VLSI Technology

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Lecture - 9
Epitaxy III –Doping during Epitaxy

In the previous class, we were talking about limitation in the epitaxial growth. That limitation comes about when the epitaxial layer gets inadvertently doped. In addition to the deliberate doping that you may want to introduce in the epitaxial layer, there is a possibility that the epitaxial layer can get inadvertently doped and that is called auto doping, auto doping or automatic doping.

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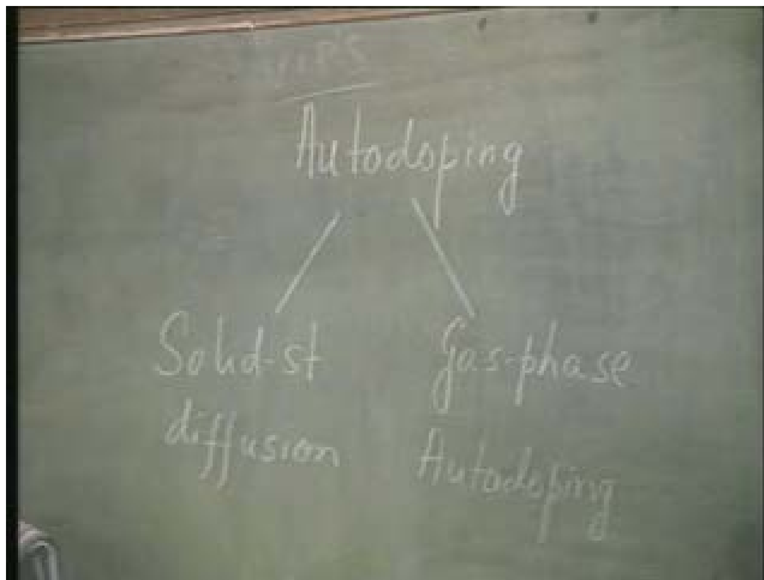

Now, there are two reasons for this inadvertent doping or auto doping. These two reasons are - one is due to solid state diffusion and the other is due to gas phase auto doping. What are these two things basically? See, before the epitaxial growth takes place the sample is being treated to high temperature. At that high temperature, it is possible for the dopants already present in the substrate to out diffuse and this will change the composition of the gas stream. The gas stream composition is controlled depending on the level of doping in the epitaxial layer that you want to grow. You want to put that

amount of boron or phosphorus or arsenic along with silicon, but the already present dopants in the substrate layer will out diffuse and modulate the composition of the gas stream, so that when the epitaxial layer is being grown, these dopants which were originally present in the substrate can now get back, reintroduced in the epitaxial layer, thereby the doping concentration of the epitaxial layer will change. It will not follow exactly the required doping level. For example, if my substrate is doped say, p-type and if I want to grow an n-type epitaxial layer near the interface, I may have a problem of having first a slightly p-type epitaxial layer growing and only then the n-type layer growth. We will explore these possibilities later.

The other thing is of course, solid state diffusion. That is as the epitaxial layer is being grown, if the doping concentration of the substrate and the epitaxial layer they are widely different, most cases it is likely to be, then there will be a diffusion from the higher concentration side to the lower concentration side and that will also modulate the doping concentration, the deliberate doping concentration of your epitaxial layer. So, both these effects will cause a change in the doping concentration of the epitaxial layer and therefore it will put a limit to how thin a layer you can grow actually with proper control of doping, because you understand there is going to be a transition layer. Between the bulk and the epitaxial layer, there is going to be a transition layer which will be determined by this effects of auto doping.

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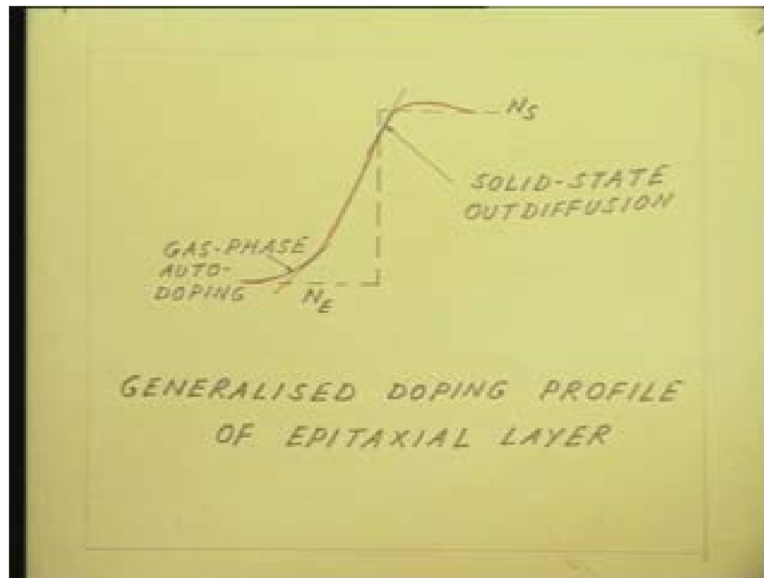

