Fundamentals of Semiconductor Devices

Prof. Digbijoy N. Nath
Centre for Nano Science and Engineering
Indian Institute of Science, Bangalore

Lecture – 40
Band diagram of heterojunctions

Welcome back. So, if you recall in the last lecture we were discussing about a compound semiconductor and heterojunctions. I have given your brief introduction I know about heterojunctions and importance of epitaxy lattice mismatch. I told you about the different kinds of hetro different kinds of compound semiconductors in group 3, 5 oxides, nitrites and so on. Every time we you know connected internet and so many other areas that compound semiconductors are widely used. So, there are lot of devices to learn about that. We will keep things simple though.

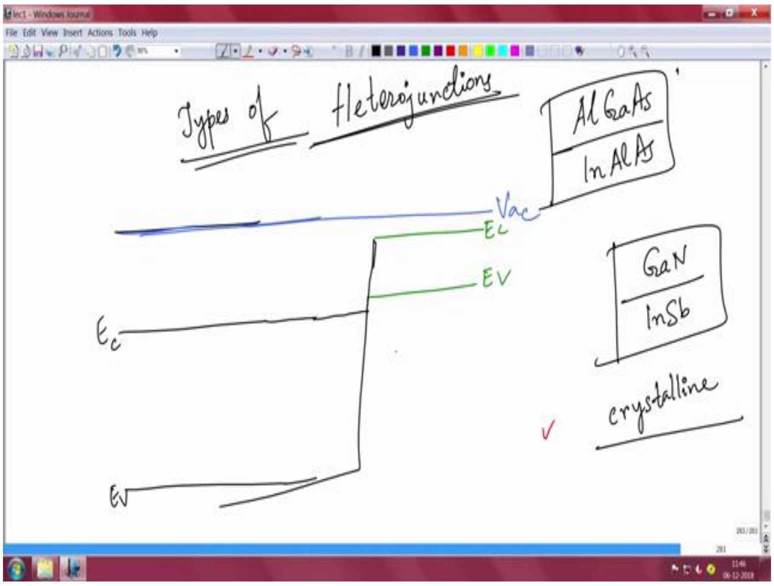
Today, we shall be starting with some Band diagrams. If you recall we have studied band diagrams of short key junction p-n junction, right MOSFET, BJTs and so on. So, what about all those structures where essentially of the same semiconductors say silicon, but if we take heterojunctions which means we have dissimilar materials with different band gaps band alignments and electron affinities, then how do you from heterojunction between a wide band gap and a narrow band gap semiconductor for example.

A p-n junction made of heterojunction all this things will study. So, that we can draw the band diagrams to understand the devices like lasers, LEDs, transistors and a many other kinds of transistors and so on. There are fascinating amount of physics that can be done I told you that a particle in a box that you might have studied in your high school or 10 plus 2 can be practically realized in a quantum well where a narrow band gap semiconductor is sandwich between two wide band gap semiconductors.

So, that such kind of things are possibly heterojunctions and we should never forget that we cannot arbitrarily stack materials on top of each other. There has to be a material science you know permissibility, you know material science has to allow that. So, the epitaxy and lattice mismatch are very important.

So, there many aspects pertaining to it which we have covered. So, today we shall start from the types of heterojunctions and how to draw band diagrams of heterojunctions. So, we will come to the whiteboard here.

(Refer Slide Time: 02:16)



So, I told you that heterojunctions are essentially the junction between two dissimilar materials, typically to have them grow on top of each other we need to have them of the same family. So, for example, you can have heterostructure of aluminium gallium arsenide on top of say indium aluminium arsenide for example, because they of the same family.

But, you cannot have a material of gallium nitride for example, on say indium antimonite randomly ok. You will not be able to get crystalline material you. Please remember that this materials have to grow crystalline in order to preserve the band structure and the band diagram. So, you cannot arbitrarily grow one metal on top of another. It has to be permitted by the material science behind it. So, those are the things we are studies.

So, now there are there are three types of heterojunctions practically speaking, you see the electron affinity rule makes of that. So, every material so, if this is a vacuum level you know you have a conduction band E_C then you have a valence band E_V suppose this is mildly n-type dope. Now, the question is in any type of p-n junction or other junction that you have studied till now the material has always been the same silicon and the band gap always has been the same mostly ok.

