Semiconductor Optoelectronics
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Lecture-13
Bandgap Engineering

Okay let us continue with the lectures and today we will discuss about band gap engineering, band gap engineering refers to or it is also called sometimes as band gap tailoring.

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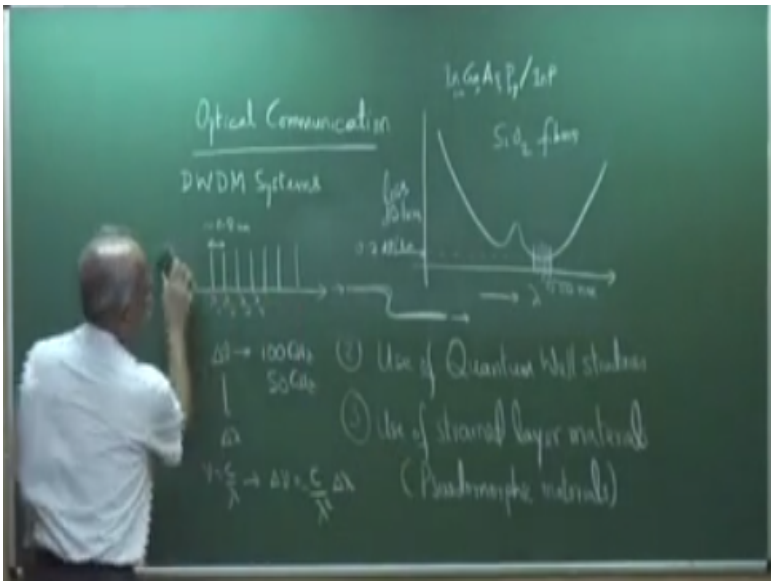

Band gap tailoring refers to the various techniques which are employ to achieve band gap modification. We have seen some of them, some of the techniques which are used are. First we have already seeing by alloying or use of alloy semi conductors use of alloy semi conductors by alloying taking different compositions you can realise materials which have different band gaps. The technique which is used is use of quantum well structures.

Use of strain layered materials these are sometimes refer to as pseudo morphic materials pseudo morphic. We have been discussing about quantum wells in the last class we will continue the discussion in this context of band gap engineering or band gap tailoring why do we need band gap tailoring or band gap engineering because we need to have materials with different band gaps.

For example with respect to optical communication in the context of optical communication today we use DWDM systems which means dense wavelength division multiplexed systems a large number of wavelengths in the low loss window of optical fibre we use a large number of wavelengths if the low loss window of the optical fibre.

So, those of you are not familiar today's communication system optical communication system uses WDM or DWDM system. If you see wavelength versus loss, loss in Dv per kilometre is a standard graph which we see fibre shows a low loss window, so this is loss low loss window cantered around 1550 nano metre. The loss here is approximately 0.2 db per kilometre this loss here is 0.2 db per kilometre silica fibre what I have plotted is the attenuation spectrum of silica fibre silica based SiO2 fibres optical fibres which are used for communication.

So, in this low loss window 1 can put large number of wavelengths in the vicinity here in this within this window. So, if you zoom this a little bit then you can have around 1550 you can have large number of wavelengths there are standard communication grid wavelengths. So, lamda 1, lamda 2, lamda 3, lamda 4 and so on, these are separated the channel separation between these. These typically the depend on what is the channel separation which is used.

In communication technology the channel separation delta mew is standard ones are 100 gigahertz or 50 gigahertz. So, corresponding to delta mew you can calculate what is delta lamda because mew is equal to c/lamda therefore delta mew this implies delta mew is equal to c/lamda square into delta lamda. So, around 1550 window for every delta mew you can find out what is delta lamda is a negative sign of course which means 100 gigahertz facing here corresponds to approximately please verify this 0.8 nano metre separation.

So, in this low loss window around 1550 you can insert large number of wavelengths with a separation of approximately 0.8 nano metres in the same fibre which means 1 fibre so the optical fibre here carries all these wavelengths at the input. The advantage is every wavelength has a certain channel capacity and you have large number of channels. So, the wavelengths are very close this 0.8 nano metre separation is quite close.

And therefore the word dense wavelength division multiplexing normally one uses WDM wavelength division multiplexing or frequency division multiplexing here it is the additional d is to say dense wavelength division multiplexing very closely spaced channels to realise such a system you also need sources which is a laser which is used as an optical source you need sources which are very closely spaced.

One can realise these lasers using the same material system but by going for band gap tailoring a little bit of tailoring of the band gap can result in wave length emission at very closely spaced lines. So, wavelength emissions which are very closely separated, so you do not have to change the material system for example in communication 1 generally uses the indium gallium arsenate phosphide or an indium phosphide substrate.