If you look at the first card we have here today, the dotted line signifies the ideal abrupt junction between the epitaxial and the bulk region. N E is the epitaxial layer doping concentration, N S is the substrate doping concentration. Let us assume that they are both same type, only the doping concentrations are different. In this particular case, I have assumed that the substrate is doped highly and the epitaxial layer is doped to a very low extent, it is almost intrinsic. The situation is analogous to the bipolar junction transistor fabrication, where you have an n plus layer diffused in the p region. So, this is actually signifying to the n plus layer diffused high doping concentration and on top of that you are trying to grow an epitaxial region of moderate doping concentration.

So, ideally speaking, this should be my abrupt junction between the epitaxial and the bulk region, the abrupt transition. In practice, however it is never like that and what you have is this red curve and this is a generalized doping profile. I call it a generalized doping profile. That is here both the effects of auto doping can be seen. That is the solid state diffusion as well as the gas phase auto doping. It is very easy for you to understand that the solid state out diffusion will be predominant actually at the interface region. This is the high concentration side, this is the low concentration side. Therefore the dopants will try to diffuse from the bulk region into the epitaxial region and therefore the doping

concentration at the epitaxial region here it will be quite high. It will not actually abruptly fall down to the level you desire. So, this portion is actually dominated by the solid state out diffusion and can be modeled by an exponential relationship.

On the other hand, the effect of the gas phase auto doping is seen as this tail. You see, if only the effect of the solid state out diffusion was present, then it would have fallen down exponentially like this. But, you find an extended tail, extending well into the epitaxial region, well away from the interface. You see, this is further away from the interface, where the effect of solid state out diffusion is minimum. This effect is due to the gas phase auto doping. That is even before the epitaxial layer growth, a lot of n-type dopant has evaporated from the substrate. It has gone and modified the gas stream and therefore the doping concentration of the epitaxial layer is affected even further off from the interface. So, this is how basically the two effects of auto doping is manifested.

Now in this particular example, I have chosen the epitaxial layer and the substrate to be of the same type. Let us say the epitaxial layer is n-type, the substrate region is n plus. So, what I have is just this extended transition region and that actually determines how thin an epitaxial layer I can grow with the proper N E doping concentration. You see, from this figure it is obvious that up to this, is my transition layer and only after that I have the epitaxial region, with the proper doping concentration. The situation can be even more serious, if the two regions are of opposite dopant type. That is to say if I have a substrate and then epitaxial layer, one is p-type and the other is n-type.

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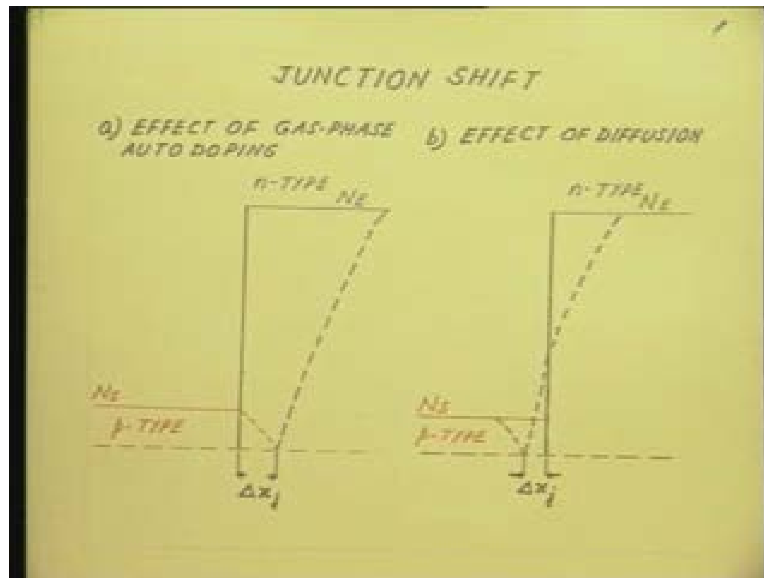

In that case, what is going to happen is called a junction shift. That is the metallurgical junction and the electrical junction will not be at the same position. By metallurgical junction what do I mean? Suppose my substrate N S that is p-type and my epitaxial region N E is n-type, then the metallurgical junction is present here, this black line that is my junction point. It should be the metallurgical junction at the, exactly at the transition point. But, because of the effects of auto doping the junction can get shifted either way.

