

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

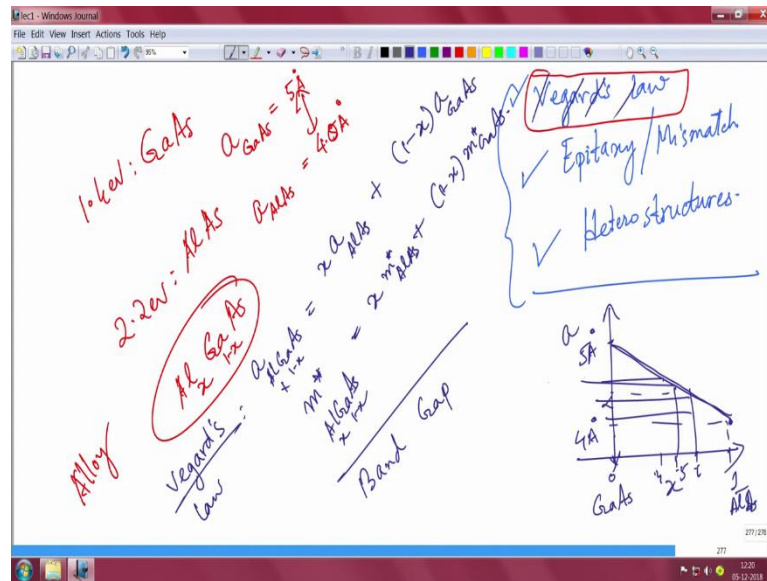
**Lecture – 39**  
**Basics of heterojunctions**

Welcome back. So, we will continue to our discussion on compound semiconductor. I told you about the introduction on compound semiconductor in the last class. We had discussed the different kinds and categories of compound semiconductor and some of the uses we had touched upon like white LEDs detector and so on. The lot of wide applications we will come to know them one by one here.

I told you in today's class we shall discuss 3 things. One is Vegard's law, one is epitaxial mismatch and one is hetero structure. We will touch them only briefly not go very deep because each of this topic is very profound. We shall understand as much as is required to understand the devices made of compound semiconductor ok. I told you that you can mix and match different types of compound semiconductor and alloy them, to tune the band gap, to tune the properties of the material that can a flexibility is not there in Silicon for example, or Germanium.

We can mix little Silicon Germanium by the way then that also will gives you limited opportunity is there. Anyways the first thing we have to understand is Vegard's law. What is Vegard's law and why this law becomes important? That is actually important when you try to understand alloys of material. Like you are taking Gallium Arsenide, you are taking Aluminium Arsenide, you are mixing them in some ratio 50-50, 40-60, 20-80 whatever and you have Aluminium Gallium Arsenide. Then the material properties can be predicted fairly you know accurately or close to accuracy using Vegard's law.

(Refer Slide Time: 01:53)



So, let us come to white board today and we will see that you know you have Vegard's law. Vegard's law what does it Vegard's law? You will see it very quickly actually. Suppose you have a Gallium Arsenide. When Gallium Arsenide has the lattice constant a  $a_{GaAs}$ . I will call it [FL] second. So, what I will do is that a Gallium Arsenide is the lattice constant of Gallium Arsenide may be it is it. May be 5 Angstrom, it may be 6 Angstrom. I do not remembered exact value, but it may be few Angstrom's ok, it is Gallium Arsenide has the lattice constant.

Now, I have Aluminium Arsenide and Aluminium Arsenide of course, this band gap is 1.4ev and this band gap is around 2.2ev. Suppose, Aluminium Arsenide has a band has a lattice constant of a Aluminium Arsenide. This is also few angstroms, for example, this can be say you know this can be say 5 Angstrom this can be 5 Angstrom. I am just giving an example I do not recall the exact value, but it can be 5 Angstrom this can be say 4.5 Angstrom or 4.0 Angstrom for example.

Now what will be the, what will be the lattice constant of Aluminium Gallium Arsenide which has say  $Al_xGa_{1-x}As$ ? It will be somewhere in between, it will be somewhere in between. Of course, it has to be in somewhere in between. So, this is an alloy right. It has to be somewhere in between.