So, this is gallium x, arsenic y, indium 1-x and p 1-y, so this is the material system which is used to realise these lasers in the 1550 window using the same composition it is possible by using the second or the third technique same exactly same value of x and y but using this second or third technique it is possible to realise lasers which emit a slightly different wavelengths. Of course by changing x and y that is the first technique which is a line we can anyhow achieve band gap modification.

But even keeping x and y constant also it is possible to vary and that is why the band gap tailoring how does this happen we will discuss in detail. So, the need for band gap engineering or band gap tailoring is to realise sources or even detectors or certain devices with a specific wavelength response we will discuss more about this at a later stage when we will discuss about the devices and tuneable laser diodes. But at this stage let us go into the technique what are the techniques that are used.

So, the first technique I do not use any further because as we know by changing the composition x of turnery compounds or by changing the composition x and y of quaternary compounds we can realise materials with different band gaps, band gap is a function of the composition of the alloys. So, let us straight away go to second technique that is use of quantum well structures this will bring us in continuity with the last class on the discussion of quantum well structures.

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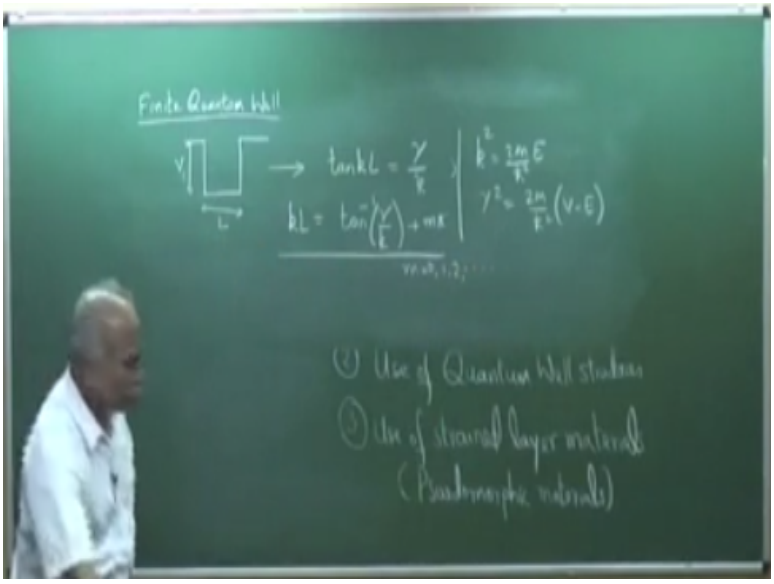

So, if we take come back to the quantum well structure if we take a finite quantum well, finite quantum well refers to the finite barrier height potential v or v0, this is the quantum well we have use notation l for the width and v is the well height. If you take a finite quantum well as we saw in the last class the energy I can value equations are given by tan kl is equal to gamma/k or you can write this as tan inverse form.

So, kl is equal to where please recall that this k is k square is 2m/ k cross square into E and gamma square was 2m/h cross square into v-E. So, kl is equal to tan inverse gamma/kappa gamma/k and + m pie if you want to get all solutions for a given l we should first write it in this form. Because tan is a multi valued function and if you write it in this form where m equal to 0, 1, 2 etc for a given l we are continuing discussion of the last class.

But in the context now of band gap engineering, band gap tailoring for a given l please see that gamma and k contain E this will give energy Eigen values and therefore for a given l you find out what is the energy Eigen value.

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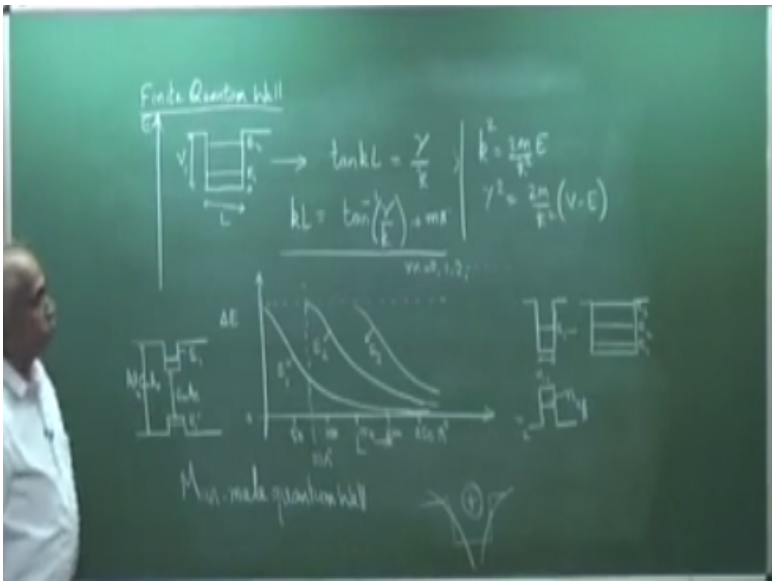

So, if you plot this as a function of well width here L versus E that is so if I have here E1, E2 and so on depending on the width it may support 1 solution or it may several solutions. So, if you plot this value E which I actually want to use the word the notation delta E because E is the total energy here axis. Now this E1, E is respect to this that is this is 0 with respect to this is E1 and with respect to this is E2.

