Semiconductor Optoelectronics

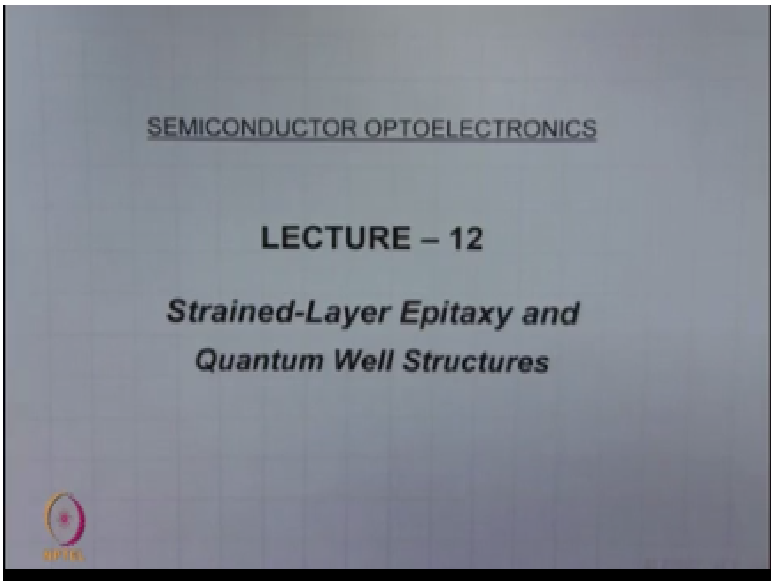
Prof. M.R. Shenoy
Department of Physics
Indian Institute of Technology-Delhi

Lecture-12

Strained-Layer Epitaxy and Quantum Well Structures

So we start with this lecture on strained layer epitaxy. In the last class I discussed about lattice mashed.

(Refer Slide Time: 00:26)



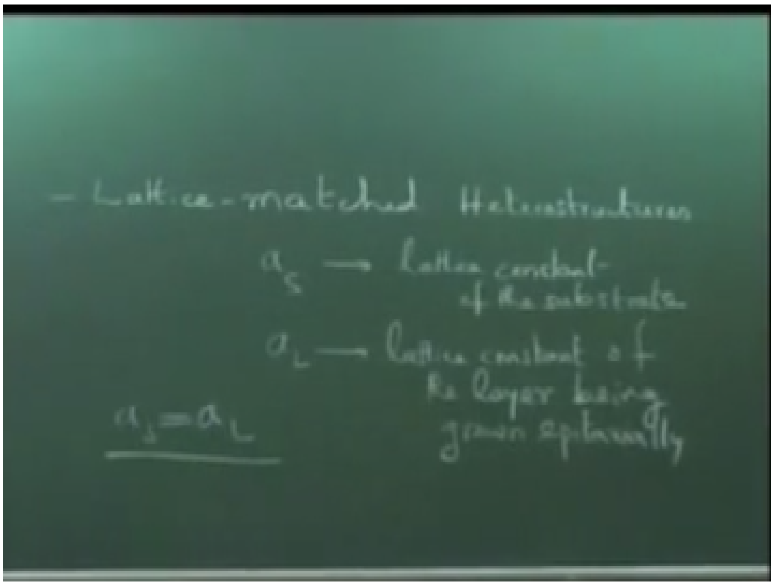
SEMICONDUCTOR OPTOELECTRONICS

LECTURE – 12

Strained-Layer Epitaxy and Quantum Well Structures

It was such growth of lattice match heterostructure. 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 As. If As is a lattice constant of the substrate and Al is the lattice constant of the layer that is being grown of the layer the epi layer actually the layer been grown epitaxially.

(Refer Slide Time: 01:26)