The figures I have here, they are not actual figures, you know. They are actually the results of computer simulation and in these two figures, we have tried to separate out the regions of auto doping. That is the first figure, if you look at that, this is the effect of gas phase auto doping. Let us look at this. What is happening? I have the substrate with a doping concentration N S. It is a p-type substrate. Gas phase auto doping is going, is that effect that is before the epitaxial layer growth, when the substrate is being heat treated, some of this p-type dopant will escape. It will evaporate and it will modulate the gas stream. So, this is what is happening.

Some of the p-type layer is escaping and getting reintroduced into the epitaxial region. This is the red dotted line showing that the p-type dopant is reintroduced in the epitaxial

region and that is why, even though I wanted to grow an n-type epitaxial region, near the junction I find that the junction has actually got shifted into the epitaxial region. The p-type region has actually extended inside the epitaxial region in figure a. You notice that the p-type region, this red region that has actually extended into the epitaxial region and therefore the junction is now here. The delta x j denotes the amount of the shift and the junction has got shifted into, inside the epitaxial region. So, this is the effect of gas phase auto doping.

Now look at figure b. This is the effect of solid state diffusion. So, the diffusion means there will be movement of dopant from higher concentration side to the lower concentration side. Now, p-type dopants are present with a higher concentration in the substrate region, so it will try to move into the epitaxial region and n-type dopant is present at a higher concentration in the epitaxial region, therefore it will try to move inside the substrate. There will be intermixing and in this particular case, since I have shown that the n-type doping concentration is very high, you can see that the junction has actually moved inside the substrate region, because there is intermixing. p-type dopant is trying to move inside, n-type dopant is also trying to move inside the substrate. So, the junction shift is at, is also here; it is also present here. But, notice that the junction has got shifted into the substrate, unlike in the previous case.

These are, as I said, the results of computer simulation in which we have tried to isolate one effect and study the effect of only that. That is either gas phase auto doping or solid state diffusion. In a practical situation you can understand that both these effects will be present. So, the junction shift will be dependant upon their relative dominants, which way the junction shifts. But, that is a very important problem. That is the junction, the electronic junction may become, may be shifted from the metallurgical junction. So, these are the effects of auto doping. In this particular case of course, we have considered only vertical auto doping. That is the region immediately above the substrate is getting doped.

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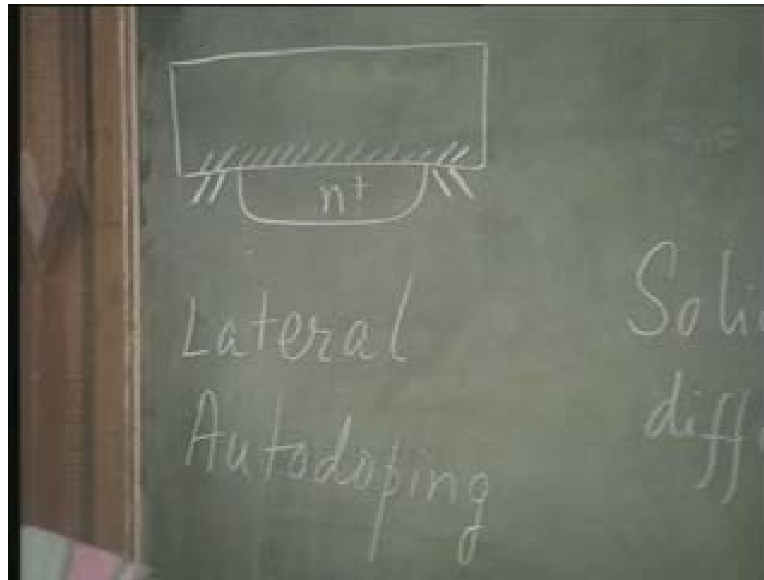

For example, if I have an n plus region and I grow an epitaxial region, then this is the portion where the effect of auto doping is going to be felt. The shaded region is the region where the effect of auto doping is going to be felt. This is vertical auto doping, but actually the effect will also be felt to a region adjacent to the substrate. In fact, all over here the doping concentration will get modulated. This is called lateral auto doping. Lateral auto doping is almost exclusively due to gas phase auto doping. The solid state out diffusion plays very little role. Here, it is almost exclusively the effect of gas phase auto doping.

