VLSI Technology

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Lecture - 4
Crystal Structure of Si

To continue with our discussion about the basic planes in a crystal lattice, you have seen that you have identified a few planes in the crystal lattice. These are 1 0 0, 1 1 0 and 1 1 1.

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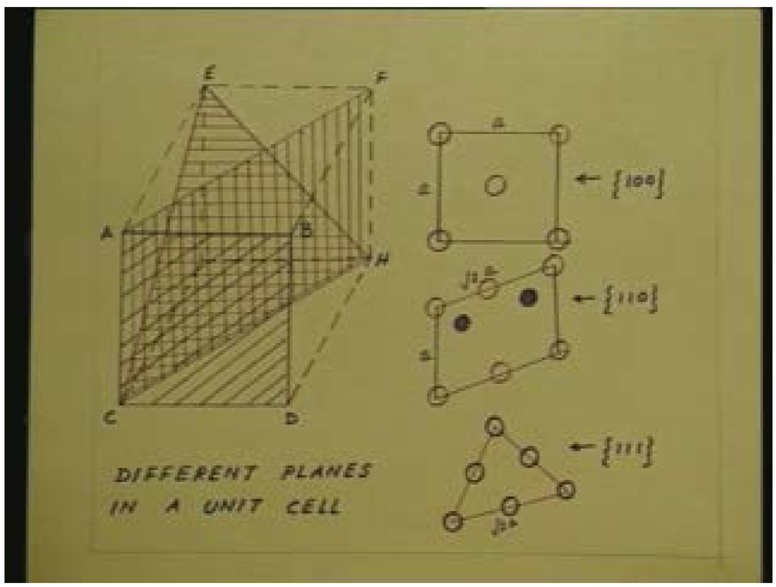

Here you can view them more clearly. See, this plane ABCD. This is actually, this black hatched plane, this is actually belonging to the family of 1 0 0 plane. What do I mean by belonging to the family of 1 0 0 planes? I mean that it makes an intercept only on one axis and is parallel to the other two axis. In this particular case, it is parallel to x and y axis and it is making an intercept on the z-axis. Similarly, if you look at this plane, the violet hatched plane that is ACHF, this plane is belonging to a family of 1 1 0 planes; ACHF, this is belonging to a family of 1 1 0 planes and if you look at the triangular plane CEH, this is actually a 1 1 1 plane. That is it makes intercepts on all the three axis, equal intercepts 1 1 1. So, these are the basic three crystal planes about which we need to concern ourselves when we are discussing silicon as a single crystal material, because these are the three planes we will encounter most often and the properties of these planes will be different.

Now, why do I say that the properties of these planes will be different? Look at this. Here, I have actually taken just this plane ABCD and put it here along with its atomic configuration.

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If you also look at this model here, this is a plane belonging to a family of a 1 0 0. This plane, right and what do you see? You see one corner atom here, one corner atom here, one corner atom here, one corner atom here and the face centered atom here. But, they are not uniquely contained in this plane. What do I mean by that? What I mean is simply this.

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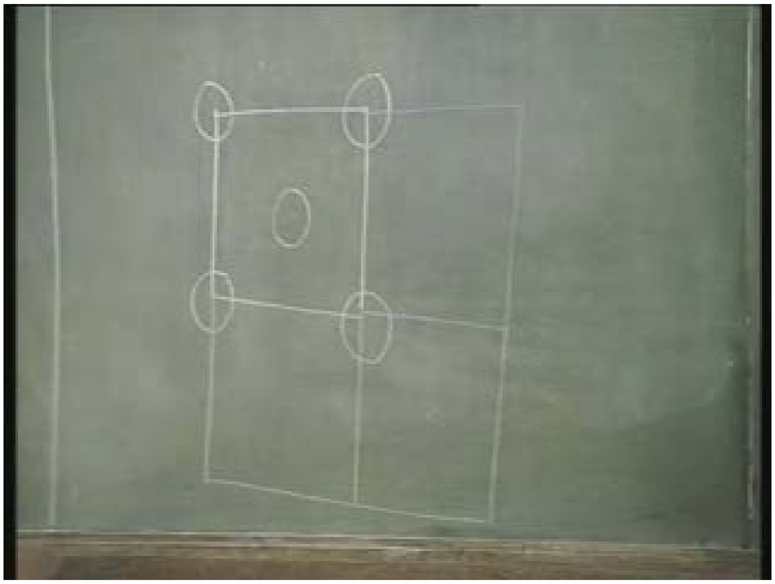

Let us consider the 1 0 0 plane. I have a corner atom here and a corner atom here and a corner atom here and one here and one at the center. Now, you can think of so many 1 0 0 planes, right. I have drawn four 1 0 0 planes here and you can see that this atom is shared by all four of them. Seems there is nothing to distinguish between this corner atom and this corner atom. It implies that all the corner atoms are shared by four of the 1 0 0 planes. So, the contribution of these corner atoms to the 1 0 0 plane, to one particular 1 0 0 plane is going to be one fourth and since I have four such corner atoms, the total contribution is going to be four into one fourth.

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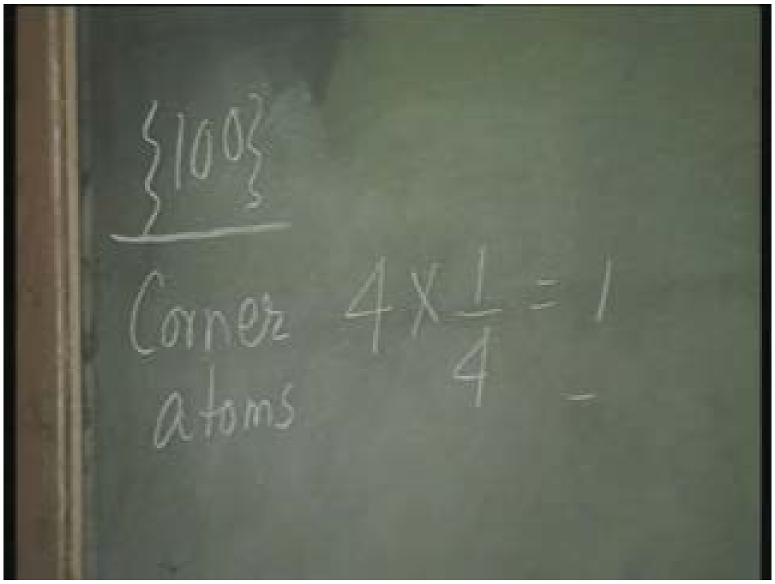

This is the contribution of the corner atoms. What about the center atom? This is uniquely contained in one 1 1 0 plane. It cannot be shared by other 1 0 0 planes. Therefore, its contribution to the 1 0 0 plane is unity. It is 1.

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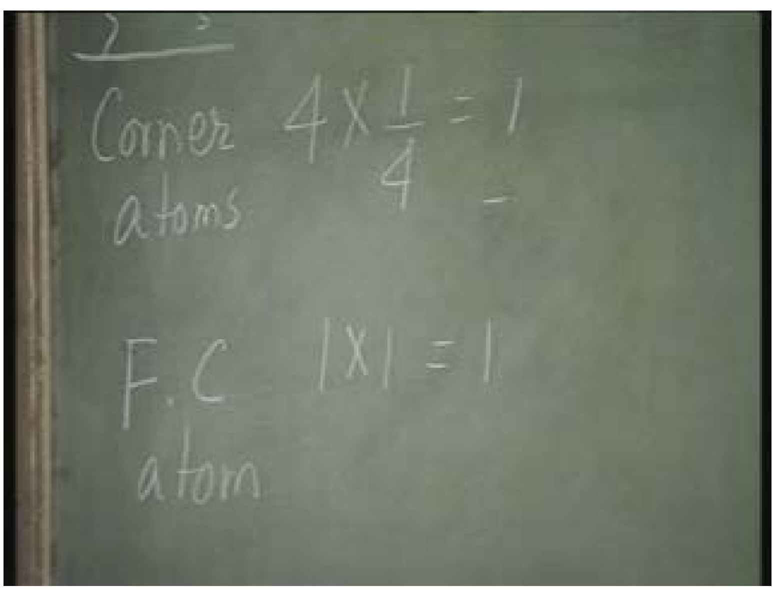

So, for the face centered atom, in other words, the total contribution of the atoms to this 1 0 0 plane is simply 2. What is the plane area now? You know that in this lattice we said that each side of the cube is a. Therefore the area of 1 0 0 plane is a square.

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So, the density of atoms in this 1 0 0 plane is 2 atoms in a square area, therefore the packing density of 1 0 0 plane is 2 by a square. Let us now think about 1 1 0 plane. You can also see it here.