- Lattice-matched Heterostructures

$a_S \rightarrow$ lattice constant of the substrate

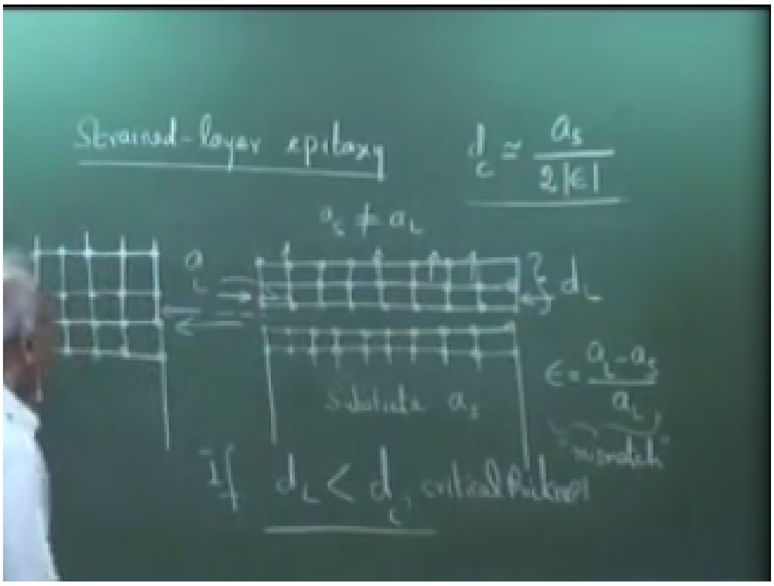
$a_L \rightarrow$ lattice constant of the layer being grown epitaxially

$a_S = a_L$

Then we wanted that Al, As must be equal to Al, so this is lattice matching, but what would happen if As is not equal to Al. In the last class in our discussion I showed that if As is not equal to Al there are some atoms which do not participate in the bonding and then there dangling bonds which are defects in the medium and the defects always increase the possibility of non radiative recombination which is detrimental to the performance of optoelectronic devices.

Is it true that we cannot grow this at all if As is not equal to Al. If As is not equal to Al even then we can grow defect free structures provided that certain conditions provided the thickness of the layer if the thickness of the layer that is being grown less than 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 called strained layer epitaxy.

(Refer Slide Time: 03:26)



It is called strained layer epitaxy because in that case there will be built in strain in the medium. So let me illustrate this strain layer epitaxy. So epitaxy is growing on top epitaxy. So if you start with the substrate as before let me show a one dimensional structure which means I have atoms setting in a one dimensional lattice which is the top monolayer that I am showing, this is the substrate which is characterized As.

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 slightly larger, so this layer has Al, the lattice constant here in 1 dimensions the separation between two atoms is Al lattice constant. This is now not matching. In the last class I had said that then this will result in dangling bonds and defects,. However if the thickness of the layer is very small what is very small 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 the lattice constant that is there would be a built in string in this direction is compressive strain from the sides which will result in a compressive strain here will lead to an elongated stain or tensile stress strain in this direction.

Compressive strain from a sides and tensile strain in this direction, so these atoms will fill a tensile strain in the vertical direct, compressive strain from here to match this atoms exactly to match this. So what would happen is this would result in a structure I will show smaller portions here I am taking a square lattice just to illustrate the point to this is square, this was also square before deformed bond.

But when they form 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 here interfaces here. So the interface has easier so it has square lattice here but what has happened in this direction is when it try to adjust itself in this direction by experience in a compressive strain then 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 As=Al before this so this was Al, so As not equal to Al, As not equal to Al, but it has adjusted itself. So that As has become equal to Al in this direction at the interface. But there is a built-in strain and hence we 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 the this is dL. Then if this thickness dL id dL is less than the critical thickness dc. So dc is the critical thickness, this critical thickness is dc is given by an empirical relation approximately equal to As/2mod epsilon.

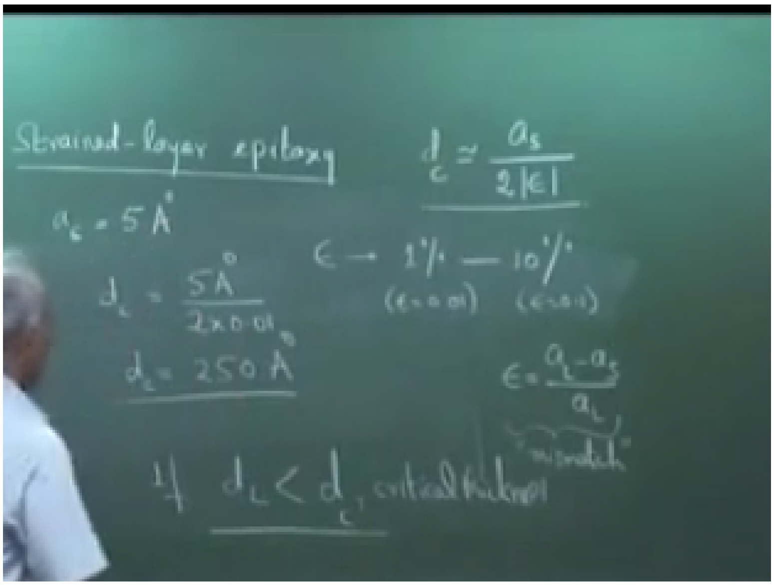
Where epsilon is called the mismatch parameter, so epsilon=aL-aS/aL is called the mismatch parameter or mismatch, it is a measure of mismatch when Epsilon=0 that means aL=aS it is perfectly lattice match structure. But when epsilon is not 0 it means aL is not equal to aS. Therefore epsilon is the mismatch parameter. If the thickness of the layer epitaxy layer which is being grown.