And therefore this is actually delta E1 and delta E2 this axis is our total energy E which has Ec, Ev and so on. So, delta E here refers to the energy of the Eigen states, so if you plot this then you will get solutions like this let me first draw the graph and then you see whether you understand whether this is alright or not. So, this is asymptotical, so what I have plotted is this is for the first state E1 this is second state E2 and third state E3 variation of E1 with the width of the well.

If you have a small well the width of the well is very small then this may support only one solution just like those who have studied optical wave guides if you take a single mode fibre. So, this is n2 this n1 you have only one solution which is an effect is here that is the ineffective of the fundamental mode. If you have a wider core then it can support the second mode third mode it becomes a multimode wave byte.

Similarly in quantum mechanics if you have a well or certain width L then depending on the value of L it may support only one solution and if the well width becomes larger it may have

many solutions. So, E1, E2, E3 and so on, so I have plotted is as the width increases this comes down this goes on dropping down E1 because from top a new solution will come E2 and similarly from a top a new solution will come E3 that is what is happening as L increases E1 is coming down this is the energy value.

So, this is 0 this delta E and after some value of L the second solution starts and E2 varies like this. So, the point here is if you look at for example this region the numbers maybe approximate numbers maybe this is 50 Armstrong this is 100 Armstrong 150 typical numbers for a semi conductor say gallium arsenate 200, 250 so L in Armstrong. So, what it means is if from 0 to 80 Armstrong let us say this is 80 Armstrong I am just giving an example to illustrate the point 80 Armstrong.

For all well width from a small value up to 80 Armstrong there is only one allowed solution there is only one E1 there is no E2,E3 if you cross this then the second solution will come. So, what has been plotted is the variation of Energy Eigen values with the well width. So, depending on your well width you will have different values for the E1. Let us focus for the time being that our well supports only one solution which well are we talking of we are talking of a quantum well which means we are looking at a double hetero structure.

In which the sandwiched layer low band gap layer has a very small as a smaller band gap. So, this is for example gallium arsenate and this is alluminum arsenate, so Alx gallium arsenate. So, we are looking at this well this is the quantum well the potential energy well in the band structure or a band diagram energy band diagram of a double hetero structure when the dimension of the sandwiched layer becomes small it is a quantum well.

So, it is this well that I have been drawing here these are called interestingly manmade quantum wells, this is manmade this structure is made by man you have made it. So, it is manmade quantum well, particle in a potential box is a standard topic in quantum mechanics and all M.Sc., physics students have studied in very detail and this existed for very long time. the particle in a box problem was basically an approximation to potential problems which one encountered.

If you have an atom here a positively charged atom then as we have discussed in our first class the potential energy varies like this and v approximate this by a box to calculate the energy Eigen values it was an approximation simplification. So, that you have analytical solutions today this is a real problem and you have real particle in a box this box is real one is no more and hypothetical approximation because these structures are real hetero structures.

Hence the name manmade quantum wells you can grow double hetero structures and you can realise quantum wells where the original results of particle in a box that which we use to study in quantum mechanics or almost directly applicable. So, we come back here that over this range if I vary the width energy Eigen value changes which means come back to the well here E1 is here and similarly there is a well here it is a barrier for electrons or well for holes which also has energy Eigen values which I call E1 dash for the valance band.

In the valance band also you have potential well or potential barrier which also have discrete energy Eigen values. The lowest allowed Eigen value is E1, the highest energy Eigen value for electrons or lowest energy for holes is E1 dash please see when we had okay I have to erase something let me draw these.

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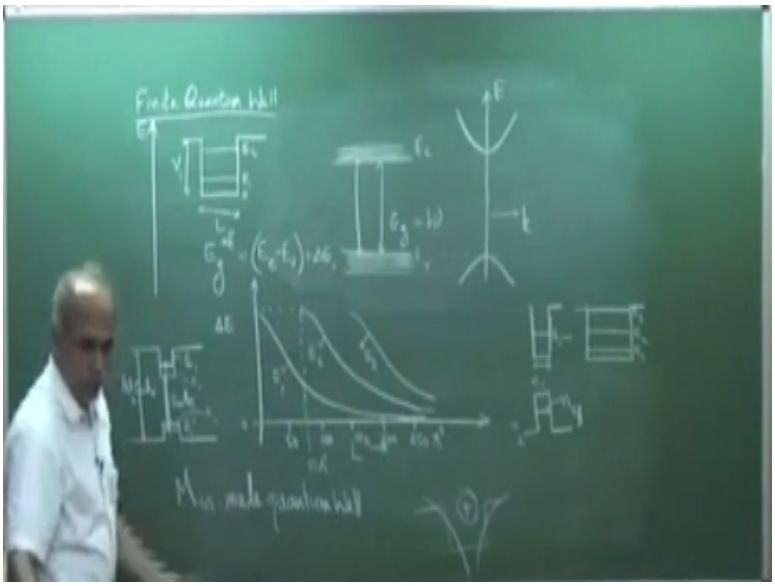