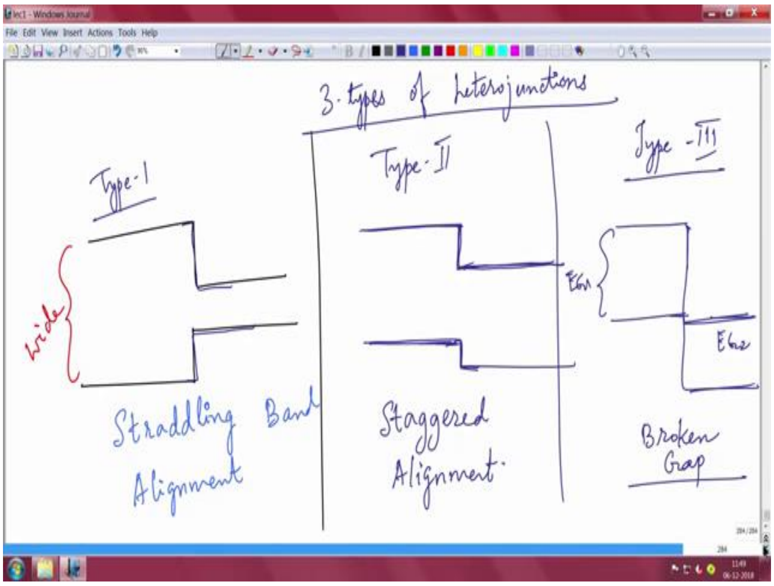
But, if the band gaps are different for example, I might have a, this is the vacuum level, right. So, this is the vacuum level. So, let me use another color for the vacuum level maybe I will use blue. So, this is your vacuum level, right and now there is another semiconductor whose conduction band might lie here and it is a narrow band gap semiconductor. So, valence band might lie here and it might be mildly n-type or mildly p-type dope let us not use the word doping as of now, let us assume that they are you know we I do not care about the doping.

You see, the case is here this is one kind of arrangement where you know you can have; you can have the conduction band of one side on above the conduction band on the other side because the electron affinity of this is lower ok. So, a junction that might be formed between them right a function that might be formed between them could be something like let me use the black color may be here; the junction might be you know if I mean I am not drawing heterojunction as of now because there will be band bending and other things, but this could be the structure, right. You know this could be structure right that could be a structure here.

But, you know this is only one possibility it is also could have been happened that the narrow band gap semiconductor would have had a different electron affinity. For example, the narrow band gap semiconductor would have this kind of E_C and E_V this kind of electron affinity where it is larger and this kind of an arrangement in which your band diagram would have looked something like this ok, that is also possible.

This is the different diagram alignment this is called different band alignment from what I have drawn in previously or it could also have happened that you know your narrow band gap semiconductor is such that is very narrow and your E_C is here, also the E_V is here, E_V is also here. So, then in that case you would have had something like this and then this.

(Refer Slide Time: 05:27)



So, there are different kinds of alignments. So, there are 3 kinds of primarily, 3 kinds of 3 types of heterojunctions are typically there ok. 3 kinds of heterojunctions are there which can be formed based on their band alignment and their electron affinity. So, you have what is call type – I and you have something call type – II and then you have something called type – III. These are three types of heterojunction.