If it is less than a critical thickness then it is possible for the atoms in the layer that is here to get adjusted although there will be a built-in string 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 sheet. If it is very thin you can stretch it, rubber you can stretch if it is think.

If I give a thick block of rubber it is just cannot stretch it, it is just like a solid you just cannot stretch it, but if the rubber sheet is think then it is possible to stretch 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 .

(Refer Slide Time: 12:40)



Let us say the substrate lattice constant aS=5 Armstrong as you know typically most of the semiconductors have aS substrate lattice constant anywhere from 5.5 to 6 Armstrong. So let me take As= 5 Armstrong. If epsilon generally people talk in terms of percentage, if epsilon is 1% to 10%, this is the kind of mismatch which is the 10% means epsilon=0.1 express in percentage is 10%.

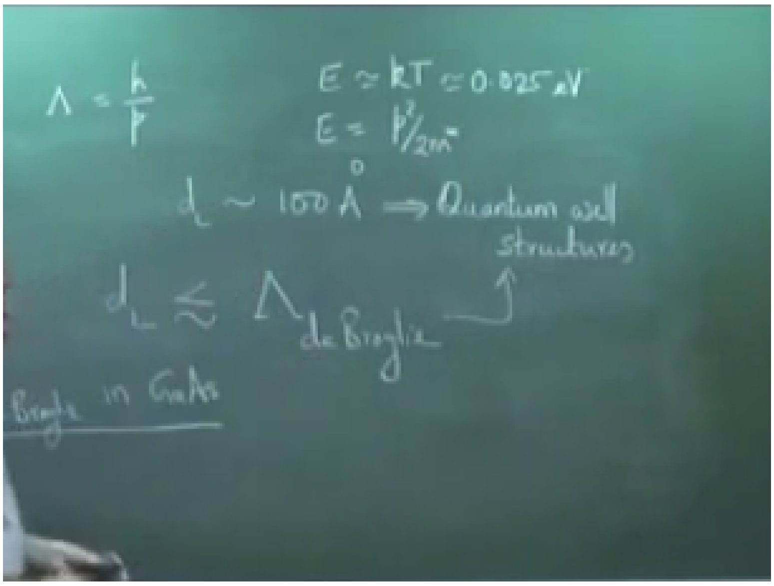
This ratio is 0.1 that is 10% mismatch one person means epsilon=0.0. So let us see what is dc the critical thickness equal to if I put 1% then As is 5 Armstrong/2*epsilon is this much that is 2*0.01 1% how much is this 250 Armstrong, the critical thickness is 250 Armstrong. So if a lattice mismatch of 1% can be tolerated provided the thickness of the layers is less than 250 Armstrong.

If you are going only a thin layer with thickness less than 250 Armstrong then that lattice mismatch can be tolerated. If you put 10% mismatch 10%, so dc will be equal to so this is for

1% for 1% for the most of the times the mismatches is talked in terms of percentage but it to remember that it means epsilon is this. So dc will be equal to 10% mismatch what we expect the thickness of the layer to be much smaller.

Because mismatch is more therefore only it has to adjust more itself there could be a thinner layer get adjusted. So dc=5 Armstrong/2*0.1 which is 25 Armstrong. So the layer that is being grown is less than 25 Armstrong then that material can stretch itself can get adjusted with a built in strain. The numbers are very small 250 Armstrong, 10 Armstrong or 25 Armstrong are these practical do they have any practical significance.