When we draw the energy band diagram Ev and Ec for a bulk semi conductor there are understand there are large number of allowed states here and it forms a band correspondingly the

EK diagram if you see then we have the conduction band and the balance band EK diagram for the band. So, these are equivalent, so this is E and k there are large number of states here right from Ec and therefore the energy band gap Eg which is here an electron which is sitting right at Ec could come down.

And recombine with a hole which is sitting at Ev and the energy of the photon which is emitted will be equal to Eg equal to h mew. Now this is Ec please see this is Ec of gallium arsenate and this is Ev of gallium arsenate bulk. But there is no state there first allowed electrons state is here and first allowed hole states is here that is the lowest energy holes state. So, the electron can sit here electron can occupy this state and this can recombine with a hole which is sitting here which means now effectively the band gap is this it is not Ec-Ev of the bulk.

But the band gap is this effective band gap, so Eg effective is equal to Ec-Ev that is the original Eg this+delta E1 that is E1 actually which I call delta E let me remove this.

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So, +E1 if I call this as E1 then this is E1 +E1 dash for the lower band, so this was Eg now we have E1 please see E1 this E1 is the difference E1 or maybe it I will be preferable that I please correct this it will be preferable that we write because we have used E1 for energy of electron in the valance band and E2 for energy of electron in the conduction band and therefore it would be preferable to use this delta E1, delta E2, delta E3.

In which this is delta E1, delta E2 kindly make this correction, so that let me show this as delta E1 dash and delta E. The delta referring to that this energies with respect to the band edge here. So, this is the effective band here which is larger than Eg, so this is 1 point that the effective band gap in quantum well structures is let me draw that again effective band gap in quantum well structure if I have an energy level here and an energy level here this is Eg effective band.

The interesting point is if you change the width of the width of the sandwiched layer that is width of this well if you change the width of the well you are moving let us say you are decreasing the width, so if you are decreasing the width then energy this is going higher. So, this comes to the new place here and this also goes to a new value and therefore the effective band gap now has increased.

So, what have we got we have tailored the band gap by simple changing the width of the quantum well or by width of the sandwiched layer this is tailoring of course one can change composition but if you see it is easier to say that we can change the composition but when you very see the fabrication process of MBE or VPE or any one of the processes it is very difficult to you can change the composition.

But it is very difficult to control the composition to the required value but controlling the thickness of the layer is very easy because in MBE technique for example today you can go layer by layer monolayer. So, you can control thicknesses to 1 monolayer, 1 monolayer is 3 to 5 Armstrong thickness, so that kind of precise control is available in fabrication and therefore by simply controlling the thickness we can change the effective band gap.

If you change the effective band gap the emission wavelength from this source when we realise a source using such structure the emission wavelength also changes. So, band gap tailoring by use of quantum well structures. You take some numbers how much what kind of change is this put some number and see let us see let me take an example just to get a field how much can really how much what is the amount that I get tuned see the maximum tuning possible of E1 is this region.

That is the width of the well from bottom of the well I can tune up to this that is the maximum variation that you can get.

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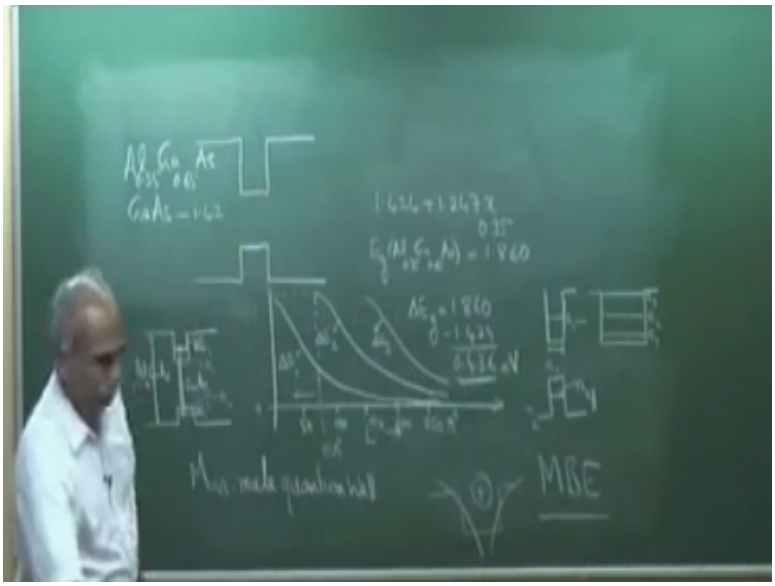

Let us say you realise a quantum well with a material let me take of familiar gallium arsenate and alluminum gallium arsenate. Let me put a composition say 0.35 gallium 0.65 and arsenic, gallium arsenate is 1.42 ev 1.42 and alluminum gallium arsenate you can calculate 1.424+1.247 into x where x is 0.35 you can substitute the numbers. So, you will have Eg, Eg of alluminum gallium arsenate 0.35 gallium 0.65 arsenate equal to you can calculate this.