So, essentially Vegard's law says that you can do a linear interpolation which means the lattice constant of this a Aluminium Gallium Arsenide  $x$  1 minus  $x$  will be equal to  $x$  times

the lattice constant of Aluminium Arsenide plus 1 minus x times the lattice constant of Gallium Arsenide.

$$a_{Al_xGaAs_{1-x}} = xa_{AlAs} + (1 - x)a_{GaAs}$$

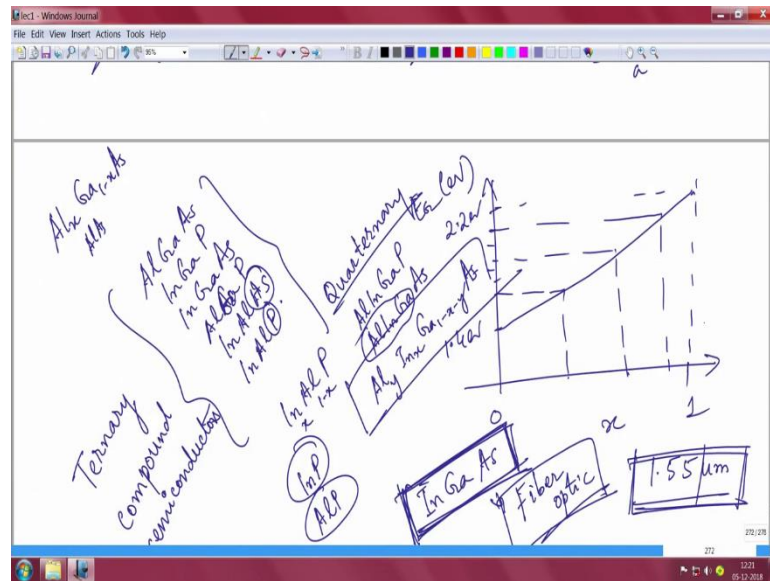
Same thing can be done for example, effective mass may be if you have an effective mass of Aluminium Gallium Arsenide x 1 minus x, it will be x times the effective mass of Aluminium Arsenide plus 1 minus x times the effective mass of Gallium Arsenide. So, it is a linear interpolation ok. So, essentially if I am plotting the lattice constant here and if I am plotting x here that is the you know fraction. So, x equal to 0 this point corresponds to 0 point corresponds to purely Gallium Arsenide and x equal to 1 that point corresponds to purely Aluminium Arsenide right. So, your lattice constant will probably go from say 5 Angstrom here to say may be this is 4 Angstrom here.

$$m^*_{Al_xGaAs_{1-x}} = xm^*_{AlAs} + (1 - x)m^*_{GaAs}$$

I am just giving an example this may not be 5 and 4 this will be something else, but this is an unique constant number by the way, it cannot be arbitrary. So, that is known. So, it will basically go as like this linear, a linear plot. So, any point here if you have x equal to 0.4, x equal to 0.5, 0.6 and so on, you can go here and look what is the value here and that has a huge implication by the way this lattice constant ok; so, similarly for effective mass. So, you can do it you know to a large extent.

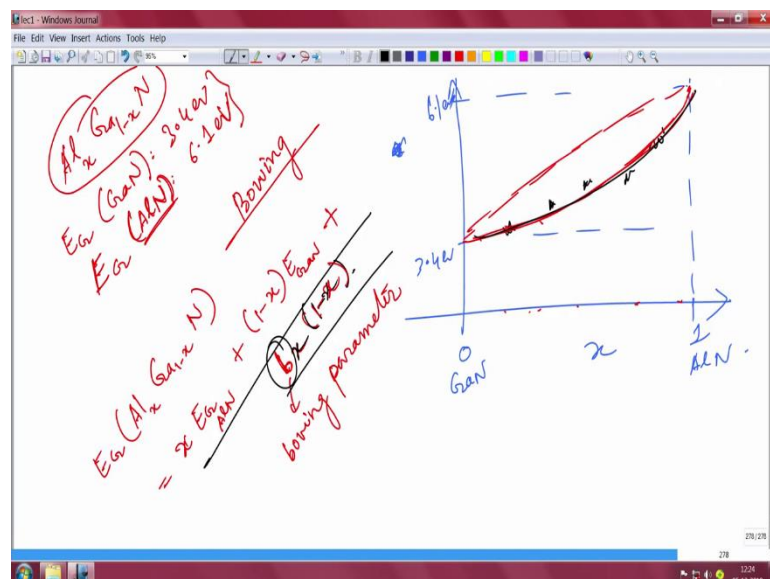
So, essentially it is a linear extrapolation between this and that is what Vegard's law says. So, it is very easy Vegard's law is very easy. However, your band gap typically will not follow a direct linear relation.

(Refer Slide Time: 05:23)



A band gap if you remember in the plot that I have drawn few slides back I did not this is the band gap. I did not draw it very linearly. A linear plot would have been like this right, but it will slightly be bent sometimes. In Aluminium Gallium Arsenide it may not be. So, much band, but in thing is that Aluminium Gallium Nitride for example, there is a lot of bending lot of bending huge number.

(Refer Slide Time: 05:44)



So, for example, I take a different material. For example, I take  $Al_xGa_{1-x}N$ , this is AlGaN, Aluminium Gallium Nitride and the band gap of Gallium Nitride is 3.4 e v; this is

the wide band gap material very wide band gap and you will be surprised actually. The band gap of Aluminium Nitride is even much larger; this is around 6.1 electron volt this is almost like insulator. It is insulator you can say, but you can actually dope Aluminium Nitride n type and that is why you sort of call it you can also merely dope it p type, but you can dope it n type definitely and. So, you can call it semiconductor because you are able to tune the conductivity ok.

