Semiconductor Device Modelling and Simulation
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Lecture - 05
Crystal Concepts (Contd.,)

Hello friends, welcome to lecture number 5. In this lecture, we will discuss about, we will continue our discussion on crystal concept and we will discuss about the Miller indices.

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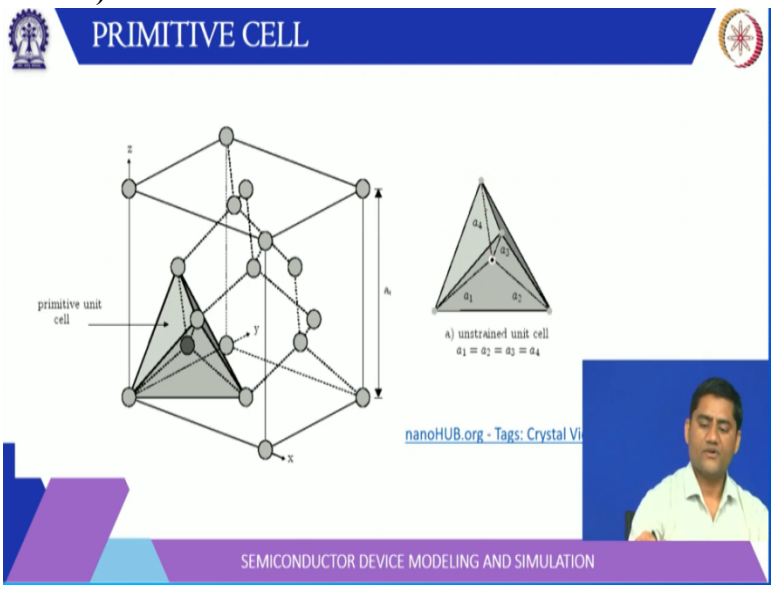

Last class, we discussed about unit cell structures. So, we discussed our simple cubic face centered cubic, body centered cubic diamond lattice. So, all these are lattice structures now, please remember the unit cell and the primitive unit cell they may not be same. So, for example, for diamond structure diamond lattice the unit cell is FCC, but the primitive unit cell is shown here certain data handling structure with the center there is 1 atom and followed by at 4 corners.

So, these are unrestrained unit cell that means, there is no strain and if you want to have a more view about the crystalline structure, there is a site here nanohub.org there you can go and view the crystalline structures. All the crystal most of the crystalline structures are available you can view them there and we have already discussed how to calculate the atom density the density of the material. So, now, we will continue how to represent a crystal through lattice vector and the Miller indices.

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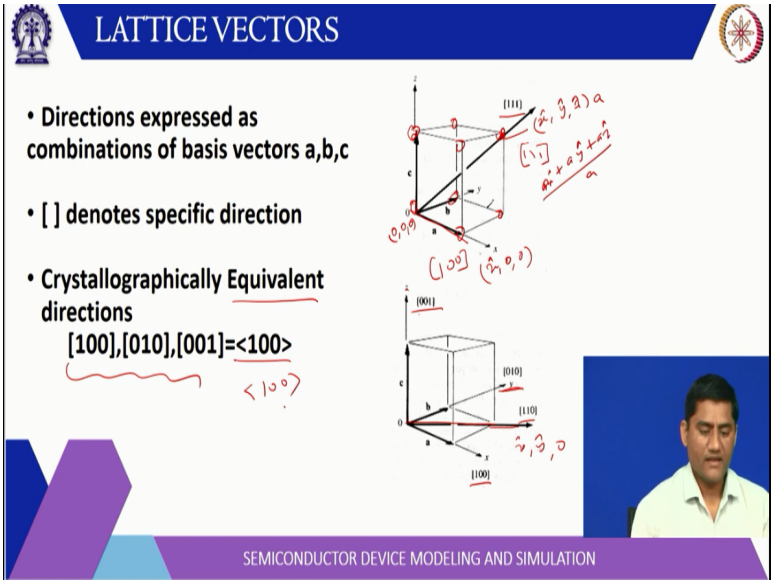

Now, let us vectors these are basically the vectors representing that direction in a semiconductor crystal. So, if you take let us say a simple cubic unit cell, there are 3 directions here a x axis y axis and z axis and simple cubic the atoms are at the corners here corners of the cube. So, if you consider the nearest atom now remember the lattice vector is drawn between or it is aligned connecting to nearest neighbours.