(Refer Slide Time: 16:01)



$\Lambda = \frac{h}{p}$

$E \simeq kT \simeq 0.025\,eV$

$E = p^2/2m^*$

$d_L \sim 100\,\overset{\circ}{A} \Rightarrow$ Quantum well structures

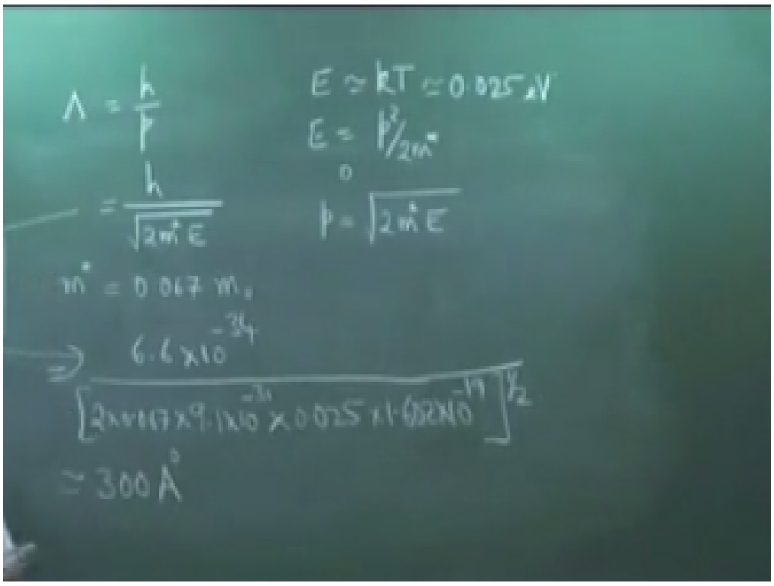
$d_L \lesssim \Lambda_{de\ Broglie}$

Broglie in GaAs

Yes if you are talking of layers with the dL of the order of 100 Armstrong, what are we talking of we are thinking of quantum well structures. If the thickness is of the order of 100 Armstrong 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 media. So structures in which the dimension that is dL 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 did the de Broglie wavelength lamda de Broglie let me calculate the Broglie for a semiconductor.

(Refer Slide Time: 17:06)



$$\lambda = \frac{h}{p} \qquad E \simeq kT \simeq 0.025\,eV$$

$$E = p^2/2m^* \qquad p = \sqrt{2m^*E}$$

$$= \frac{h}{\sqrt{2m^*E}}$$

$$m^* = 0.067\,m_0$$

$$\Rightarrow \frac{6.6\times10^{-34}}{\left[2\times0.067\times9.1\times10^{-31}\times0.025\times1.602\times10^{-19}\right]^{1/2}}$$

$$\simeq 300\,\mathring{A}$$

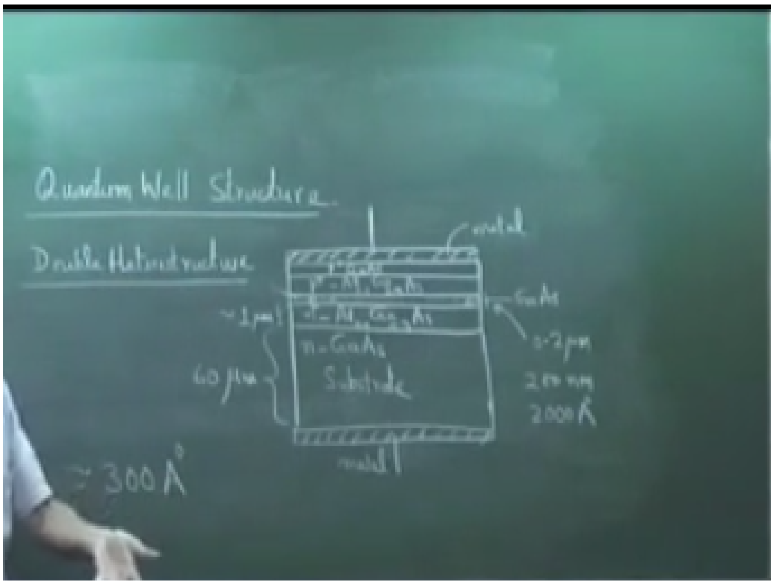
Let us say e for example in gallium arsenide I want to calculate lamda de Broglie of electrons in the semiconductor gallium arsenide. How to calculate de Broglie, so we know that lamda=h/p the p is the momentum, h is the Planck's constant, the thermal energy of electrons electrons has thermal energy E is of the order of kT corresponding to these electrons thermal electronic I want to find out what is the corresponding de Broglie wavelength.