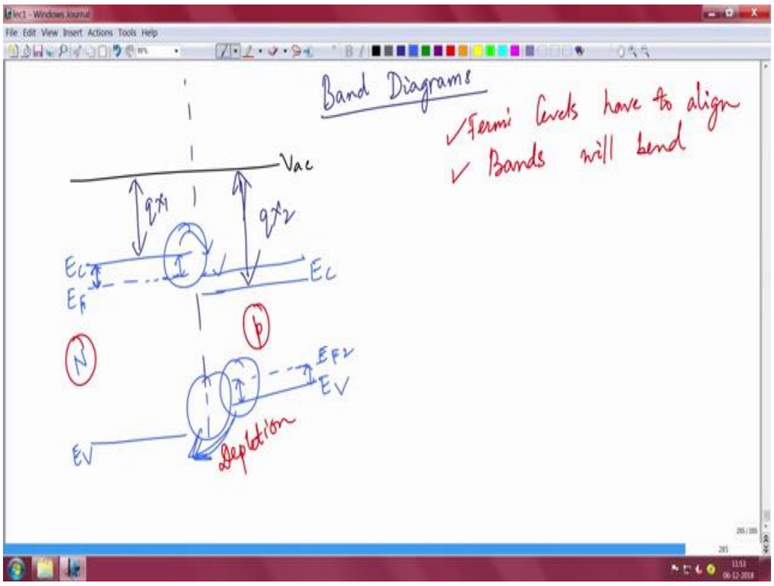
So, in the first type of heterojunction, you have heterojunctions like this and I am not very good at drawing here, but actually this is a narrow band gap you see this is a narrow band gap semiconductor right and this is a wide band gap semiconductor right that is possible. So, this kind of alignment is there and this is call type – I alignment or it is also called straddling. It is called a straddling band alignment; not bang, it is a band ok. Straddling band alignment, this is called type – I ok. This is called type – I. This type of alignment is called type – I alignment.

Then we have type – II. What is type – II? In type – II, you will have something called staggered. So, you will have something like this and then you will have something like this probably. You see the here you know you have a step in the conduction band coming down, the valance when also has a step here. Here also you have a step, but your band is such that the second, the second layer, the second material ok, the second materials electron affinity is little higher. So, that you know you have a step like this, but the valence band also steps down.

So, in a way you have a band that is aligning here. This depends on electron affinity by the way nothing to do otherwise. So, it depends on electron affinity of this is called type – II and this is called staggered band gap a staggered band alignment, staggered alignment which calls staggered alignment. And you can see that, but this is not a this is not have in a real dope semiconductor you will have depletion and other things which I have not shown here, but I will show that.

And, the third one is the type – III and this is broken gap. So, you will have something like this and as I told you something like this maybe. These 2 bands are 2 band gaps you know this is band gap 1 and this is band gap 2, they are completely now like not aligned in a way. So, when you joined them together you from something like that. This is also called broken gap alignment. It is called broken gap alignment or also we can call type – III. So, these are the 3 types of heterojunctions that are possible depends on what you are looking at.

(Refer Slide Time: 08:07)



So, if we do simple you know band diagrams because for making any devices we should be able to draw heterojunction band diagram and heterojunction band diagrams. If you understand heterojunction band diagrams then you can understand actually any types of devices at semiconductor devices including homojunction and heterojunction, but many of the text books and many of the, you know the courses do not focus and do not teach the band diagrams of heterojunctions very well.

So, we will make sure that are you basically understand everything. So, you know let us considered very simple one. Suppose I have a vacuum level here; [FL] please, pay attention you will see that is very easy to draw. Suppose, I have the vacuum level here and then I have a wide band gap material here I will sorry, wide band gap material here I will call it E_C , E_V and wide band gap I will use capital letter and for small band gap value small letter.

This is mildly N-type dope; this is the Fermi level on the wide band gap side. So, I call this is N-type and I will use capital N for wide band gap on the other side I have a narrow band gap semiconductor, suppose this is the type – II a sort of type I sort of an alignment straddling sort of an alignment. So, I have a narrow band gap which is E_C for example, and then I have E_V and this is mildly this is E_{F1}, this is E_{F2}. This is mildly p-type dope that is mildly N-type dope. We can see that the electron affinity here sorry, the electron affinity here q_{X2} is actually more than the electron affinity here which is q_{X1} that is where is alignment is happen.

Now, the moment you joined them actually the moment you joined them what will happen is that please remember that because their mildly doped, you will have at the junction you have some depletion here, because the bands will try to band and the Fermi level is to align in equilibrium and there will be some depletion here because the Fermi level because your Fermi level has to align, right. Your Fermi level that you know from the other basics Fermi levels have to align in equilibrium, they cannot have a change in position. The Fermi levels have to align. So, the bands will band to make the Fermi level align.

What is happening is that practically speaking, what is happening is the electrons and holes are flowing from one material to the other material. Electrons are flowing from the left side wide and gap material to the to the left the right side narrow band gap material and holes that are here in the narrow band gap; narrow band gap rights material on the right side holes are trying to move to the left side where the holes are not are in minority right.