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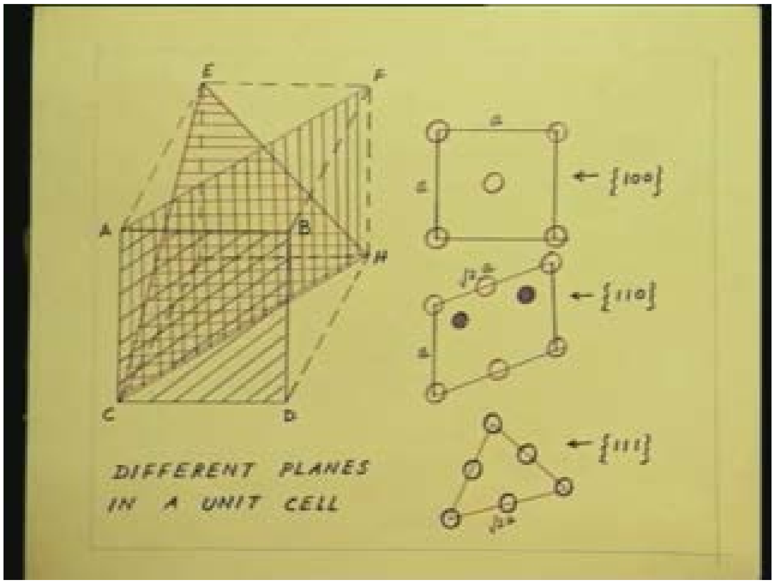

This is the 1 1 0 plane. In fact, it might be clearer if you look at this. Look at the model.

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This is my 1 1 0 plane if I draw a big diagonal here and this is my 1 1 0 plane. Let me try to look at it here.

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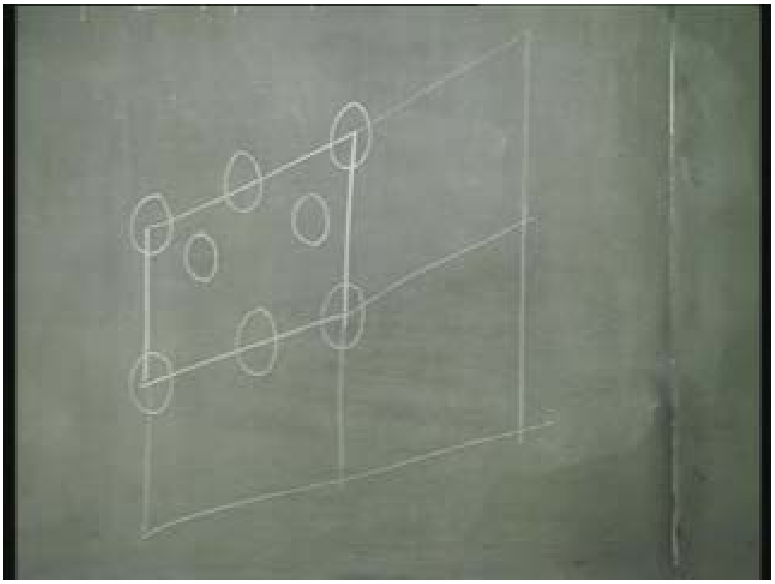

This is this big diagonal and this is the side of the crystal. Now, I have a corner atom here, a corner atom here, a corner atom here, a corner atom here and I have the face centered atoms here. These two atoms are actually this one and the one at below, right, these two atoms. What I mean is this and this and in addition to that I also have the two atoms from the second sub lattice sitting on the plane, one fourth three fourth three fourth and three fourth one fourth three fourth. So, what about the atomic contribution? Again, as before if I try to extend it, you can see each corner atom is shared by four 1 1 0 planes.

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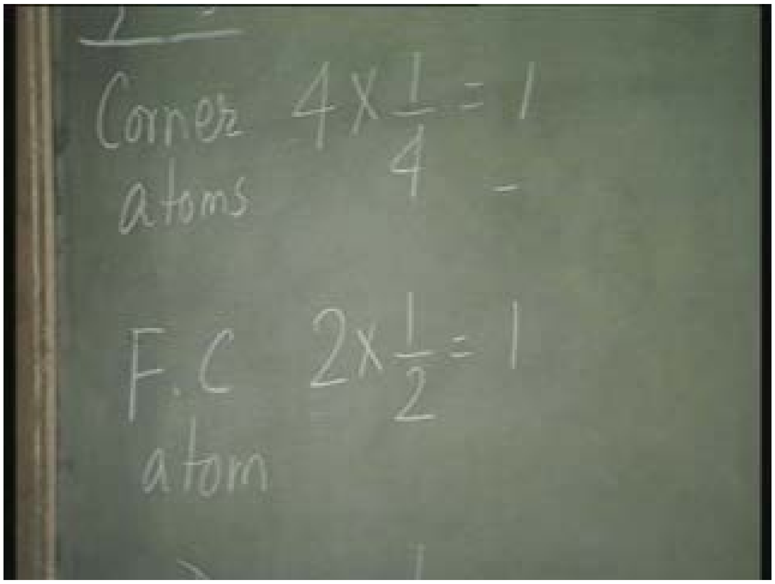

Therefore, the contribution of the corner atoms is 4 into one fourth that is 1.What about the face centered atom? This is one of the face centered atom and it is shared by two planes. Therefore the contribution is half and since I have two such face centered atoms, it is 2 into half equal to 1. In addition, I have two atoms of the second sub lattice which is uniquely sitting on this 1 1 0 plane. It is not shared by any other 1 1 0 planes.

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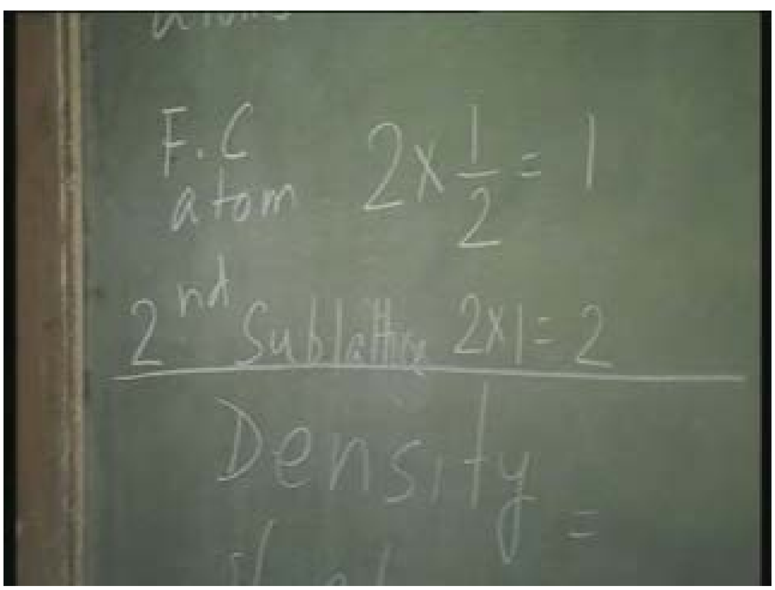

Therefore, the contribution is going to be unity for each one of them and for two such second sub lattice atom I have, therefore the total atomic contribution to the 1 1 0 plane is 4 and what about the area of this 1 1 0 plane?

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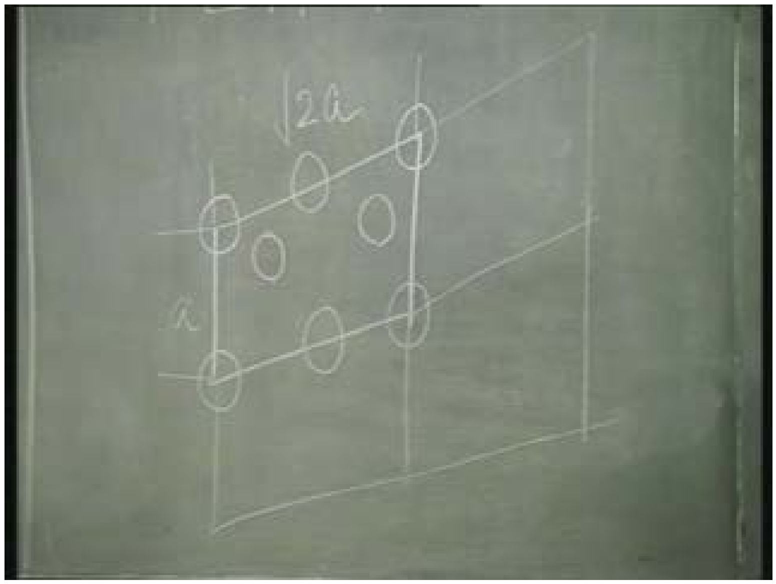

You know, this side is actually a and this is root 2a. Therefore the area is root 2 a squared.

