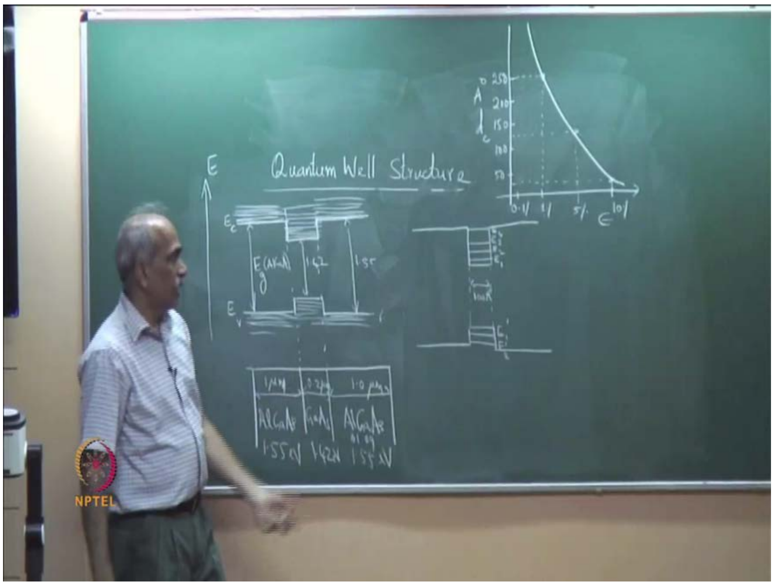

And we have a situation where now this well dimension is very small. Let us say for example, 100 angstrom, this potential well is now a quantum well and in this we do not have so many allowed states, there are very few allowed states. So we have energy levels E 1, E 2, E 3, E 4 similarly, in the lower level allowed states for holes so we have E 1 dash, E 2 dash and so on. Now with this picture what is a potential quantum well? A quantum well structure is a double hetero structure where the intermediate layer, the active layer, the thickness of the active layer is of the order of 100 angstroms or 10 nanometers, why the number has come? It is not 100 and of the order, it could be a 150, it could be 200, it could be 20 angstrom, this is a quantum well structure.

Why did I bring it here? Because we saw that in the case of strained-layer epitaxy the kind of thickness of the layers which were required where after order of 50 to 250 angstroms and that indeed correspond to the thicknesses of quantum well structures. Hence the title strained-layer epitaxy and quantum well structures, in fact there are many devices which are called strained-layer quantum well devices, strained-layer quantum well devices because strained-layer epitaxy works out well without any defects only when the dimensions become very small. So if you plot for example, if you plot epsilon here versus the critical thickness d C. So let us say epsilon 0.01, 0.1, 0.0 let me take a smaller values that is 0.1 percent, 1 percent and 10 percent, 5 percent somewhere in between, just I want to find the plot. So what kind of numbers will we get? 50, 100, 150, 200, 250 angstroms these are all in angstrom. I had calculated already for 1 percent and 10 percent, for 1 percent it was 25, for 1 percent it was 250 250 angstroms. I have taken example just now with the layers is equal to 5 angstrom so you saw this is d C critical thickness was 250 angstrom, here for 1 percent 250 is it? Please check? 250 angstrom and for 10 percent we had 25 angstrom, for 5 percent you will have 125 angstrom actually I should have taken even smaller, you could also find out for 0.1 percent so this will go to 2500 angstrom which means basically if you plot such a curve this will come down rapidly d C versus epsilon.

Use a proper scale, the critical layer the critical thickness, thickness of the layer critical thickness of the layer drops rapidly with increase in strain, but the numbers involved are of the order of 100 angstrom and strained-layer epitaxy, therefore always goes along with quantum well structures. If you want defect free layers and what is a quantum well structure? It is basically a double hetero structure where the thickness of the active layer is of the order of 100 angstroms.