So, here there are 2 nearest neighbours, so 1 vector can we along x axis 1 lattice vector can we along y axis 1 lattice vector can we along z axis therefore, our lattice vector will be this can be written as x cap 0, y cap 0, z cap like this and so on. And the direction is denoted by this kind of bracket. So, if you look at the diagonal so, diagonal of a cube, if you look here, this point has position x cap, y cap, z cap and all have unit a. So, a times x cap a times y cap a times z cap or you can write this point is a times x cap + a times y cap + a times z cap.

Now, the vector connecting this origin which is 0 0 0 is ax cap ay cap az cap so, every all the x, y, z they have a here. So, if you divide by a you have 1 1 1. So, this direction is called 1 1 1 and is represented through a closed bracket. Similarly, for this line you can write 1 0 0 again a closed bracket, this z axis is 0 0 1 y axis is 0 1 0 the diagonal at the bottom face, this is x cap y cap and z is 0 so, it is become 1 1 0.

So, these are now if you notice in our cubic structure 0 0 1, 0 1 0 and 1 0 0 they are equivalent because whether you look in 1 0 0 direction or 0 1 0 direction or 0 0 1 direction, you will see the

same configuration, there is no difference in the view. So, when there is no difference in the view, we call them equivalent directions and all these 3 equivalent direction they can be represented through a triangular bracket so this 1 0 0.

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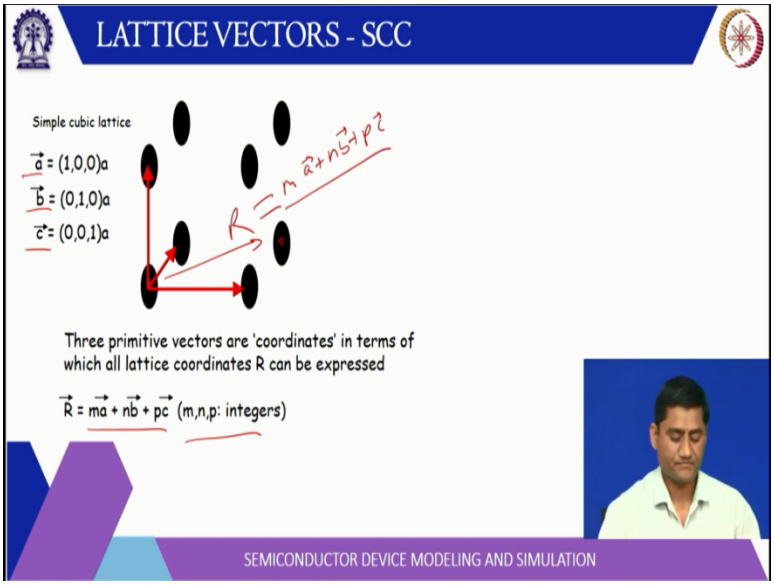

Now, we can find out the lattice vector for other cubic structures cubic cells, so of course in a simple cubic it is 1 0 0, 0 1 0 and 0 0 1 and many (())(05:11) of course, now, idea is that any lattice side any lattice point can be represented in terms of origin a distance is let us say R. So, R can be represented as a combination of these 3 primary or primitive vectors with some integer so, m is an integer times a, n is an integer times b plus p is integer times c.

So that means whole crystal can be reproduced by choosing different values of m n and p. So, if you take positive you will construct the write up if you take these values negative you can construct the write up.