I have done a small calculation you will see that this comes out to be 1.860 and therefore delta Eg is the band gap difference between this and this delta Eg is 1.860 -1.424 which is 6, 3 and 4, 0.436ev is the delta Ego hay very quick estimation that how much he will be able to tune what is the wavelength range over which you can tune you will see that the number is really very big you can tune over a relatively wide range for all from the practical point of view.

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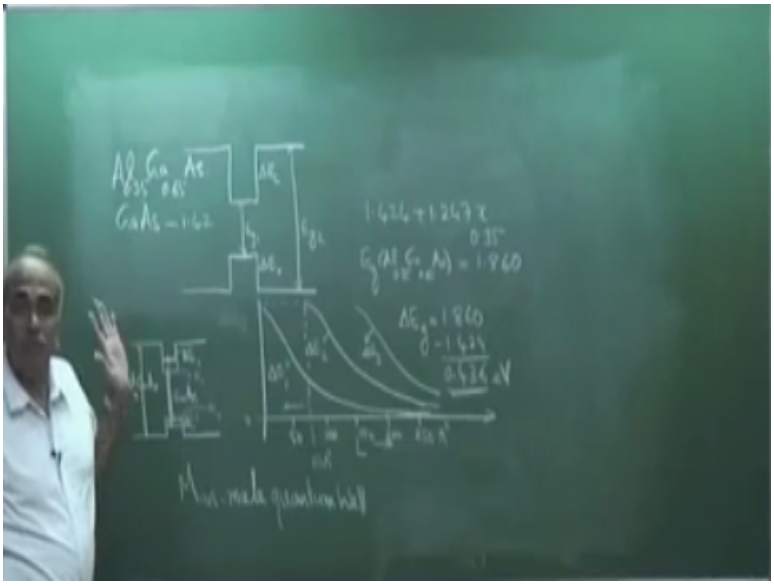

There is something here this was Eg of gallium arsenate and this is Eg of alluminum gallium arsenate, so Eg 1 and Eg 2 delta Eg is the difference where how much will appear here and how much will appear here what is the discontinuity that will be the point is I have shown the that is the discontinuity here and the discontinuity here. It could have been that these are aligned and only the discontinuity heels here.

But note in fact is there is a discontinuity band gap discontinuity here and here this is called as delta Ec discontinuity and this is this discontinuity is called delta Ev this has been determined by experiments that this delta Ec is approximately 65% that is 0.65 times delta Eg and delta Ev the discontinuity at the valance band here is about 35% of the total delta Eg and this is 65% in in the early 80s this number was 85 and 15 85% delta Ec and 15.

But so subsequently advanced experiments have determined that this discontinuity is approximately 65% and 35 %, why this is this is a bigger issue, this is question this the question is whether the 65 and 35 is the universal for all materials know it depends on the material system but for most materials which are used in opto-electronics it is approximately in this region.

Sometimes you will see 33 and 67 people are using 33 and 67, 30 and 70 but it is around this value but it depends on the material system dependents on doping also depend it on doping module which will depend on dependence on doping the question is whether it depends on

doping also the dependence on doping is much small the primary dependence is on the material itself. So, let us assume this number.

So, if you assume 65% and 35% please see our delta Eg is here then this discontinuity that we have why we are interested in this discontinuity because that is the maximum change that you can get from here to here this is delta Ec the maximum variation of E1 can be from the bottom of the well up to the top of the well. So, delta Ec is 65% of this, so you know delta Eg so you can calculate what is delta Ec you can calculate what is delta Ev.

This is I think delta Ec is approximately you can see some numbers 0.29ev and delta ev is approximately 0.15ev approximate number you can multiply n c. Therefore the total band gap total effective band gap can vary 1.4 24 up to 1.860 the maximum variation possible you can calculate the wavelength of emission that is lamda g corresponding to 1.424 you can calculate check what is the number we know immediately 1.24/1.424 will give you approximately 0.88 micrometre.