So this is E=p square/2m m* in the medium or p=square root of twice m*E and lamda=h/p. So this is equal to h/square root of 2m*E I am calculating the average de Broglie wavelength of electron in a semiconductor and if I take gallium arsenide for example then we know m* for the conduction band electrons is equal to 0.067*m0. So if I substitute in this expression here h=6.6*10 to the power of -34/square root of to the power 1/2*m*067*m0 which is 9.1*10 to the power of -31 kg.

M* is this much into m0*E kT=0.025 Ev but rest all are in Si units, so you have to convert this into Joules 1.602*10 to the power of -90 whole to the power 1/2 simplify this and you will see that this comes out to be approximately I think 297 Armstrong, so approximately 300 Armstrong I think 297 please check use the calculator and check approximately 300 Armstrong. The de Broglie wavelength 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 Armstrong of the order of 300 Armstrong we have a quantum well structure, a structure in which quantum size effects become important. So quantum size effect referred to the effect which leads to discrete energies for electrons.

(Refer Slide Time: 21:46)



Let me go a little bit further therefore what is a quantum well structure and how does the quantum well structure form. We have talked about double hetro structures where you had a substrate a substrate on top of this you grow earlier let me put typical material say gallium arsenide on which and gallium arsenide n+ and taking a typical structure which is used in laser diode. For example n+gallium arsenide or aluminium gallium arsenide aL 0.1 example.

Al 0.1 gallium 0.9 and arsenide, so n+aluminium 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 60-100 microns so let us say 60 microns, this not to scale and on top of this you grow earlier here generally 1-2 micron, ok so let say 1 micron or 2 micron, 3 micron thus the kind of numbers one micro this layer.

And on top of this we grow a thin layer that is gallium arsenide intrinsic or lightly doped PR lightly doped n gallium arsenide, this layer thickness is generally I am drawing the layer thickness of a double heterostructure gallium arsenide thickness of 0.2 micrometre some numbers will make it will give you a good idea. So this layer here intermediate these 0.2 micrometer.

On top of this we grow another layer which is p p+or p aluminium gallium arsenide aL 0.1 gallium 0.9 arsenide 0.9. This is again let us say about 1 micron ok almost 1 micron. On top of this generally 1 grows a p+ layer of gallium arsenide p+gallium arsenide why do one need all this layers is a technological reasons and also physics involved and on top of this you have the metal for contacts at the bottom metal electrode.

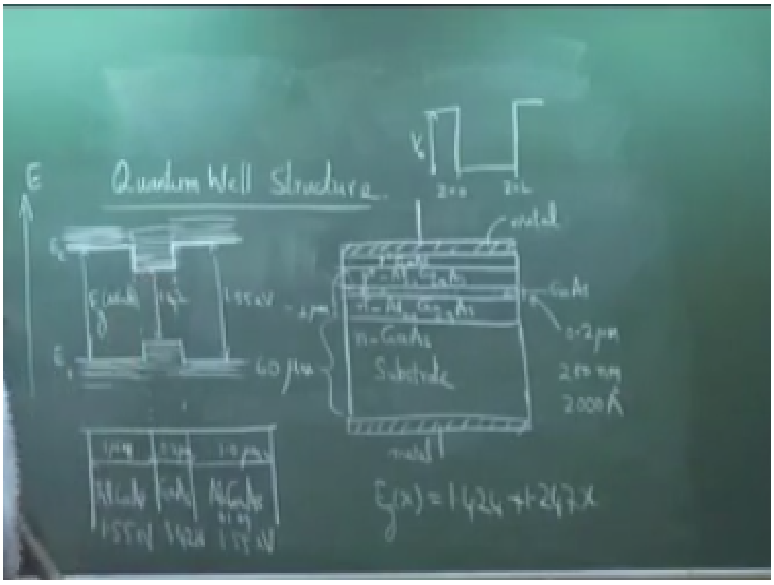
This is also metal and top electrode here, top contact then w have a p+ layer will discuss this forms an only contact, there are shortly contacts and only contacts, so this founds the only contact is p+ and metal and n+ metal and this si double electrode structure and it got heterojunction as we already discussed, we can see here so this is p gallium arsenide then pn junction here there is pp junction here.

So there is one heterojunction here and 1 heterojunction here, heterojunction is junction between 2 dissimilar semiconductors. So we have 2 heterojunctions hence this there are this is a double heterostructure. 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 nanometre or 2000 Armstrong.

This is a double heterostructure, if we reduce this dimension of the active layer if we go on reducing bring down to 200 Armstrong or 100 Armstrong what results is a quantum well structure, it is a double heterostructure where the thickness of the active layer is very thin or very small, the thickness is very small, so thickness is very small. It is of the order of 100 times. So it varies the quantum well structure.