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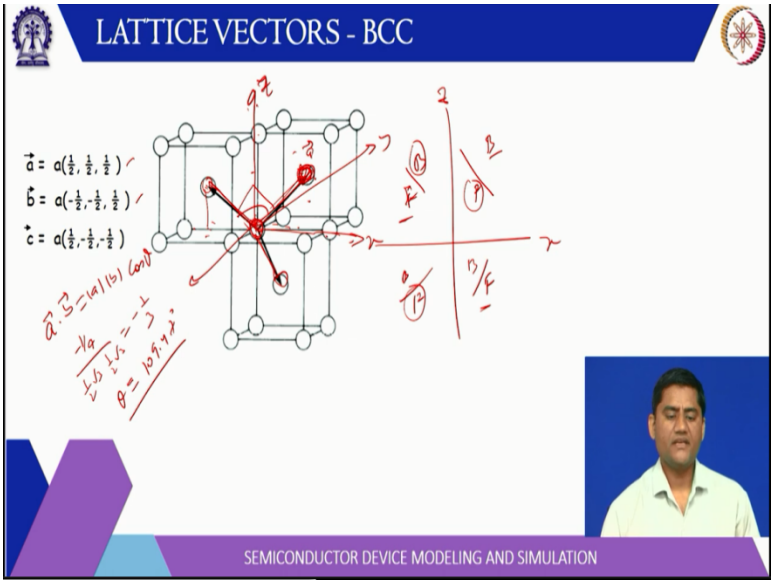

For a BCC now, you notice here is not a long x y z this lattice vector connects the nearest atoms. So, in a BCC it is a body's atom or the atom in the center at the center of the body which is nearest to the atoms as the edges. So, if you put let us 3 units cell together, so and connect this corner atom to body element of 1 body element of 2 and body element of 3. So, of course, first one will be this is let us say x this is let us say y and this is let us say this is z.

So, this will be x a by 2 y a by 2 and z a by 2 so, this is vector a then this is vector b which is x is now here is –x so, -a by 2 along the x axis then y is again same. So, it is +1 by 2 -1 by 2 y it is opposite direction and z is +1 by 2 z and similarly, for the third one is x is half y is minus half and that is also minus half so these 3 other. So, basically you can look like this I can maybe show you let us say this is your plane.

So, there is a 1 cubic cell lying here and then 1 cubic cell lying here slightly staggered like this and other one lying here. So, these 3 is basically they are constituting the line connecting the body centers of these 3 unit cell are the 3 basis vector. Now, it is not that you know you can have only these 3 vectors, there are other possibilities also you can take other unit cells, for example, if you take beside the top unit cell.

So, if you draw like this, z axis. So, let us say this is back this is front so, there are 2 then back front here also back front back front. So, here if you see this one is the back this is x axis this is the z axis. So, y is positive here y is negative here, so, this is front and here, this is also front y is

negative here z is negative. So, you can choose this front here this back here and then you have to choose from this one.

So, basically the idea is that these angles they are at the connecting in the body diagonals and you can find the angle between these 2 vectors also. So, you can if you recall your formula that 2 vectors a vector and b vector, so, a dot product of 2 vectors is magnitude a magnitude b times cosine theta. So, if you calculate the angle between these 2 vectors, you can take the dot product and that value comes out to be a dot b is -1 by 4 -1 by 4 and 1 by 4.

So, that comes out to around -1 by 4 divided by magnitude of a is 1 by 2 times root 3, magnitude of b is also 1 by 2 times root 3. So, that comes out to around -1 by 3. So, your theta comes out to be 109.47 degree. So, that is the angle between these 2 vectors. So, unlike simple cubic, they are not at 90 degree. So, these 3 are the lattice vector for BCC.

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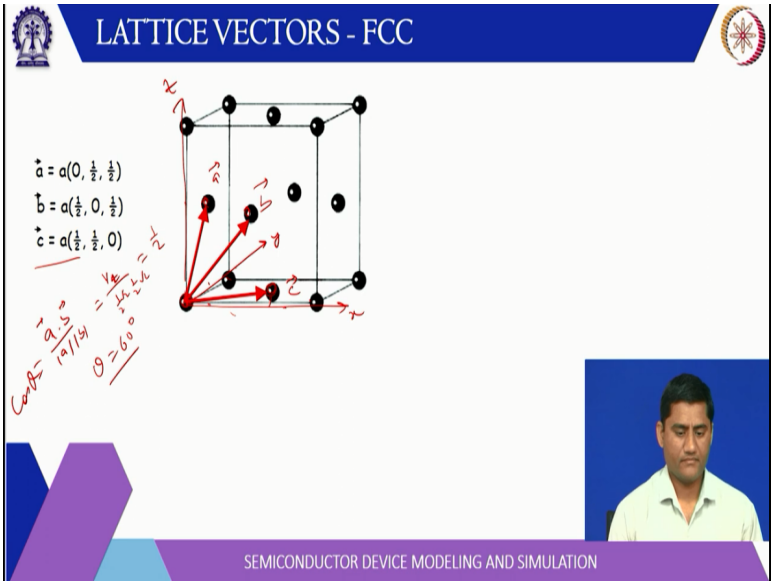