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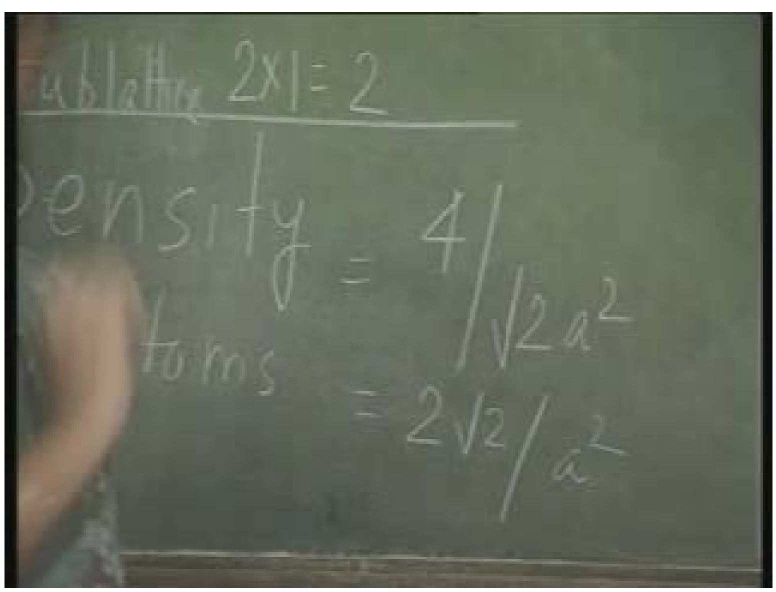

Therefore, the density is going to be 4 by root 2a square which is equal to 2 root 2 by a square. Am I correct? So, you see for 1 0 0 plane, the atomic density was 2 by a square. For 1 1 0, the atomic density is 2 root 2 by a square. Therefore, atomic density is larger in case of 1 1 0 planes. Now, let us take the case of 1 1 1.

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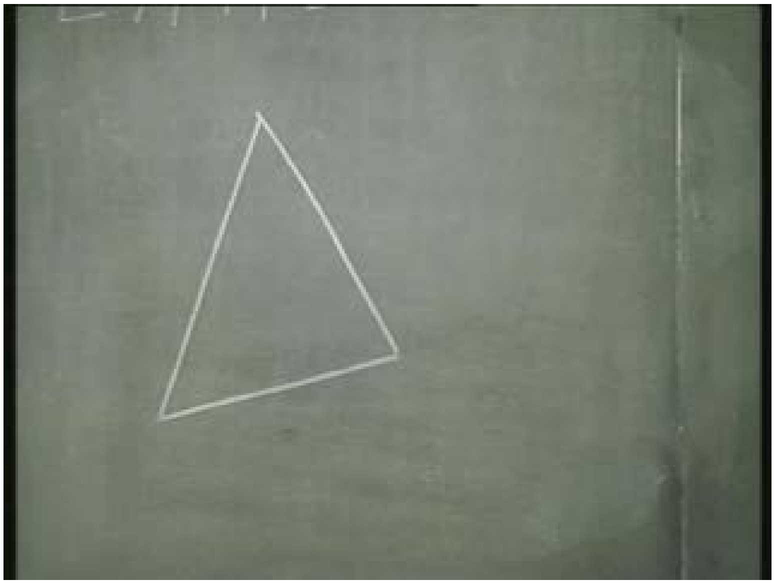

This is the 1 1 1plane, as you can also see here, this plane ECH.

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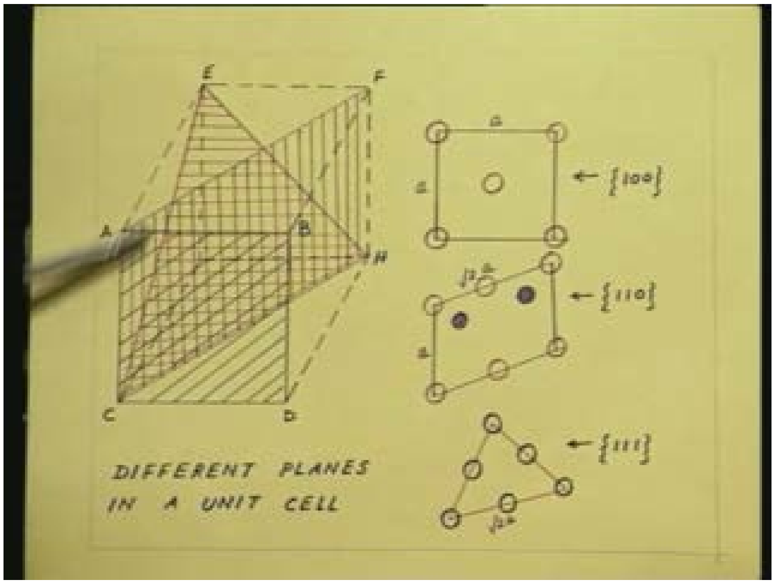

Where are the atoms located?

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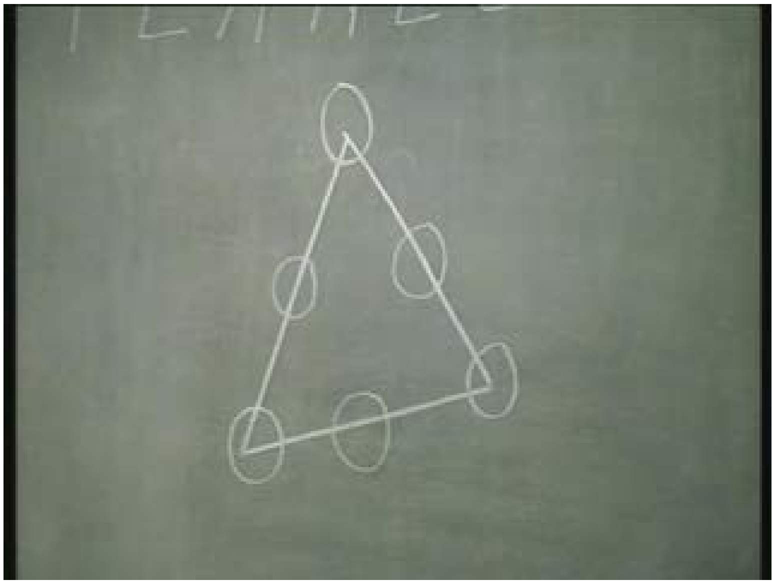

At the three corners. These are the three corner atoms and the three face centered atoms. We can also look in here.

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It is going through this diagonal, through this diagonal and through the base diagonal. So, you see this corner atom and this corner atom and in the middle there is a face centered atom, at the bottom here. Similarly, on this diagonal there is this corner atom, this corner atom and this face centered atom here. So, again let us look at the atomic contribution to this particular plane.

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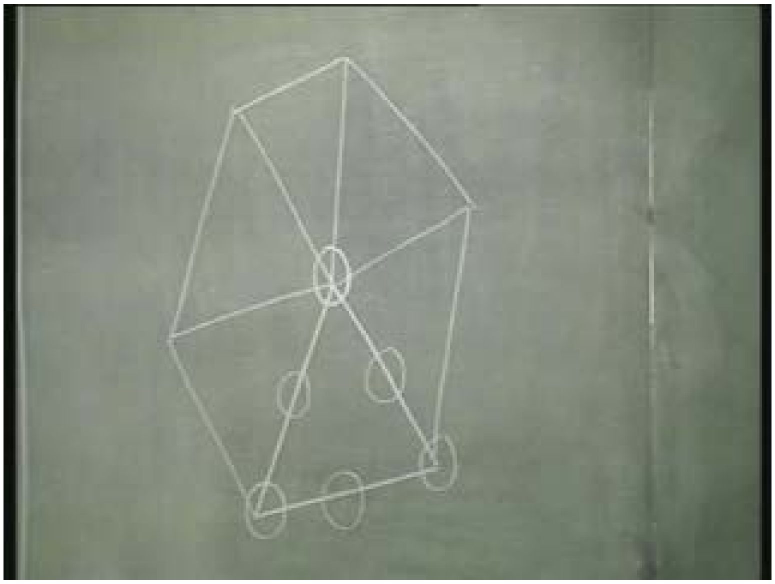

These are all the possible 1 1 1 planes passing through this point. That is I have 1 2 3 4 5 6, 6 planes. It is a hexagon. It has to be, because this is actually an isosceles, an equilateral triangle, each triangle having 60 degrees. So, I have six such triangles, basically. So, for each corner atom it is shared by six 1 1 1 planes.