So, you know your band gap of Aluminium Nitride this and band gap of Gallium Nitride is this. So, a band gap of Aluminium Gallium Nitride has to be between this, but it so, turns out that it will not be linear. So, what I mean to say is that if I plot band gap here and if I plot x here, so, x equal to 0 will correspond to Gallium Nitride and x equal to 1 will correspond to Aluminium Nitride. So, the band gap of Gallium Nitride is 3.4 e v and band gap of Aluminium Nitride is 6.1ev ok. It will not go linearly like this that is not going to happen.

So Vegard's law actually [FL] it has to you have to you have to modify the Vegard's law. It will go something like this oh sorry it will go something like this. There is the curve here there is the curve here and that is called the bowing, the bowing bow. It is like a bow right. It is a bowing and there is a bowing parameter that is why. So, the band gap and this is true for many compound semiconductor by the way. I am just giving an example of Aluminium Gallium Nitride, but band gap typically has something called bowing parameter.

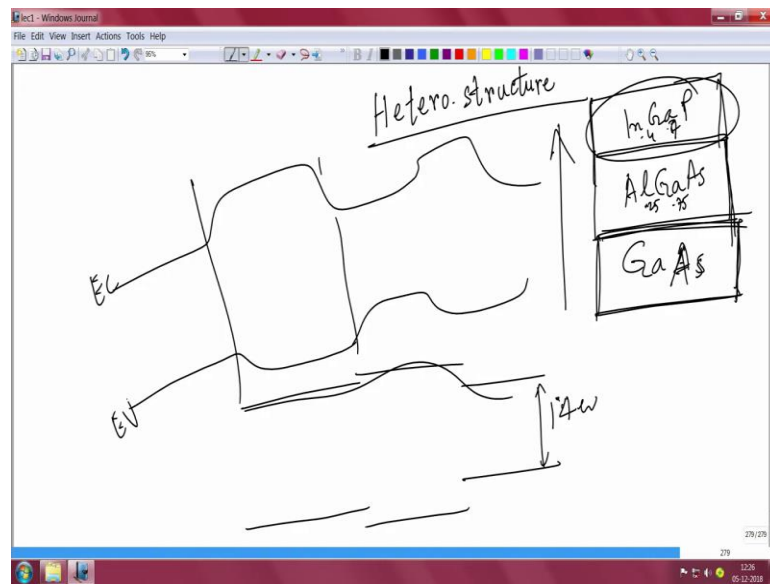
So, what happens is that the band gap of Aluminium Gallium 1 minus x Nitride will be x times the band gap of Aluminium Nitride you are right plus 1 minus x times the band gap of Gallium Nitride, but there is a bowing parameter you know if this is the equation and you will get something like this ok; so, so straight line there; is a bowing parameter here. So, essentially what will happen is that you have to plus some bowing parameter b x into 1 minus x that gives a non-linearity. This b is called the bowing parameter bowing parameter.

$$E_G(\text{Al}_x\text{Ga}_{1-x}\text{N}) = xE_{G_{\text{AlN}}} + (1 - x)E_{G_{\text{GaN}}} + bx(1 - x)$$

And this b is experimentally determined, you cannot do otherwise you just experimentally determined. you grow Aluminium Gallium Nitride have different composition 10 percent, 20, 40, 50, 60 and you measure them the band gap experimentally optical whatever and

then you have this you can do this experimental data fitting you know like this and then you do this plot and you get this bowing parameter experimentally ok. So, this  $x$  into  $x$  minus 1 minus 1 minus  $x$  bowing parameter comes here. So, this is called bowing parameter and this is important in many compound semiconductor band gap InGaN, InGaS and so on. This bowing parameter comes ok. So, that is Vegard's law [FL]. So, if you do not know the values of something, you can always use Vegard's law ok.

(Refer Slide Time: 08:57)