Similarly, we can calculate the lattice vector for FCC. So, for FCC, the 3 the nearest neighbor of the for this corner element, nearest neighbours of the face centers, so, this is the bottom face, this is the front face, this is the left face. So, the vector connecting the bottom phase, let us say this is x axis, this is y axis and this is z axis. So, bottom face will be a by 2 x + a by 2 y. So, this is c vectors then the front face x y along x a by 2 along z a by 2. So, this is b vector and the left face along y a by 2 along z by 2 so, this is a vector.

So, these are 3 vectors that describe the FCC lattice again you can find the angle between these 2 vectors a dot v divided by magnitude a magnitude b and that is cos theta and that comes out to around 1 by 2 divided by 1 by 2 root 2 times 1 by 2 root 2 and that is around 1 by 4 that is 1 by 2, so, that theta is will be 60 degree. So, that will be the angle between these lattice vectors for FCC case.

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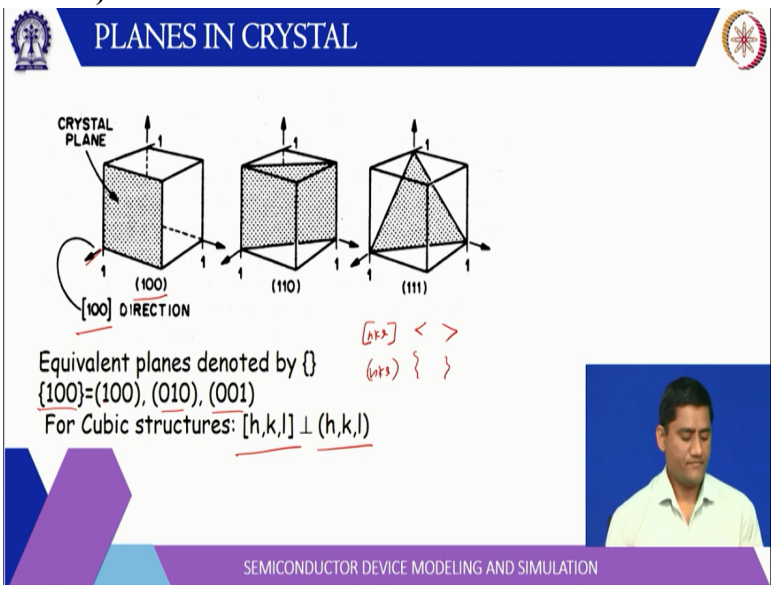

Now, once we know the lattice vectors, we can also describe the lattice planes in the crystal. So, a lattice plane is designated by the direction perpendicular to it. So, if the direction perpendicular to a plane is let us say 1 0 0 then the plane will also recall 1 0 0 the difference in the notation will be direction is represented by a square bracket and plan is represented by simple brackets and of course, similar to the equivalent direction which were represented by triangular brackets.

Similarly, the equivalent planes are represented by curly brackets. So, for example, if you see a simple cubic then 1 0 0 which is perpendicular to x axis 0 1 0 perpendicular to y axis 0 0 1 perpendicular to z axis they will equal and plane and then you can write within curly bracket 1 0 0. Now another thing to note here if these 3; values are represented by a number h k and l. So, a general notice and for any plane or direction we use h k l notation h k l. So, h k l direction is perpendicular to h k l plan for cubic structures it may not be true for other structures.