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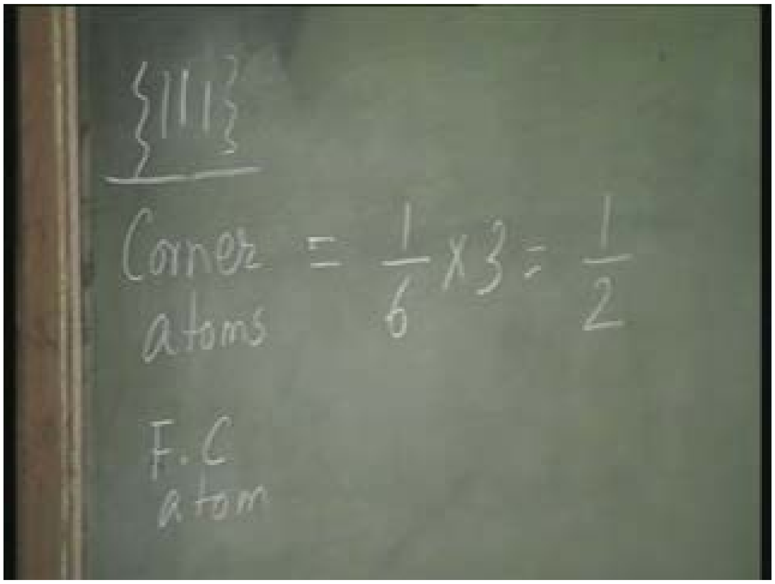

Therefore the contribution to one particular, there are three such corner atoms. Each is shared by 6 cells. Therefore, the total contribution of these corner atoms is 3 into 1 by 6 that is half. What about the face centered? Half; it is shared by two planes.

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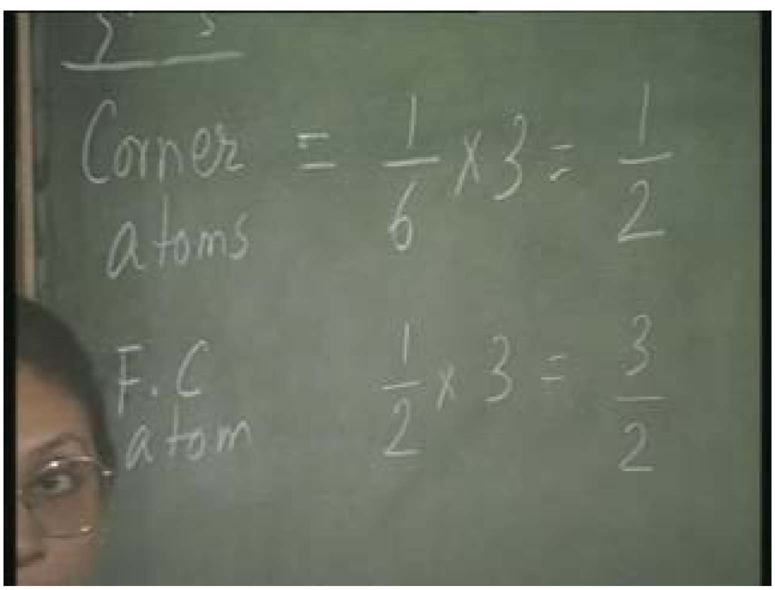

Therefore, the sum is 2 again. What about the area of this 1 1 1 plane? As you know, this is an equilateral triangle. The area of the triangle can be given by half base into altitude. Therefore, let us do a little bit of high school geometry.

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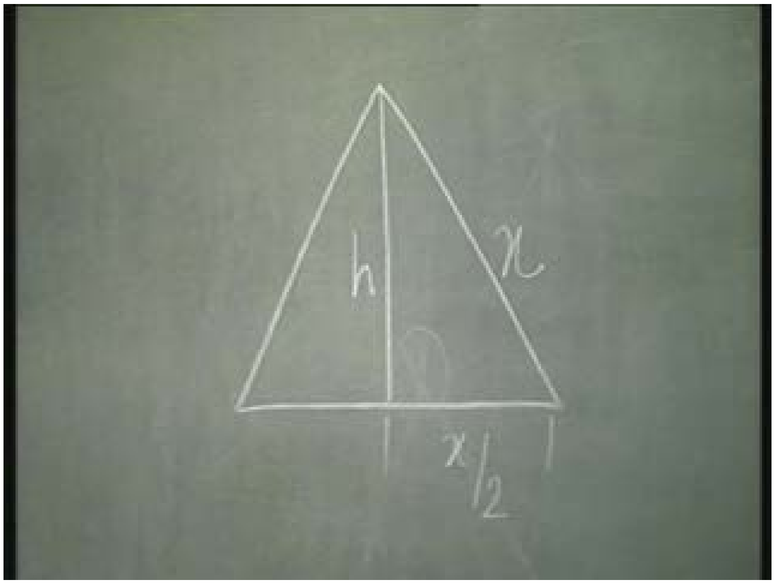

I have this equilateral triangle. Its side, let us call it x. I drop an altitude from here. This is h.

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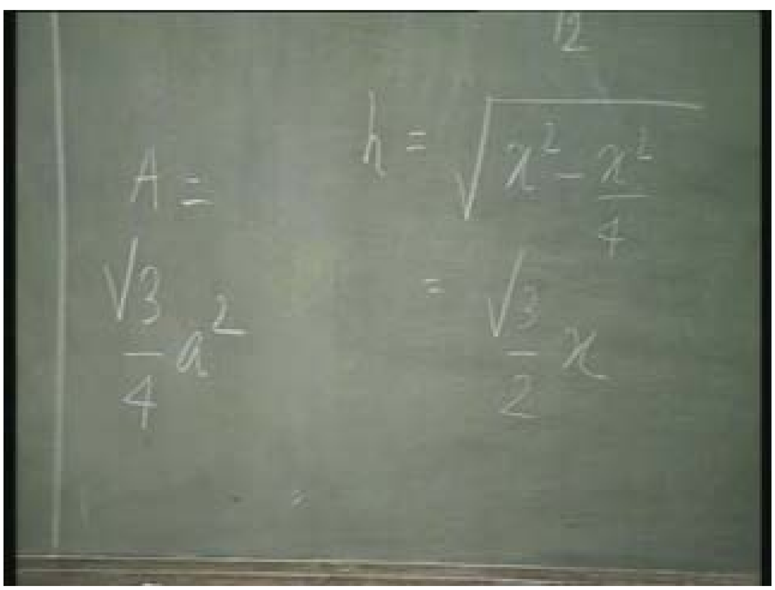

Since this is an equilateral triangle, this is going to be actually x by 2 and this is x. Therefore, h is root 3 by 2 x. Therefore, the area of this triangle will be given by root 3 by 4 a square. That is the area, because x is actually root 2 a. I think, I will just redo this once again; may be the step should be worked out.

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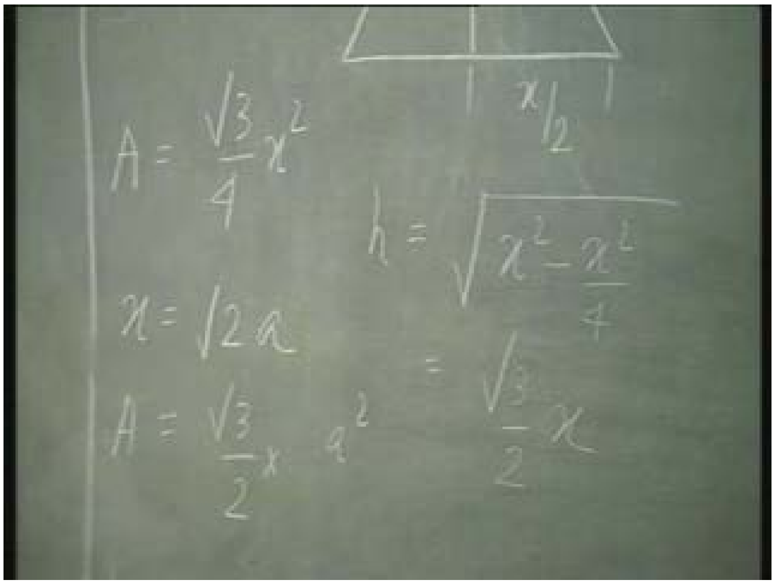

So, I have half, base, base is actually my x into root 3 by 2 x. So, I have root 3 by 4. Area is actually root 3 by 4 x squared and since my x is actually twice, x is root 2 a, therefore area is root 3 by 4 into 2 a squared, so, root 3 by 2 a square.