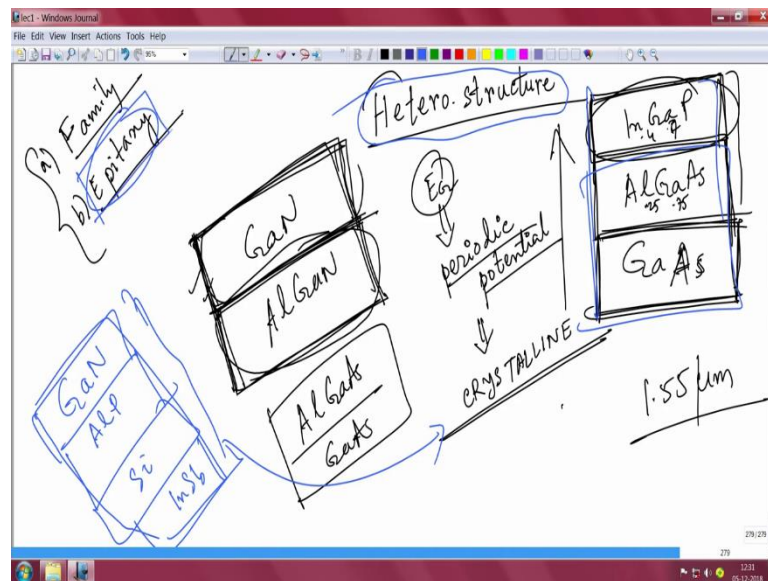
Now, one of the unique things that compound semiconductor allows which Silicon cannot do is doing something called hetero structures ok. Epitaxy will come between the hetero structure only. Hetero structure, it means there are 2 dissimilar materials that you are combining. So, suppose you have a layer of Gallium Arsenide when I say layer I am talking about a bulk material. It is not a single atomic layer, it is a thick crystal maybe it is a wafer it can be few hundred micron few hundred nanometer thick, its Gallium Arsenide ok.

On top of that you can make an Aluminium Arsenide, you can grow it is that is called epitaxy I will come to that. You can make this structure or even you can make a structure is up to you. You can make, but it is not always random ok. You can make Aluminium Gallium Arsenide and maybe this is 25 percent, this is 75 percent whatever right anything; Aluminium Gallium Arsenide you made. May be on top of that you want to make an Indium Gallium Phosphide may be Indium 40 percent Gallium, 70 percent and so on right, you can make the structures.

So, if I look at the band diagram along this direction you have you know Gallium Arsenide which has a band gap of 1.4eV then you have Aluminium Gallium Arsenide whose band gap will be slightly more than Gallium Arsenide because it is Aluminium Arsenide is 2.2. So, this will be slightly larger band gap like this right. Then Indium Gallium Phosphide might have a smaller slightly smaller band gap, may be even slightly small. You can tune of course, depends on Indium. So, you see your band diagram actually changing. So, you can have different kinds of band diagram like this right, different band diagrams can be done sorry.

You know different band diagrams can be done depends on the; this is conduction band for example, this is valance band. This kind of things are not possible in Silicon [FL] these are these kind of things are not possible with Silicon.

(Refer Slide Time: 10:53)



And hetero structures is basically the structure of this dissimilar materials that your piling up, that you are actually growing on stack one top of another. This is hetero structure and it you can make the variety of devices. Your semiconductor laser is based on similar hetero structures, not exactly this hetero structure, sort of hetero structure ok. Your white light LED, your RF transistors if many of these devices that you are looking at in your real time your mid diode detectors your 1.55 micron lasers and detectors that you are using for optical fibre communication; all these are actually made on hetero structures.

They are used on hetero structures like LEDs and all that. They all use hetero structures of different kinds of hetero structures, these are basically stacks or structures of dissimilar material. Of course, there are many rules that you have to follow. You cannot physically practically speaking you cannot randomly grow or get materials on top of another material just like that for. These are the hetero structures by the way. So, remember that right.

So, if I have a material of Gallium Arsenide I cannot arbitrarily put Gallium Nitride here that will not work. What do I mean by not work? When I say it will not work it means you cannot deposit Gallium Nitride and Gallium Arsenide such that both of these are crystalline. You see a semiconductor band diagram semiconductor, band structure semiconductor band gap and all the device physics your drift diffusions scattering everything is dependent on band gap band structure.

And everything comes from periodic potential, if you recall periodic potential from very first lectures k space, E-K diagram. And this needs a crystalline material. If you do not have a crystalline material if you have a polycrystalline or an amorphous material you do not have a periodic potential, you cannot define a band gap. Your all the analysis will breakdown ok. So, for a device to work you need everything crystalline. When I say crystalline you understand what is crystalline right.

You have the order the long range order your atoms are arranged in a definite fashion in all you know it will for a large for infinite long ok. No matter where you look you will always get the same arrangement of atoms the same spacing of atoms, they are not oriented grains there, it is repetitive the lattice is repetitive and it is a crystal structure ok.