Before the epitaxial layer is grown, when the substrate was being subjected to heat treatment, the dopants have diffused out and they can be reintroduced all over this place and from there can get reintroduced into the epitaxial region. So, these are the effects of auto doping and lateral auto doping is something one should be very careful about, because it may cause us an electrical short, an electrical short between two adjacent devices. See, this is a n plus region. The next n plus region may be further off here, but because of the lateral auto doping all the n plus regions can get connected. So, unless you take proper precaution to isolate between the two n plus regions, with a boron diffusion

something like that, then there is a possibility of getting an electrical short due to lateral auto doping.

Now, there is another interesting aspect associated with epitaxy.

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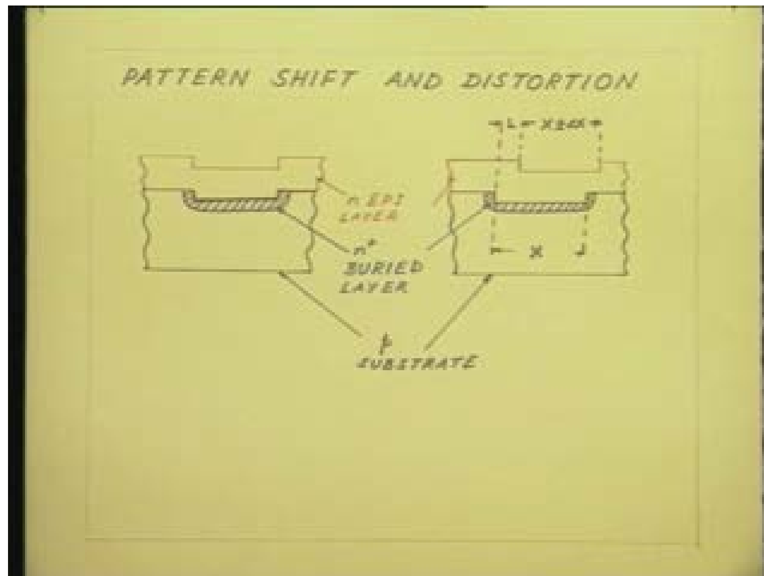

You see, normally I would assume that when there is an indentation on the surface that is a step on the surface and if I am growing an epitaxial layer that same step will be transformed into the epitaxial region also. That is what I expect is something like this. See, what I have drawn here is simply the process steps involved in a bipolar junction transistor fabrication. I started out with the p-type substrate, then I have made the n plus buried layer. Then, I have stripped the oxide and in doing so, I have created a step here. The step is visible to all of you, you can see the step, right. So, now if I grow an epitaxial layer, I would expect it to be aligned with this step, so that the epitaxial layer should also be formed like this, because everywhere I expect that, ok, I am growing say, 5 micron from the substrate. So, this height should be 5 micron. I should expect it to be properly aligned.

Now, this proper alignment is going to play a very important role in my further processing, because this step, once the epitaxial layer is formed you see, I have no way of knowing where the underlined buried layer is. So, this step is only going to tell me where the underlying buried layer is, so that I can properly put my base mask and the emitter mask, so that the transistor is fabricated in this active region and not this way or that way. So, this is what I want. But, unfortunately what in most cases I am going to get is this figure. Here you see that the step is not aligned. It has got shifted. Also, the size of this, the buried layer mask, the size of this may not be the same. Like here, I have shown that this was x, the length of the buried layer diffusion, that was x and the length of this step may be x plus or minus delta x. So, the pattern on the substrate may get shifted by an amount l and it can also get distorted by an amount plus minus delta x. This is called pattern shift and pattern distortion.