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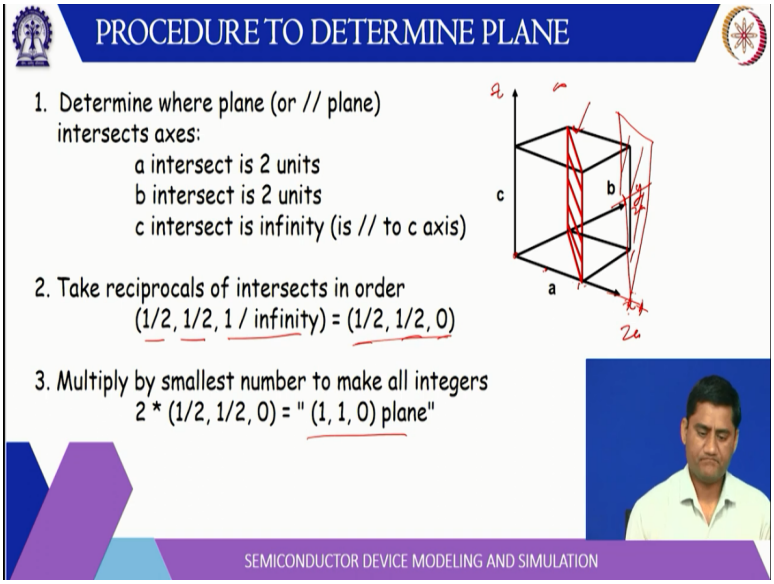

Now, how to determine the plane? So, if a given plan is given how do we name it? So, the standard procedure for naming the plane is first we find what are the intersects do to that plane on the x axis and y axis. Now, 2 planes if they are parallel and they can be said they are you know same plane basically except in certain situation. So, you can choose the origin nearby and then find the intersect.

So, the for example, the planes on here intersect x axis y axis and z axis. So, in intersect the x axis let us say at some lesser 2 units and y axis a 2 unit and z axis it is not intersecting. So we can set is intersecting the z axis at infinity then what we do? We take the inverse of the intersect. So, intersect is 2 the inverse will be 1 by 2, 1 by 2 and the 1 by infinity. So, that was 1 by 2, 1 by 2 and 0 then we multiply with certain number integer, so that all the numbers in the bracket with an integer.

So, here we can easily see if we multiply by 2, we get 1 1 0 plane. So, now, you see here if let us say, you take a plane here, this distance is a so the example as so on is basically intersecting at 2 a. So this is a this is 2a this is also 2a so, these 2 plane will be actually parallel and they are basically same plane both are 1 0 0 plane the exception will come when intersect is half of the a. Then of course, we can name it 2 0 0 plane those things will you know discuss in examples.

But the procedure is that you find out what is the intersect? Due to a plane at the x axis y axis and z axis then invert it and make them integer and that will tell you the name of the plane.

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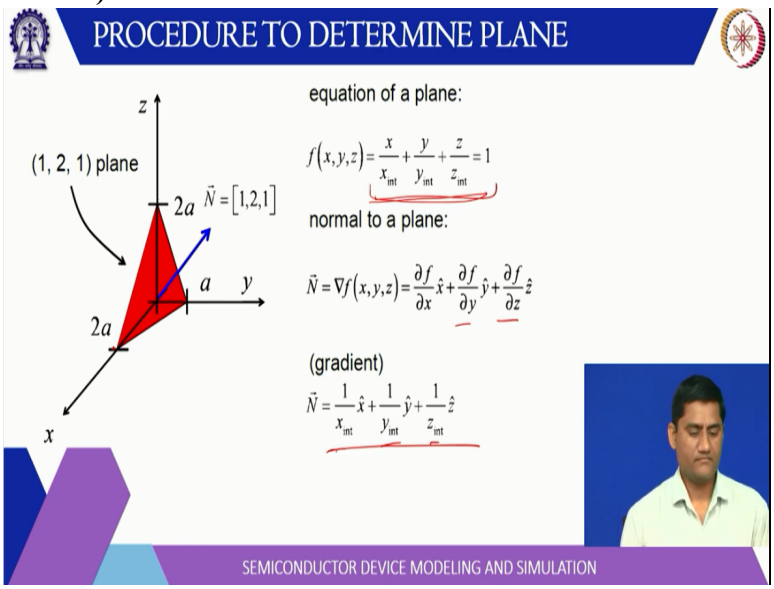

Now, from where we get this procedure, if you recall your class 12 mathematics, the equation of the plane, equation of the plane is written like this x divided by x intersect + y divided by y intersect + z divided by z intersect = 1 and you can verify it that x intersect y and z both are 0. So, this will be 1 at y intersect x and z both are 0 and y = y intersect so that is again 1. Similarly, a z intersect x and y both are 0 so z by z intersect will be 1.