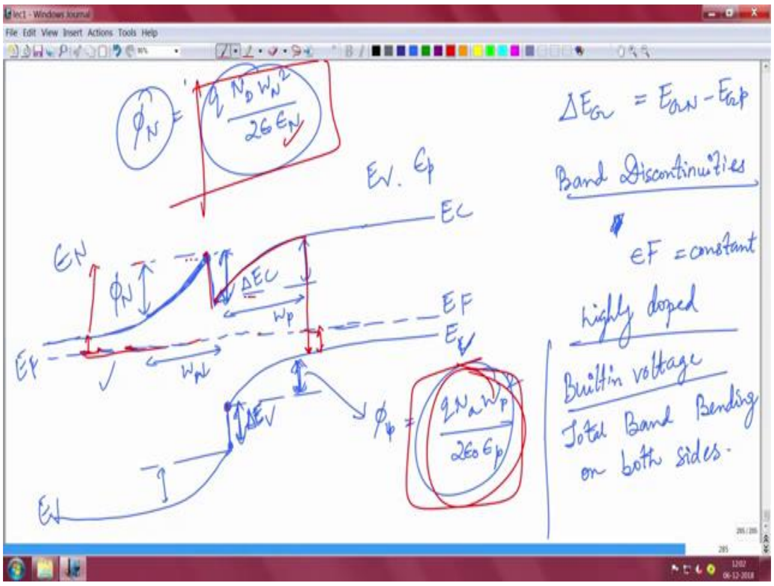
So, this is N-type semiconductor and this is small p, I will give p type material this is an wide band gap and narrow band gap p-type and band given N and p-type heterojunction at the depletional form p-n junctional from just like what we have studied earlier for silicon except that there will be some band discontinuities here because your band gap is not the same. So, the way you draw it essentially is that and this is the most important part. This part will have ok; so, let me draw it completely here; so, you this, right this.

So, you see this part will be essentially deplete now because electrons will go from this side to that side. So, that part will not slightly deplete and holes will come from here to here. So, this part will is also deplete as the hole will come. So, essentially when I say depletion what I mean? When I say depletion I mean that; one I say depletion I mean that your Fermi level sorry, your Fermi level position your Fermi level and this electron the conduction band edge the spacing the spacing will basically increase if the electrons are coming from here to here and depleting, right.

Similarly, the spacing ,the gap between Fermi level and the valence band on this side also has to increase because holes are coming from the right to the left and so, it is getting depleted. So, essentially your Fermi level and the valence band edge also have to I means that the spacing also has to increase but far away from the junction. The spacing between the Fermi level and the valence band will not change and far away from the junction the valence conduction band and the Fermi level here on the N side also will not change just like in a p-n junction in silicon.

Only around this point and this point your bands will band, your bands will band in order to form a p-n junction. So, and the Fermi level has to align. So, let me rub it up again so that you know you can basically get an idea what I am talking about here.

(Refer Slide Time: 12:12)



So, before joining; so, before joining what will happen is that I have this sorry, I have this conduction band, right. It will not be bend of course will be straight line. So, I have this; I have this conduction band here, it is mildly doped. So, Fermi level is here and then I have the valence band here. On the other side I have the conduction band here, the valence band here and the mildly dopes the p-type Fermi level E_{F2} is also here, this is E_{F1}.

So, at the junction what will happen is that you draw it is actually too long here. So, so at the junction you will have depletion now, right that is what you know. So, the bands will bend the Fermi level has to align. So, the Fermi level has to align. So, essentially this whole thing will try to come down and this whole thing will try to go up. So, that the Fermi levels will align, making sure that this far away from the junction this $E_C - E_F$, this $E_F - E_V$ will be constant ok.

So, what do you do is that one thing is that you see this point; this point corresponds to this point here, the conduction band where it is meeting with this interface. You fix this point in your mind and this conduction band on the other side is fix this point in the mind ok. Now, with that being in mind you have to bend the band. So, this conduction band over here this conduction band over here essentially you fix this point and now you bend it ok; it has to bend like this.