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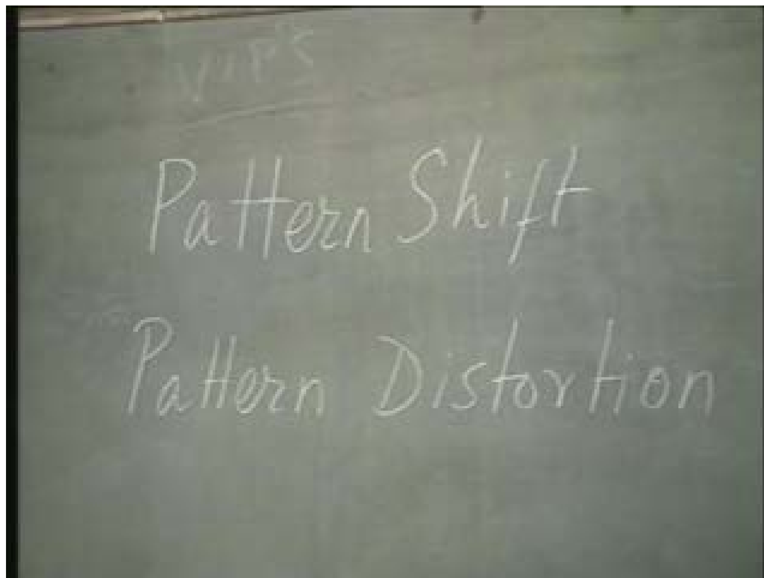

Now the question is, why should this happen? Why should this pattern shift and distortion take place? It takes place because, as you already know, that the crystal growth is extremely dependant on the crystal orientation. What is epitaxy after all? It is growth of a crystalline layer.

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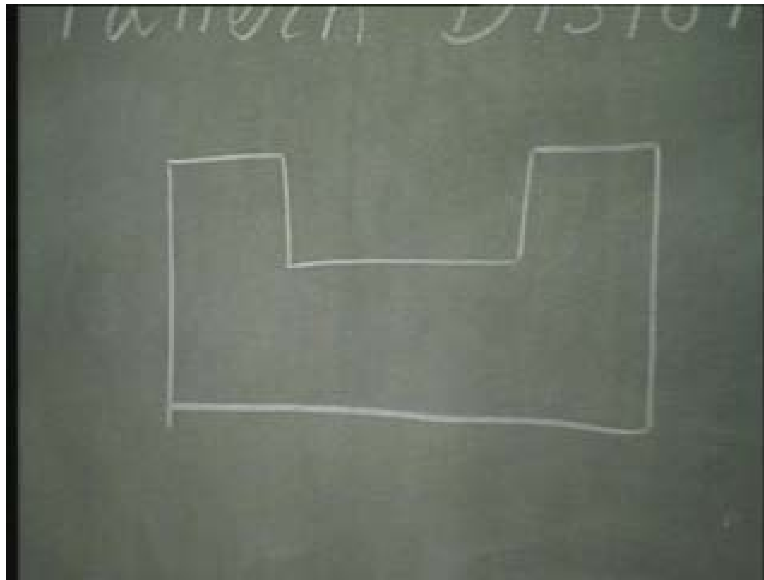

So, whenever there is a step on the surface, whenever there is a step on the surface, you are exposing a number of crystal planes at this step. So, the surface may be 1 0 0 or 1 1 1 or whatever. But whenever there is a step, a number of crystal planes are going to be exposed and when epitaxial growth is taking place, it is taking place anisotropically. That is the growth rate is going to be dependant on the crystal orientation. That is why you do not have uniform growth rate. If you had uniform growth rate, this step will get translated into the epitaxial layer, no problem. But because this growth rate is not isotropic, it is anisotropic, you get all these problems of pattern shifting and pattern distortion.

How does one minimize this pattern shift? See, minimizing this pattern shift and distortion is going to be quite a crucial point, because this will tell on my further processing. This will determine my, the alignment of my further processing steps. So, a lot of research has gone in, to connect the pattern shift and distortion with the epitaxial growth parameters and these are some of the findings. That is pattern shift is minimized at high deposition temperature. Why should it be so? Remember, high deposition temperature means the mobility, the surface mobility is high. Whenever the surface mobility is high, the growth tends to be isotropic. That is on all the phases, the incoming molecules, they have enough time to orient themselves. Therefore, on all the crystal

planes the growth rate tends to be same. So, if you have high deposition temperature, pattern shift will be minimized.