So, you it is impossible to get Gallium Nitride which is crystalline on top of Gallium Arsenide just by depositing Gallium Nitride and Gallium Arsenide ok. So, you cannot arbitrarily have materials. You can have Gallium Nitride for example, on top of Aluminium Gallium Nitride. So, you see a trend you need to grow it on the same family of materials ok. The family of materials has to be same. Even then there are some very important conditions and boundaries conditions and stringent criteria. Even when you grow Gallium Nitride and Aluminium Gallium Nitride or you grow Aluminium Gallium Arsenide on Gallium Arsenide there are rules that you have to follow ok. Any



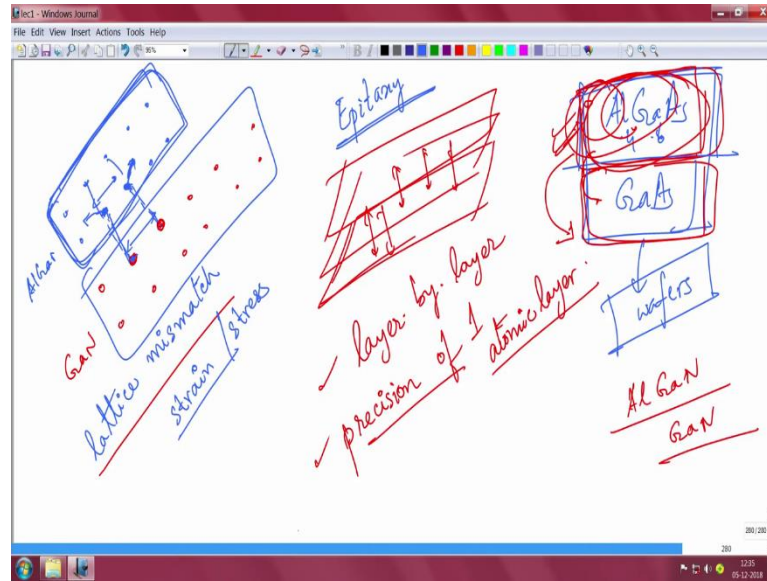
heterostructure for that matter; [FL] one thing is that it has to be within the same family of materials.

Now, growing dissimilar family of materials is possible, but that is special in some cases only. You cannot grow Gallium Arsenide and Gallium Nitride for example, and all these things right. And so, the thing and this growth of these materials that you are depositing this process is called epitaxy, I will come to that quickly ok. An epitaxy is there and essentially your hetero structure device depends on device performance and everything depends on whether you are able to grow or deposit this material whatever material as per your desire as per how you have planned that is why hetero structure is also about material science as much as about devices. If you do not have a materials understanding to a basic extent you will not be able to design devices.

Because I might arbitrarily say oh you know what I will put Gallium Nitride on top of you know Aluminium Phosphide on top of Silicon on top of you know some random thing like Indium antimonite this kind of structure cannot physically exist. I mean they can exist, but it will be amorphous, you cannot have this crystalline ok, it will not be crystalline ok. So, you need to have a materials basic materials understanding to allow you to think as to what kind of hetero structure and what kind of stacks are possible. So, that you can design and you know come up with device ideas new type of device ideas ok.

You cannot arbitrarily do this that's because this is limited by epitaxy. So, now, I hope you understand, what is hetero structure. Hetero structure essentially is you know you have stacking of different materials it. It can be 2 just 2 material 2 stack it can be 3 it can be multi it can be 100 who cares, it is hetero structure ok. There are different kinds of hetero structure by the way, the way the band gaps are aligned it will come in sometime later. But here I am talking about epitaxy. Epitaxy is basically you have to, when you want to grow a material on top of another material.

(Refer Slide Time: 16:00)



Say you want to grow Aluminium Gallium Arsenide and this can be say 40, 60 on top of you want to grow on top of Gallium Arsenide. So, Gallium Arsenide wafers are available you can buy Gallium Arsenide wafers commercially ok. So, you buy Gallium Arsenide wafer and you want to deposit Aluminium Gallium Arsenide crystalline that is a very advanced sophisticated costly expensive and time consuming process actually ok. It is not very easy. You have to do epitaxy for that.

What is epitaxy? Epitaxy is essentially the process, the physics or material science of growing a material for example, this material on top of another material such that this material, the crystal structure of this Aluminium Gallium Arsenide mimics the crystal structure of the layer below of the substrate below. So, Aluminium Gallium Arsenide cannot have an arbitrary crystal structure. It has to mimic the crystal structure of the material below that is called epitaxy. And typically it is done by couple of techniques in which you can deposit one layer by one layer of Aluminium Gallium Arsenide. One layer, the next layer then next layer of course, they have a vertical strong vertical bonding these are not like 2D materials where the vertical bonding is weak.

These are strong bonded materials and you will have grow them layer by layer. You grow them layer by layer which means you have which means you have you need to have a precision. You have when you deposit the material, when you deposit the material you have to deposit it has precision of 1 atomic layer which is very insane right. At the

precision of one atomic layer you have to deposit this material. In such a way that the materials that is growing or depositing should be mimicking the crystal structure of the material below which means if Gallium Arsenide has a lattice constant of you know whatever the lattice constant Aluminium Arsenide, Aluminium Gallium Arsenide might have a smaller lattice constant, slightly smaller lattice constant.