But, far away from the junction your Fermi level has to align; that means, far away from the junction far away from the junction E_C and E_F this spacing has to be constant, but you keep you are imagining that this point you are fixing the band and you are pulling the band down here. So, let us Fermi level will align. Similarly, you fix this point here, right you in your in your mind and you pull this valance band up. You pull this valence band up so that you know it is something like this; this is the valance band.

So, I will have to remove this valence band here now right ok. This is the valence band. This point is the fix point where the valence band was supposed to meet the junction and this was the point where the conduction was suppose to meet the junction. So, it will also bend. The band gap has to remain same on the right side, that is the narrow band gap this point this has to remain same, right. On the similarly on the left side the band gap has to remain same right the band gap has to remain same. This was the point where the valence band on the left side was there and it has to go like this because this band gap will remain the same, no questions about.

And the Fermi level of course, has to align. So, far away from junction this gap has to be same, this gap has to be same. So, the Fermi level is aligning here. You see far away from the junction this gap has to be same the p-type, right and far away from junction this gap has to be same the n-type right. Only at the junction you see the Fermi level and the valence band and conduction band spacing has increased; that means, there is the depletion. Similarly, Fermi level and the valence band distance is increased; that means, there is a depletion near the junction; from both sides their appropriate depletion that have formed. So, please that keep that in mind.

And what will happen is now that what will happen now is that you will have to join this two points like that and then you have to join this points to like that you have to join this two points like that. So, your band diagram looks like this ok; your band diagram essentially looks like that. So, you have this Fermi level, right. If this Fermi level and you have it is band bending this is E_C, this is E_V this is your common Fermi level everywhere now. This is E_C on the left side, this is E_V on the left side, this is the wide band gap material, it is a narrow band gap material. So, this is your p-n junction that has formed, this is your p-n junction that has formed.

So, remember here if the band gap on this side is suppose I am just saying, 3 electron volt and the band gap on this side is suppose 2 electron volt then the difference of the band gap is called the band gap difference you know ΔE_G that will be 1 volt, right; 1 electron volt. So, essentially that ΔE_G essentially is the band gap on the bigger side here minus the band gap on the lower side small p ok. So, that is what happening.

$$\Delta E_G = E_{GN} - E_{Gp}$$

And this point this gap that is straight that is formed is actually ΔE_C and this is called ΔE_V. These are called band discontinuities band discontinuities. This is called conduction band discontinuity and this is called excuse me this is called valence band discontinuity ok. And you can see that the there is a band bending here it is happened. This band bending that has happened that and there is a band bending that is happen also here. This is the same as this band bending. This band bending is the happening which is the same as this band bending that is happening which is same as this.

So, to this band bending essentially again if this band bending I will call it as $\emptyset_N$ then $\emptyset_N$ will essentially be q the doping that is on this side which is N_D and the depletion which is like say W_N; W capital N, W_N^2, epsilon naught epsilon N because the dielectric constant on this side to be epsilon N dielectric constant on this side could be epsilon small p and the dielectric constants could be different.

$$\emptyset_N = \frac{qN_D W_N^2}{2 \in_0 \in_N}$$

So, you remembered a electric field has to be continuous everywhere. Actually it is the electric field times dielectric constant that has to be constant which is the displacement vector in a way we can say. So, this is the band bending on this side and the band bending on this side this quantity is actually $\emptyset_p$that is given by qN_a that is the doping on this side times W; this is the depletion for example, W small p. So, W small p square by 2 epsilon naught epsilon small p ok. So, that is the band bending that has happened on both sides and the built in potential.