What is the quantum well structure you can define it in different ways quantum well structure is a double heterostructure it is a semiconductor double heterostructure where the thickness of the active layer is of the order of 100 times volts, that the thickness is less than the de Broglie wavelength of electrons in the medium. So quantum well structure is basically a double heterostructure but the thickness has been reduced.

(Refer Slide Time: 28:22)



If you see the now why quantum well structure where is 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. So let us see where is the well the potential well. If you zoom this what I am doing is I will rotate this to 90 degree and zoom only this region zoom this region only, aluminium gallium arsenide has a larger band gap compared to gallium arsenide.

You remember that Eg of x=1.424+1.247 at go to 25 and 25 x which means for x greater than 0 it is greater than that of gallium arsenide. This is that the gallium, therefore these layers have higher value, so 2 things I am doing I am rotating this to 90 degree I am showing the layers here, this is the gallium arsenide here which was 0.2 micron and this is 1 micron. So I have rotated this to 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 aluminium gallium arsenide 0.1, 0.9 arsenide, what is the band gap corresponding to x=0.1. So we calculated this it was 1.55. So this is 1.55 Ev, this is 1.42 Ev, 1.55 E, I plot the band diagram here corresponding to each of this media the energy band diagram. So I have this is Eg, so this is Ec, Ev and this is Eg of aluminium gallium arsenide that is 1.55 and this is 1.4.

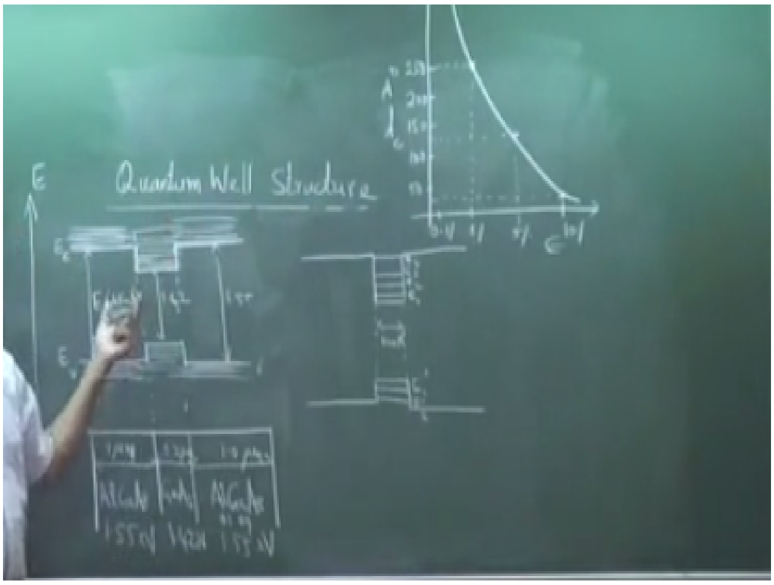
So this is gallium arsenide, so this is 1.4 and this is again 1.5, what is this axis E, there is a difference in band gap energy and what we have here is if you see this conduction band here what we have is finite potential well famous problem in quantum mechanics particle in a potential box. This is V0 so x=0 particle in a potential box. If it is a infinite potential than this goes continuously.

Otherwise this is a finite potential value. So what you have here is the potential well and this well is quantum well. This potential energy there is a potential energy well, so that is that quantum well, when will this become a quantum well, this will become a quantum well the structure in thin enough so that quantum size is coming to play. Right now number of allowed states here.

Because it is a bulk semiconductor, here also very large number of allowed states here also you have very large number of allowed states. Allowed states for electron, electrons can occupy any of the state, similarly you have large number of allowed states for holes and large number of allowed states. This is a double heterostructure, this is not a quantum well, right now this is a double heterostructure.

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 that allowed electron energy values are finite and we have a situation there.

(Refer Slide Time: 34:38)



Now this well dimension is very small, let us say for example 100 times, this potential well is now a quantum well and this we do not have so many allowed states there are very few allowed states. So we have energy levels E1, E2, E3, E4, similarly in the lower level allowed states for holes we have E1 dash, E2 dash, and so on. So now with this picture what is a potential well quantum well.