We will talk a little bit more on this, this have very important advantages of strained-layer epitaxy. In the mean time let me recall little bit of quantum mechanics that we have studied and see how the energy varies allowed electron energy varies with the well thickness.

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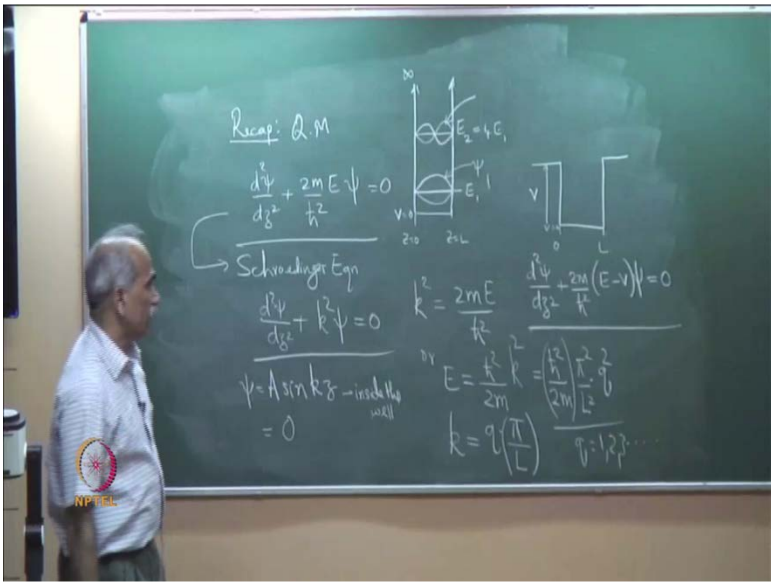

Recall your recap, your basic quantum mechanics. Quantum mechanics of particle in a potential box, first we have an infinite well. So this is V equal to 0 as going to infinity. The first problem that we so this is z equal to 0 and z equal to L the solution of one dimensional solution so d square psi by d z square plus 2 m by h cross square into E into psi equal to 0, the one dimensional Schrodinger equation the one dimensional Schrodinger equation. So this I can write as d square psi by d z square plus let me call this as k square. So k square psi equal to 0, where k square is equal to 2 m E by h cross square or E is equal to h cross square by 2 m into k square h cross square k square by 2 m E is equal to the allowed energies so where k this k's are given by q times pi by L z L at this is we have already seen this k is equal to q times pi by L, where L is the dimension of the structure.

So this gives energy values here, please see that if you substitute this here this is h cross square by 2 m, h cross square by 2 m into q square or pi by pi square by L square into q square and what is q? q is equal to 1, 2, 3 integers. So if you put q is equal to 1 this is the first one that is E 1. So E 1 is here and next will be 4 times q equal to 2. So q square so you will have E 2 here, this is E 2 is equal to 4 times one 1.

And what kind of wave functions if you solve this what will you get? You will get solutions of the form psi is equal to a sine kappa z, a sine k z a sine k z and this is inside the well here and outside, inside the well and outside field is equal to 0 because it is a infinite rigid wall. rigid wall boundary condition means, the field has to go to 0 the wave function has to go to 0 there and therefore, the wave function if you see they look like this the first solution of course, this is this is the second solution a very quick recap. So these are the psi, this is psi 1 and this is sinusoidal as you can see it is sinusoidal and k contains a q there and therefore, you have various solutions.

So these values can be directly obtained you see in this expression if I give you a well of dimension 100 angstrom all others are constants, h cross is constant, m is constant for the given material only L. So depending on dimension we have different values of E, this is the basic problem of a infinite potential well, what about finite potential well? So if we next go to the problem of a finite potential well same 0 same L but now this is not infinite but this height is V always the vertical axis is energy. So this is now V so this is V equal to 0 and this is V is equal to V

What kind of solutions will we get? Same Schrodinger equation you have to solve but there is a difference now that outside also there is a there is a finite potential here V, earlier we had only V equal to 0 and there is no field outside because of the rigid wall boundary condition but now there is a finite value of V. So you have to write the equation for the outer region which is d square psi by d z square plus 2 m by h cross square into E minus V into psi equal to 0, there is a V which has come, potential energy E minus V psi equal to 0.