Now, if you want to find the normal to a plane whose equation is known, we will take the gradient of that equation to the plane. So, if you take the gradient, so, if this is function f then df by dx along x direction df by dy along y direction df by dz along z direction. So, what you will get? You will get 1 by x intersect times x cap + 1 over y intersect and y cap + 1 over z intersect times z cap. So, this is precisely what we have done, we find out the x intersect y intersect z intersect, take the inverse and we say this is the plane.

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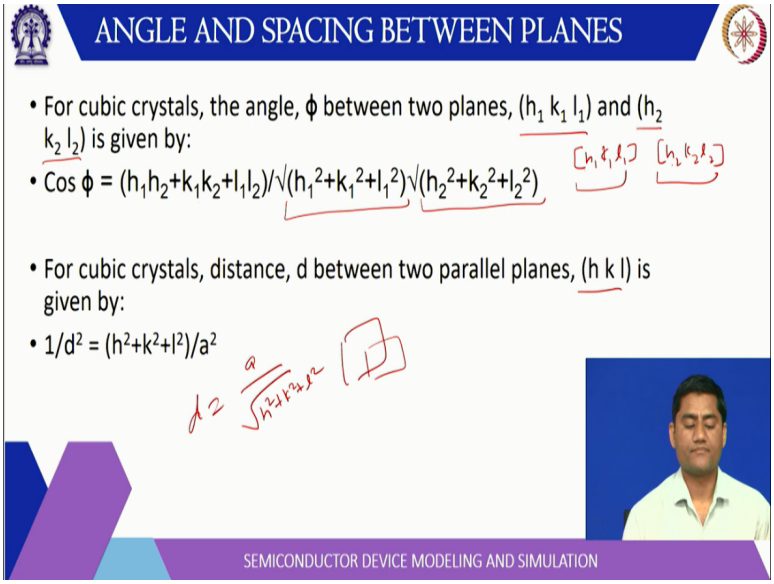

Now, for the cubic crystal, the angle between 2 planes is same as the angle between the perpendicular directions of those planes. So, let us say you have h 1 k 1 l 1 is 1 plane h 2 k 2 l 2 is another plane. So, corresponding direction will be h1 k1 l1, h2 k2 l2. So, if you want the angle between 2 vectors again a dot b is ab cosine phi. So, cosine phi will be a dot b, a dot b h1 h 2 + k 1 k 2 + l 1 l 2 divided by magnitude of individual vectors.

That is the square root of h 1 square + k 1 square + l 1 square and multiplied by the square root of h2 square + k 2 square + l 2 square. So, that way we can determine the angle between any 2 arbitrary planes of a cubic crystal and also the distance between 2 parallel planes is given by d = a divided by square root of h square + k square + l square that we can find because this h k l direction is perpendicular to the plane. So, that line will intersect the 2 consecutive planes at a by square root of h square + k square + l square.

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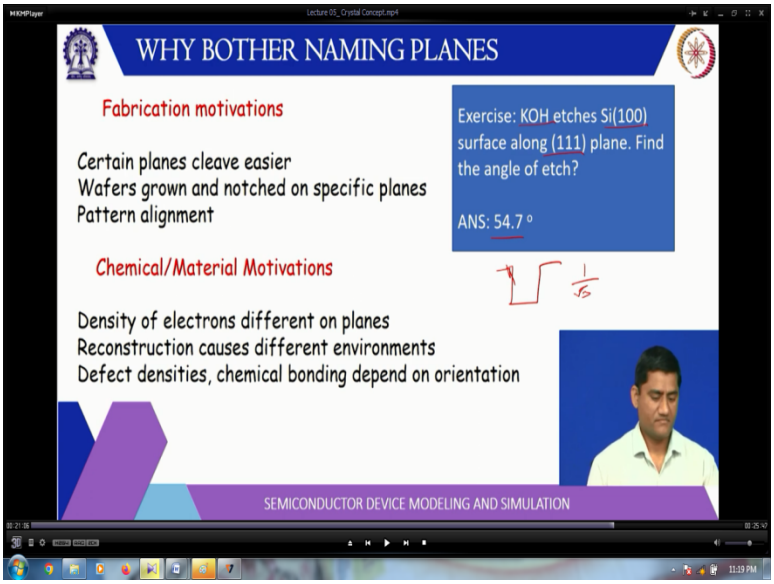