A quantum well structure is a double heterostructure where the intermediate layer the active layer the thickness of the active layer is of the order of 100 Armstrong or 10 nanometres, why the number has 100 of the order it could be 150, it could be 200, it could be 20 Armstrong, this is the quantum well structure. Why did I bring it here because we saw that in the case of strain the layer epitaxy.

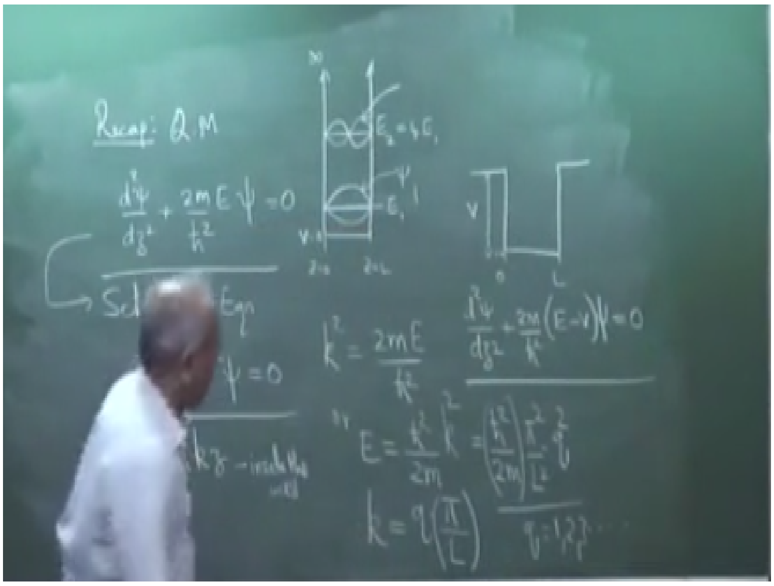
The kind of thickness of the layers which were required where of the order of 50 to 250 Armstrong and that indeed correspond to the thickness of quantum well structures hence the type of strained layers epitaxy and quantum well structures, in fact there are many devices which are called strained layer 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 epsilon here verses a critical thickness Dc, so let us say epsilon 0.01, 0.1, soothe 0.0 let me a smaller value that is 0.1%, 1% and 10%, 5% somewhere in between because I want to find a plot, so what kind of numbers will we get 50, 100, 150, 200, 250 Armstrong. These are all Armstrong. I had calculated already for 1% and 10% for 1% it was 25, for 1% it was 250, 250 Armstrong.

I taken an example just now with the As=5 Armstrong, so you saw this is Dc critical thickness was 250 Armstrong here, so 1% 250 thee please check 250 angstrom and for 10% we had 25 Armstrong and 5% will have 125 Armstrong , so I should have taken even smaller you could also find out for 0.1% so this will go to 2500 Armstrong, it means basically if you plot such a curve this will come down rapidly Dc verses epsilon.

Gives a proper scale the critical layer thickness of the layer critical thickness of the layer drops rapidly with increasing strain, but the numbers involve of the order of 100 Armstrong and the strained layer epitaxy therefore always goes along with quantum well structure. If you want to defect 3 layers and what is quantum well structure it basically a double heterostructure where the thickness of the active layer is of the order of 100 Armstrong.

(Refer Slide Time: 40:40)



We will talk a little bit more on this these are very important advantages of strained layer epitaxy. In the mean time let me recall little bit of quantum mechanics that we have study and see how the energy released allowed electron energy varies with the well thickness, recall your recap the basic quantum mechanics. Quantum mechanics of particle in a potential box, first we have an infinite well.

So this is V=0 and going to infinity let see this is z=0 and z=l, the solution of 1 dimensional solutions so these were size by dz square+2n/h cross square*E*shy=0. The one dimensional Schrodinger equation. So this I can write as d2 shy/dz square+ let me call this k square, so k square shy=0 where k square=2mE/h cross square or E=h cross square/2m*kc h cross square k square/2m= the allowed energies.

So where k these ks are given by few times phy/lz l that is we have already seen this k=q times phy/l where l is the dimension of the structure. So this is energy values please see that we substitute this here this is h cross square/2m q square or phy/phy square/l square*q square and what is 1, q=1, 2, 3 infinities. So if you put q=1 this is the first one that is E1, that El is here.