Their spacing might be small slightly smaller than this. This is called lattice mismatch; this is called lattice mismatch. When you grow Aluminium Arsenide on top of Gallium Arsenide, Aluminium Gallium Arsenide on top of Gallium Arsenide right; this is Gallium Arsenide for example, then you have a slight difference in the lattice it is called lattice mismatch. Aluminium Gallium Arsenide, Gallium Arsenide have very negligible lattice mismatch. They are almost lattice matched. So, that is not a good example ok. They are called lattice matched assume like Aluminium Gallium Arsenide and Gallium Arsenide have almost the same lattice constant.

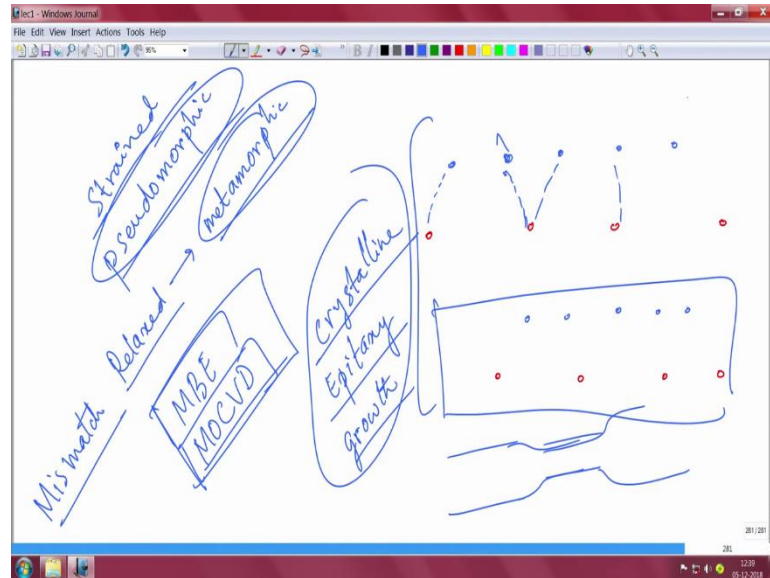
So, they are called almost lattice matched. Let us take an example of something else say Aluminium Gallium Nitride and Gallium Nitride ok. So, if this is Gallium Nitride and this is Aluminium Gallium Nitride, it has a smaller lattice constant of Gallium Nitride. When I say you have to do epitaxy, you want to actually mimic you want AlGa<sub>N</sub>, this layer to mimic the crystal structure below which means when you grow one on top of the another, this lattice constant that you have here has to mimic or match the lattice constant here which means this atom and this atom will be pull apart little bit so that they can be one on one on top of them right.

This is called there is a strain that is developing a strain or a stress is developing in the Aluminium Gallium Nitride layer because the spacing here is slightly slower lower and the spacing is slightly bigger. When you are growing one layer of Aluminium Gallium Nitride on top of Gallium Nitride this lattice spacing has to match this lattice spacing. So, [FL] you are pulling this Ga<sub>N</sub>, Ga<sub>N</sub> will basically pull this atom slightly away.

So, that the spacing increases and you are able to deposit them one on one. This is called strain Aluminium Gallium Nitride, but if you keep growing this Aluminium Gallium Nitride strain on top of this will become very strained and stress. So, the energy will increase even. So, it will try to relax. It will try to relax. If you grow a sufficiently thick AlGa<sub>N</sub> it will try to relax because you are straining it know you are straining you have you

have this is epitaxy and of course, and you have to make sure that this is crystalline that is why it is very important.

(Refer Slide Time: 20:28)



You know you have this this this this for example, that is the Gallium Nitride spacing I am talking about. An Aluminium Nitride spacing is suppose this this this this this like that right. So, this has to strain. So, that this can be mimic this can form you know one on one the bonding can be formed right. This can form a bonding here right. You have to it is very difficult actually that you have to strain up. This Aluminium Gallium Nitride layer on top gets strained, but it can only accommodate the strain up to sometime. After a few layers or few thickness this Aluminium Nitride will Gallium Nitride become so much of strain energy that it will relax. Once it relax it will go back to it is original you know it will go back to it is original spacing ok. Once it is strain when it is strained it is strain to Gallium Nitride.

So, what will happen is that you will have Gallium Nitride like this ok, your Aluminium Gallium Nitride also is one on one you will have, but that is highly strained. This layer is highly strained because that is not it is natural spacing. If you grow thick sufficiently thick it will basically relax, it will basically give away and then it will come back to it is original position ok; it will come back to it is original position like the smaller spacing. So, when the top layer is strained, you call it that layer you call it pseudomorphic pseudomorphic.

You can have this Indium Gallium Arsenide on Gallium Phosphide and all the things which are you know you can have certain things which are pseudomorphic.