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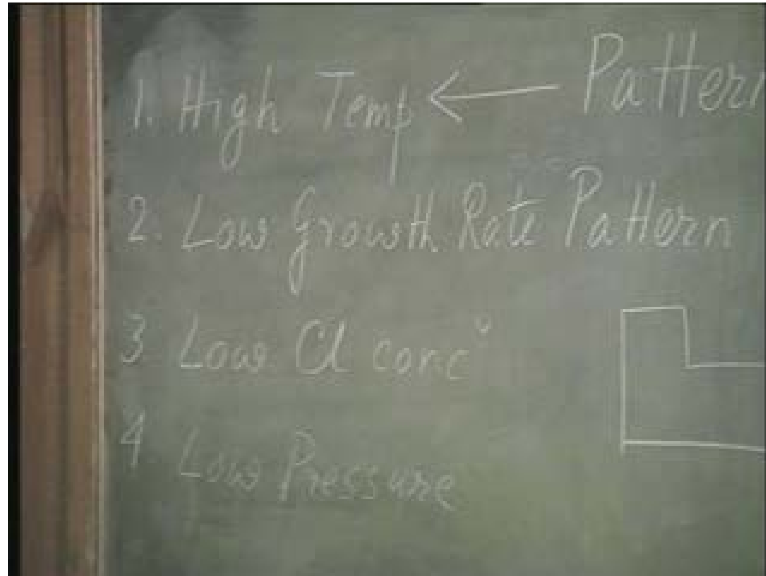

Also, if I operate in the region of low growth rate, remember, last class we showed a graph that is the silicon tetra chloride concentration, as you increase the concentration of silicon tetrachloride, the growth rate increases and if the growth rate is too high, you do not want that, because you get poly crystalline layer. So, you see, again this sort of follows as a corollary. If you have a reduced growth rate that means the crystal quality is better, the layer quality is better, so, again the growth tends to be isotropic. So, the second point is you should operate in a low growth rate region and it is also seen that the amount of chlorine, the more the amount of chlorine you have, the more is the pattern shift. Again, it can be related. You see, the more amount of chlorine you have, the growth rate tends to be high. Therefore, anisotropy tends to be more. Therefore, reduce the amount of chlorine and you are going to have lesser problem of pattern shift.

A corollary of this third point is that, with lower pressure, the pattern shift will be less. If you have lower pressure you can vent out the chlorine or the HCl faster. Therefore the pattern shift will be less. In addition to this, how the substrate is oriented during epitaxial

growth also seems to play a major role. That is it is found that if you have an 1 0 0 substrate, keep the substrate perfectly oriented to its crystal plane, place it perfectly oriented. That is the gas flow should come perfectly along the sample surface, should be perfectly oriented. On the other hand, if you have an 1 1 1 wafer, then misorient it slightly, misorient it by 2 degrees or 4 degrees. That has been seen to minimize the pattern shift problem. So, this is universally done. If you have 1 0 0 samples, keep it perfectly oriented; if you have 1 1 1 sample misorient it by a couple of degrees, 2 degrees to 4 degrees in order to minimize the pattern shift.

Let me just mention one thing that which you can see as a corollary of point number 3, remember, silicon epitaxy can be carried out by using two routes. One is the chlorosilane route, the other is the silane route. So, as a corollary of point number 3, if you are using silane route, then the problem of pattern shift should be minimized. It should be very low, because you have no chlorine. It is absolutely free of chlorine, but even though silane does not give you a problem of pattern shift, the pattern distortion problem is present there. So, one aspect is that we have to minimize the pattern shift by carefully controlling the process parameters. The other aspect is in spite of all these precautions, if you have pattern shift and pattern distortion, then your subsequent masking steps should take care of this defect. That is you must be able to identify how much pattern shift there will be.

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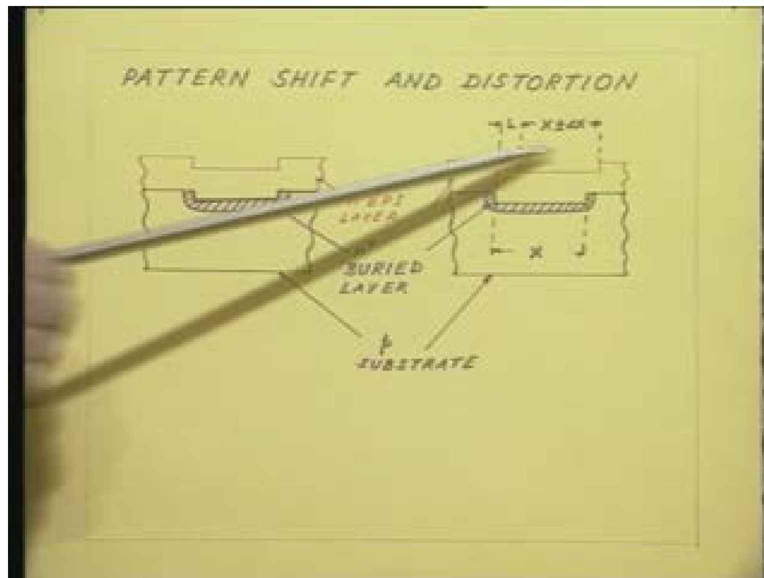

So, even if the step gets, if the step gets shifted by an amount l in this direction, then your next mask should actually be shifted in a direction minus l, in order to take care of the alignment problem.