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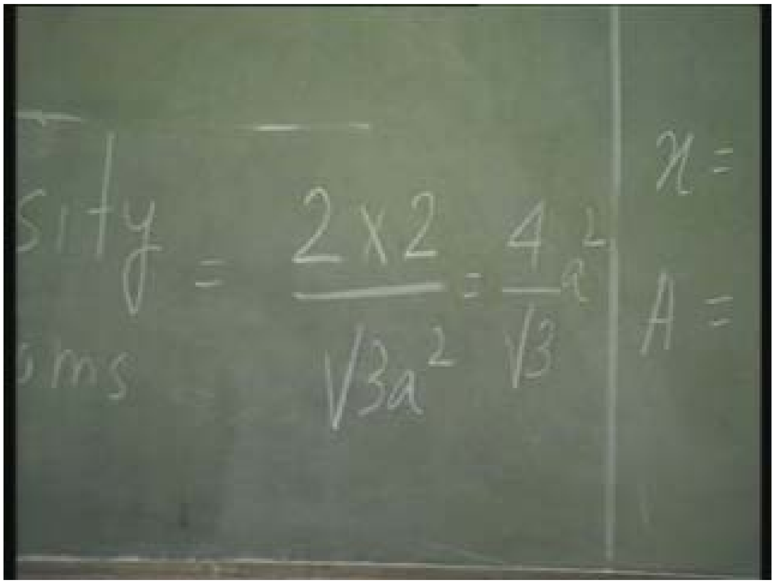

So you see, the density of atoms therefore is going to be 2 into 2 by root 3 a square. That is 4 by root 3 a square. So, we have calculated the packing density of the three most important planes for our purpose. That is 1 0 0, 1 1 0 and 1 1 1 and you have seen that the packing density in 1 0 0 plane is 2 by a square, packing density in 1 1 0 plane is 2 root 2 by a square and packing density in 1 1 1 plane is 4 by root 3 a square.

Why am I harping on this packing density? Because, the packing density controls certain important properties of the particular planes. So, let us note this point that the packing density in 1 0 0 plane is the lowest; it is the lowest. We will look at some of the other properties of these planes and then we will try to correlate how the material properties are governed by this atomic configurations in the planes.

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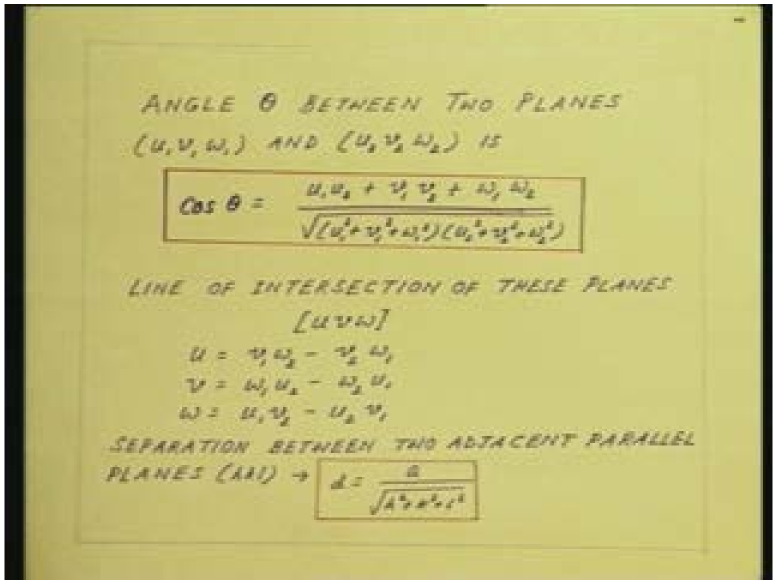

You can see here some of the basic geometric considerations of the planar structure. First of all see that when I have two planes, two planes are meeting. The angle between the two planes if I call this angle theta, theta between two planes u 1 v 1 w 1, by u v w actually I mean the miller indices, so it can be 1 0 0, 1 1 1, etc. So, between these two planes u 1 v 1 w 1 and u 2 v 2 w 2 is given by this relationship cos theta is equal to u 1 u 2 plus v 1 v 2 plus w 1 w 2 divided by square root of u 1 square plus v 1 square plus w 1 square multiplied by u 2 square plus v 2 square plus w 2 square. Also, these planes will intersect at a line. The line direction is given by uvw, where u is v 1 into w 2 minus v 2 into w 1, v is w 1 into u 2 minus w 2 into u 1 and w is u 1 v 2 minus u 2 v 1. This is a line of intersection between two planes and finally, the separation between two adjacent parallel planes that is when I say two adjacent parallel planes what I mean is, you see, this is one plane.

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This is its adjacent parallel plane, the front plane and the back plane or you can say this and this or the top and the bottom. This is what I mean by two adjacent parallel planes, the two planes are parallel to each other. So, what is the separation between these two planes is given by this relationship.

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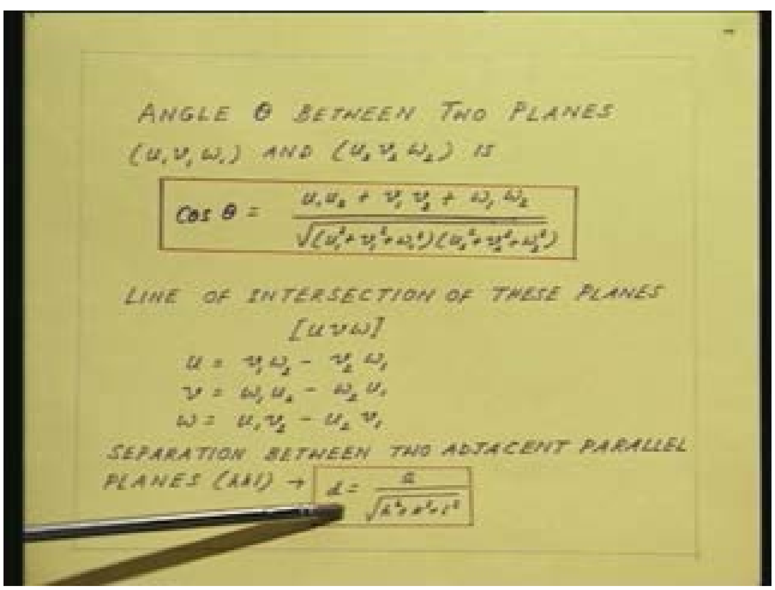

d is equal to a divided by square root of h square plus k square plus l square, where h k l and the miller indices of this plane. So, these two relations, the relation of the angle between two planes and the separation between two planes are going to be quite important along with the atomic density of each plane, in determining the properties of each particular plane and that will tell us for any particular application what should be the crystal orientation.

Let us explore it a little further. You know that the separation between two planes are given by this relationship d is a by root over h square plus k square plus l square. Therefore if I have two 1 0 0 planes that is this front plane and this back plane, the separation between them is simply a. You can see it from here, the separation between them is a.

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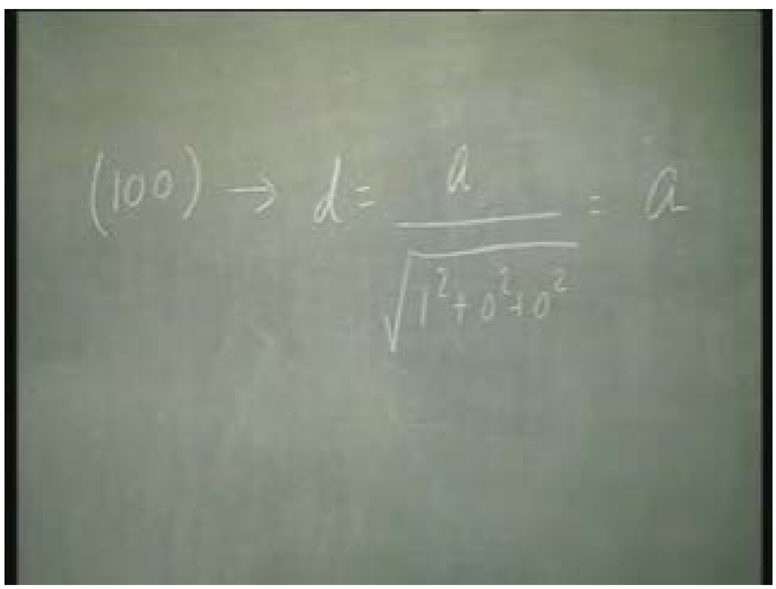

I can work it out for 1 0 0 planes, agreed, for 1 1 0 planes and for 1 1 1 planes.