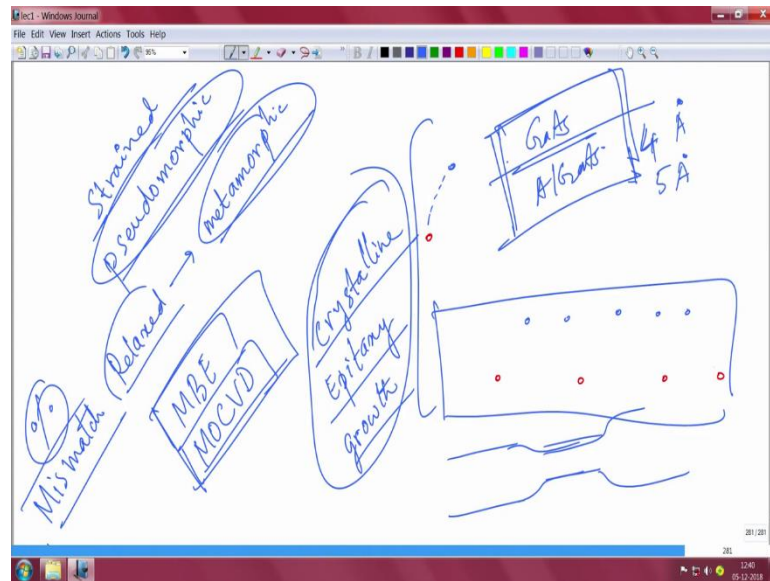
And if it is relaxed; that means, it has got an enough thickness and so the material is now unable to get strained to the layer below. It will relax. It is called metamorphic ok. Even otherwise, even otherwise when it relaxes it does not mean that the crystal structure is violated, it is just relaxed. Everything will mimic the structure it is growing crystalline only ok, it is growing crystalline only and that's why that is called you call epitaxy. You have to and we do not use the term deposit so much. We call it epitaxy or growth you can call it growth ok, it is a terminology difference that is growth.

So, you have a substrate, you have a background layer essentially it is called substrate on which you are doing this. Here you are using GaN for example, ok. Similarly, you can have Gallium Phosphide or you know whatever substrate on top of that you might be growing Indium Gallium Arsenide or Indium Gallium Phosphide and so on. This epitaxy or the growth will ensure that your growing crystalline material and 2 important techniques are MBE called Molecular Beam Epitaxy and MOCVD which is Metal Organic Chemical Vapor Deposition.

These are techniques that are used to grow these materials layer by layer in a crystalline fashion. It is a very advanced and sophisticated techniques that are precision of one atomic layer. You can do one atomic layer by one atomic layer deposition and that is why you can essentially change the structure very abruptly from one layer to another layer and you can get this band diagrams which are you know unique and these kind of enables the band diagrams and band structure which are not possible otherwise that allows you to have different functionalities that is what is you should remember.

So, this MBE and MOCVD are techniques that can do this epitaxy and crystalline growth. It can eventually be pseudomorphic or it can be metamorphic and these are dependent on the lattice mismatch. What is the lattice mismatch? For example, if one layer has a lattice constant of you know I am talking about just an example.

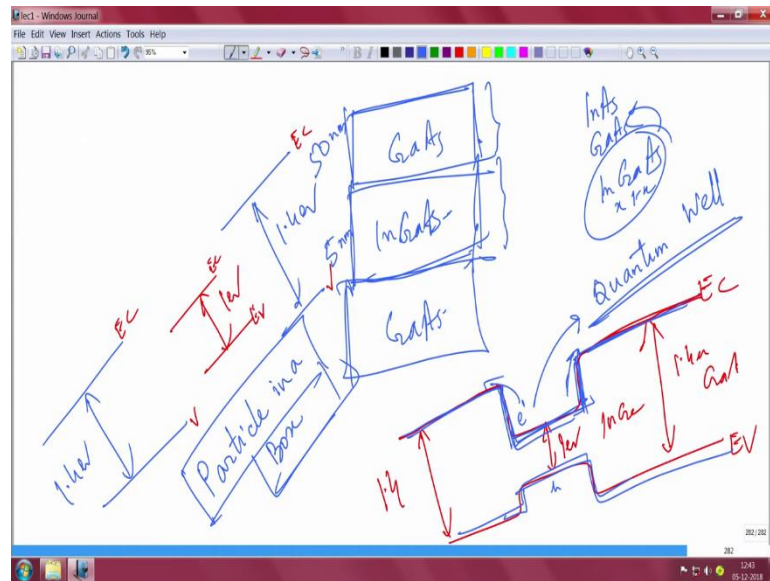
(Refer Slide Time: 24:01)



If the the bottom layer has a lattice constant of 5 Angstrom and the top layer that you are growing has a lattice constant of 4.9 Angstrom and it is a very small lattice mismatch, you would be able to grow little thicker until the material relaxes. If on the other hand the lattice mis constant is 4 Angstrom on top and 5 Angstrom on bottom then you will be getting so much of strain that in a few layers it will basically relax [FL]. So, lattice mismatch the degree the percentage of lattice mismatch dictates how much you can grow pseudomorphic or strain ok.