If you put for lamda g corresponding to 1.860 so this is 1.24/1.860 the number will be much smaller so this will come out to be how much will it come 1.24/1.86 approximately 1/3 2/3 approximately 2/3 if I drop this and this it is 12/18 which is 2/3, so it is approximately 0.65. the point is you can tune the emission from 880 nano metre to 650 nano metre maximum tuning variation.

But this is a very when I talked about optical communication window we need wavelength to the varied by 0.8 nano metre less than 1 nano metre is the variation that is that we are talking. So, therefore tuning that is changing the emission wavelength by controlling the thickness is the easiest ways because compositions the gas mixture gas flow rate in the fabrication process are kept constant simply the thickness is controlled.

In one case you may have some 50 Armstrong and then next time for the next layer you may take 55 Armstrong, 60 Armstrong. So, you change the thickness by 5 Armstrongs and the emission wavelength will change. So, this is band gap engineering or tailoring this tailoring it is adjusting

the dimension, so that is why the name tailoring band gap tailoring by use of quantum well. We will talk little bit more about these when they come to quantum well lasers the devices quantum well lasers and stained quantum well lasers.

The third point let me briefly talk about the third point that is strained quantum well structure these are the 3 important techniques which are used for band gap tailoring or band gap engineering.

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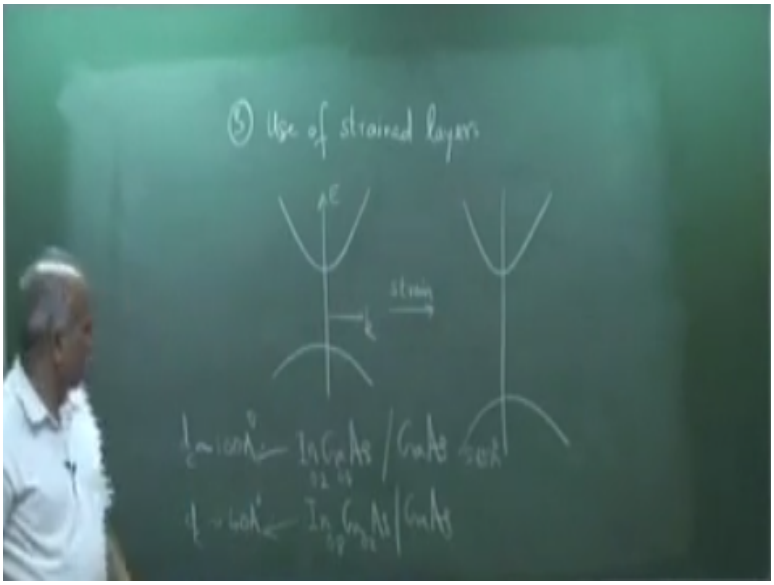

So, the third point is use of strained layers in the last class we talked about strained layer epitaxy strain layers when you introduce strain in a medium, so normally you have the EK diagram here this is the band structure in the presence of a strain what strain are we talking of at the inter phase there could be compress your strain or tensile strain, tensile strain is where it is elongated in the compressive strain it is compressed and this is done automatically.

The layer adjust itself so that bonds are complete when bonds are complete the energy of the system is minimum that is why it tries to do that it tries to do even if the layer is thick but is not able to do and then it leads to cracks in the system in the cracks in the material and therefore if the layer of the semi conductor which is being grown is less than the critical thickness then it is possible to grow strained epitaxial layer without any defects.

Now one of the important implications of this are consequences of this is change in so, due to strain the band gap changes first the simple picture, so the band gap could change which means it could become larger or it could become smaller depending on in a system in a given material system if the strain is compressive and then if the band gap becomes larger then if the strain is tensile then the band gap becomes smaller.

So, by control of strain how can you control strain, strain can be controlled by choosing the lattice mismatch, so you can choose for example indium gallium arsenate on gallium arsenate let us say indium gallium arsenate you could choose 0.2, 0.8 arsenate or you could choose indium 0.8, gallium 0.2, arsenate on gallium arsenate. The critical thickness in this case which one do we expect thickness please see gallium arsenate has 5.65 Armstrong as the lattice constant, indium arsenate has 5.87 as the lattice constant.

Here only 0.2 fraction of gallium is replaced therefore this will have a lattice constant closer to this, this will have a lattice constant closer to indium arsenate means further from gallium arsenate indeed if you put some numbers you will see that the dc the critical thickness in this case is about approximately 100 Armstrong approximate numbers of the order of 100 Armstrong. And in this scale I am sorry in this case dc because so we expected to be more or less critical thickness is expected to be less.

So, dc is of the order of 40 Armstrong because the mismatch is higher, so one can put the numbers and we have seen that you can calculate dc is equal to As/2 mod epsilon and c. So, by changing the composition you can change the strain by the changing the strain you can change the band gap. So, one can choose a proper combination to change the band gap. Now you could also argue if you want to change the composition why go for strain we could directly change the composition and change the band gap yes.