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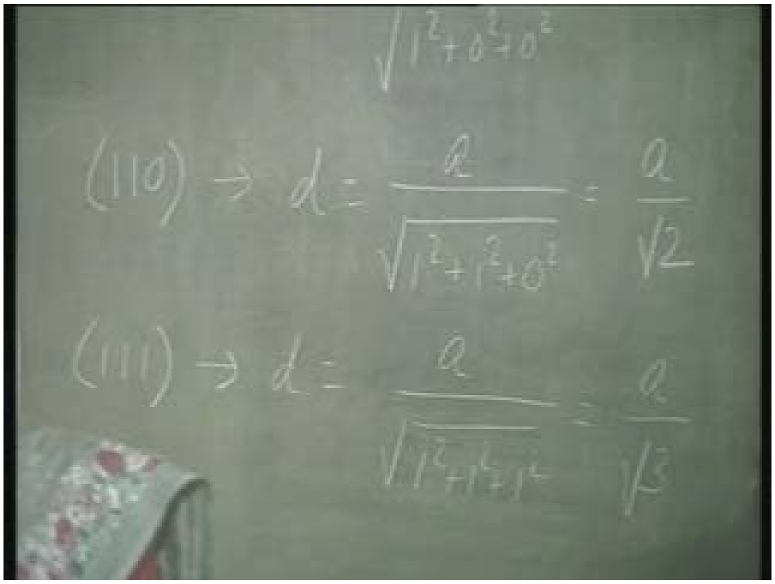

So, from this what do we see? We see that the 1 1 1 planes are, they have the least spacing between two adjacent parallel planes. In other words, 1 1 1 planes are most closely spaced together. This is quite an important observation, the fact that 1 1 1 planes are spaced most closely together. In order to fabricate any device we will first need to have a block of single crystal silicon. Single crystal silicon is generally grown from the melt and when you are solidifying the melt under controlled conditions, it is easiest to grow it in the 1 1 1 direction because, the 1 1 1 planes are most closely spaced together. It is easier for the crystal to grow in that direction with the least spacing between adjacent planes. It can just grow very easily in that particular direction. So, it is very simple to grow. Let us not say it is very simple. It is much simpler to grow 1 1 1 crystal than if you want to grow the crystal in 1 0 0 or 1 1 0 direction.

What does that mean? See, finally as engineers, you must always realize that everything boils down to the cost. It is easier to grow silicon in 1 1 1 direction; corollary - 1 1 1 crystals will be cheaper. That is one of the major reasons why almost all bipolar junction transistors were fabricated on 1 1 1 wafers, because they are readily available and they are cheaper. Therefore, the cost of your fabricated device can also get low. Finally, you will have to sell. Whatever integrated circuit you make, you have to sell it. Therefore, it is easier to grow and it is also cheaper. But, there are other considerations which we will consider later for certain particular applications. For example, for MOSFETs you may not want a 1 1 1 crystal. We will consider that in a few minutes.

While on the subject of this least spacing between adjacent parallel planes, let me also tell you that because of this reason it is most difficult to etch silicon in 1 1 1 direction, least spacing between them. Therefore, they want to stay put, it is difficult to etch them off. There are many chemical etchants. When silicon is subjected to that, those chemical etchants, it etches it selectively. That is it will etch other planes, but it will not etch 1 1 1 planes. Therefore when you are etching, 1 1 1 planes will be exposed. The etching will stop when it encounters an exposed 1 1 1 planes. This again has some very interesting fall outs.

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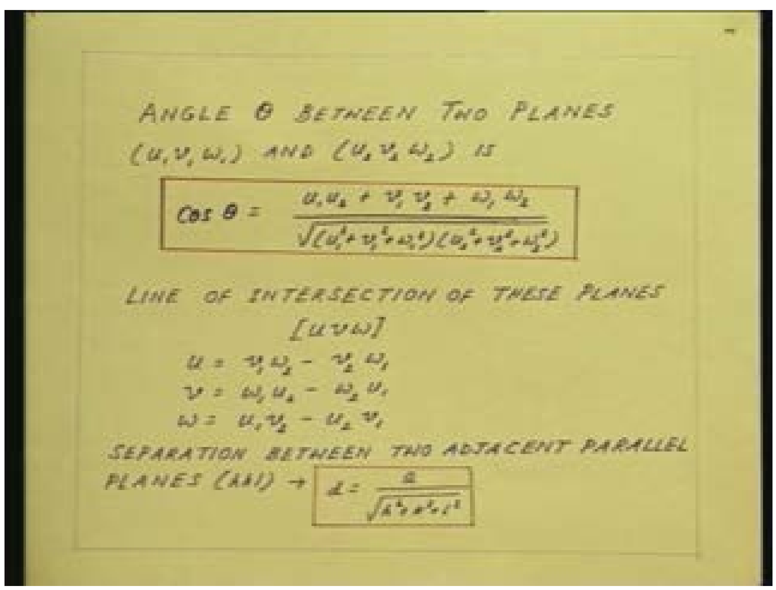

Look at the angle between two planes. Cos theta is given by this relationship. Now suppose you have an 1 0 0 wafer, suppose you have an 1 0 0 wafer. You have exposed it to a selective etchant, which is going to expose the 1 1 1 planes. Now, the angle between the 1 0 0 plane on the surface and the 1 1 1 plane which we are going to expose is going to be given by this relationship.

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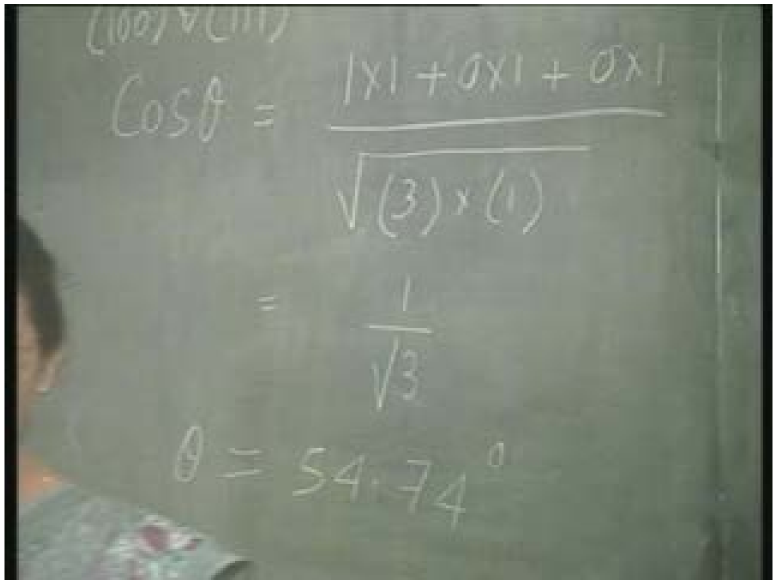

So, if you work out, cos theta will be given as u 1 u 2 plus v 1 v 2 plus w 1 w 2. Cos theta is going to be 1 upon root 3. This works out to be an angle of 54.74 degrees approximately 54.735 or something; 54.74 degrees. What do I mean by this? What I mean is something like this.

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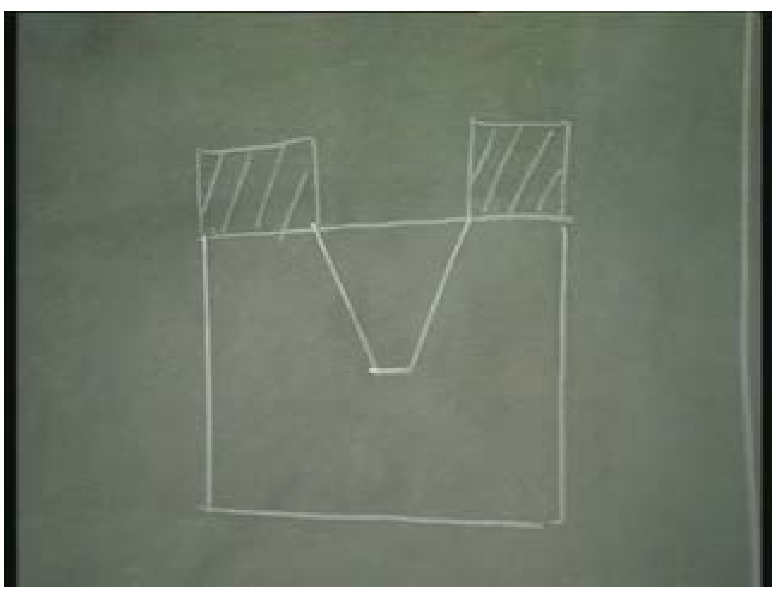

You have the 1 0 0 wafer. This is the cross sectional diagram. You have the 1 0 0 wafer. Now, you have exposed it to the etching through a window, let us say. I have protected this by means of oxide and you are subjecting it to etching. So, what is going to happen? The etching is going to proceed like this and the angle that is this angle is going to be 54.74 degrees. Do you realize? This surface is actually my 1 0 0 plane and this, what I have exposed is 1 1 1 plane. So, this 1 1 1 plane meets the 1 0 0 plane at the surface at an angle of 54.74 degrees. So, you see there are some very interesting facts associated with this particular properties of the 1 0 0 and the 1 1 1 planes.