Now that you have grown an epitaxial layer, next point is how good is its crystal quality? Let me tell you something. The epitaxial layer is only as good as the bulk crystal is, because you are growing something on top of an already existing layer and as I said, the term epitaxy itself means arranged upon. The crystalline quality of the epitaxial layer comes about because of the underlying crystalline symmetry of the bulk layer. So, unless the bulk layer shows a very good crystalline symmetry, you cannot expect anything to be arranged upon that. So, the quality of an epitaxial layer is critically dependent on the quality of the bulk layer. It is only as good as the bulk layer and very often the quality is really inferior to the bulk crystal. That is because, the bulk crystal defects will get translated into the epitaxial layer.

During the epitaxy, some additional defects will come into the picture. Therefore, the final crystal quality is likely to be inferior to the bulk crystal quality.

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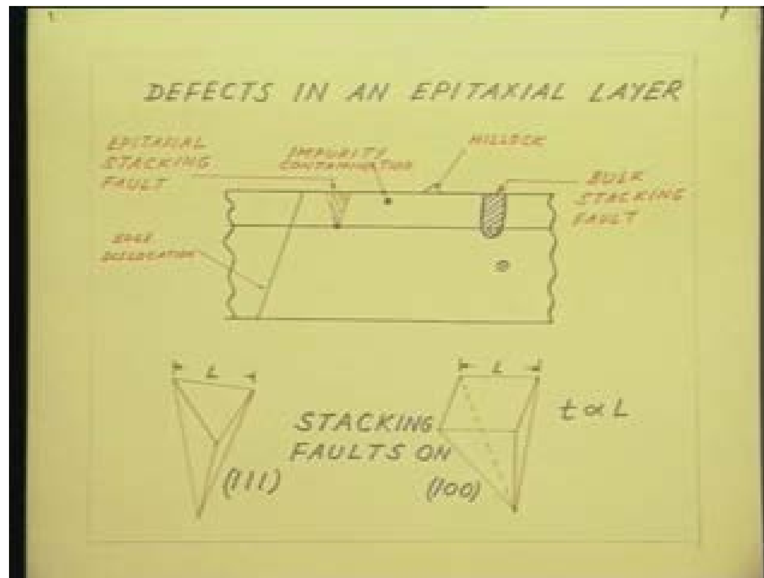

Now, here I have a schematic representation of some of the defects in the epitaxial region. First of all let us look at this line. By this line, I want to represent an edge dislocation. You know, an edge dislocation is an extra half plane of atoms which can be viewed in two dimension as an extra line. So, if this edge dislocation is present in the bulk crystal, as the epitaxial layer grows, this dislocation will simply carry on into the epitaxial region also; it will extend all the way into the epitaxial region. Second point is, if there is something on the surface, that something most often is a small patch of native oxide. Then, a stacking fault may originate from that and the stacking fault actually grows in size. As the epitaxial region grows, you see, the area of the stacking fault is growing in size. We will discuss more about the stacking fault in a few minutes.

The other point is during the epitaxial growth, you may introduce some contamination due to some impurity present in the gas stream or present in a reactor chamber, which is incorporated into the epitaxial layer. The other problem is the growth may not be uniform and you may have hillocks and if you have hillocks, a dent is also possible. You may have a hillock or a valley present in the epitaxial layer and finally, if there is a bulk stacking fault which is crossing the epitaxial region, then that will grow into the epitaxial region and form a layer of stacking fault. Of all these defects, the most important one is

the stacking fault. This is most commonly present. They are the most important type of defects associated with the epitaxial layer and they can be examined by etching the epitaxial surface in a selective etching technique.