Strain has strain induced changes have many other advantages a little bit more complication some amount of a quantum mechanics has to be brought in here but okay let me very briefly introduce the balance band in a semi conductor is more complicated it is not simple we have been always drawing a simple EK diagram in the valance band.

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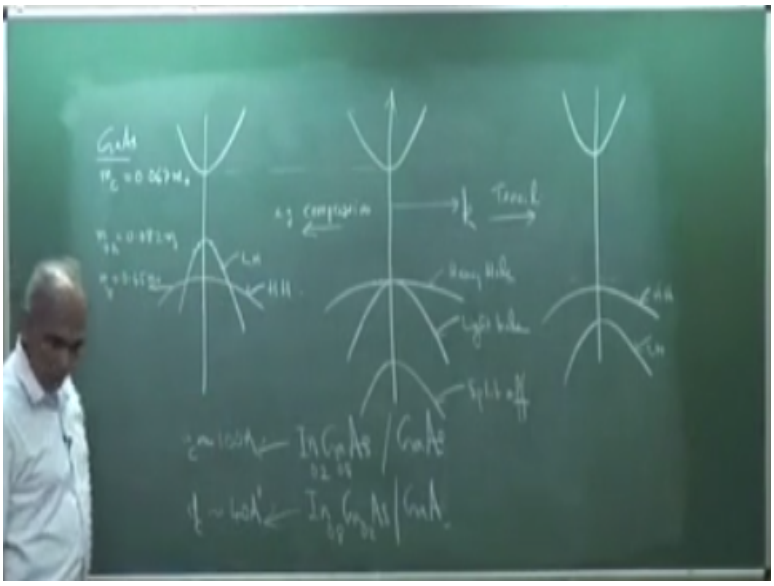

The valance band is actually more complicated it comprises of a light hole band, a heavy hole band and a split off band. So, I am now making it little bit more complicated and a split off band this is called this is the heavy hole band this is the light hole band and this is split off band the same EK diagram all the earlier was drawing I was drawing the upper most band because the electrons will get the firs field here of the holes which are interacting will be the holes which are here.

And therefore it is this band which is most important in normal circumstances but when you introduced strain what happens in this material is at k equal to 0 this is k at k equal to 0 the degeneracy between light hole and heavy hole breaks and the 2 bands separate out depending on the strain it could be like this. So, it could take so the light hole could come up and the heavy hole band could still remain there heavy hole band and the light hole bands.

Depending on the type strain whether it is tensile strain or compressive strain you could have a picture which is like this, so light hole band is here heavy hole band is here I will tell what is this heavy hole and light hole in a minute but let me first talk about band gap tuning. So, you can see that the effective band gap has been tuned and the holes which are now interacting with electrons or in this band light hole band.

The band gap has changed and the effective mass of holes mv has changed because this band is very rapidly, so if you find out for example for gallium arsenate we know that mc is equal to 0.067 and 0 and maybe I have given you what is mv was 0.45 m0 the light hole has a mass mv of light hole is approximately 0.082 times m0, it is light compare to this first point heavy hole it is heavy in mass this is light this is very simple level of talking light.

But basically it is because of the band variation here, so now the carriers which are participating are electrons here and holes in the light hole band in my original diagram here it is the holes which have energy it because they are coming first, so they are the once which we are interacting with this now it is this. So, the property of the semi conductor changes very much this has certain implications later we will discuss in realising ultra low threshold semi conductor lasers.

We will go bring those complications a little later for the time being in this context the band gap has changed and the effective mass of the carriers have changed by strain if you had let us say for example this is compressive strain if you use tensile strain the opposite will have that is this remains here this changes a little bit and the degeneracy is broken but and of course forget split off is quite deep.

So, now the light hole band is here and heavy hole band is here, so if you use tensile strain for the same material system the band gap has increased here the effective band gap has decreased. So, please remember that the purpose is not just to decrease or increase the band gap there are additional benefits which will come because of the effective mass of holes instead of heavy holes now light hole will be participating.

This we will appreciate when we discuss about devices because that has an implication on the movement Fermi level under injection and the movement for Fermi level under injection conditions determines the threshold you will see this at a later state but for the time being by use of strain you have a band gap modification and change in the carrier mass effective mass of the carriers. Now we have a few more minutes what are this light holes and heavy holes very quickly but you may have to refer to some more basic books.