$$\emptyset_p = \frac{qN_a W_p^2}{2 \in_0 \in_p}$$

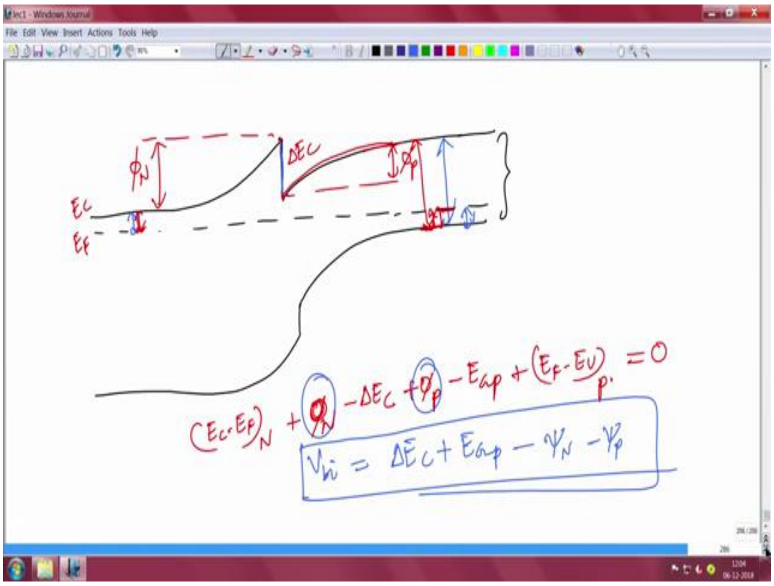
And other things actually you cannot you know you cannot just like that use the existing p-n equation that equation to come up with the built in potential because you see the depletion approximation may not always hold true in a heterojunction. You will see in very special cases that in a heterojunction you may not have depletion at the edge. I will show you some examples pertaining to that and also remember that if one side is very highly doped then that of course, the same thing happens the depletion side will predominantly beyond the other side ok. Even in a heterojunction the band bending will not happen on one side essentially it will be only on the lightly dope side, right.

So, the built in potential here you know the built in potential the built in voltage that we have studied you know classic p-n junction also is actually the total band bending is actually that total band bending ok, on both sides, the total band bending on both sides. So, in a way this is actually this plus this is the total built in potential ok, is the total built in potential. You can see that you can actually derive that; you can actually derive that by you know starting from the Fermi level here. You can do this or you can also do it by other ways and that is I will tell you.

So, you start from the Fermi level here, you go up this quantity which is $E_F - E_C$ that you $E_C - E_F$ on the n side that you know if you know the doping, then you go again this much which is $\emptyset_N$ you reach this point, right then you back here which is minus ΔE_C. Then you go up this point which is this quantity that is the band bending then you come back fully the band gap of the p-side, then again you go up by this quantity which is $E_F - E_C$ and you come back again the Fermi level.

You understand my point? I am starting from the Fermi level, I am doing one circle essentially one motion around the band diagram and I am coming back again to the Fermi circle Fermi this thing. So, I will use the another slide and I will show you what I am talking about actually. Remember, that this quantity plus this quantity is actually the total built in voltage, but you can also derive it in you know same thing you can actually find these values in a function the function of band gaps.

(Refer Slide Time: 20:32)



And, also what was I was telling you is that you know I have a Fermi level here for example, this is a Fermi level and if I look at the band diagram there, it is looks like this, this, this, right; then it has like this, this, this and this right sorry this is little bit not so correct ok.

So, this is the band gap on the p side; I will call it E_G and small p, that is. So, you see if I start from; if I start from this from this Fermi level this point, suppose I go up by this quantity what is that quantity? That is $E_C - E_F$ on the N side, right. So, that is $E_C - E_F$ on the N side which is very easy to find out if you know the doping by the way, Maxwell-Boltzmann ok.

Then, I starts from this point and then I go up by this band bending this is the band bending you know if I go up by band that is $\emptyset_N$. So, plus $\emptyset_N$ that is the band bending I reach this point now. I come down by this quantity which is ΔE_C, right; so, minus ΔE_C that is that this continuity, then I again go up by this quantity which is your band bending on the p-side, this is called $\emptyset_p$ that I wrote the expression in the previous slide. So, I will again go up by plus $\emptyset_p$ then I reach this point and I come back the full band gap of to p side.