Even then either a pseudomorphic or metamorphic you will be able to grow crystalline materials and only when you grow crystalline materials you will be able to get these hetero structure of Gallium Arsenide, Aluminium Gallium Arsenide and so on. So, this structures you cannot arbitrarily assume and then you can that you can grow and you can do. These have a material limitations and this have a you know from the materials point of view you should be able to justify where are such a structure is possible ok. One such a structure is possible then you can do fanciful things ok. One such a structure is possible then you can do many things.

(Refer Slide Time: 25:04)



For example, you might take a layer of say for example, Indium Arsenide has a lower band gap than Gallium Arsenide. So, if you take Indium Gallium Arsenide you so, whatever  $x$ ,  $1 - x$ , the band gap will be lower than Gallium Arsenide ok. So, suppose I have a layer of Gallium Arsenide on top of say Indium Gallium Arsenide thin layer and then there is also a Gallium Arsenide layer below ok. And what are the thicknesses of this epitaxial layers? They can be as low as 1 to 2 nanometer, 2, 2 nanometer sorry not micron.

Even you can grow one nanometer using MBE one to 2 nanometer. Of course, you can grow 1 nanometer using MBE or you can sub one nanometer by the way. And you can be few times of nanometer; 20, 30 nanometer, you can grow few hundreds of nanometer 100 to 500 nanometer, you can even grow micron. Anyways typically this can be thin. So, when I am talking about the structure, suppose I am talking about a very small structure suppose this is only 5 nanometer and this is suppose 50 nanometer, this is substrates it can be much thicker also does not matter now, because Indium Gallium Arsenide has a smaller band gap than Gallium Arsenide.

So, if I draw the band diagram it will look like Gallium Arsenide is this say 1.4 eV. There is also Gallium Arsenide on the other side 1.4 eV. In between I have Indium Arsenide this is by the way conduction band, conduction band, conduction band this is valence band, valence band, valence band. In between you have Indium or Gallium Arsenide whose band gap is small. So, the band gap here might be say 1 eV. If you join them together you will

have a band diagram like this. This is conduction band, this is valence band, this is conduction band, this is valence band this is 1.4 eV of Gallium Arsenide.

This is again 1.4 eV of Gallium Arsenide in between you have say 1 eV of Indium Gallium Arsenide. You will see the structure where you have a this is conduction band. So, this is the potential. You have a potential profile like this you have potential profile like this. Do you know what it looks like? It looks like a quantum well. If you have probably read about your quantum confinement, you have read about in your high school physics in your 10 plus 2 physics you might have read about particle in a box in of physics in a particle in a box. This is the practical realization of a particle in a box. If you put an electron here it is like a box. There is a there is a potential profile on either side that will not allow the electron to escape.

It is not infinitely higher potential that is ok, but it will not be able to escape outside right or a hole here is confined here right. And electron and hole will not be able to escape outside, it is like a well. It is like particle in a box, a quantum well. And these are used not only in optical devices like LEDs and laser diodes, this also used in transistors, high speed transistors we used them. So, particle in a box that you have learnt in your high school or 10 plus 2 physics can be practically realized in hetero structure only ok. So, this hetero structure allows you to get that particle in a box out of a configuration ok. So, this is the beautiful thing actually.

So, let us end the class here today. We have had sufficient orientation and knowledge of compound semiconductor. So, we have talked about Vegard's law, epitaxy, why you need epitaxy that you have to mimic the crystal structure below, lattice mismatch is a big issue and you have to make sure that you cannot arbitrarily it come up with device ideas, but putting any arbitrary material on any arbitrary substrate. It has to follow lattice mismatch and this crystalline it has to be crystalline. So, you have to do epitaxy and the material science will put a restriction on what kind of things you can do. Once you can do those things you can also apply Vegard's law to extrapolate the alloy composition and other things.

The band gap of course, does not follow the Vegard's law. Exactly you need to have a non-linear factor that is the bowing parameter and I told you things like particle in a box of quantum well can be realized in a proper hetero structure ok. It can be realized in a



proper hetero structure and your material science will always dictate: what is the realistic estimate of your device you are making you know. It is not like just Silicon that you have a Silicon material and you can do things, doping is another thing by the way that I did not discuss here.

So, the next class I will tell you about the different kinds of hetero structures. I told you about the different materials; Arsenide, Phosphide, antimonite oxide, Nitride. I am talking about different classes of hetero structure. When you have 2 structures hetero structures how do they align in their band diagram that is what I am talking about ok. We will talk about hetero structure alignments and we will talk about hetero structure band diagrams in the next class and we will start also talk a talk about devices from there after ok.

So, thanks for a time. We will meet you soon.