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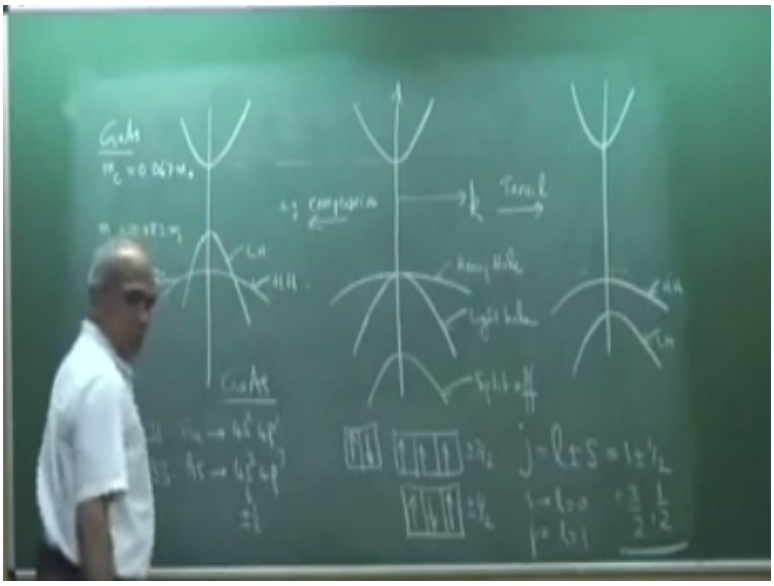

If you take gallium arsenate every time I take gallium arsenate because one it is most widely materials reason number 1, reason number 2 is we become familiar with one particular material so that for any other material you can always extend the arguments. We know that this has 4 s2 , 4p1 gallium is 31 atomic number and outer valance has 4s2 4p1 arsenate atomic number 33 has 4s24p3, s2 means spin it has +- half spin.

Please see s2 means there can be 2 electrons in p there are 3 shell, so the 3 electrons could be on like this or it could be, so the total spin in this case is 3/2 and in this case it is half +- is possible depending on whether all of them are down or all of them are up this is the total spin and the angular momentum j is given by L+-s this is called LS coupling L+-S L is orbital quantum number S is the spin quantum number.

L for s shells L equal to 0 for p Shells L equal to 1 this is the value of spin, so L equal to 0 and L equal to 1 therefore the total quantum number here will become you can take values so 1 **1**+-half the total spin which means this can become 3/2 and half. The angular momentum can take values 3/2 and half very quickly and therefore you have 3 combinations now please s can take values 3/2 and +- half, j can take 3/2 and half.

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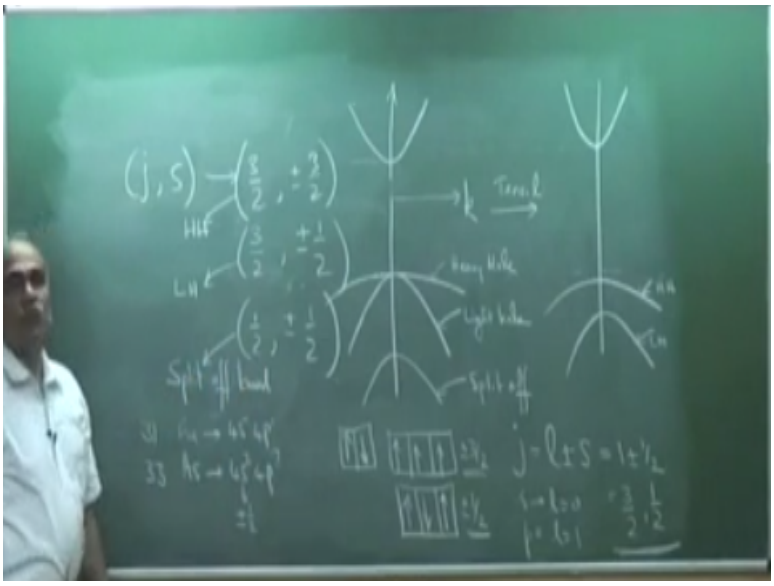

And therefore we have combination of states which are S which are J, S the states are represented by J,S which gives the combinations possible are 3/2, +-3/2 **3/** 3/2 here and +-3/2, 3/2 +- half and the last one is half, +-half the first number is J, J takes values 3/2 and half S takes values +-3/2 and +-half so we the combinations which are possible are these. This is nothing but the heavy hole band this corresponds to the light hole band.

And this corresponds to the split off band those of you interested you can read more about this but I thought because I have drawn them what do they really represent these represent the allowed quantum states of electron. So, depending on the quantum state of an electron they may occupy this band or this band or this band. So, this is light hole and heavy hole the concept of light hole and heavy hole is a quantum mechanical concept.

Please refer to certain books if you wish to know more about this but our objective has been to see the band gap variation due to strain due to tailoring of quantum well structures and due to composition. So, let me stop at this point we have covered most of the material aspects in the next class we will discuss about p-n junctions you have studied p-n junctions but my interest will be to see hetero structure p-n junctions how would be a p-n junction or what is the energy band diagram of a hetero structure p-n junction.

Because most of the devices we will see are p-n hetero structures it is not the simple p-n junction which we normally study in electronics. So, we will see how they are because that has lot of implications in the final device characteristics.