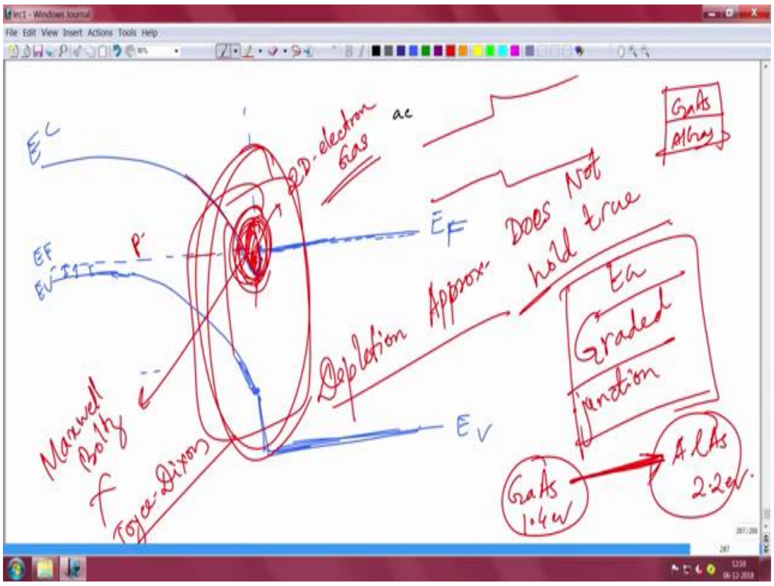
$$(E_C - E_F)_N + \emptyset_N - \Delta E_C + \emptyset_p - E_{Gp} + (E_C - E_F)_p = 0$$

So, minus E_{Gp}, I come here I reach this point I again go up by this quantity which is plus $(E_F - E_V)$ on the p side then I reach the Fermi level only you know. So, I started from here reached here. So, the total equation has to be 0. So, your built in potential is actually this quantity plus this quantity. So, that will built in potential will be equal to you can take the other things the other side ΔE_C plus the that is this plus this whole band gap, the entire band gap I mean E_{Gp} minus this quantity and this quantity ok. I can call it as like you know $\varphi_N - \varphi_p$ this is this quantity and this quantity which is easy to find out that is kT by q ln of N C by N D on the N side similarly NB by NA on the on the NA on the other side. So, this is very easy to understand.

$$V_{bi} = \Delta E_C + E_{Gp} - \varphi_N - \varphi_p$$

So, this quantity will also give you the built in potential which I have told you in the previous slide is essentially this quantity plus this quantity, that is the built in. Now, this is only one type of heterojunction by the way. There could be many other types of heterojunction you know heterojunctions that where depletion approximations actually breakdown.

(Refer Slide Time: 23:06)



There can be many types of heterojunction. So, for example, if I talk about heterojunction where you know I have suppose I have vacuum level. So, I will use the black color for the vacuum level. Suppose, this is the vacuum level E_{vac} and suppose, I have a narrow band gap semiconductor here, I will use the blue color probably a narrow band gap semiconductor here E_C and E_V.

There is a narrow band gap semiconductor it is lightly p-type doped here and on the other side I have a wide band gap semiconductor E_C and then I have E_V and this is very highly dope. So, the Fermi level is almost touching the conduction band which means on the N side you are not going to get any you are not going to get any depletion for example, you are not going to get any depletion on the N side.

And how will the band diagram look here now? So, essentially your entire depletion will be on this side, right. So, essentially your p type semiconductor will bend in order to make the Fermi levels align. So, this Fermi level has to align with that right. So, what will happen is that the p-types semiconductor will move up if this whole thing will move up essentially to align the band. So, and far away from the junction it has to be the same and you should keep in mind that at the junction you know at the junction, you should actually fix this point which is this point and this point.

So, the this conduction band will actually get fixed here, but it will move up like that ok, this is conduction band. And your Fermi level is to align right and the valence band also has to this point will fix up, this point will fix up and it will go away. So, eventually your Fermi level has to align and far away from the Fermi level will align like this. You see this side will have no depletion because this is very very highly dope right this will be no depletion here by the way ok.

So, this is the Fermi level eventually that is the global Fermi level that will form here and this point of the valence band of semiconductor far away from the junction it has to be same. So, it goes like this, the band gap has to be same everywhere on the left side, so, anyways. So, you know you ok so, it sorry. So, it has to go like that it is to go like that. The band gap is same of course everywhere far away from the junction this point has to be this spacing $E_C - E_F - E_V$ has to be constant and there is a huge depletion here you can see the whole band gap it is actually inversion that is forming here you can say. Even remember the inversion of silicon MOSFET same thing is happening here actually in a way.