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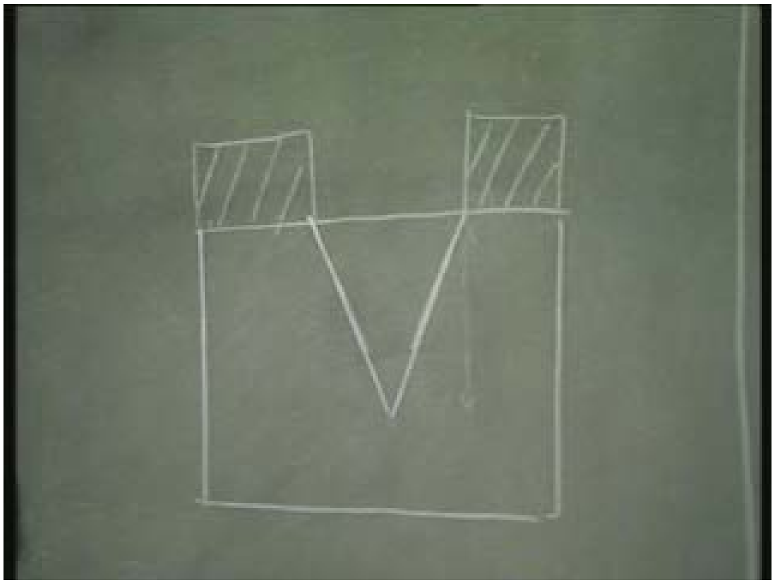

First of all, if I keep on etching, continue the etching, finally what I am going to have is, etching cannot proceed any further. It is going to stop here and this height will be determined by the width of the window, because you see this angle is fixed. Therefore I am governed by this window opening to know finally how much I can etch. It will be a self limiting etching. Etching will finally stop at a point, no matter how long I keep etching it. So, this is actually a very, very useful property of 1 0 0 wafer and this is, this particular thing it has various application.

Incidentally this is called a V groove etching. The name is self explanatory. You are making a V groove in 1 0 0 wafer. So, this V groove etching has various interesting applications. One such application is you have a device called a VMOS or a UMOS. Very briefly let me tell you what that is.

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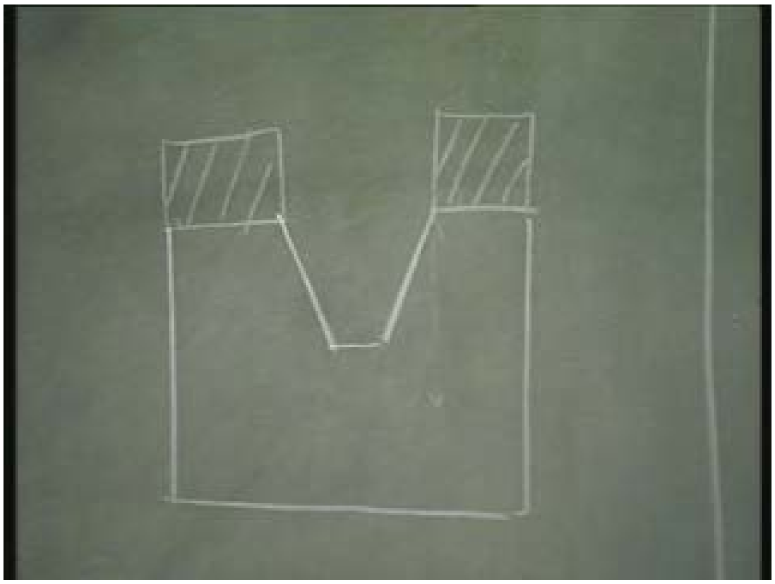

For that UMOS, you have a structure like this. You have etched it down and you a structure like this. So now, this portion can be the source and the drain and you can have your gate here. So, what have you achieved? You have achieved a MOSFET with a very small channel without actually having to have very crucial photolithography. By deciding the time of etching and by keeping this window dimension, you can actually realize a channel length which is going to be much smaller than your original window opening. So, it is used in VMOS. It can also be used in isolation between two devices. If you can etch it down, you can have one device here and other device here. It is also used, nowadays there are a lot of interest generated in micro machining of silicon and this selective etching is very much used for micro machining of silicon. These topics we will cover later on as the course progresses, but let me tell you that this is a very, very interesting fact that the, that first of all it is difficult to etch 1 1 1 planes, because of its least spacing between adjacent parallel planes and secondly, it is very interesting that 1 0

0 and 1 1 1 meets each other at this particular angle of 54.74 degrees which makes a lot of interesting possibilities.

Now, 1 1 1 plane also has another interesting property. It has the highest tensile strength and modulus of elasticity; highest tensile strength and modulus of elasticity among the other planes. So, what is the fall out of that? That means it is very hard to crack. Now you see, when I am making a device, I have a big disc of silicon, a big silicon wafer like this; big disc of silicon.

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I would like to cut pieces from here. How does one cut? Usually what is done is you scribe using a diamond tipped tool; you scribe like that and then you try to cleave it, break it along the scribe lines. So, the natural tendency of silicon will be to break along its natural cleavage plane and what is that natural cleavage plane? Obviously 1 1 1, because 1 1 1 has the highest modulus of elasticity and the highest tensile strength. Therefore, when you cleave a silicon, the plane you expose is going to be 1 1 1, agreed. So, 1 1 1 is the natural cleavage plane of silicon. If I have a 1 0 0 wafer, let us say that this surface is actually 1 0 0 and when I am cleaving, I am going to expose 1 1 1 planes here. The plane I am going to expose here is actually going to be 1 1 1.

We have already seen that the 1 1 1 plane is going to meet the 1 0 0 plane at the surface at this angle of 54.74 degrees. That means it never cleaves vertically, it always cleaves at an angle of 54.74 degrees. That is one observation. The other observation is when I am doing the scribing, I must know how to scribe. That is along which direction to scribe.

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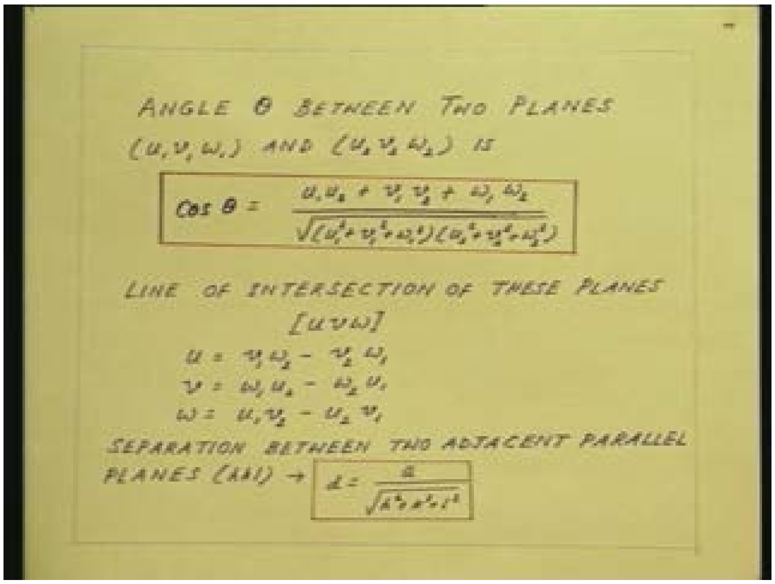

Again, this formula tells me what is the line of intersection of these two planes by this, u v w. These are the directions of the line and between 1 0 0 and 1 1 1, if you work it out, you will find that the direction of the line is going to be 1 1 0. That is this, along this 1 1 0 directions the planes are going to meet. So, it is common practice to provide this direction on a silicon wafer. How does one provide this direction?

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Simply, see this is otherwise a circular disc. One side, we provide a flat. This flat is along the 1 1 0 direction. This simply signifies that I am going to specify one scribe line for you. So, this flat is provided on the wafer. Your first scribe line is perpendicular to this flat. These are the first two scribe lines, perpendicular to the flat you can scribe. Fortunately in 1 0 0 wafer, we have an advantage. That is the 1 1 0 lines meet at a mutually perpendicular direction and you can cut out rectangular chips from a circular wafer. All the four lines that I have drawn are the four 1 1 0 directions which are meeting in mutually perpendicular direction and therefore we can easily cut rectangular chips. Why did I say that this is an advantage of 1 0 0 wafer, simply because this advantage does not exist, if I have for example, an 1 1 1 wafer.

What happens in an 1 1 1 wafer?