Now, why bother naming the planes? Whenever we process a semiconductor the planes will cleave along certain planes easily or you know certain planes are notched or marked. So, that you know for better pattern alignment, so, the each surface will have its own properties. So, for example, if you x silicone using KOH solution, it will basically edge along certain times direction because that direction is more reactivity. So, if you see that KOH etches silicon 1 0 0 surface along 1 1 1 plane.

So, if you find the angle between these 2 planes 1 0 0 and 1 1 1 you will get around 1 divided by square root of 3. So, that will be around 54.7 degree. So, that is the angle between the planes along which line this k which will edge so, it will not act vertically as you expect, but at certain angle 54.7 degree then of course, along the planes, different planes, there are different density of atoms or that means different density of electrons and different planes since there are different density of atoms there will be different density of defects and the possibility of chemical bonding will depend on the surface orientation.

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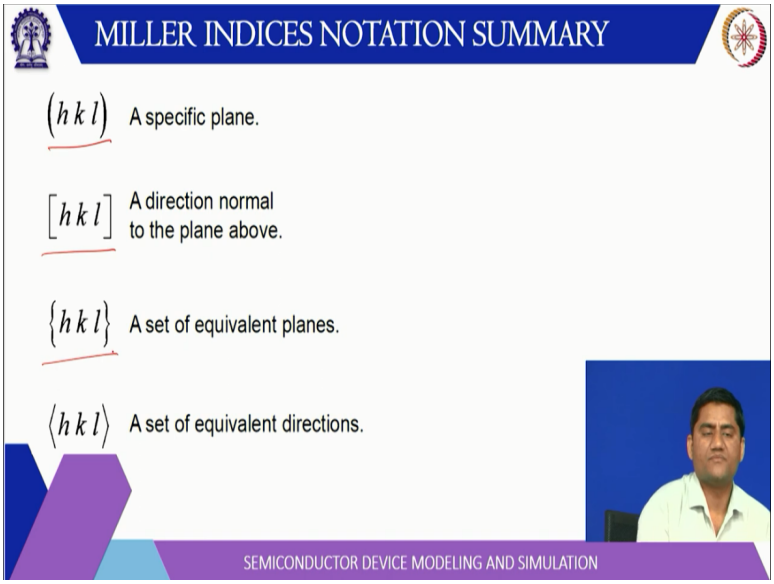

So, in summary we have discussed the miller indices notation we represent a plane by a simple bracket we represent a direction by a rectangular bracket we represent equivalent planes by curly brackets and we represent a set of equivalent directions by triangular brackets.

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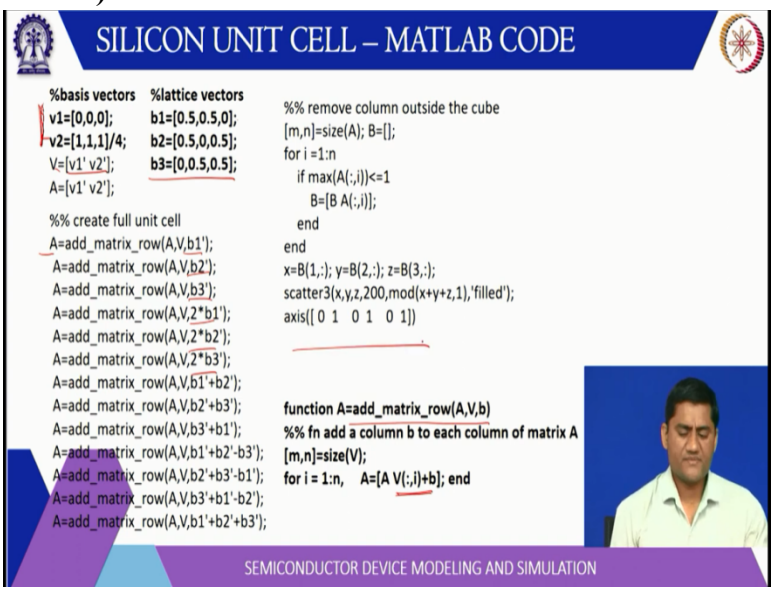