And then you will have this ΔE_V like this ok, it will not bend. So, much this will not bend and this will from like this and this is Fermi level this is going above the conduction band. You see this conduction band, this is the conduction band. This conduction band is going below the Fermi level here this is the Fermi level which means this part has a very high density of what we call 2D electron gas just like your silicon MOSFET except the there is no SiO_2 silicon dielectric constant here, but it is only semiconductor on both side.

But, the bands have band so much that there is inversion here this is a p-type semiconductor because this is the Fermi level here in p-type semiconductor identifies you are getting a very high density of electron gas. It is actually and very high density of electron gas it is inverting actually you know.

So, there different kinds of hetrostructures you can found depending on the band diagram, Alignment, electron affinity and the band gap. You see because there is a very high density of electron gas this is highly-highly conducting. So, in this junction your depletion approximation cannot hold true. Depletion approximation that we use in our conventional p-n junction does not hold true in this case ok, does not hold true you can see that the depletion approximation cannot hold true because in the junction you have a very high density of electron gas.

This high density of electron gas make sure that although this is depleted you have very high conductivity here. So, the whole thing is not depleted that is why approximation breaks down and in such cases you also cannot apply your classical Maxwell Boltzmann approximation cannot be applied because this is high density you have to use something called Joyce-Dixon that I had mention to you long back if you remember Joyce-Dixon. So, there is many kind of things that you have to you know take into account when you draw heterojunctions. There can be many types of heterojunctions you know it depend on the alignment, you can have inversion you can have accumulation and so on.

So, there is a this kind of things right and these are used actually in practical devices by the ways. I will tell you about the devices very soon I will tell you about the devices what kind of the devices can be made and I already told you that particle in a well box can be made LEDs and other things are definitely taking advantage of such hetrostructures, but in an transistor also you will see a lot of actually applications that use this kind of hetrostructures ok.

And now and the next we will start what we will start next time is called the graded heterojunction, graded junction. Graded junction is in the band is graded actually you can change the band gap as you go over a position ok. I will tell you how to do that because you know if you are having gallium arsenide which is 1.4 electron volt and you have suppose having aluminium arsenide which is 2.2 electron volt. You can either make heterojunction like gallium arsenide, aluminium gallium arsenide. So, the heterojunction will look something like you know like this of course and like this.

But, you can also you can increasingly grade it. You can, as you grow the material you can linearly change or a exponentially change the band gap of the material and that is the beauty you can actually use that and that is routinely used in your devices like HPTs that are actually used in your cell phones by the way. So, this is not something fancy this actually practically used in the cell phones and stuff ok.

So, let us wrap the class here today for this lecture. We have talked about heterojunctions and hetro structures, we introduced the band diagram concept p-n junction and other things how the band alignments are there. I hope you are now familiar with heterojunction a band diagrams there can be different alignments, different dopings, different band gaps and band alignment. So, depending on that you have to think and draw the band diagram. It can be p-p, it can be n-n, n-p-p and the wide and narrow they can have different combinations and you remembered a straddling, staggered and the broken gap alignments depending on the electron affinity.

So, when you are given a new heterojunction to make on both sides you just do that thing. You see if both are doped moderately then depletion will be on both side. So, depletion [FL] your Fermi level and the conduction band or Fermi level and the valence band depending n-n-p, n or p we will increase that gap will increase, but far away from the junction it will not be any influence that you remember.

And secondly, you draw a hypothetical line vertical line you fix the points where the conduction and valence bands are supposed to be there and hooking that you know clutching that to that point you shift the band up or down. And let the Fermi level move up and down so that the Fermi level becomes aligned everywhere there is no step in Fermi function, right. And those points where you fix the conduction and valence band should be in position and you join those edges eventually you will get a $\Delta E_C, \Delta E_V$ that the discontinuity is a band diagram ok.

Any questions you can always email me, chat with me you know for this heterojunction band diagram is very important because the device is based on heterojunctions are very exciting because you have a lot of lot more things to do and a lot of research is going on those things. So, in the next class we will start with graded heterojunction which will be advantageous in many applications that you will see. So, we will end the class here.

Thank you for your time.