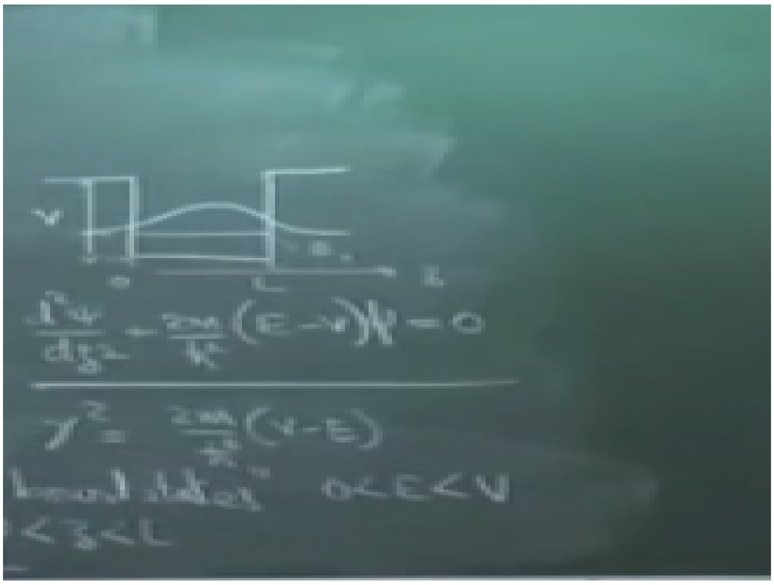
And next will be 4 times q=2, so q square will have E2 yes E2=4 times and what kind of wave functions if you solve this what will you get solutions the form shy=a sin top of k sin kz and this is inside the well here and outside inside it, and outside field is equal to 0 because it is a infinite rigid wall visit wall boundary condition is the field has to go to 0 the wave function has to go to 0 there.

And therefore the wave functions if you see they look like this the first solution of course this is, this is the second solution, the very quick recap so these are the sin, this is shy 1 and this is shy as you can it is shy order k contains q there and therefore you have various solutions. So these values can be directly obtain you seen this expression if I give you a well of dimensions 100 Armstrong all others are constants that is gross is constant M is constant for the given material only l.

So depending on dimension we have different values of offer, this is the basic problem of infinite potential, what about finite potential band, so if you next go to the problem of a finite potential values, same 0, same l, but now this is not infinite but this height is we always the vertical axis is energy this is v=0 and this v=0 what kind of solutions will be get same Schrodinger equation you have to solve.

But there is a difference now that outside also there is a finite potential here v or here we are had only v=0 and there is no field outside because of the rigid wall bounding condition, but now there is a finite value of V, so you have to write equation for outer region which is dsquarephy/dz square+2my h cross square*E-V*shy=0. Let the v which has come potential energy E-vshy=0.

(Refer Slide Time: 46:36)



$$\frac{d^2\psi}{dz^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0$$

$$\gamma^2 = \frac{2m}{\hbar^2}(V-E)$$

bound states" $0<E<V$

$<z<L$

And what kind of solution to we get, you if you write the fields I am not going to solve this, this is only the quick recap, so if you 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 gamma square

=2m/h cross square*v-E is this term here with a negative sign why negative sign because v is higher, we are looking for bound states.

What are bound states, we are looking for bound states, bound states means the energy remains within this, it is back into the well which means you have oscillatory solutions inside and exponentially decaying solutions outside. They are the bound states that is 0 less than v 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 shy=some constant Armstrong

This is just as revision v to the power of gama z, this si B*sin constant kx kz+delta you can write it in different form+delta delta is a constant and c e to the power-gamma z. This is for z less than 0 that is this side this z axis, z less than 0 this is the solution for 0 less than that z, less than l and the solution for z greater than m, which clearly tells you the solutions are exponentially decaying.

So if you see the solution here now E1, this corresponds to E1 you will get field variation if wave function variation which is like it is finite the continuity of see boundary condition continuity of shy and its derivative gives you a field which is off this form, the wave function has exponential tales outside in a finite infinite potential well as compared to an infinite potential well where the wave function is 0 outside.

The energy E1 if you apply the boundary conditions to this at every interface at Z=0, z=l if you apply continuity of field and its derivatives continuity of wave function and its derivative you get it Eigen value equations which is n alpha d alpha l and aL=gamma bites, this is a transcendental equation you have to solve this numerical to get the solution. Solution means this is called the E, this is called Eigen value equation and the solutions will give you the energy Eigen values.

That E1, E2 here and that will also give you the wave functions, so this is how we determine the energy in a potential well the particle in a potential well, the standard problem that which we had in quantum mechanics, there is something interesting which I want to tell but I think top 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.