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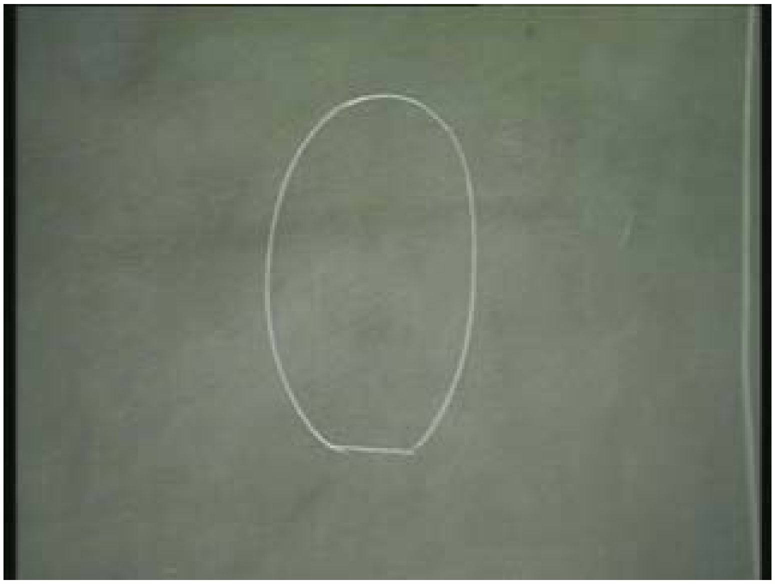

Suppose you have 1 1 1 wafer. Again, your natural cleavage plane is going to be 1 1 1. The surface 1 1 1 plane must meet the bulk 1 1 1 plane. That is when I say 1 1 1 plane, I mean a family of such planes 1 1 1 and 1 minus 1 1 or minus 1 1 1. Here also if you work out that detection of the line, you will find that they meet in the direction of 1 1 0.

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The angle however is going to be different and the angle is going to be, cos theta is going to be, if it is 1, say if I have for example, 1 minus 1 and 1 and 1 1 1, this is how it is represented - 1 1 bar 1. This 1 bar signifies that this is making a y intercept of minus 1. So, these two planes if they have to cut, it will be and this angle will work out to be 70.53 degrees. So, theta is different. Notice that even here it is not really vertical. It is not 90 degrees, it is 70.53 degrees.

So, whenever you cleave a silicon you do not really have a vertical block. It is always the bulk plane that you are exposing. It is always making a non 90 degree angle with the surface. If the surface is 1 0 0, this angle is going to be 54.74 degrees, if the surface is 1 1 1, it is going to make an angle of 70.53 degrees. But, the important point is even these two planes they are going to meet in 1 1 0 direction and where are these 1 1 0 direction?

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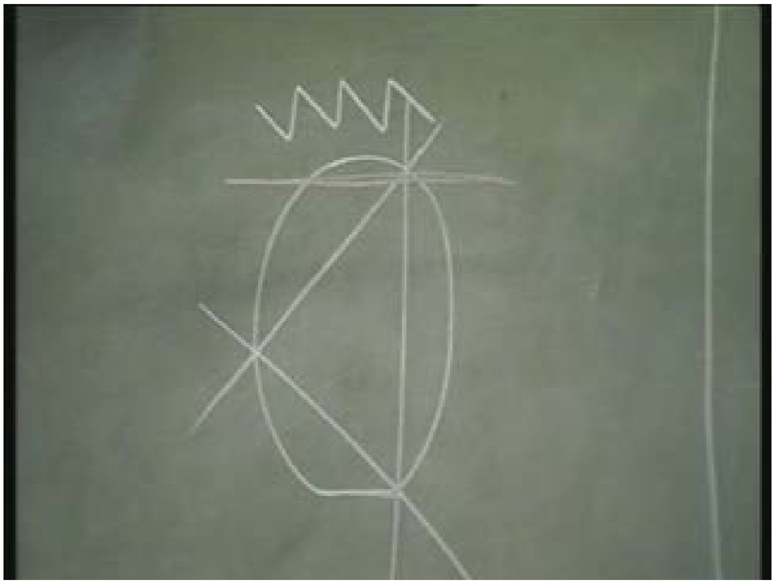

See, I have provided a flat. Therefore my first scribe line is going to be perpendicular to this flat. So, this is one 1 1 0 direction. Where are the other two 1 1 0 direction? You know, it is going to be like this. Remember the 1 1 1 plane, it is bound by the three 1 1 0 lines and they are constituting a triangle and the angle between these two, any two 1 1 0 lines is not 90 degree, but 60 degrees. It is an isosceles, sorry it is an equilateral triangle. So, you have a small problem here.

What is that small problem? When I want to scribe silicon, I would like to get as many square or rectangular chips as possible. But, in this particular case, you see, I cannot scribe in a mutually perpendicular direction. I will nevertheless try. That is I have put my first scribe line here. So, automatically I am going to try to scribe it. The next scribe line I am going to put like this. But, this is not the natural cleavage direction. So, it will resist. Silicon will resist scribing along that line. So, what I will have is not a clean break along this line. Instead I will have a zigzag cut with each zig and each zag along the 1 1 0 directions.

So, you will find that along this direction it is breaking cleanly, because it is cleaving along a natural direction of 1 1 0, but when you try to cleave in a direction perpendicular to your first scribe line, it is not going to cleave cleanly. Instead you are going to have a fine zigzag pattern with each line referring to this 1 1 0 or this 1 1 0 lines. That is what I meant, each zig and each zag corresponding to 1 1 0 directions. So, it is a bit difficult to cleave the 1 1 1 wafer in mutually perpendicular direction.

If I have 1 1 0 silicon, if I have 1 1 0 silicon, it is going to be very interesting. Again you see, the first point is common. When I am cleaving, it is going to be 1 1 1 planes. Cleavage plane is going to be 1 1 1 plane. I will leave it for you to work it out. Find out the angle cos theta. You will find that you have 1 1 1 planes meeting the surface 1 1 0 plane in, I mean at 90 degrees.

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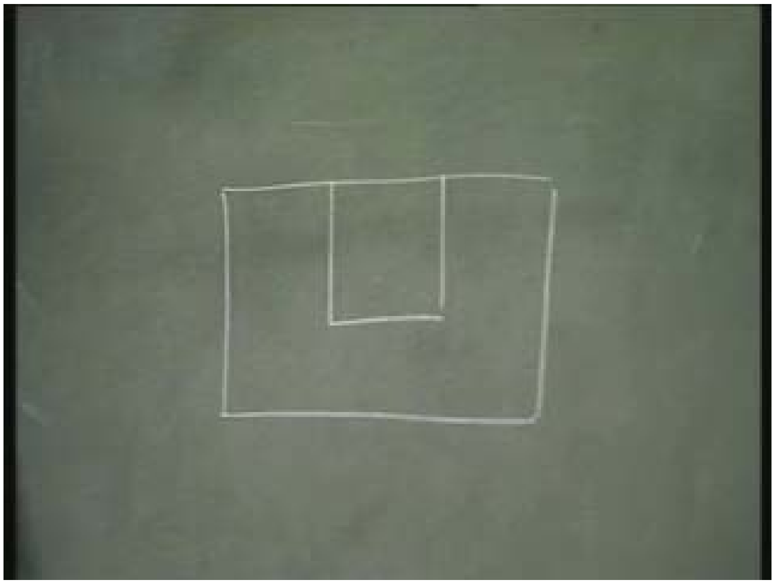

That is again if I refer to a cross sectional diagram, if the surface is actually 1 1 0 and if you cleave, it is going to be like this or if you etch for example, if you expose it to a selective etchant, the selective etchant is going to expose 1 1 1 planes and these 1 1 1 planes are going to meet the 1 1 0 planes at the surface at 90 degrees. So, if you have 1 1 0 wafer, you can have deep vertical grooves, not the V grooves like you had in case of 1 0 0 wafer, but you are going to have deep vertical grooves. You can etch deep vertical grooves only in 1 1 0 wafers.

So, what have we seen so far? We have seen that since 1 1 1 has the least spacing between two planes, it is easier to grow the crystal along that direction, also because it has the highest tensile strength, it is the natural cleavage plane for silicon and we have seen the angle between the 1 1 1 plane thus exposed and the surface plane, whatever the surface plane may be 1 0 0 or 1 1 0 or 1 1 1 and you have seen how the scribing is going to be done.

Finally, let me tell you that there are some other processing steps like oxidation and diffusion, which will also be influenced by the properties of these individual planes. For example, the atomic density. You have noticed that the atomic density was lowest in 1 0

0 plane. Therefore, when you subject them to oxidation for the same time, for the same temperature, under identical condition you will find the oxide thickness on 1 1 1 plane is more than that on 1 0 0 planes, simply because the 1 1 1 planes have more density of silicon atoms. Therefore it is easier for oxygen to find silicon, available silicon and react with it. You have enough supply of oxygen. Therefore the more number of silicon you have, the more density of silicon you have, the easier it is to grow the oxide. So, when you are subjecting your wafers for any processing, you must know what the crystal orientation is, because the oxidation thickness will depend on the crystal orientation. Let us stop here today.