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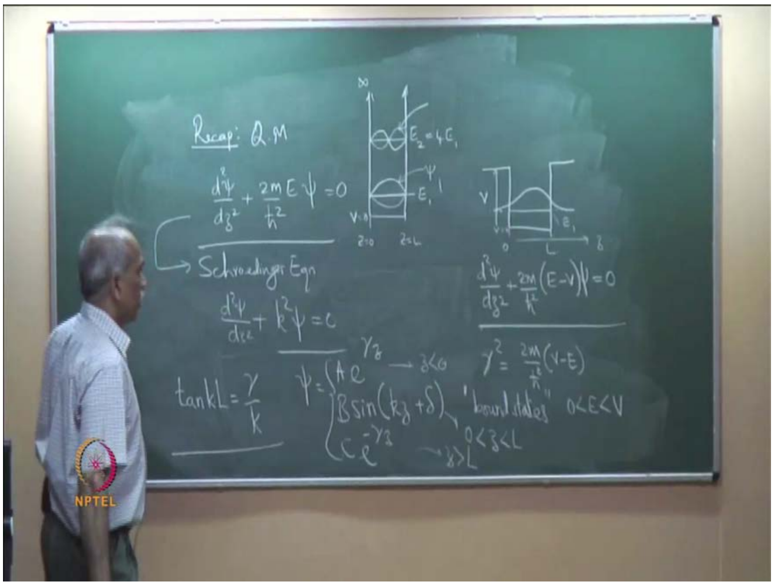

And what kind of solutions do we get? You if you write the fields I am not going to solve this it is only a quick recap, those of you who have not done please see any of the basic quantum mechanics books. So you can write the fields if I call this as if I call this as 2 m gamma square equal to 2 m by h cross square into V minus E. If this term here with a negative sign why negative sign? Because V is higher, we are looking for bound states what are bound states? So we are looking for bound states.

Bound states means the energy remains within this, it is bound to the wall which means you have oscillatory solutions inside and exponentially decaying solutions outside they are the bound states, that is 0 less than E less than V are the bound states therefore, V is greater than E and therefore, I flip this and then you write the field solutions you can write psi is equal to some constant a this is just as a revision E to the power of gamma z, this is B into sine some constant k x k z plus delta. You can write it in different form plus delta, where delta is a constant and C e to the power minus gamma z. This is for z less than 0, that is this side that this is z axis, z less than 0 this is a solution for 0 less than z, less than L and this is the solution for z greater than L which clearly tells you the solutions are exponentially decaying.

So if you see the solution here now E 1. So this corresponds to E 1 you will get a field variation, a wave function variation which is like this. It is finite a continuity of field boundary conditions we continuity of psi and it is derivative gives you a field which is of this form, the wave function has exponential tails outside in a finite in a finite potential well as compared to an infinite potential well where the wave function is 0 outside.

The energy E 1s are obtained if you apply the boundary conditions to this at every interface at z equal to 0 and z equal to L if you apply continuity of field and its derivatives continuity of wave function and its derivatives you get a Eigen value equation which is tan kappa d, kappa L, tan k L is equal to gamma by k this is a transcendental equation. You have to solve this numerically to get the solutions. Solution means to get the value of E this is called the Eigen value equation and the solutions will give you the energy Eigen value the E 1, E 2 here and that will also give you the wave function side.

So this is how we determine the energy in a potential well, a particle in a potential well, a standard problem that which we had in quantum mechanics. There is something interesting which I want to tell that I think we will stop here and continue in the next class and we will see how the energy depends on the dimensions of the well and how this is used for band gap tailoring or band gap engineering. So this will be our next topic.