Here is one simple program which you can write in MATLAB. So, this is for silicone or diamond lattice so, here we define with this basis vector v1 and v2. Now, these are 2 items which form the basis. So, one is at 0 0 0 other is at A by 4 A by 4 A by 4. So, here we have taken equal to 1 because it is for representation purpose so, these to form the basis. So, now basis vector can be written as a combination of these 2 positions. Now, these 2 vectors can be combined these will be 2 positions.

Now, lattice vectors are the vectors of the FCC lattice and each lattice point is occupied by these 2 basis vectors. So, this is again half, half, 0 half, 0, half 0, half, half. So, these are 3 lattice vectors. Now, what we do we can add the matrix rows. So, if you row this code here, functions are add matrix row a, b. So, what it will do? It will add a column to each column of matrix A. So, matrix A is initially I think blank here.

So, this will first add this vector v1, so, v1 is a lattice vector then add vector v2 then add vector v3 so, this is for the second one twice of v1 v2 v3 and then for each vector it is basically adding 2 atoms because if you see here the vector v it contains v1 and v2. So, for each lattice point we are adding 2 atoms there and then of course, if you want to view a particular unit cell then you could remove the atoms which are outside the cube. So, the simple code for that one.

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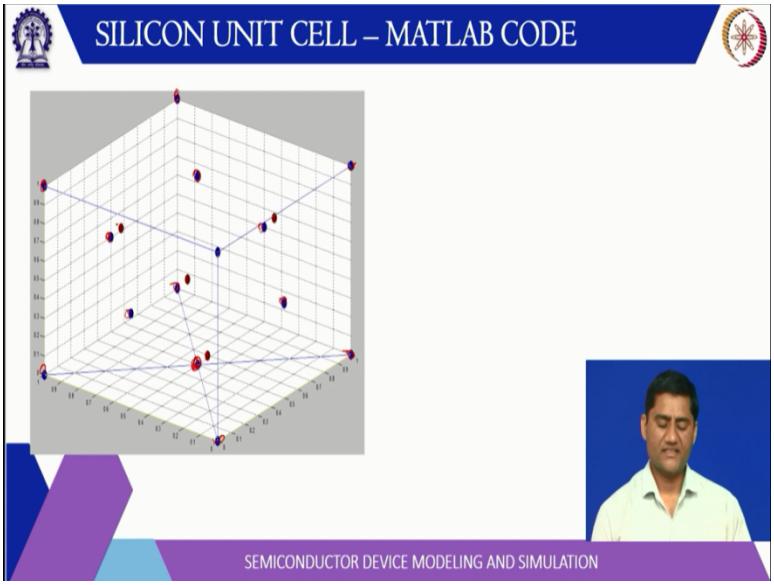

And then if you display it, you can view the unit cell so, these are the obviously corner atoms 8 corners here then you can use different colors. So, color can be represented with certain this has filled. And you can choose the color while plotting it basically. So, this is the top bottom face, this is the top face, this is a side face the right face, then there is a front face this is the front face. Then there is a back face and then these 4 are the body atoms 1 2 3 4. So, that way you can basically visualize yourself write your own code you can practice for writing for BCC or SCC, let us say and see the crystal structure.

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So, we have discussed about the lattice vectors and the Miller indices to so particular unit cell and the unit cell a cubic unit cell simple cubic FCC and VCC these are the unit cells, but the lattice vectors are written for the primitive unit cell and the primitive unit cell is basically the lattice vector length of the primitive universal is not exactly the side length of the cube, but it is the distance between 2 nearest atoms. So, we have discussed how to identify the lattice vectors Miller indices and how to write a simple code where we can visualize the crystal structure. Thank you very much.