After the growth of the epitaxial region, see, the usual practice is along with your processing wafers, you also put a dummy wafer for this characterization testing in the epitaxial reactor. So, on the dummy wafer you carry out some selective etching. If you carry out the selective etching, then these stacking faults can be viewed as small pits on the surface. The etching will take place in a preferential manner along around this stacking faults and we will see them as pits on the surface. Now, the funny thing is this. That if you have 1 1 1 surface, then this pit will be viewed as a triangle. See the top view of this. This is actually, what I have drawn here is a pyramid with a base, which is a triangle. So, when you are etching and you are viewing the surface from the top, then the top view will look like a triangle. So, you will find a triangular pit.

On the other hand, if the sample surface is 1 0 0, then we will find a rectangular or a square pit. You know why this is so? The answer lies in the crystal orientation itself, right. On 1 1 1, what I find is an equilateral triangle. Each side of the triangle is actually in 1 1 0 direction and on the 1 0 0 surface, what I find is a square or the rectangle, again with each side in the 1 1 0 mutually perpendicular direction and exposing the 1 1 1 faces in the bulk. That is what this signifies. As I told you that the most important reason for this stacking faults is the presence of small patches of native oxide on the surface.

See if you remember, in the silicon crystal, the silicon-silicon spacing was related to the lattice constant. The value is 2.35 Angstrom. On the other hand, the silicon-oxygen-silicon that spacing is 3.05 Angstrom. They are not equal. So, if you have a silicon-oxygen-silicon, small region on the substrate surface like here, then when you are growing the epitaxial layer, it is growing by steps and that does not match with the step already present there. So, this will cause a fault. This is a fault we see manifested in the epitaxial region as a stacking fault and a proof of this is, experimental verification is that

the number of stacking faults is proportional to the effectiveness of the hydrogen cleaning of the silicon surface before epitaxy.

Remember, before epitaxial growth, there is an in situ cleaning step. In that in situ cleaning step, first silicon is flushed in dry hydrogen at a high temperature and this is done in order to reduce the surface to remove all traces of native oxide. So, unless that is done, you will have a large number of stacking faults in the epitaxial region. So, it goes to prove that the stacking faults are closely associated with the traces of native oxide present on the silicon surface. The hillocks can of course be viewed without etching. There is a good fallout of these stacking faults, provided they are within reasonable lengths. The good fallout is that this offers a way of measuring the thickness of the epitaxial layer.

This is again by geometric consideration. You see, what you have exposed here is an equilateral triangle and then it goes into the pyramid. So, actually the height of this pyramid is your epitaxial layer thickness. It is extending all the way down to the substrate point. Isn't it? So, under the microscope, you can measure what the side of the pit is, what the length of the side of the pit is and that is going to be proportional to the thickness. The proportionality constant of course is going to be different for the different crystal surfaces, but it is going to be proportional. So, once I know what the surface crystal, the substrate crystal orientation is you can easily calculate what the epitaxial layer thickness is, simply by looking at these stacking faults under the microscope and measuring the side. In both cases, this is true. Here, the side of triangle I am calling it L, here I am calling the side of the square or the rectangle as L. This will give you a good idea of what the epitaxial layer thickness is going to be without having to resort to other techniques, simple ready to use way.

So, so far we have been talking about vapour phase epitaxy in general and vapor phase epitaxy of silicon in particular. I could continue on this topic for some more time like, you know, there are possibility of having selective epitaxy. That is selective epitaxy is something like this.

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Suppose you have a substrate. You want to grow an epitaxial layer, but you do not want to grow it all over the place. You only want to grow it somewhere here. So, this is called a selective epitaxy. This is usually done by covering the region where you do not want epitaxy to take place, by covering that with silicon dioxide or sometimes poly crystalline silicon and then carrying out the epitaxial process, controlling the temperature and the growth rate, so that the epitaxial growth is only taking place on the exposed silicon.

See, it is quite simple to understand. Suppose you have the surface covered with oxide. Only there are some windows in which the underlying silicon is present. You remember the chlorosilane reaction is actually surface catalyzed. So, only where it is coming in contact with the silicon surface, epitaxial growth will take place. Similarly on poly crystalline, if you are covering it with poly crystalline silicon, then also it is quite simple to achieve, because on poly crystalline the growth will not be epitaxial, but it will tend to be amorphous or poly crystalline. So, selective epitaxy is quite an attractive technique, because you can have islands of silicon epitaxial region. So, the isolation between the devices is going to be quite simple. You have one transistor here another transistor here like that.

They are automatically isolated, they can be .... automatically isolated. But, in principle they are all the same. They all come under the category of vapor phase epitaxy. There is a another technique of growing thin crystalline layers, which is, which has become very important nowadays and that is called molecular beam epitaxy.